Full wwPDB X-ray Structure Validation Report (i)

May 13, 2020 – 10:58 am BST

PDB ID	:	1GTH
Title	:	DIHYDROPYRIMIDINE DEHYDROGENASE (DPD) FROM PIG, TERNARY COMPLEX WITH NADPH AND 5-IODOURACIL
Authors	:	Dobritzsch, D.; Ricagno, S.; Schneider, G.; Schnackerz, K.D.; Lindqvist, Y.
Deposited on	:	2002-01-15
Resolution	:	2.25 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

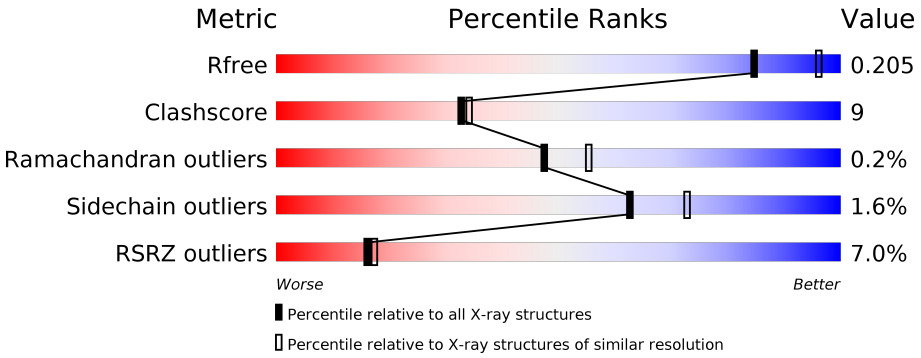
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.25 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	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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

Mol	Chain	Length	Quality of chain
1	A	1025	5% 84% 15%
1	B	1025	5% 83% 15%
1	C	1025	7% 83% 16%
1	D	1025	10% 81% 17%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SF4	B	1027	-	-	X	-
2	SF4	C	1027	-	-	X	-
2	SF4	D	1027	-	-	X	-
6	IDH	B	1034	-	-	X	-
7	IUR	C	1034	-	-	X	-

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 34762 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.

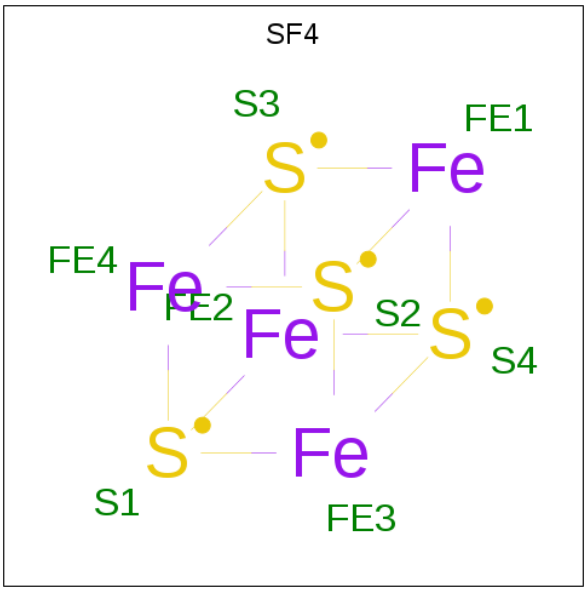
- Molecule 1 is a protein called DIHYDROPYRIMIDINE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1019	Total	C	N	O	S	0	0	0
			7770	4927	1317	1470	56			
1	B	1012	Total	C	N	O	S	0	0	0
			7719	4892	1309	1462	56			
1	C	1015	Total	C	N	O	S	0	0	0
			7740	4905	1313	1466	56			
1	D	1019	Total	C	N	O	S	0	0	0
			7770	4927	1317	1470	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 (three-letter code: SF4) (formula: Fe_4S_4).



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

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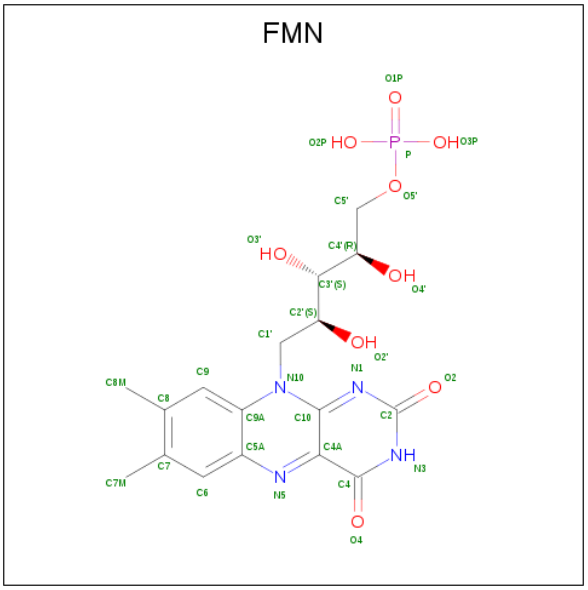
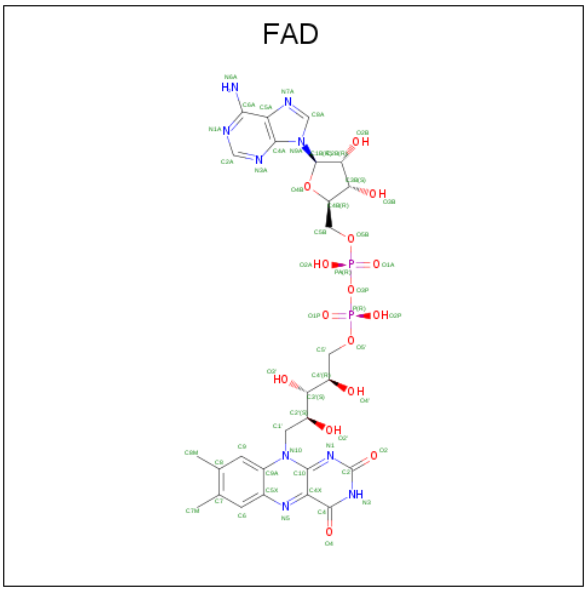
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total Fe S 8 4 4	0	0
2	D	1	Total Fe S 8 4 4	0	0

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



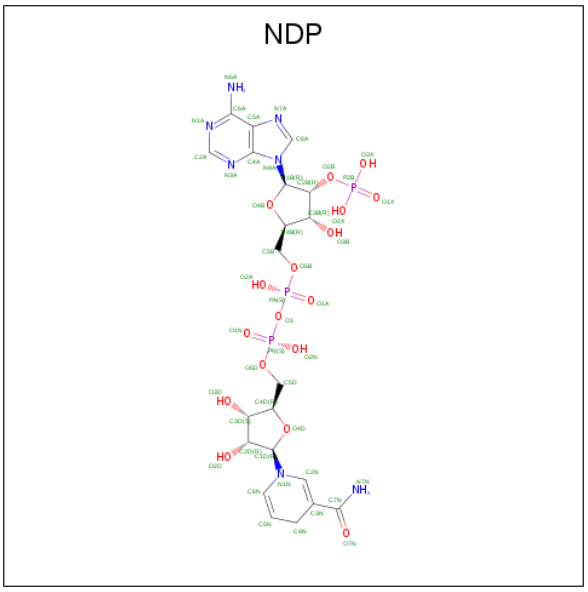
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O P 31 17 4 9 1	0	0
3	B	1	Total C N O P 31 17 4 9 1	0	0
3	C	1	Total C N O P 31 17 4 9 1	0	0
3	D	1	Total C N O P 31 17 4 9 1	0	0

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



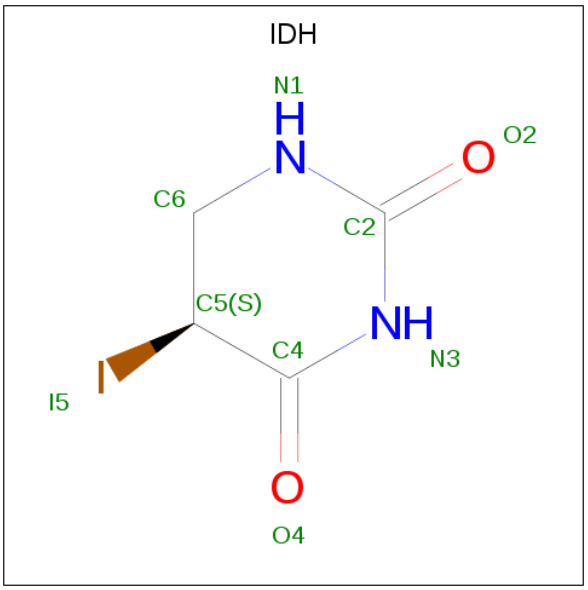
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
4	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
4	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
4	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

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



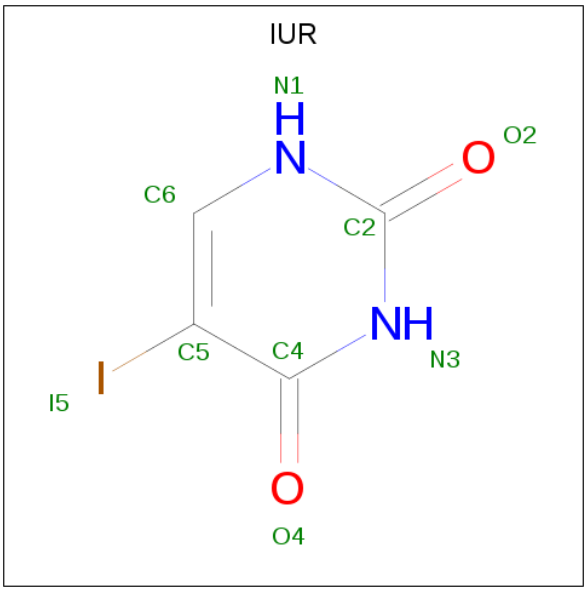
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O P 48 21 7 17 3	0	0
5	B	1	Total C N O P 48 21 7 17 3	0	0
5	C	1	Total C N O P 48 21 7 17 3	0	0
5	D	1	Total C N O P 48 21 7 17 3	0	0

- Molecule 6 is (5S)-5-IODODIHYDRO-2,4(1H,3H)-PYRIMIDINEDIONE (three-letter code: IDH) (formula: $C_4H_5IN_2O_2$).



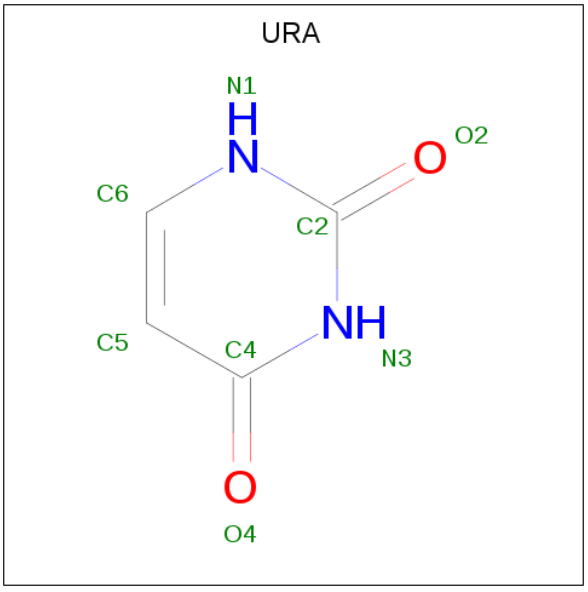
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C N O 8 4 2 2	0	0
6	B	1	Total C I N O 9 4 1 2 2	0	0

- Molecule 7 is 5-IODOURACIL (three-letter code: IUR) (formula: $C_4H_3IN_2O_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	C	1	Total	C	I	N	O	0	0
			9	4	1	2	2		

- Molecule 8 is URACIL (three-letter code: URA) (formula: $C_4H_4N_2O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	D	1	Total	C	N	O	0	0
			8	4	2	2		

- Molecule 9 is water.

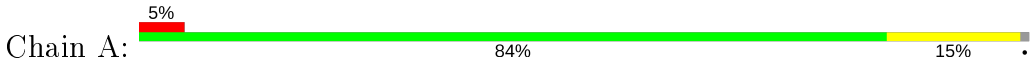
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	839	Total O 839 839	0	0
9	B	869	Total O 869 869	0	0
9	C	701	Total O 701 701	0	0
9	D	664	Total O 664 664	0	0

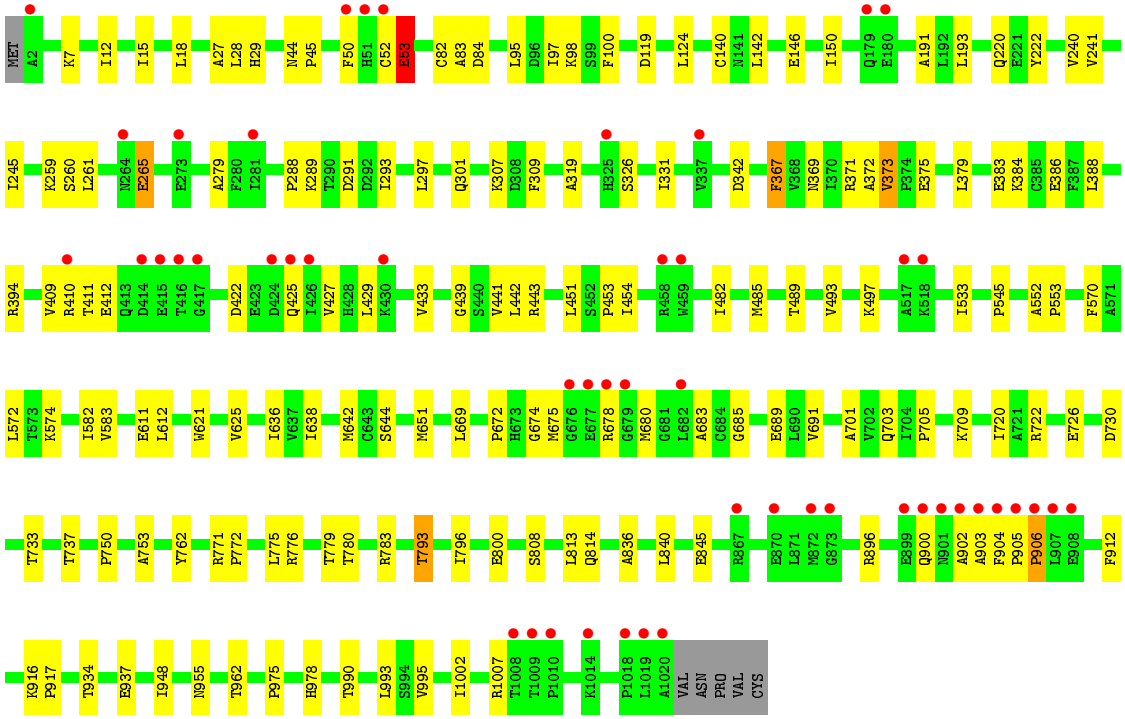
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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

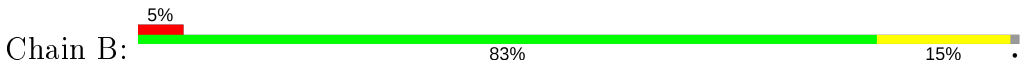
Chain A:

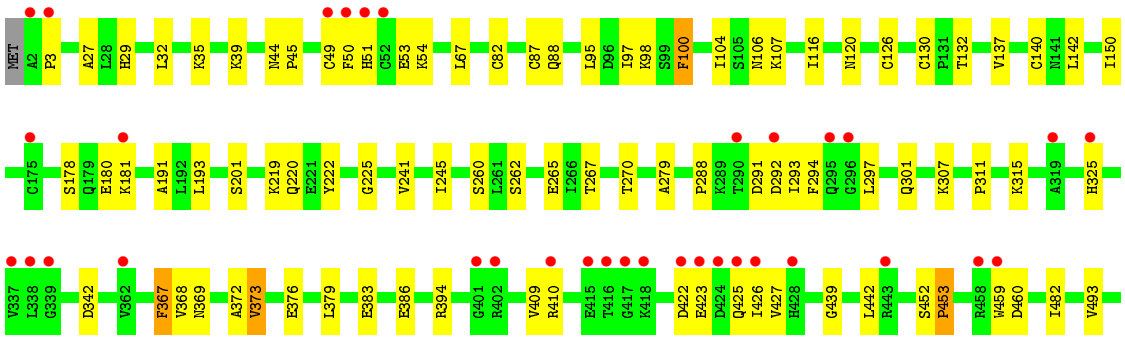


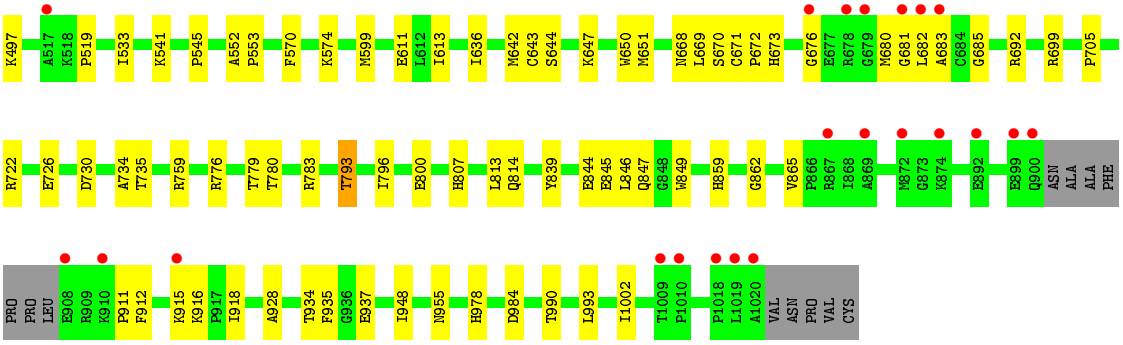


- Molecule 1: DIHYDROPYRIMIDINE DEHYDROGENASE

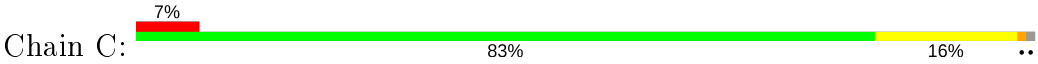
Chain B:

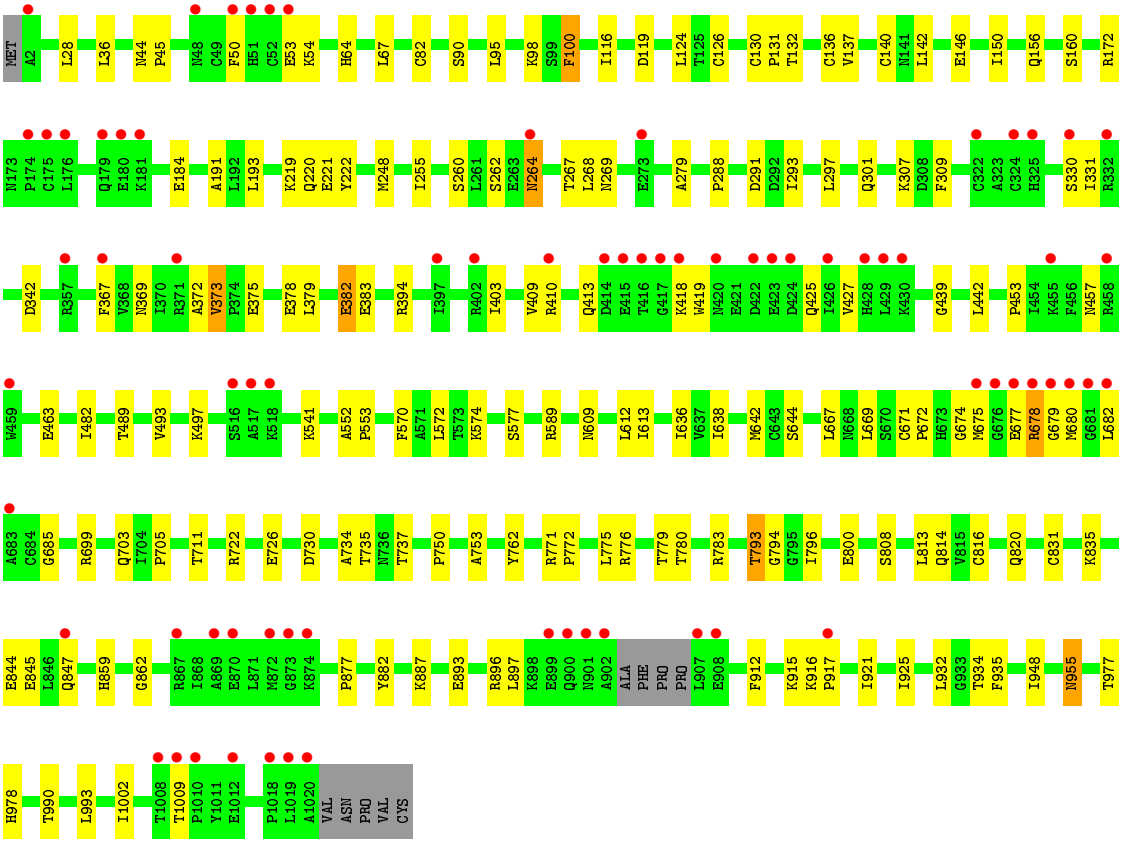




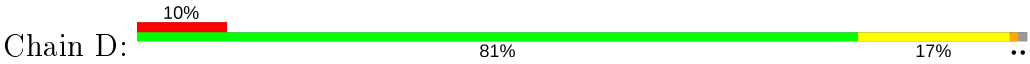


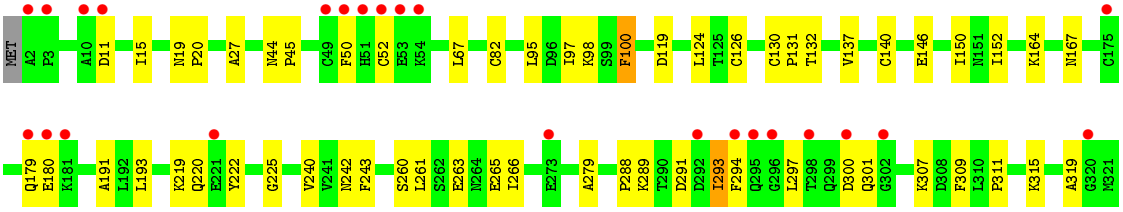
• Molecule 1: DIHYDROPYRIMIDINE DEHYDROGENASE

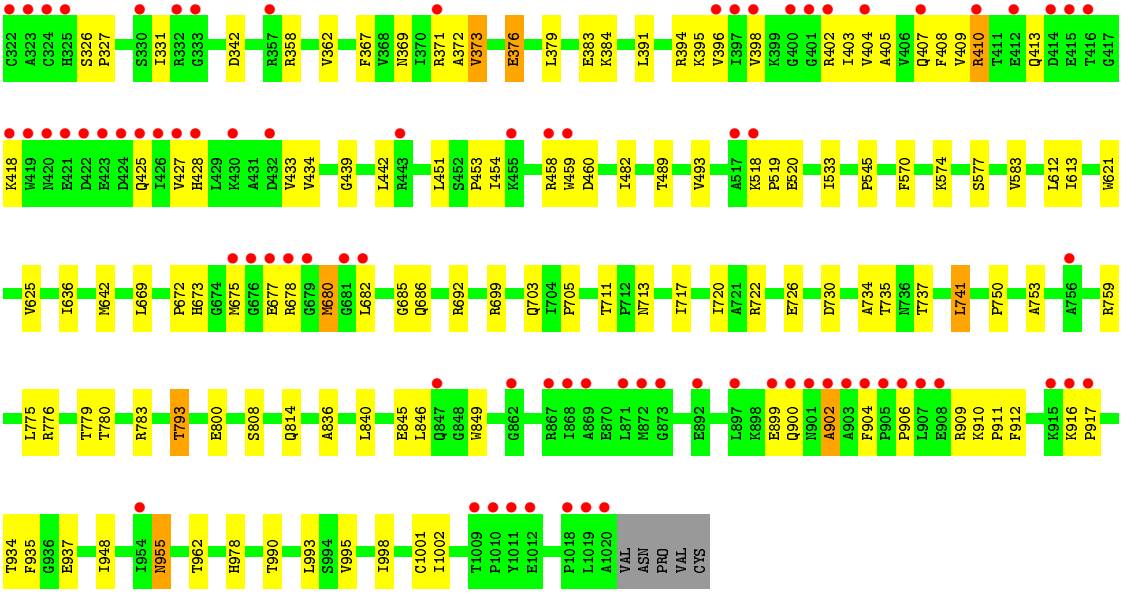




• Molecule 1: DIHYDROPYRIMIDINE DEHYDROGENASE






C322 A323 C324 H325 S326 P327 S330 I331 R332 G333 D342 R357 R358 V362 F367 V368 N369 I370 R371 A372 V373 E376 L379 E383 K384 L391 R394 K395 V396 I397 V398 K399 G400 G401 R402 I403 V404 A405 V406 Q407 F408 V409 R410 T411 E412 Q413 D414 E415 T416 G417
K418 W419 N420 E421 D422 E423 D424 Q425 I426 V427 H428 L429 K430 A431 D432 V433 V434 G439 L442 R443 L451 S452 P453 I454 K455 R458 W459 D460 I482 T489 V493 A517 K518 P519 E520 I533 P545 F570 K574 S577 V583 L612 I613 W621
V625 I636 M642 L669 P672 H673 G674 M675 G676 E677 R678 G679 M680 G681 L682 G685 Q686 R692 R699 Q703 I704 F705 T711 P712 N713 I717 I720 A721 R722 E726 D730 A734 T735 N736 T737 L741 P750 A753 A756 R759
L775 R776 T779 T780 R783 T793 E800 S808 Q814 A836 L840 E845 L846 Q847 G848 W849 G862 R867 I868 A869 E870 L871 M872 G873 E892 L897 K898 E899 Q900 N901 A902 A903 F904 P905 P906 L907 E908 R909 K910 P911 F912 K915 K916 P917
T934 F935 G936 E937 I948 I954 N955 T962 H978 T990 L993 S994 V995 I998 C1001 I1002 T1009 P1010 Y1011 E1012 P1018 L1019 A1020 VAL ASN PRO VAL CYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	82.21Å 159.69Å 167.59Å 90.00° 97.11° 90.00°	Depositor
Resolution (Å)	25.00 – 2.25 25.00 – 2.25	Depositor EDS
% Data completeness (in resolution range)	98.1 (25.00-2.25) 98.3 (25.00-2.25)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.16 (at 2.26Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.177 , 0.209 0.175 , 0.205	Depositor DCC
R_{free} test set	3984 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å^2)	25.7	Xtriage
Anisotropy	0.624	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 52.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	34762	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.26% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.34	0/7932	0.58	0/10751
1	B	0.34	0/7877	0.59	0/10672
1	C	0.33	0/7898	0.58	0/10701
1	D	0.33	0/7932	0.59	0/10751
All	All	0.34	0/31639	0.58	0/42875

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7770	0	7797	131	0
1	B	7719	0	7747	139	0
1	C	7740	0	7769	163	0
1	D	7770	0	7798	190	0
2	A	32	0	0	2	0
2	B	32	0	0	2	0
2	C	32	0	0	2	0
2	D	32	0	0	3	0
3	A	31	0	19	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	31	0	19	1	0
3	C	31	0	19	1	0
3	D	31	0	19	0	0
4	A	53	0	31	0	0
4	B	53	0	31	1	0
4	C	53	0	31	0	0
4	D	53	0	31	1	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	5	0
6	A	8	0	4	1	0
6	B	9	0	5	4	0
7	C	9	0	3	4	0
8	D	8	0	3	0	0
9	A	839	0	0	16	0
9	B	869	0	0	21	0
9	C	701	0	0	15	0
9	D	664	0	0	21	0
All	All	34762	0	31430	551	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 9.

All (551) 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:427:VAL:HG21	1:D:410:ARG:HH21	1.25	1.02
1:C:264:ASN:H	1:C:264:ASN:HD22	1.17	0.91
1:D:904:PHE:O	1:D:906:PRO:HD3	1.70	0.90
1:C:410:ARG:NH1	1:D:427:VAL:HG13	1.87	0.89
1:C:410:ARG:HH12	1:D:427:VAL:HG22	1.36	0.88
1:D:909:ARG:HG2	1:D:909:ARG:HH11	1.39	0.87
1:D:319:ALA:CB	1:D:904:PHE:HB2	2.05	0.87
1:B:681:GLY:HA2	9:B:2602:HOH:O	1.74	0.86
1:D:291:ASP:OD1	1:D:293:ILE:HG13	1.77	0.84
1:C:613:ILE:HG22	7:C:1034:IUR:I5	2.48	0.84
1:C:410:ARG:NH1	1:D:427:VAL:HG22	1.92	0.84
1:A:427:VAL:HG22	1:B:410:ARG:NH2	1.94	0.83
1:D:319:ALA:HB1	1:D:904:PHE:HB2	1.60	0.83
1:C:410:ARG:HH22	1:D:427:VAL:HG22	1.42	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:427:VAL:CG2	1:D:410:ARG:HH21	1.90	0.82
1:A:410:ARG:HH21	1:B:427:VAL:HG22	1.43	0.82
1:A:582:ILE:HD12	9:A:2256:HOH:O	1.77	0.82
1:B:669:LEU:HD23	9:B:2601:HOH:O	1.79	0.82
1:A:342:ASP:HB3	5:A:1032:NDP:H42N	1.63	0.81
1:B:859:HIS:HD2	1:B:862:GLY:H	1.28	0.81
1:C:410:ARG:NH2	1:D:427:VAL:HG22	1.96	0.81
1:D:776:ARG:O	1:D:780:THR:HG23	1.80	0.81
1:C:859:HIS:HD2	1:C:862:GLY:H	1.28	0.80
1:C:369:ASN:HA	1:D:50:PHE:HE2	1.46	0.79
1:D:682:LEU:HD13	9:D:2465:HOH:O	1.81	0.79
1:D:398:VAL:HG22	1:D:403:ILE:HA	1.66	0.77
1:D:398:VAL:HG13	1:D:402:ARG:O	1.85	0.77
1:D:410:ARG:HD3	1:D:425:GLN:OE1	1.85	0.77
1:A:427:VAL:HG22	1:B:410:ARG:HH21	1.50	0.77
1:B:39:LYS:HG3	9:B:2075:HOH:O	1.85	0.76
1:C:342:ASP:HB3	5:C:1032:NDP:H42N	1.65	0.76
1:B:54:LYS:HB3	9:B:2105:HOH:O	1.85	0.76
1:B:262:SER:HB3	1:B:265:GLU:OE1	1.85	0.76
1:C:410:ARG:HH12	1:D:427:VAL:CG2	1.98	0.75
1:A:50:PHE:CE2	1:B:369:ASN:HA	2.22	0.75
1:D:373:VAL:HG22	1:D:376:GLU:HB2	1.68	0.75
1:D:342:ASP:HB3	5:D:1032:NDP:H42N	1.69	0.75
1:B:342:ASP:HB3	5:B:1032:NDP:H42N	1.70	0.73
1:C:613:ILE:CG2	7:C:1034:IUR:I5	3.07	0.73
1:D:301:GLN:O	1:D:403:ILE:HG22	1.88	0.73
1:B:671:CYS:SG	6:B:1034:IDH:I5	3.17	0.72
1:C:410:ARG:HE	1:D:410:ARG:NH2	1.87	0.72
1:C:642:MET:HE1	1:C:675:MET:HG3	1.71	0.72
1:D:711:THR:HG22	9:D:2454:HOH:O	1.89	0.72
1:A:441:VAL:HG21	1:A:443:ARG:HD2	1.70	0.72
1:A:369:ASN:HA	1:B:50:PHE:CE2	2.24	0.71
1:C:410:ARG:CZ	1:D:427:VAL:HG22	2.20	0.71
1:C:369:ASN:HA	1:D:50:PHE:CE2	2.26	0.71
1:C:762:TYR:CZ	1:D:780:THR:HG22	2.26	0.70
1:A:422:ASP:OD2	1:A:425:GLN:HG3	1.90	0.69
1:D:410:ARG:HG3	1:D:410:ARG:HH11	1.55	0.69
1:A:410:ARG:HH21	1:B:427:VAL:CG2	2.05	0.69
1:A:50:PHE:HE2	1:B:369:ASN:HA	1.58	0.68
1:C:410:ARG:NH2	1:D:410:ARG:NH1	2.41	0.68
1:A:574:LYS:HE3	9:A:2520:HOH:O	1.93	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:410:ARG:HD2	1:C:425:GLN:OE1	1.95	0.67
1:A:410:ARG:CZ	1:B:410:ARG:NH2	2.58	0.67
1:C:820:GLN:O	1:D:962:THR:HG22	1.94	0.67
1:D:395:LYS:HD2	1:D:407:GLN:OE1	1.95	0.66
1:C:672:PRO:HG2	1:C:737:THR:OG1	1.95	0.66
1:C:378:GLU:O	1:C:382:GLU:HG3	1.96	0.66
1:B:442:LEU:HD22	1:B:482:ILE:HD11	1.76	0.65
1:B:291:ASP:OD1	1:B:293:ILE:HG12	1.96	0.65
1:D:394:ARG:HG3	1:D:409:VAL:HG13	1.77	0.65
1:C:671:CYS:SG	7:C:1034:IUR:I5	3.23	0.65
1:A:410:ARG:NH2	1:B:427:VAL:CG2	2.60	0.65
1:C:410:ARG:HH12	1:D:427:VAL:CB	2.09	0.65
1:D:720:ILE:CD1	9:D:2454:HOH:O	2.46	0.64
1:D:720:ILE:HD12	9:D:2454:HOH:O	1.97	0.64
1:A:369:ASN:HA	1:B:50:PHE:HE2	1.62	0.64
1:D:583:VAL:HG12	1:D:678:ARG:HH11	1.62	0.64
1:A:582:ILE:HA	9:A:2256:HOH:O	1.96	0.63
1:C:775:LEU:O	1:C:779:THR:HG23	1.98	0.63
1:A:896:ARG:HH21	1:A:900:GLN:HE22	1.45	0.63
1:B:410:ARG:HD2	1:B:425:GLN:OE1	1.98	0.63
1:C:644:SER:HB3	1:C:680:MET:HE2	1.81	0.63
1:D:319:ALA:HB2	1:D:904:PHE:HB2	1.81	0.63
1:C:410:ARG:HH21	1:D:410:ARG:CZ	2.11	0.63
1:C:877:PRO:HD2	1:C:882:TYR:CG	2.33	0.63
1:D:410:ARG:HH11	1:D:410:ARG:CG	2.12	0.63
1:B:682:LEU:HD12	9:B:2605:HOH:O	1.97	0.63
1:A:410:ARG:NH1	1:B:410:ARG:HH12	1.97	0.62
1:D:167:ASN:OD1	1:D:909:ARG:NH1	2.33	0.62
1:A:427:VAL:CG2	1:B:410:ARG:NH2	2.62	0.62
1:A:948:ILE:HG12	1:A:1002:ILE:HG12	1.81	0.62
1:A:260:SER:HB3	1:A:265:GLU:OE1	2.00	0.61
1:D:52:CYS:HB3	1:D:384:LYS:HG2	1.82	0.61
1:D:909:ARG:HH11	1:D:909:ARG:CG	2.13	0.61
1:C:762:TYR:OH	1:D:780:THR:HG22	2.00	0.61
1:A:442:LEU:HD22	1:A:482:ILE:HD11	1.82	0.60
1:A:691:VAL:HG21	1:A:720:ILE:HG23	1.82	0.60
1:D:722:ARG:O	1:D:726:GLU:HG3	2.01	0.60
1:C:932:LEU:HD21	1:D:741:LEU:HD11	1.83	0.60
1:A:934:THR:OG1	1:A:937:GLU:HG3	2.02	0.60
1:A:583:VAL:HG12	1:A:678:ARG:NH1	2.17	0.60
1:D:583:VAL:HG12	1:D:678:ARG:NH1	2.17	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:990:THR:HG22	1:A:990:THR:O	2.02	0.59
1:B:574:LYS:HE3	9:B:2549:HOH:O	2.00	0.59
1:B:409:VAL:HG22	1:B:422:ASP:O	2.02	0.59
1:B:422:ASP:OD2	1:B:425:GLN:HG3	2.02	0.59
1:D:180:GLU:CD	1:D:180:GLU:H	2.05	0.59
1:D:682:LEU:HD11	1:D:686:GLN:NE2	2.18	0.59
1:A:689:GLU:OE2	1:D:327:PRO:HG3	2.02	0.59
1:A:439:GLY:HA2	5:A:1032:NDP:O2N	2.02	0.59
1:D:909:ARG:HG2	1:D:909:ARG:NH1	2.15	0.58
1:D:642:MET:HE1	1:D:675:MET:HG3	1.85	0.58
1:D:775:LEU:O	1:D:779:THR:HG23	2.03	0.58
3:B:1030:FMN:C4A	6:B:1034:IDH:H5	2.33	0.58
1:C:54:LYS:HB3	9:C:2079:HOH:O	2.03	0.58
1:C:410:ARG:HH12	1:D:427:VAL:HG13	1.66	0.58
1:A:793:THR:HB	1:A:814:GLN:HB2	1.85	0.58
1:C:172:ARG:HG3	9:C:2191:HOH:O	2.04	0.58
1:C:990:THR:O	1:C:990:THR:HG22	2.03	0.58
1:D:379:LEU:O	1:D:383:GLU:HG3	2.04	0.58
9:A:2140:HOH:O	1:B:29:HIS:HB2	2.04	0.58
1:C:439:GLY:HA2	5:C:1032:NDP:O2N	2.04	0.58
1:C:779:THR:HG22	1:C:808:SER:HB3	1.85	0.58
1:B:611:GLU:O	1:B:673:HIS:HE1	1.87	0.58
1:A:410:ARG:NE	1:B:410:ARG:NH2	2.52	0.57
1:C:36:LEU:HB3	9:C:2064:HOH:O	2.03	0.57
1:D:442:LEU:HD22	1:D:482:ILE:HD11	1.85	0.57
1:D:82:CYS:O	1:D:98:LYS:HD2	2.05	0.57
1:B:439:GLY:HA2	5:B:1032:NDP:O2N	2.05	0.57
1:A:572:LEU:HD13	1:A:638:ILE:HB	1.86	0.57
1:C:269:ASN:HB2	9:C:2243:HOH:O	2.04	0.57
1:C:672:PRO:HA	1:C:682:LEU:HD22	1.86	0.57
1:C:146:GLU:HG2	1:D:67:LEU:HD23	1.84	0.57
1:A:443:ARG:NH1	9:A:2401:HOH:O	2.38	0.57
9:C:2507:HOH:O	1:D:775:LEU:HD12	2.03	0.57
1:C:948:ILE:HG12	1:C:1002:ILE:HG12	1.86	0.57
1:B:379:LEU:O	1:B:383:GLU:HG3	2.04	0.57
1:C:410:ARG:NH1	1:D:427:VAL:CG1	2.65	0.57
1:D:779:THR:HG22	1:D:808:SER:HB3	1.85	0.57
1:A:29:HIS:HB2	9:B:2161:HOH:O	2.05	0.56
1:C:845:GLU:HG3	1:C:912:PHE:CE2	2.40	0.56
1:A:342:ASP:CB	5:A:1032:NDP:H42N	2.34	0.56
1:C:410:ARG:NH2	1:D:410:ARG:CZ	2.68	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:395:LYS:HB2	1:D:407:GLN:HB2	1.86	0.56
1:B:342:ASP:OD1	1:B:372:ALA:HB1	2.05	0.56
1:A:1007:ARG:HD3	9:A:2812:HOH:O	2.06	0.56
1:A:342:ASP:OD1	1:A:372:ALA:HB1	2.06	0.56
1:D:948:ILE:HG12	1:D:1002:ILE:HG12	1.87	0.56
1:A:220:GLN:HG3	1:A:222:TYR:CZ	2.41	0.56
1:D:705:PRO:HA	1:D:730:ASP:OD2	2.06	0.56
1:D:846:LEU:HD22	1:D:849:TRP:CE2	2.41	0.56
1:A:552:ALA:HB3	1:A:553:PRO:HD3	1.87	0.55
1:B:955:ASN:HB3	1:B:978:HIS:HB3	1.88	0.55
1:C:955:ASN:HB3	1:C:978:HIS:HB3	1.88	0.55
1:D:909:ARG:NH1	9:D:2572:HOH:O	2.39	0.55
1:C:877:PRO:HG3	1:C:977:THR:HB	1.89	0.55
1:A:683:ALA:HB1	9:A:2567:HOH:O	2.06	0.55
1:D:678:ARG:HD3	9:D:2374:HOH:O	2.07	0.55
1:D:489:THR:O	1:D:493:VAL:HG23	2.06	0.55
1:D:955:ASN:HB3	1:D:978:HIS:HB3	1.89	0.55
1:D:439:GLY:HA2	5:D:1032:NDP:O2N	2.07	0.55
1:C:264:ASN:H	1:C:264:ASN:ND2	1.97	0.54
1:D:916:LYS:HB2	1:D:917:PRO:HD2	1.89	0.54
1:C:410:ARG:HH12	1:D:427:VAL:CG1	2.20	0.54
1:D:669:LEU:O	1:D:685:GLY:HA3	2.07	0.54
1:A:896:ARG:NH2	1:A:900:GLN:HE22	2.05	0.54
1:B:409:VAL:HG21	1:B:423:GLU:HA	1.89	0.54
1:B:668:ASN:O	9:B:2601:HOH:O	2.18	0.54
1:B:613:ILE:HG22	6:B:1034:IDH:I5	2.77	0.54
1:C:291:ASP:OD1	1:C:293:ILE:HG12	2.08	0.54
1:C:722:ARG:O	1:C:726:GLU:HG3	2.06	0.54
1:A:410:ARG:NH2	1:B:427:VAL:HG21	2.23	0.54
1:A:611:GLU:O	6:A:1033:IDH:H6C2	2.08	0.54
1:A:722:ARG:CZ	1:D:300:ASP:HB3	2.38	0.54
1:D:962:THR:HG21	1:D:995:VAL:HG11	1.90	0.54
1:B:132:THR:HB	1:B:137:VAL:HG23	1.90	0.53
1:B:990:THR:O	1:B:990:THR:HG22	2.08	0.53
1:C:342:ASP:OD1	1:C:372:ALA:HB1	2.08	0.53
1:A:642:MET:HE1	1:A:675:MET:HG3	1.90	0.53
1:A:410:ARG:CZ	1:B:410:ARG:CZ	2.86	0.53
1:D:408:PHE:HB2	1:D:427:VAL:HB	1.91	0.53
1:D:759:ARG:HH11	1:D:759:ARG:HG2	1.73	0.53
1:C:845:GLU:HG3	1:C:912:PHE:CD2	2.43	0.53
1:B:95:LEU:HD21	1:B:116:ILE:HG23	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:288:PRO:HB3	1:D:307:LYS:HB2	1.91	0.53
1:A:394:ARG:HG3	1:A:409:VAL:HG13	1.90	0.53
1:B:669:LEU:O	1:B:685:GLY:HA3	2.09	0.53
1:C:44:ASN:HB2	1:C:45:PRO:CD	2.39	0.53
1:C:672:PRO:HG3	9:C:2490:HOH:O	2.07	0.53
1:D:289:LYS:HD3	9:D:2664:HOH:O	2.09	0.53
1:D:95:LEU:HD23	1:D:119:ASP:HB2	1.90	0.53
1:A:410:ARG:CZ	1:B:410:ARG:HH22	2.22	0.53
1:B:342:ASP:CB	5:B:1032:NDP:H42N	2.37	0.53
1:B:722:ARG:O	1:B:726:GLU:HG3	2.09	0.53
1:B:948:ILE:HG12	1:B:1002:ILE:HG12	1.91	0.53
1:A:485:MET:HE1	1:B:32:LEU:HB2	1.90	0.52
1:A:82:CYS:O	1:A:98:LYS:HD2	2.09	0.52
1:B:844:GLU:O	1:B:847:GLN:HG3	2.08	0.52
1:A:644:SER:HA	1:A:680:MET:HG2	1.91	0.52
1:B:342:ASP:HB2	5:B:1032:NDP:C5N	2.40	0.52
1:D:342:ASP:CB	5:D:1032:NDP:H42N	2.38	0.52
1:B:650:TRP:HH2	9:B:2601:HOH:O	1.91	0.52
1:C:410:ARG:NE	1:D:410:ARG:NH2	2.56	0.52
1:D:458:ARG:NH1	9:D:2301:HOH:O	2.42	0.52
1:D:845:GLU:HG3	1:D:912:PHE:CD2	2.44	0.52
1:C:342:ASP:CB	5:C:1032:NDP:H42N	2.38	0.52
1:C:301:GLN:O	1:C:403:ILE:HG13	2.09	0.52
1:C:844:GLU:O	1:C:847:GLN:HG3	2.09	0.52
1:D:993:LEU:HD23	1:D:993:LEU:O	2.10	0.52
1:A:288:PRO:HB3	1:A:307:LYS:HB2	1.91	0.52
1:A:379:LEU:O	1:A:383:GLU:HG3	2.08	0.52
1:A:410:ARG:HG3	1:A:425:GLN:OE1	2.10	0.52
1:B:288:PRO:HB3	1:B:307:LYS:HB2	1.92	0.52
1:A:291:ASP:OD1	1:A:293:ILE:HG12	2.10	0.52
1:C:262:SER:HB3	1:C:264:ASN:ND2	2.25	0.52
1:A:388:LEU:CD1	1:A:429:LEU:HD21	2.39	0.52
1:A:53:GLU:HB2	9:A:2084:HOH:O	2.09	0.51
1:B:670:SER:HA	1:B:682:LEU:HD23	1.91	0.51
1:D:713:ASN:ND2	9:D:2465:HOH:O	2.36	0.51
1:D:993:LEU:HD23	1:D:993:LEU:C	2.30	0.51
1:B:409:VAL:CG2	1:B:422:ASP:O	2.58	0.51
1:B:672:PRO:HG2	1:B:673:HIS:CD2	2.46	0.51
1:C:267:THR:HG22	9:C:2321:HOH:O	2.11	0.51
1:C:711:THR:HG22	9:C:2491:HOH:O	2.10	0.51
1:C:410:ARG:HE	1:D:410:ARG:CZ	2.22	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:845:GLU:HG3	1:A:912:PHE:CD2	2.45	0.51
1:C:394:ARG:HG3	1:C:409:VAL:HG13	1.92	0.51
1:C:613:ILE:HG23	7:C:1034:IUR:I5	2.80	0.51
1:C:796:ILE:HD13	1:C:813:LEU:HB3	1.93	0.51
1:C:916:LYS:HB2	1:C:917:PRO:HD2	1.92	0.51
1:D:394:ARG:HG3	1:D:409:VAL:CG1	2.39	0.51
1:C:442:LEU:HD22	1:C:482:ILE:HD11	1.91	0.51
1:C:221:GLU:HG2	9:C:2211:HOH:O	2.09	0.51
1:C:859:HIS:HD2	1:C:862:GLY:N	2.05	0.51
1:A:289:LYS:HA	9:A:2401:HOH:O	2.11	0.51
1:C:705:PRO:HA	1:C:730:ASP:OD2	2.11	0.51
1:A:720:ILE:HG13	9:A:2568:HOH:O	2.11	0.51
1:D:682:LEU:O	1:D:686:GLN:HG3	2.10	0.51
1:D:717:ILE:HG13	1:D:720:ILE:HD11	1.93	0.51
1:A:27:ALA:O	1:B:497:LYS:HE2	2.11	0.50
1:C:95:LEU:HD23	1:C:119:ASP:HB2	1.92	0.50
1:C:410:ARG:HH22	1:D:427:VAL:CG2	2.20	0.50
1:A:779:THR:HG22	1:A:808:SER:HB3	1.94	0.50
1:C:896:ARG:HG2	1:C:896:ARG:HH11	1.75	0.50
1:D:404:VAL:O	1:D:405:ALA:HB2	2.12	0.50
1:A:193:LEU:HD12	1:A:261:LEU:HB2	1.93	0.50
1:D:391:LEU:HD22	1:D:427:VAL:HG21	1.93	0.50
1:A:669:LEU:O	1:A:685:GLY:HA3	2.11	0.50
1:C:131:PRO:HB3	1:C:373:VAL:HG11	1.93	0.50
1:D:293:ILE:CG2	1:D:394:ARG:O	2.60	0.50
1:A:612:LEU:HD11	1:B:935:PHE:CE2	2.45	0.50
1:A:955:ASN:HB3	1:A:978:HIS:HB3	1.93	0.50
1:D:219:LYS:HG3	1:D:260:SER:OG	2.12	0.50
1:C:262:SER:HB3	1:C:264:ASN:HD21	1.77	0.50
1:C:669:LEU:O	1:C:685:GLY:HA3	2.11	0.50
1:A:410:ARG:NE	1:B:410:ARG:HH22	2.10	0.50
1:A:411:THR:O	1:A:412:GLU:HB3	2.11	0.49
1:A:95:LEU:HD23	1:A:119:ASP:HB2	1.93	0.49
1:C:267:THR:HG22	1:C:268:LEU:N	2.27	0.49
1:D:44:ASN:HB2	1:D:45:PRO:CD	2.42	0.49
1:D:909:ARG:NH1	1:D:909:ARG:CG	2.74	0.49
1:A:779:THR:O	1:A:783:ARG:HG3	2.11	0.49
1:B:95:LEU:HD11	1:B:120:ASN:HB2	1.93	0.49
1:A:52:CYS:HB2	1:A:384:LYS:HG2	1.95	0.49
1:B:267:THR:OG1	1:B:270:THR:HG23	2.12	0.49
1:C:410:ARG:CZ	1:D:410:ARG:NH1	2.75	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:220:GLN:HG3	1:B:222:TYR:CZ	2.48	0.49
1:A:44:ASN:HB2	1:A:45:PRO:CD	2.43	0.49
1:B:552:ALA:HB3	1:B:553:PRO:HD3	1.95	0.49
1:A:722:ARG:NH1	1:D:300:ASP:HB3	2.28	0.49
1:A:497:LYS:HE2	1:B:27:ALA:O	2.13	0.49
1:C:288:PRO:HB3	1:C:307:LYS:HB2	1.93	0.49
1:B:459:TRP:O	1:B:460:ASP:HB2	2.13	0.49
1:D:735:THR:N	1:D:793:THR:HG23	2.28	0.49
1:B:796:ILE:HD13	1:B:813:LEU:HB3	1.95	0.48
1:D:342:ASP:OD1	1:D:372:ALA:HB1	2.13	0.48
1:B:180:GLU:H	1:B:180:GLU:CD	2.17	0.48
1:B:82:CYS:O	1:B:98:LYS:HD2	2.13	0.48
1:D:309:PHE:CE1	1:D:331:ILE:HD11	2.49	0.48
1:B:643:CYS:HB2	1:B:650:TRP:CE2	2.48	0.48
1:D:672:PRO:HG3	1:D:737:THR:OG1	2.13	0.48
1:B:676:GLY:HA2	1:B:680:MET:O	2.13	0.48
1:C:410:ARG:HH11	1:D:427:VAL:HG13	1.71	0.48
1:B:672:PRO:HA	1:B:682:LEU:CD1	2.43	0.48
1:B:699:ARG:HA	1:B:699:ARG:NE	2.28	0.48
1:A:410:ARG:CZ	1:B:410:ARG:NH1	2.76	0.48
1:D:672:PRO:HG2	1:D:673:HIS:ND1	2.28	0.48
1:A:705:PRO:HA	1:A:730:ASP:OD2	2.14	0.48
1:B:132:THR:HB	1:B:137:VAL:CG2	2.44	0.48
1:B:779:THR:O	1:B:783:ARG:HG3	2.14	0.48
1:C:193:LEU:HD22	1:C:193:LEU:N	2.29	0.48
1:B:294:PHE:HA	1:B:297:LEU:HD12	1.96	0.47
1:C:379:LEU:O	1:C:383:GLU:HG3	2.14	0.47
1:B:178:SER:OG	1:B:181:LYS:HG3	2.14	0.47
1:B:734:ALA:HA	1:B:735:THR:HA	1.65	0.47
1:C:877:PRO:HD2	1:C:882:TYR:CB	2.44	0.47
1:D:220:GLN:HG3	1:D:222:TYR:CZ	2.49	0.47
1:C:220:GLN:HG3	1:C:222:TYR:CZ	2.49	0.47
1:A:259:LYS:HE2	9:A:2287:HOH:O	2.13	0.47
1:B:325:HIS:HA	9:B:2363:HOH:O	2.14	0.47
1:A:386:GLU:OE1	1:B:367:PHE:HB2	2.14	0.47
1:C:126:CYS:HB3	1:C:130:CYS:SG	2.55	0.47
1:D:294:PHE:HA	1:D:297:LEU:HD12	1.97	0.47
1:B:44:ASN:HB2	1:B:45:PRO:CD	2.45	0.47
1:D:293:ILE:HG21	1:D:394:ARG:O	2.15	0.47
1:D:990:THR:HG22	1:D:990:THR:O	2.14	0.47
1:A:621:TRP:O	1:A:625:VAL:HG23	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:ALA:CB	1:A:904:PHE:HB3	2.45	0.47
1:C:612:LEU:HD11	1:D:935:PHE:CE2	2.50	0.47
1:A:373:VAL:HG23	1:A:375:GLU:OE1	2.15	0.47
1:D:396:VAL:HG13	1:D:403:ILE:CD1	2.45	0.47
1:D:750:PRO:O	1:D:753:ALA:HB2	2.14	0.47
1:C:497:LYS:HE2	1:D:27:ALA:O	2.15	0.47
1:C:67:LEU:HD23	1:D:146:GLU:HG2	1.95	0.47
1:B:845:GLU:HG3	1:B:912:PHE:CE2	2.50	0.47
1:C:410:ARG:NE	1:D:410:ARG:CZ	2.78	0.47
1:D:845:GLU:HG3	1:D:912:PHE:CE2	2.50	0.47
1:C:50:PHE:CE2	1:D:369:ASN:HA	2.50	0.47
1:C:734:ALA:HA	1:C:735:THR:HA	1.70	0.47
1:A:845:GLU:HG3	1:A:912:PHE:CE2	2.49	0.46
1:B:241:VAL:O	1:B:245:ILE:HG12	2.16	0.46
1:D:191:ALA:O	1:D:279:ALA:HA	2.16	0.46
1:D:307:LYS:HE3	9:D:2281:HOH:O	2.15	0.46
1:A:442:LEU:HD22	1:A:482:ILE:CD1	2.45	0.46
1:B:846:LEU:HD22	1:B:849:TRP:CE2	2.50	0.46
1:C:413:GLN:HG3	1:C:419:TRP:CE2	2.50	0.46
1:A:451:LEU:O	1:A:454:ILE:HG12	2.16	0.46
1:B:126:CYS:HB3	1:B:130:CYS:SG	2.55	0.46
1:C:896:ARG:NH1	1:C:896:ARG:HG2	2.30	0.46
1:D:131:PRO:HB3	1:D:373:VAL:HG11	1.97	0.46
1:D:793:THR:HB	1:D:814:GLN:HB2	1.97	0.46
1:A:326:SER:HB3	9:A:2345:HOH:O	2.15	0.46
1:B:839:TYR:HA	1:B:918:ILE:HD12	1.98	0.46
1:C:64:HIS:HE1	1:C:382:GLU:OE2	1.98	0.46
1:D:371:ARG:HB2	1:D:371:ARG:HE	1.48	0.46
1:C:750:PRO:O	1:C:753:ALA:HB2	2.14	0.46
1:A:775:LEU:HD12	9:B:2646:HOH:O	2.16	0.46
1:A:783:ARG:HD3	9:A:2623:HOH:O	2.15	0.46
1:B:533:ILE:O	1:B:545:PRO:HD3	2.16	0.46
1:B:915:LYS:HG3	9:B:2702:HOH:O	2.16	0.46
1:C:735:THR:N	1:C:793:THR:HG23	2.31	0.46
1:D:642:MET:HG2	1:D:680:MET:SD	2.56	0.46
1:C:644:SER:HA	1:C:679:GLY:O	2.16	0.46
1:C:82:CYS:O	1:C:98:LYS:HD2	2.16	0.46
1:A:331:ILE:HG23	1:A:433:VAL:HG21	1.98	0.46
1:C:100:PHE:C	1:C:100:PHE:CD1	2.90	0.46
1:A:191:ALA:O	1:A:279:ALA:HA	2.16	0.45
1:B:297:LEU:HA	1:B:301:GLN:OE1	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:219:LYS:HG3	1:C:260:SER:OG	2.17	0.45
1:D:899:GLU:OE1	1:D:899:GLU:HA	2.15	0.45
1:A:342:ASP:HB2	5:A:1032:NDP:C5N	2.46	0.45
1:B:140:CYS:HA	2:B:1027:SF4:S3	2.57	0.45
1:B:191:ALA:O	1:B:279:ALA:HA	2.16	0.45
1:B:613:ILE:CG2	6:B:1034:IDH:I5	3.35	0.45
1:C:934:THR:HB	1:D:677:GLU:OE2	2.15	0.45
1:D:132:THR:HB	1:D:137:VAL:HG23	1.98	0.45
1:C:776:ARG:O	1:C:780:THR:HG22	2.16	0.45
1:A:342:ASP:CB	5:A:1032:NDP:C5N	2.94	0.45
1:B:735:THR:N	1:B:793:THR:HG23	2.32	0.45
1:C:267:THR:HG22	1:C:269:ASN:H	1.80	0.45
1:A:12:ILE:O	1:A:15:ILE:HG22	2.16	0.45
1:B:570:PHE:HB3	1:B:636:ILE:HB	1.99	0.45
1:B:859:HIS:CD2	1:B:862:GLY:H	2.19	0.45
1:C:53:GLU:HG2	1:C:54:LYS:N	2.32	0.45
1:D:917:PRO:HA	9:D:2577:HOH:O	2.17	0.45
1:D:362:VAL:HG11	1:D:408:PHE:CE2	2.52	0.45
1:D:342:ASP:HB2	5:D:1032:NDP:C5N	2.47	0.45
9:A:2431:HOH:O	1:B:35:LYS:HE2	2.17	0.45
1:C:457:ASN:HB3	1:C:463:GLU:OE1	2.17	0.45
1:C:820:GLN:O	1:D:962:THR:CG2	2.64	0.45
1:A:796:ILE:HD13	1:A:813:LEU:HB3	1.99	0.45
1:B:845:GLU:HG3	1:B:912:PHE:CD2	2.52	0.45
1:C:410:ARG:HH21	1:D:410:ARG:NE	2.15	0.45
1:D:621:TRP:O	1:D:625:VAL:HG23	2.17	0.45
1:D:934:THR:OG1	1:D:937:GLU:HG3	2.17	0.45
1:A:533:ILE:O	1:A:545:PRO:HD3	2.17	0.44
1:B:759:ARG:HG2	1:B:759:ARG:HH11	1.82	0.44
1:D:19:ASN:OD1	1:D:20:PRO:HD2	2.17	0.44
1:D:242:ASN:ND2	9:D:2215:HOH:O	2.50	0.44
1:A:750:PRO:O	1:A:753:ALA:HB2	2.17	0.44
1:C:552:ALA:HB3	1:C:553:PRO:HD3	2.00	0.44
1:A:783:ARG:NE	9:A:2624:HOH:O	2.49	0.44
1:C:574:LYS:HE3	9:C:2386:HOH:O	2.17	0.44
1:C:572:LEU:HD13	1:C:638:ILE:HB	1.99	0.44
1:A:722:ARG:HD3	1:D:300:ASP:HB3	1.98	0.44
1:D:699:ARG:NE	1:D:699:ARG:HA	2.32	0.44
1:A:140:CYS:HA	2:A:1027:SF4:S3	2.56	0.44
1:A:309:PHE:CE1	1:A:331:ILE:HD11	2.53	0.44
1:A:776:ARG:O	1:A:780:THR:HG22	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:142:LEU:HD23	1:C:142:LEU:HA	1.87	0.44
1:D:140:CYS:HA	2:D:1027:SF4:S3	2.57	0.44
1:D:326:SER:HA	1:D:327:PRO:HD3	1.83	0.44
1:C:132:THR:HB	1:C:137:VAL:HG23	1.99	0.44
1:C:375:GLU:HG2	9:C:2151:HOH:O	2.17	0.44
1:D:703:GLN:HG3	9:D:2461:HOH:O	2.18	0.44
1:A:28:LEU:HD22	1:B:519:PRO:HB3	1.98	0.44
1:A:902:ALA:O	1:A:903:ALA:C	2.55	0.44
1:A:993:LEU:HD23	1:A:993:LEU:C	2.38	0.44
1:D:225:GLY:HA2	4:D:1031:FAD:H3B	2.00	0.44
1:A:146:GLU:HG2	1:B:67:LEU:HD23	2.00	0.44
1:A:771:ARG:N	1:A:772:PRO:CD	2.80	0.44
1:C:644:SER:N	1:C:680:MET:HE2	2.33	0.44
1:A:7:LYS:HE3	9:B:2563:HOH:O	2.17	0.44
1:B:150:ILE:HB	2:B:1027:SF4:S4	2.58	0.44
1:B:793:THR:HB	1:B:814:GLN:HB2	1.99	0.44
1:D:301:GLN:HA	1:D:402:ARG:HA	2.00	0.44
1:D:413:GLN:HA	1:D:418:LYS:O	2.18	0.44
1:B:692:ARG:HD2	9:B:2615:HOH:O	2.18	0.43
1:C:191:ALA:O	1:C:279:ALA:HA	2.18	0.43
1:C:53:GLU:CD	1:C:887:LYS:HB3	2.38	0.43
1:B:570:PHE:CB	1:B:636:ILE:HB	2.48	0.43
1:D:265:GLU:HB3	1:D:266:ILE:H	1.48	0.43
1:D:642:MET:HE3	1:D:675:MET:CE	2.48	0.43
1:C:779:THR:O	1:C:783:ARG:HG3	2.17	0.43
1:D:451:LEU:O	1:D:454:ILE:HG12	2.19	0.43
1:D:900:GLN:HB3	9:D:2570:HOH:O	2.17	0.43
1:B:934:THR:OG1	1:B:937:GLU:HG3	2.18	0.43
1:D:459:TRP:O	1:D:460:ASP:HB2	2.19	0.43
1:A:371:ARG:NH1	1:A:371:ARG:HB2	2.33	0.43
1:B:642:MET:HE2	9:B:2602:HOH:O	2.17	0.43
1:C:427:VAL:HG21	1:D:410:ARG:NH2	2.10	0.43
1:C:915:LYS:HG3	9:C:2560:HOH:O	2.19	0.43
1:C:993:LEU:C	1:C:993:LEU:HD23	2.39	0.43
1:D:570:PHE:HB3	1:D:636:ILE:HB	2.00	0.43
1:B:219:LYS:HG3	1:B:260:SER:OG	2.19	0.43
1:B:373:VAL:HG22	1:B:376:GLU:H	1.84	0.43
1:C:771:ARG:N	1:C:772:PRO:CD	2.82	0.43
1:C:793:THR:HB	1:C:814:GLN:HB2	2.00	0.43
1:D:759:ARG:NH1	1:D:759:ARG:HG2	2.33	0.43
1:A:570:PHE:HB3	1:A:636:ILE:HB	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:LYS:HE2	9:B:2259:HOH:O	2.19	0.43
1:A:905:PRO:HA	1:A:906:PRO:HD3	1.92	0.43
1:B:201:SER:HB2	1:B:493:VAL:HG13	2.00	0.43
1:C:140:CYS:HA	2:C:1027:SF4:S3	2.59	0.43
1:C:342:ASP:CB	5:C:1032:NDP:C5N	2.97	0.43
1:C:677:GLU:CD	1:D:934:THR:HB	2.39	0.43
1:B:847:GLN:HG2	9:B:2706:HOH:O	2.19	0.43
1:D:998:ILE:HB	1:D:1001:CYS:HB2	2.01	0.43
1:A:675:MET:HE1	1:A:678:ARG:HD2	2.00	0.42
1:B:859:HIS:HA	1:B:865:VAL:HG23	2.01	0.42
1:B:993:LEU:HD23	1:B:993:LEU:C	2.39	0.42
1:D:779:THR:O	1:D:783:ARG:HG3	2.19	0.42
1:C:342:ASP:HB2	5:C:1032:NDP:C5N	2.50	0.42
1:C:675:MET:HE1	1:C:678:ARG:HD3	2.00	0.42
1:D:734:ALA:HA	1:D:735:THR:HA	1.71	0.42
1:A:342:ASP:HB3	5:A:1032:NDP:C4N	2.41	0.42
1:B:670:SER:N	9:B:2602:HOH:O	2.52	0.42
1:C:378:GLU:O	1:C:382:GLU:CG	2.66	0.42
1:D:533:ILE:O	1:D:545:PRO:HD3	2.18	0.42
1:A:916:LYS:HB2	1:A:917:PRO:HD2	2.01	0.42
1:B:88:GLN:HG3	1:B:95:LEU:O	2.19	0.42
1:C:577:SER:HB2	9:C:2405:HOH:O	2.19	0.42
1:C:893:GLU:O	1:C:897:LEU:HG	2.19	0.42
1:D:97:ILE:HA	1:D:100:PHE:CD2	2.53	0.42
1:D:613:ILE:HD13	1:D:642:MET:HE2	2.01	0.42
1:B:342:ASP:CB	5:B:1032:NDP:C5N	2.97	0.42
1:B:644:SER:N	1:B:680:MET:HE2	2.35	0.42
1:C:90:SER:HB2	1:C:136:CYS:HA	2.00	0.42
1:C:267:THR:HG21	9:C:2320:HOH:O	2.20	0.42
1:C:570:PHE:HB3	1:C:636:ILE:HB	2.01	0.42
1:D:319:ALA:HB2	1:D:904:PHE:CB	2.49	0.42
1:B:311:PRO:O	1:B:315:LYS:HG3	2.20	0.42
1:C:150:ILE:HB	2:C:1027:SF4:S4	2.60	0.42
1:C:642:MET:HE3	1:C:675:MET:CE	2.49	0.42
1:B:541:LYS:HB3	9:B:2499:HOH:O	2.19	0.42
1:B:682:LEU:O	1:B:683:ALA:C	2.58	0.42
1:B:705:PRO:HA	1:B:730:ASP:OD2	2.20	0.42
1:C:877:PRO:CG	1:C:977:THR:HB	2.48	0.42
1:D:132:THR:HB	1:D:137:VAL:CG2	2.49	0.42
1:D:711:THR:CG2	9:D:2454:HOH:O	2.58	0.42
1:D:836:ALA:O	1:D:840:LEU:HG	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:367:PHE:HB2	1:B:386:GLU:OE1	2.20	0.42
1:A:836:ALA:O	1:A:840:LEU:HG	2.19	0.42
1:C:699:ARG:NE	1:C:699:ARG:HA	2.33	0.42
1:C:771:ARG:HD2	9:D:2384:HOH:O	2.18	0.42
1:D:342:ASP:CB	5:D:1032:NDP:C5N	2.98	0.42
1:D:150:ILE:HB	2:D:1027:SF4:S4	2.60	0.42
1:B:100:PHE:CD1	1:B:100:PHE:C	2.93	0.42
1:B:671:CYS:SG	1:B:673:HIS:O	2.78	0.42
1:C:262:SER:CB	1:C:264:ASN:ND2	2.83	0.42
1:C:64:HIS:CE1	1:C:382:GLU:OE2	2.73	0.42
1:B:442:LEU:HD22	1:B:482:ILE:CD1	2.48	0.41
1:C:342:ASP:HB3	5:C:1032:NDP:C4N	2.43	0.41
1:D:574:LYS:HE3	9:D:2358:HOH:O	2.20	0.41
1:A:97:ILE:HD11	2:A:1026:SF4:S4	2.60	0.41
1:A:142:LEU:HD12	1:A:150:ILE:HG12	2.02	0.41
1:A:297:LEU:HA	1:A:301:GLN:OE1	2.21	0.41
1:B:647:LYS:O	1:B:651:MET:HG3	2.20	0.41
1:D:164:LYS:O	1:D:909:ARG:NH2	2.53	0.41
1:C:935:PHE:CE2	1:D:612:LEU:HD11	2.55	0.41
1:A:962:THR:OG1	1:A:995:VAL:HG21	2.20	0.41
1:B:106:ASN:O	1:B:107:LYS:HB2	2.20	0.41
1:B:142:LEU:HA	1:B:142:LEU:HD23	1.87	0.41
1:C:116:ILE:HD13	1:C:156:GLN:HG3	2.02	0.41
1:C:541:LYS:HD3	9:C:2096:HOH:O	2.20	0.41
1:C:816:CYS:HB3	3:C:1030:FMN:O1P	2.20	0.41
1:D:261:LEU:HD21	1:D:451:LEU:HD21	2.00	0.41
1:D:44:ASN:HB2	1:D:45:PRO:HD2	2.02	0.41
1:D:900:GLN:C	1:D:902:ALA:H	2.23	0.41
1:B:49:CYS:SG	1:B:51:HIS:CE1	3.13	0.41
1:C:375:GLU:CD	1:C:375:GLU:H	2.23	0.41
1:D:243:PHE:HD1	1:D:909:ARG:HE	1.68	0.41
1:D:910:LYS:HA	1:D:911:PRO:HD3	1.93	0.41
1:A:241:VAL:O	1:A:245:ILE:HG12	2.21	0.41
1:A:651:MET:HG2	1:A:701:ALA:HB2	2.02	0.41
1:D:126:CYS:HB3	1:D:130:CYS:SG	2.61	0.41
1:D:124:LEU:HG	1:D:240:VAL:HG13	2.03	0.41
1:D:402:ARG:HG3	9:D:2286:HOH:O	2.20	0.41
1:A:691:VAL:HG21	1:A:720:ILE:CG2	2.50	0.41
1:B:452:SER:HA	1:B:453:PRO:HA	1.87	0.41
1:B:644:SER:HA	1:B:680:MET:HG2	2.03	0.41
1:C:831:CYS:O	1:C:835:LYS:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:672:PRO:HG3	1:A:737:THR:OG1	2.21	0.41
1:A:709:LYS:HA	1:A:733:THR:HB	2.03	0.41
1:C:589:ARG:O	1:C:609:ASN:HA	2.21	0.41
1:D:331:ILE:HG23	1:D:433:VAL:HG21	2.02	0.41
1:B:845:GLU:H	1:B:845:GLU:CD	2.21	0.41
1:C:132:THR:HB	1:C:137:VAL:CG2	2.49	0.41
1:D:319:ALA:CB	1:D:904:PHE:CB	2.90	0.41
1:A:371:ARG:HB2	1:A:371:ARG:HH11	1.86	0.41
1:B:100:PHE:O	1:B:104:ILE:HG13	2.21	0.41
1:B:911:PRO:HG2	9:B:2760:HOH:O	2.21	0.41
1:C:264:ASN:N	1:C:264:ASN:HD22	1.95	0.41
1:C:28:LEU:HD22	1:D:519:PRO:HB3	2.03	0.41
1:D:403:ILE:HG12	1:D:404:VAL:N	2.36	0.41
1:A:489:THR:O	1:A:493:VAL:HG23	2.20	0.41
1:A:18:LEU:HD11	1:A:975:PRO:HB3	2.02	0.41
1:C:413:GLN:HA	1:C:418:LYS:O	2.21	0.41
1:C:44:ASN:HB2	1:C:45:PRO:HD2	2.02	0.41
1:C:921:ILE:O	1:C:925:ILE:HG13	2.21	0.41
1:D:692:ARG:HG2	9:D:2458:HOH:O	2.20	0.41
1:A:722:ARG:O	1:A:726:GLU:HG3	2.21	0.41
1:B:671:CYS:O	1:B:682:LEU:HG	2.22	0.41
1:A:762:TYR:CE1	1:B:780:THR:HG22	2.55	0.41
1:C:309:PHE:CE1	1:C:331:ILE:HD11	2.56	0.41
1:A:703:GLN:HG3	9:A:2578:HOH:O	2.20	0.40
1:A:83:ALA:O	1:A:84:ASP:C	2.59	0.40
1:B:225:GLY:HA2	4:B:1031:FAD:H3B	2.04	0.40
1:B:776:ARG:NE	9:B:2663:HOH:O	2.53	0.40
1:B:807:HIS:HB3	1:B:928:ALA:HB2	2.02	0.40
1:C:124:LEU:HD13	1:C:160:SER:HB2	2.03	0.40
1:D:193:LEU:HD22	1:D:193:LEU:N	2.36	0.40
1:D:403:ILE:HD13	1:D:434:VAL:HG23	2.01	0.40
1:C:410:ARG:NH1	1:D:427:VAL:CG2	2.68	0.40
1:D:911:PRO:HG2	9:D:2220:HOH:O	2.20	0.40
1:C:248:MET:CE	1:C:255:ILE:HD11	2.51	0.40
1:A:124:LEU:HG	1:A:240:VAL:HG13	2.02	0.40
1:B:193:LEU:HD22	1:B:193:LEU:N	2.36	0.40
1:B:87:CYS:SG	1:B:97:ILE:HD12	2.61	0.40
1:D:577:SER:HB2	9:D:2415:HOH:O	2.21	0.40
1:C:297:LEU:HA	1:C:301:GLN:OE1	2.20	0.40
1:C:682:LEU:CD1	1:C:711:THR:HG21	2.51	0.40
1:D:311:PRO:O	1:D:315:LYS:HG3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:410:ARG:NH1	1:D:410:ARG:CG	2.76	0.40
1:D:518:LYS:O	1:D:520:GLU:HG3	2.21	0.40
1:C:489:THR:O	1:C:493:VAL:HG23	2.21	0.40
1:D:152:ILE:HD11	2:D:1027:SF4:S4	2.62	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1017/1025 (99%)	974 (96%)	40 (4%)	3 (0%)	41	46
1	B	1008/1025 (98%)	961 (95%)	45 (4%)	2 (0%)	47	55
1	C	1011/1025 (99%)	973 (96%)	36 (4%)	2 (0%)	47	55
1	D	1017/1025 (99%)	968 (95%)	48 (5%)	1 (0%)	51	60
All	All	4053/4100 (99%)	3876 (96%)	169 (4%)	8 (0%)	47	55

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	53	GLU
1	A	53	GLU
1	A	906	PRO
1	C	674	GLY
1	B	3	PRO
1	D	902	ALA
1	A	674	GLY
1	C	794	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	848/854 (99%)	840 (99%)	8 (1%)	78	86
1	B	843/854 (99%)	830 (98%)	13 (2%)	65	75
1	C	845/854 (99%)	830 (98%)	15 (2%)	59	68
1	D	848/854 (99%)	830 (98%)	18 (2%)	53	62
All	All	3384/3416 (99%)	3330 (98%)	54 (2%)	62	73

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	GLU
1	A	100	PHE
1	A	265	GLU
1	A	367	PHE
1	A	373	VAL
1	A	453	PRO
1	A	793	THR
1	A	800	GLU
1	B	100	PHE
1	B	292	ASP
1	B	367	PHE
1	B	368	VAL
1	B	373	VAL
1	B	394	ARG
1	B	426	ILE
1	B	453	PRO
1	B	599	MET
1	B	793	THR
1	B	800	GLU
1	B	916	LYS
1	B	984	ASP
1	C	100	PHE
1	C	184	GLU
1	C	264	ASN

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Mol	Chain	Res	Type
1	C	330	SER
1	C	367	PHE
1	C	373	VAL
1	C	382	GLU
1	C	453	PRO
1	C	667	LEU
1	C	678	ARG
1	C	703	GLN
1	C	793	THR
1	C	800	GLU
1	C	955	ASN
1	C	1009	THR
1	D	11	ASP
1	D	15	ILE
1	D	100	PHE
1	D	179	GLN
1	D	263	GLU
1	D	293	ILE
1	D	358	ARG
1	D	367	PHE
1	D	373	VAL
1	D	376	GLU
1	D	410	ARG
1	D	428	HIS
1	D	453	PRO
1	D	680	MET
1	D	741	LEU
1	D	793	THR
1	D	800	GLU
1	D	955	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	847	GLN
1	A	900	GLN
1	B	51	HIS
1	B	64	HIS
1	B	269	ASN
1	B	407	GLN
1	B	487	ASN
1	B	673	HIS

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Mol	Chain	Res	Type
1	B	859	HIS
1	C	64	HIS
1	C	170	GLN
1	C	264	ASN
1	C	487	ASN
1	C	859	HIS
1	D	269	ASN
1	D	487	ASN
1	D	686	GLN

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 carbohydrates 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	$\#\|Z\| > 2$
3	FMN	B	1030	-	31,33,33	3.08	10 (32%)	40,50,50	3.67	14 (35%)
5	NDP	B	1032	-	45,52,52	1.60	7 (15%)	53,80,80	1.59	10 (18%)
3	FMN	A	1030	-	31,33,33	3.11	11 (35%)	40,50,50	3.62	13 (32%)
2	SF4	D	1026	-	0,12,12	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	SF4	C	1027	-	0,12,12	0.00	-	-		
6	IDH	B	1034	-	6,9,9	1.87	2 (33%)	10,12,12	2.35	4 (40%)
2	SF4	A	1026	-	0,12,12	0.00	-	-		
4	FAD	B	1031	-	51,58,58	2.62	19 (37%)	60,89,89	1.77	10 (16%)
4	FAD	C	1031	-	51,58,58	2.58	21 (41%)	60,89,89	1.75	8 (13%)
2	SF4	A	1029	-	0,12,12	0.00	-	-		
2	SF4	D	1028	-	0,12,12	0.00	-	-		
5	NDP	D	1032	-	45,52,52	1.61	6 (13%)	53,80,80	1.59	10 (18%)
2	SF4	C	1026	-	0,12,12	0.00	-	-		
7	IUR	C	1034	-	7,9,9	1.53	1 (14%)	6,12,12	10.95	5 (83%)
5	NDP	A	1032	-	45,52,52	1.61	7 (15%)	53,80,80	1.59	10 (18%)
6	IDH	A	1033	1	8,8,9	2.23	3 (37%)	9,10,12	1.18	0
2	SF4	B	1026	-	0,12,12	0.00	-	-		
2	SF4	C	1028	-	0,12,12	0.00	-	-		
2	SF4	A	1028	-	0,12,12	0.00	-	-		
2	SF4	B	1027	-	0,12,12	0.00	-	-		
2	SF4	B	1029	-	0,12,12	0.00	-	-		
2	SF4	D	1029	-	0,12,12	0.00	-	-		
4	FAD	D	1031	-	51,58,58	2.64	20 (39%)	60,89,89	1.77	10 (16%)
3	FMN	D	1030	-	31,33,33	3.06	10 (32%)	40,50,50	3.61	14 (35%)
3	FMN	C	1030	-	31,33,33	3.13	11 (35%)	40,50,50	3.63	13 (32%)
2	SF4	A	1027	-	0,12,12	0.00	-	-		
2	SF4	C	1029	-	0,12,12	0.00	-	-		
2	SF4	D	1027	-	0,12,12	0.00	-	-		
8	URA	D	1034	-	6,8,8	2.24	2 (33%)	4,10,10	11.54	3 (75%)
2	SF4	B	1028	-	0,12,12	0.00	-	-		
5	NDP	C	1032	-	45,52,52	1.61	8 (17%)	53,80,80	1.57	10 (18%)
4	FAD	A	1031	-	51,58,58	2.56	22 (43%)	60,89,89	1.72	9 (15%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FMN	B	1030	-	-	1/18/18/18	0/3/3/3
5	NDP	B	1032	-	-	5/30/77/77	0/5/5/5
3	FMN	A	1030	-	-	1/18/18/18	0/3/3/3
2	SF4	D	1026	-	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SF4	C	1027	-	-	-	0/6/5/5
6	IDH	B	1034	-	-	-	0/1/1/1
2	SF4	A	1026	-	-	-	0/6/5/5
5	NDP	D	1032	-	-	6/30/77/77	0/5/5/5
4	FAD	C	1031	-	-	4/30/50/50	0/6/6/6
2	SF4	A	1029	-	-	-	0/6/5/5
2	SF4	D	1028	-	-	-	0/6/5/5
4	FAD	B	1031	-	-	6/30/50/50	0/6/6/6
2	SF4	C	1026	-	-	-	0/6/5/5
7	IUR	C	1034	-	-	-	0/1/1/1
5	NDP	A	1032	-	-	6/30/77/77	0/5/5/5
6	IDH	A	1033	1	-	-	0/1/1/1
2	SF4	B	1026	-	-	-	0/6/5/5
2	SF4	C	1028	-	-	-	0/6/5/5
2	SF4	A	1028	-	-	-	0/6/5/5
2	SF4	B	1027	-	-	-	0/6/5/5
2	SF4	B	1029	-	-	-	0/6/5/5
2	SF4	D	1029	-	-	-	0/6/5/5
4	FAD	D	1031	-	-	4/30/50/50	0/6/6/6
3	FMN	D	1030	-	-	1/18/18/18	0/3/3/3
3	FMN	C	1030	-	-	1/18/18/18	0/3/3/3
2	SF4	A	1027	-	-	-	0/6/5/5
2	SF4	C	1029	-	-	-	0/6/5/5
2	SF4	D	1027	-	-	-	0/6/5/5
8	URA	D	1034	-	-	-	0/1/1/1
2	SF4	B	1028	-	-	-	0/6/5/5
5	NDP	C	1032	-	-	5/30/77/77	0/5/5/5
4	FAD	A	1031	-	-	4/30/50/50	0/6/6/6

All (160) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1031	FAD	C4X-C10	9.96	1.48	1.38
4	B	1031	FAD	C4X-C10	9.77	1.48	1.38
4	A	1031	FAD	C4X-C10	9.38	1.48	1.38
4	C	1031	FAD	C4X-C10	9.28	1.48	1.38
3	B	1030	FMN	C1'-N10	-9.24	1.38	1.48
3	A	1030	FMN	C1'-N10	-9.02	1.39	1.48
3	D	1030	FMN	C1'-N10	-8.71	1.39	1.48
3	C	1030	FMN	C1'-N10	-8.68	1.39	1.48
3	C	1030	FMN	C4A-C10	6.77	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1031	FAD	C9A-N10	6.66	1.47	1.38
4	C	1031	FAD	C9A-N10	6.64	1.47	1.38
4	B	1031	FAD	C9A-N10	6.64	1.47	1.38
3	A	1030	FMN	C4A-C10	6.62	1.45	1.38
4	A	1031	FAD	C9A-N10	6.43	1.47	1.38
3	B	1030	FMN	C4A-C10	6.25	1.45	1.38
3	D	1030	FMN	C4A-C10	6.11	1.44	1.38
3	C	1030	FMN	C9A-N10	6.08	1.46	1.38
3	B	1030	FMN	C9A-N10	5.99	1.46	1.38
3	D	1030	FMN	C9A-N10	5.76	1.46	1.38
3	A	1030	FMN	C9A-N10	5.69	1.46	1.38
3	C	1030	FMN	C4-N3	5.27	1.42	1.33
3	C	1030	FMN	C4A-N5	5.13	1.40	1.33
3	A	1030	FMN	C4A-N5	5.11	1.40	1.33
3	D	1030	FMN	C4A-N5	5.11	1.40	1.33
5	B	1032	NDP	C4N-C3N	-5.01	1.40	1.49
3	D	1030	FMN	C4-N3	4.99	1.41	1.33
3	A	1030	FMN	C4-N3	4.95	1.41	1.33
3	B	1030	FMN	C4-N3	4.93	1.41	1.33
5	D	1032	NDP	C4N-C3N	-4.84	1.40	1.49
5	A	1032	NDP	C4N-C3N	-4.84	1.40	1.49
5	C	1032	NDP	C4N-C3N	-4.83	1.40	1.49
8	D	1034	URA	C4-N3	4.77	1.41	1.33
3	B	1030	FMN	C4A-N5	4.69	1.40	1.33
4	D	1031	FAD	O4B-C1B	4.62	1.47	1.41
4	A	1031	FAD	O4B-C1B	4.24	1.47	1.41
5	B	1032	NDP	C4N-C5N	-4.24	1.37	1.48
3	C	1030	FMN	C7M-C7	4.23	1.59	1.51
5	C	1032	NDP	C4N-C5N	-4.21	1.37	1.48
4	C	1031	FAD	O4B-C1B	4.21	1.47	1.41
3	C	1030	FMN	C4-C4A	4.17	1.48	1.41
4	B	1031	FAD	PA-O2A	-4.17	1.35	1.55
4	A	1031	FAD	C4-N3	4.17	1.40	1.33
5	A	1032	NDP	C4N-C5N	-4.17	1.38	1.48
5	D	1032	NDP	C4N-C5N	-4.14	1.38	1.48
3	A	1030	FMN	C7M-C7	4.10	1.59	1.51
3	A	1030	FMN	C4-C4A	4.09	1.48	1.41
4	B	1031	FAD	C4-N3	4.09	1.40	1.33
4	D	1031	FAD	PA-O2A	-4.03	1.36	1.55
4	C	1031	FAD	C4-N3	4.02	1.40	1.33
4	A	1031	FAD	PA-O2A	-4.01	1.36	1.55
3	D	1030	FMN	C7M-C7	4.01	1.59	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1030	FMN	C4-C4A	4.00	1.48	1.41
4	C	1031	FAD	PA-O2A	-3.98	1.36	1.55
3	B	1030	FMN	C4-C4A	3.97	1.48	1.41
3	B	1030	FMN	C7M-C7	3.94	1.58	1.51
4	D	1031	FAD	C4-N3	3.90	1.39	1.33
4	D	1031	FAD	C4-C4X	3.88	1.48	1.41
4	C	1031	FAD	C4-C4X	3.84	1.48	1.41
6	A	1033	IDH	O2-C2	3.82	1.31	1.23
4	B	1031	FAD	C4-C4X	3.79	1.47	1.41
4	B	1031	FAD	O4B-C1B	3.77	1.46	1.41
5	D	1032	NDP	C2N-C3N	3.76	1.45	1.34
4	D	1031	FAD	C10-N1	3.74	1.38	1.33
6	A	1033	IDH	O4-C4	3.71	1.30	1.23
5	A	1032	NDP	C2N-C3N	3.70	1.45	1.34
5	B	1032	NDP	C2N-C3N	3.68	1.45	1.34
5	C	1032	NDP	C2N-C3N	3.68	1.45	1.34
4	D	1031	FAD	C4X-N5	3.58	1.38	1.33
4	B	1031	FAD	C10-N1	3.52	1.37	1.33
4	B	1031	FAD	C4X-N5	3.45	1.38	1.33
4	B	1031	FAD	P-O2P	-3.43	1.39	1.55
4	A	1031	FAD	C10-N1	3.41	1.37	1.33
3	A	1030	FMN	C10-N1	3.41	1.37	1.33
3	D	1030	FMN	C4'-C3'	3.39	1.59	1.53
4	C	1031	FAD	P-O2P	-3.38	1.39	1.55
3	D	1030	FMN	C10-N1	3.36	1.37	1.33
3	A	1030	FMN	C4'-C3'	3.31	1.59	1.53
4	C	1031	FAD	C10-N1	3.30	1.37	1.33
4	A	1031	FAD	P-O2P	-3.29	1.39	1.55
3	C	1030	FMN	C4'-C3'	3.29	1.59	1.53
4	C	1031	FAD	C4X-N5	3.27	1.38	1.33
4	D	1031	FAD	P-O2P	-3.26	1.40	1.55
3	C	1030	FMN	C10-N1	3.23	1.37	1.33
4	A	1031	FAD	C4X-N5	3.23	1.38	1.33
3	B	1030	FMN	C10-N1	3.22	1.37	1.33
4	A	1031	FAD	C4-C4X	3.20	1.46	1.41
4	B	1031	FAD	C8-C7	3.10	1.48	1.40
7	C	1034	IUR	C4-N3	3.09	1.38	1.33
4	A	1031	FAD	C2-N3	3.03	1.44	1.38
4	A	1031	FAD	C8-C7	3.02	1.48	1.40
4	C	1031	FAD	C8-C7	2.99	1.48	1.40
4	C	1031	FAD	O5'-C5'	2.97	1.56	1.44
4	A	1031	FAD	O5'-C5'	2.96	1.56	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1030	FMN	C5A-N5	2.96	1.40	1.35
3	B	1030	FMN	C4'-C3'	2.95	1.59	1.53
3	D	1030	FMN	C5A-N5	2.91	1.40	1.35
4	D	1031	FAD	C8-C7	2.89	1.48	1.40
3	C	1030	FMN	C5A-N5	2.89	1.40	1.35
4	C	1031	FAD	C2-N3	2.87	1.43	1.38
4	B	1031	FAD	C4A-N3A	2.85	1.39	1.35
4	B	1031	FAD	C2-N3	2.84	1.43	1.38
4	D	1031	FAD	C2A-N3A	2.83	1.36	1.32
4	B	1031	FAD	O5'-C5'	2.80	1.55	1.44
4	C	1031	FAD	C2B-C1B	-2.79	1.49	1.53
3	B	1030	FMN	C5A-N5	2.77	1.39	1.35
4	B	1031	FAD	C2A-N1A	2.76	1.39	1.33
4	D	1031	FAD	O5'-C5'	2.74	1.55	1.44
4	D	1031	FAD	O4B-C4B	2.74	1.51	1.45
6	B	1034	IDH	C6-N1	2.72	1.49	1.46
4	D	1031	FAD	C2-N3	2.71	1.43	1.38
4	C	1031	FAD	C2A-N3A	2.71	1.36	1.32
4	C	1031	FAD	O4B-C4B	2.69	1.51	1.45
4	A	1031	FAD	O4B-C4B	2.68	1.51	1.45
4	A	1031	FAD	C4A-N3A	2.68	1.39	1.35
4	B	1031	FAD	O4B-C4B	2.66	1.51	1.45
4	A	1031	FAD	C2A-N3A	2.65	1.36	1.32
4	C	1031	FAD	C5X-N5	2.63	1.39	1.35
4	D	1031	FAD	C2A-N1A	2.60	1.38	1.33
4	B	1031	FAD	C2A-N3A	2.60	1.36	1.32
6	B	1034	IDH	O4-C4	-2.60	1.18	1.23
4	C	1031	FAD	C4A-N3A	2.55	1.39	1.35
4	B	1031	FAD	C5X-N5	2.54	1.39	1.35
4	D	1031	FAD	C4A-N3A	2.51	1.39	1.35
4	A	1031	FAD	C2A-N1A	2.50	1.38	1.33
4	B	1031	FAD	C2B-C1B	-2.46	1.50	1.53
5	A	1032	NDP	C4A-N3A	2.46	1.39	1.35
5	D	1032	NDP	C4A-N3A	2.42	1.39	1.35
4	C	1031	FAD	C2A-N1A	2.40	1.38	1.33
5	A	1032	NDP	C6N-C5N	2.36	1.37	1.33
5	C	1032	NDP	C6N-C5N	2.35	1.37	1.33
5	D	1032	NDP	C6N-C5N	2.35	1.37	1.33
4	D	1031	FAD	C5X-N5	2.34	1.39	1.35
5	C	1032	NDP	C4A-N3A	2.33	1.38	1.35
4	A	1031	FAD	C2B-C1B	-2.30	1.50	1.53
6	A	1033	IDH	C5-C4	2.29	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1032	NDP	C5D-C4D	2.29	1.58	1.51
5	B	1032	NDP	C6N-C5N	2.27	1.37	1.33
4	A	1031	FAD	C5X-N5	2.25	1.39	1.35
5	A	1032	NDP	C5D-C4D	2.24	1.58	1.51
4	A	1031	FAD	C2-N1	-2.24	1.33	1.38
5	B	1032	NDP	C5D-C4D	2.15	1.58	1.51
5	C	1032	NDP	O4B-C1B	2.14	1.44	1.41
5	C	1032	NDP	P2B-O2B	-2.13	1.55	1.59
5	B	1032	NDP	C4A-N3A	2.12	1.38	1.35
5	D	1032	NDP	C5D-C4D	2.10	1.58	1.51
3	C	1030	FMN	C6-C7	2.09	1.43	1.37
4	B	1031	FAD	C5B-C4B	2.08	1.58	1.51
5	B	1032	NDP	PA-O1A	-2.08	1.43	1.50
4	D	1031	FAD	P-O5'	-2.08	1.50	1.59
3	A	1030	FMN	C6-C7	2.08	1.43	1.37
4	D	1031	FAD	PA-O5B	-2.07	1.50	1.59
5	A	1032	NDP	P2B-O2B	-2.06	1.55	1.59
4	C	1031	FAD	PA-O5B	-2.05	1.51	1.59
4	A	1031	FAD	C9-C8	2.05	1.42	1.37
8	D	1034	URA	C6-N1	2.04	1.38	1.34
4	C	1031	FAD	C2-N1	-2.03	1.34	1.38
4	A	1031	FAD	C5B-C4B	2.03	1.57	1.51
4	D	1031	FAD	C2B-C1B	-2.02	1.50	1.53
4	A	1031	FAD	C3B-C4B	2.00	1.58	1.53
4	C	1031	FAD	C5B-C4B	2.00	1.57	1.51

All (143) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	C	1034	IUR	N1-C2-N3	-18.61	113.64	128.43
7	C	1034	IUR	C4-N3-C2	17.39	129.82	115.14
8	D	1034	URA	N1-C2-N3	-16.90	114.99	128.43
3	B	1030	FMN	C4-N3-C2	15.95	128.61	115.14
3	A	1030	FMN	C4-N3-C2	15.75	128.44	115.14
3	D	1030	FMN	C4-N3-C2	15.51	128.24	115.14
3	C	1030	FMN	C4-N3-C2	15.46	128.19	115.14
8	D	1034	URA	C6-N1-C2	14.61	121.62	114.42
3	B	1030	FMN	C4A-C4-N3	-9.60	110.30	123.43
3	A	1030	FMN	C4A-C4-N3	-9.55	110.37	123.43
3	C	1030	FMN	C4A-C4-N3	-9.52	110.41	123.43
3	D	1030	FMN	C4A-C4-N3	-9.42	110.55	123.43
4	D	1031	FAD	C4-N3-C2	8.09	121.98	115.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	1031	FAD	C4-N3-C2	7.98	121.88	115.14
4	C	1031	FAD	C4-N3-C2	7.78	121.71	115.14
4	A	1031	FAD	C4-N3-C2	7.67	121.62	115.14
7	C	1034	IUR	C5-C4-N3	-7.44	113.32	123.27
3	D	1030	FMN	C4-C4A-C10	6.47	124.23	119.95
3	A	1030	FMN	C4-C4A-C10	6.38	124.17	119.95
3	C	1030	FMN	C4-C4A-C10	6.29	124.12	119.95
3	B	1030	FMN	C4-C4A-C10	6.23	124.07	119.95
3	C	1030	FMN	C1'-N10-C9A	5.91	122.94	118.29
3	B	1030	FMN	C1'-N10-C9A	5.70	122.78	118.29
3	D	1030	FMN	C1'-N10-C9A	5.70	122.78	118.29
8	D	1034	URA	C5-C4-N3	-5.60	111.00	123.31
3	A	1030	FMN	C1'-N10-C9A	5.46	122.59	118.29
5	B	1032	NDP	PN-O3-PA	5.20	150.68	132.83
5	D	1032	NDP	PN-O3-PA	5.15	150.51	132.83
5	A	1032	NDP	PN-O3-PA	5.09	150.31	132.83
5	C	1032	NDP	PN-O3-PA	5.03	150.09	132.83
6	B	1034	IDH	C4-N3-C2	-4.81	119.81	126.25
5	A	1032	NDP	C3N-C2N-N1N	-4.77	116.28	123.10
5	B	1032	NDP	C3N-C2N-N1N	-4.76	116.30	123.10
5	C	1032	NDP	C3N-C2N-N1N	-4.72	116.36	123.10
5	D	1032	NDP	C3N-C2N-N1N	-4.67	116.43	123.10
4	B	1031	FAD	C4X-C4-N3	-4.61	117.13	123.43
4	C	1031	FAD	C4X-C4-N3	-4.56	117.19	123.43
4	D	1031	FAD	C4X-C4-N3	-4.51	117.26	123.43
4	A	1031	FAD	C4X-C4-N3	-4.48	117.30	123.43
6	B	1034	IDH	C5-C4-N3	4.09	121.76	116.19
3	A	1030	FMN	O4'-C4'-C3'	4.06	118.97	109.10
3	B	1030	FMN	O4'-C4'-C3'	3.97	118.75	109.10
3	D	1030	FMN	C4A-N5-C5A	3.91	120.68	116.77
3	C	1030	FMN	O3'-C3'-C2'	-3.85	99.51	108.81
4	D	1031	FAD	C4-C4X-C10	-3.84	117.41	119.95
3	B	1030	FMN	O3'-C3'-C2'	-3.79	99.65	108.81
3	D	1030	FMN	O4'-C4'-C3'	3.79	118.31	109.10
4	B	1031	FAD	C4-C4X-C10	-3.76	117.46	119.95
3	C	1030	FMN	O4'-C4'-C3'	3.73	118.17	109.10
3	B	1030	FMN	C4A-N5-C5A	3.72	120.49	116.77
3	C	1030	FMN	O2'-C2'-C1'	3.71	118.51	109.59
4	C	1031	FAD	C4-C4X-C10	-3.70	117.50	119.95
3	A	1030	FMN	C4A-N5-C5A	3.66	120.43	116.77
4	A	1031	FAD	C4-C4X-C10	-3.66	117.53	119.95
3	C	1030	FMN	C4A-N5-C5A	3.64	120.41	116.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	1032	NDP	C1D-N1N-C2N	-3.60	115.12	121.11
5	B	1032	NDP	C1D-N1N-C2N	-3.58	115.14	121.11
5	A	1032	NDP	C1D-N1N-C2N	-3.51	115.27	121.11
4	A	1031	FAD	O2A-PA-O1A	3.49	129.48	112.24
3	D	1030	FMN	O3'-C3'-C2'	-3.48	100.39	108.81
4	D	1031	FAD	O2A-PA-O1A	3.48	129.44	112.24
5	C	1032	NDP	C1D-N1N-C2N	-3.45	115.37	121.11
4	B	1031	FAD	O2A-PA-O1A	3.44	129.26	112.24
4	C	1031	FAD	O2A-PA-O1A	3.43	129.19	112.24
3	B	1030	FMN	O2'-C2'-C1'	3.41	117.80	109.59
3	D	1030	FMN	O2'-C2'-C1'	3.40	117.78	109.59
3	D	1030	FMN	P-O5'-C5'	3.39	127.63	118.30
3	A	1030	FMN	O3'-C3'-C2'	-3.34	100.74	108.81
3	A	1030	FMN	O2'-C2'-C1'	3.33	117.61	109.59
3	C	1030	FMN	P-O5'-C5'	3.32	127.43	118.30
3	B	1030	FMN	P-O5'-C5'	3.30	127.38	118.30
3	A	1030	FMN	P-O5'-C5'	3.20	127.11	118.30
3	B	1030	FMN	C5'-C4'-C3'	-3.07	106.27	112.20
4	C	1031	FAD	C5X-C9A-N10	-3.02	115.53	117.72
3	C	1030	FMN	C5'-C4'-C3'	-3.01	106.39	112.20
3	B	1030	FMN	C4-C4A-N5	-2.97	115.20	118.60
3	A	1030	FMN	C5'-C4'-C3'	-2.94	106.53	112.20
7	C	1034	IUR	C6-N1-C2	2.86	120.08	115.36
3	D	1030	FMN	C5'-C4'-C3'	-2.83	106.73	112.20
3	C	1030	FMN	C4-C4A-N5	-2.83	115.36	118.60
4	A	1031	FAD	C5X-C9A-N10	-2.82	115.67	117.72
3	D	1030	FMN	C4-C4A-N5	-2.81	115.39	118.60
3	A	1030	FMN	C4-C4A-N5	-2.79	115.40	118.60
4	D	1031	FAD	C5X-C9A-N10	-2.79	115.69	117.72
4	B	1031	FAD	C5X-C9A-N10	-2.69	115.77	117.72
5	D	1032	NDP	O7N-C7N-N7N	-2.60	116.79	122.88
5	B	1032	NDP	O7N-C7N-N7N	-2.56	116.89	122.88
5	C	1032	NDP	O5B-C5B-C4B	-2.56	100.19	108.99
5	C	1032	NDP	O7N-C7N-N7N	-2.54	116.94	122.88
7	C	1034	IUR	C6-C5-I5	2.53	122.45	118.68
3	D	1030	FMN	O3'-C3'-C4'	2.49	114.84	108.81
5	A	1032	NDP	O7N-C7N-N7N	-2.49	117.06	122.88
5	D	1032	NDP	O5B-C5B-C4B	-2.44	100.60	108.99
6	B	1034	IDH	N3-C2-N1	2.44	119.46	116.61
5	A	1032	NDP	O2A-PA-O1A	2.43	124.28	112.24
5	A	1032	NDP	O5B-C5B-C4B	-2.42	100.67	108.99
3	C	1030	FMN	O3'-C3'-C4'	2.41	114.63	108.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	1032	NDP	O5B-C5B-C4B	-2.40	100.73	108.99
6	B	1034	IDH	C6-C5-I5	-2.39	107.52	110.59
5	A	1032	NDP	O2B-C2B-C3B	2.38	120.31	111.68
4	A	1031	FAD	C5'-C4'-C3'	-2.37	107.62	112.20
3	B	1030	FMN	C7-C6-C5A	-2.37	117.87	121.22
5	B	1032	NDP	O2B-C2B-C3B	2.37	120.25	111.68
5	D	1032	NDP	O2A-PA-O1A	2.36	123.88	112.24
4	D	1031	FAD	C2A-N1A-C6A	2.35	122.78	118.75
5	C	1032	NDP	O2B-C2B-C3B	2.35	120.20	111.68
4	D	1031	FAD	C5'-C4'-C3'	-2.34	107.69	112.20
4	C	1031	FAD	C5'-C4'-C3'	-2.34	107.69	112.20
4	B	1031	FAD	C5'-C4'-C3'	-2.33	107.70	112.20
4	C	1031	FAD	C5A-C6A-N1A	-2.33	115.07	120.35
4	C	1031	FAD	C2A-N1A-C6A	2.32	122.72	118.75
5	D	1032	NDP	O2B-C2B-C3B	2.31	120.04	111.68
4	B	1031	FAD	C5A-C6A-N1A	-2.30	115.14	120.35
4	B	1031	FAD	C2A-N1A-C6A	2.30	122.68	118.75
5	B	1032	NDP	O2A-PA-O1A	2.29	123.57	112.24
5	A	1032	NDP	O4B-C1B-C2B	2.28	110.55	106.59
3	B	1030	FMN	O3'-C3'-C4'	2.28	114.33	108.81
5	C	1032	NDP	O2A-PA-O1A	2.28	123.49	112.24
4	D	1031	FAD	C5A-C6A-N1A	-2.27	115.20	120.35
3	C	1030	FMN	C7-C6-C5A	-2.26	118.03	121.22
5	C	1032	NDP	O4B-C1B-C2B	2.23	110.45	106.59
3	A	1030	FMN	O3'-C3'-C4'	2.22	114.18	108.81
3	A	1030	FMN	C7-C6-C5A	-2.22	118.07	121.22
5	A	1032	NDP	N3A-C2A-N1A	-2.22	125.20	128.68
4	A	1031	FAD	C5A-C6A-N1A	-2.21	115.34	120.35
5	A	1032	NDP	O5D-PN-O1N	2.18	117.58	109.07
5	D	1032	NDP	N3A-C2A-N1A	-2.16	125.30	128.68
3	B	1030	FMN	C6-C5A-C9A	2.16	121.88	119.05
5	D	1032	NDP	O4B-C1B-C2B	2.14	110.31	106.59
4	A	1031	FAD	P-O3P-PA	2.13	140.14	132.83
5	B	1032	NDP	O5D-PN-O1N	2.12	117.35	109.07
3	D	1030	FMN	C7-C6-C5A	-2.11	118.23	121.22
4	B	1031	FAD	C4A-C5A-N7A	2.11	111.60	109.40
5	D	1032	NDP	O5D-PN-O1N	2.11	117.30	109.07
4	A	1031	FAD	C2A-N1A-C6A	2.10	122.35	118.75
5	C	1032	NDP	N3A-C2A-N1A	-2.10	125.39	128.68
5	B	1032	NDP	N3A-C2A-N1A	-2.10	125.40	128.68
4	D	1031	FAD	P-O3P-PA	2.09	140.01	132.83
5	C	1032	NDP	O5D-PN-O1N	2.08	117.20	109.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	1031	FAD	P-O3P-PA	2.04	139.84	132.83
3	D	1030	FMN	C6-C5A-C9A	2.03	121.72	119.05
5	B	1032	NDP	O4B-C1B-C2B	2.01	110.07	106.59
4	D	1031	FAD	C5A-C6A-N6A	2.01	123.41	120.35

There are no chirality outliers.

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	1032	NDP	PN-O3-PA-O5B
5	B	1032	NDP	O4D-C1D-N1N-C2N
4	B	1031	FAD	C5B-O5B-PA-O1A
4	B	1031	FAD	PA-O3P-P-O5'
4	C	1031	FAD	C5B-O5B-PA-O1A
5	D	1032	NDP	PN-O3-PA-O5B
5	D	1032	NDP	O4D-C1D-N1N-C2N
5	A	1032	NDP	PN-O3-PA-O5B
5	A	1032	NDP	O4D-C1D-N1N-C2N
4	D	1031	FAD	C5B-O5B-PA-O1A
5	C	1032	NDP	PN-O3-PA-O5B
5	C	1032	NDP	O4D-C1D-N1N-C2N
4	A	1031	FAD	C5B-O5B-PA-O1A
5	B	1032	NDP	C3B-C2B-O2B-P2B
5	D	1032	NDP	C3B-C2B-O2B-P2B
5	A	1032	NDP	C3B-C2B-O2B-P2B
5	C	1032	NDP	C3B-C2B-O2B-P2B
5	B	1032	NDP	C1B-C2B-O2B-P2B
5	D	1032	NDP	C1B-C2B-O2B-P2B
5	A	1032	NDP	C1B-C2B-O2B-P2B
5	C	1032	NDP	C1B-C2B-O2B-P2B
4	C	1031	FAD	PA-O3P-P-O5'
4	D	1031	FAD	PA-O3P-P-O5'
4	A	1031	FAD	PA-O3P-P-O5'
4	B	1031	FAD	C5B-O5B-PA-O3P
4	C	1031	FAD	C5B-O5B-PA-O3P
3	B	1030	FMN	C4'-C5'-O5'-P
3	A	1030	FMN	C4'-C5'-O5'-P
3	D	1030	FMN	C4'-C5'-O5'-P
3	C	1030	FMN	C4'-C5'-O5'-P
4	B	1031	FAD	O4B-C4B-C5B-O5B
4	C	1031	FAD	O4B-C4B-C5B-O5B
4	D	1031	FAD	O4B-C4B-C5B-O5B

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Mol	Chain	Res	Type	Atoms
4	D	1031	FAD	C5B-O5B-PA-O3P
4	A	1031	FAD	C5B-O5B-PA-O3P
5	B	1032	NDP	O4B-C4B-C5B-O5B
5	D	1032	NDP	O4B-C4B-C5B-O5B
5	D	1032	NDP	O4D-C4D-C5D-O5D
5	A	1032	NDP	O4B-C4B-C5B-O5B
5	A	1032	NDP	O4D-C4D-C5D-O5D
5	C	1032	NDP	O4B-C4B-C5B-O5B
4	A	1031	FAD	O4B-C4B-C5B-O5B
4	B	1031	FAD	P-O3P-PA-O2A
4	B	1031	FAD	C3B-C4B-C5B-O5B

There are no ring outliers.

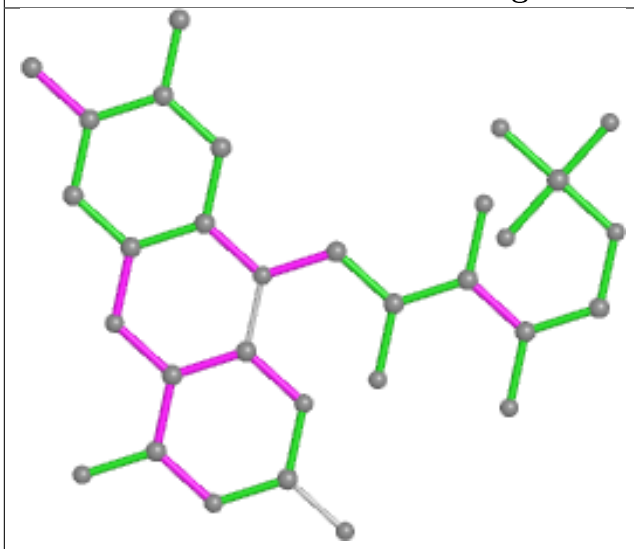
16 monomers are involved in 43 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1030	FMN	1	0
5	B	1032	NDP	5	0
2	C	1027	SF4	2	0
6	B	1034	IDH	4	0
2	A	1026	SF4	1	0
4	B	1031	FAD	1	0
5	D	1032	NDP	5	0
7	C	1034	IUR	4	0
5	A	1032	NDP	6	0
6	A	1033	IDH	1	0
2	B	1027	SF4	2	0
4	D	1031	FAD	1	0
3	C	1030	FMN	1	0
2	A	1027	SF4	1	0
2	D	1027	SF4	3	0
5	C	1032	NDP	6	0

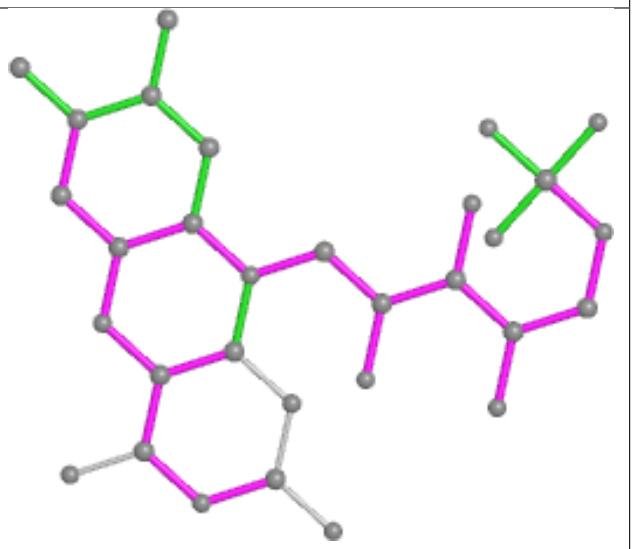
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

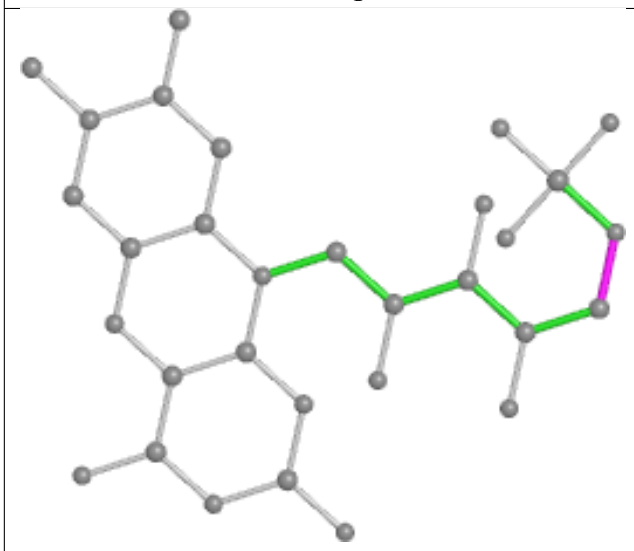
Ligand FMN B 1030



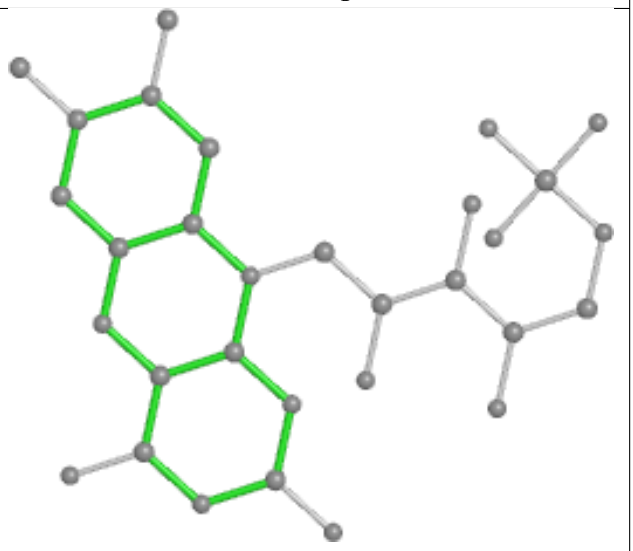
Bond lengths



Bond angles

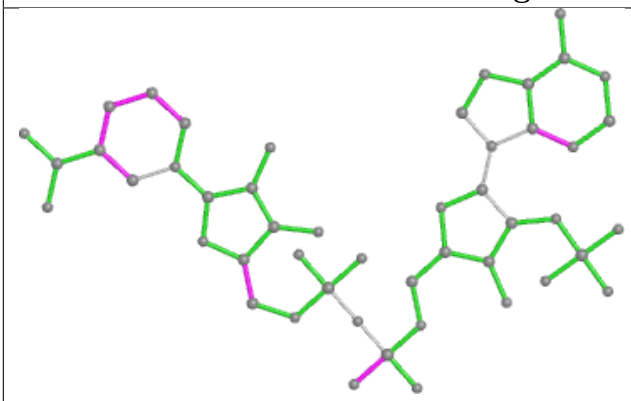


Torsions

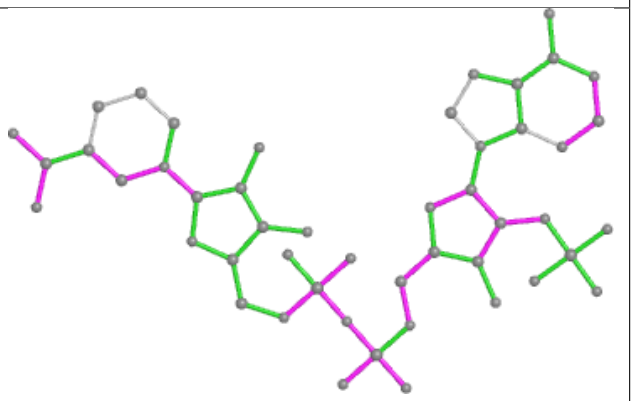


Rings

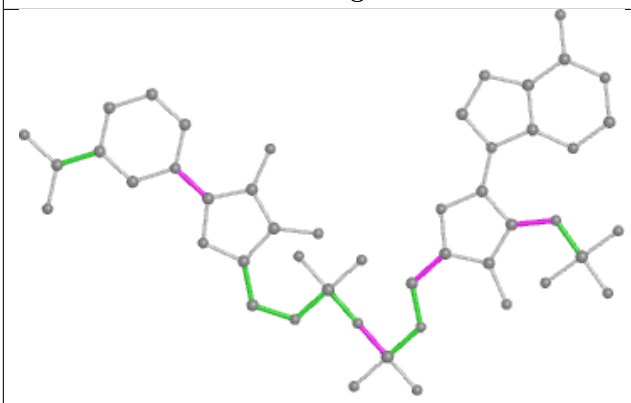
Ligand NDP B 1032



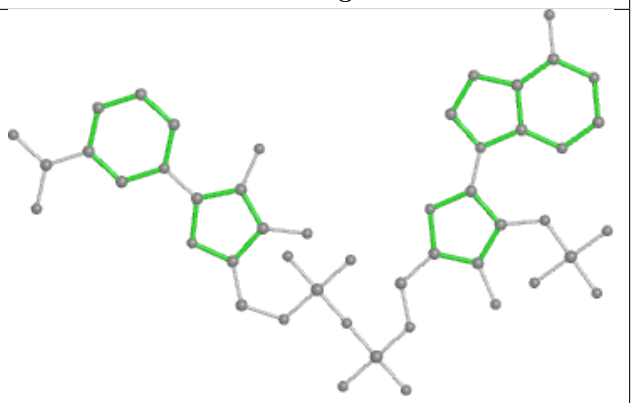
Bond lengths



Bond angles

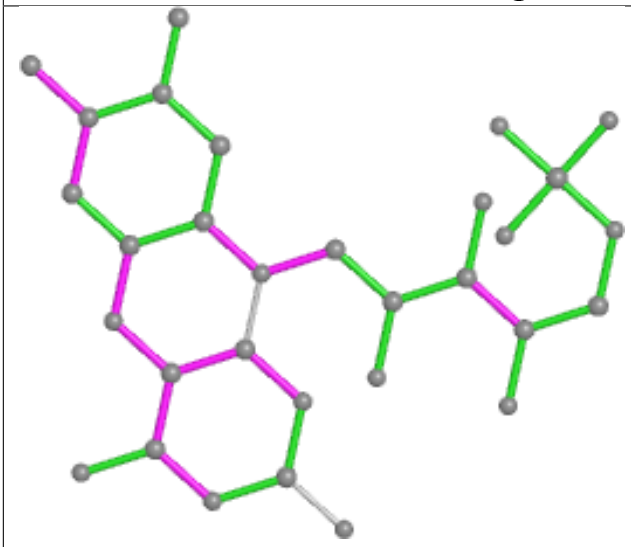


Torsions

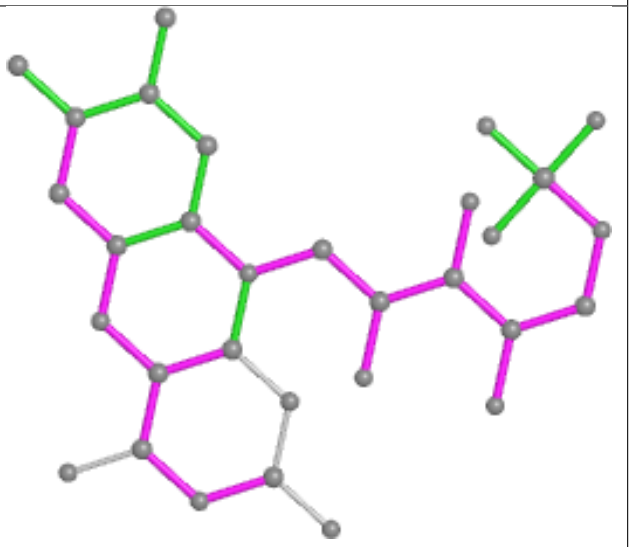


Rings

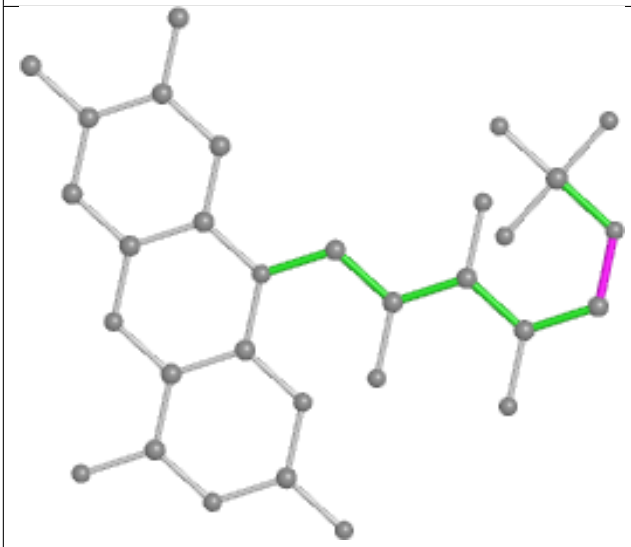
Ligand FMN A 1030



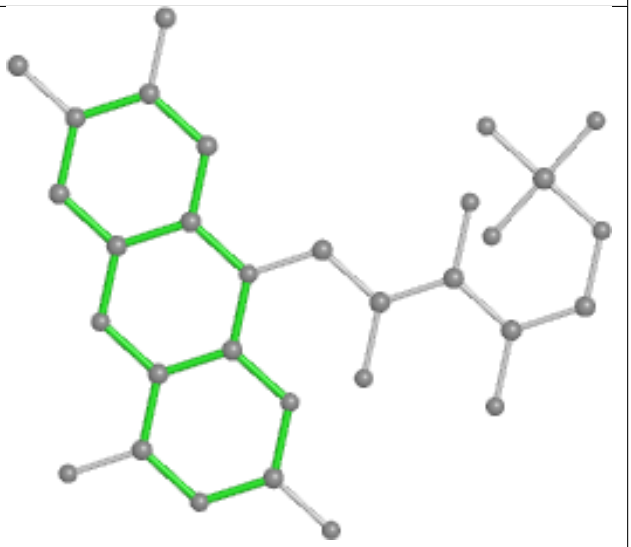
Bond lengths



Bond angles

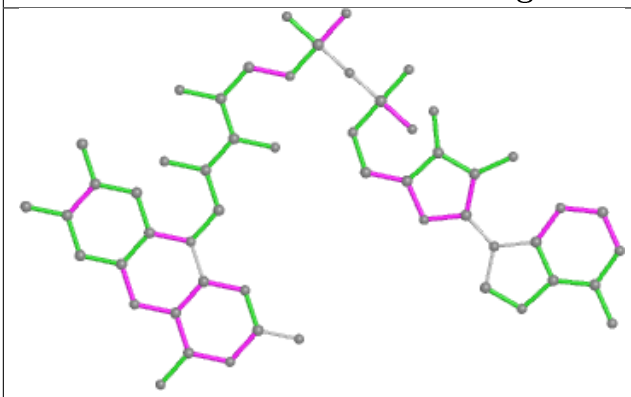


Torsions

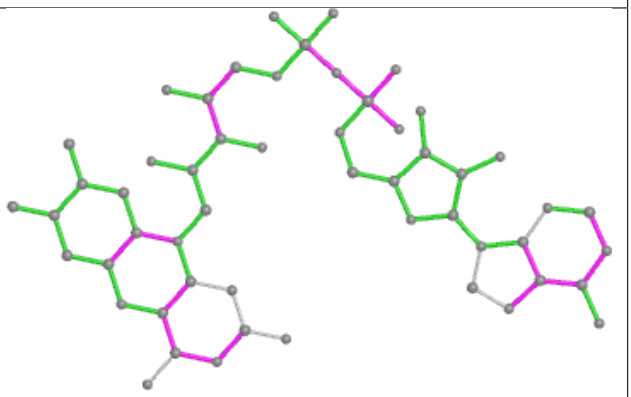


Rings

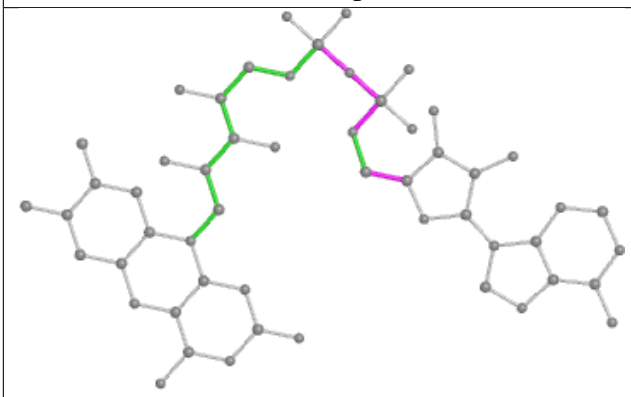
Ligand FAD B 1031



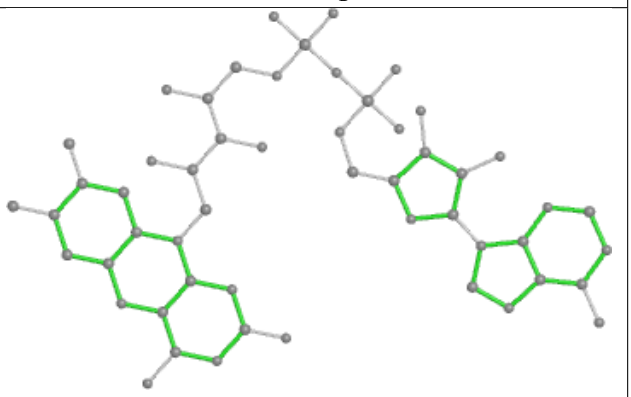
Bond lengths



Bond angles

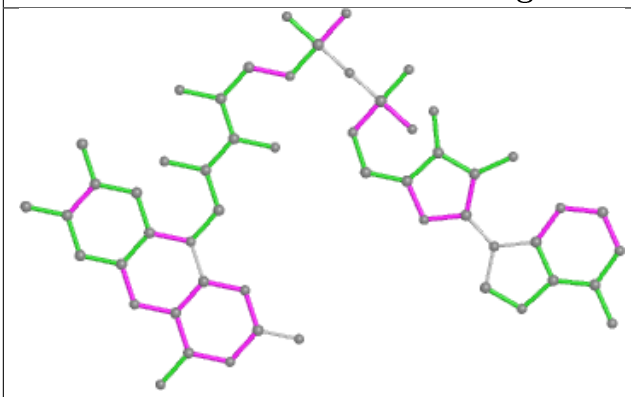


Torsions

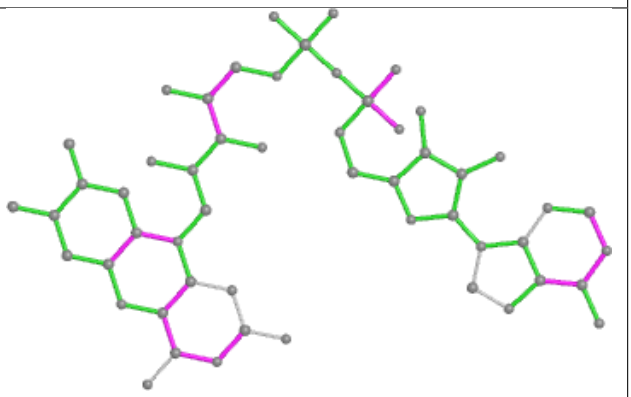


Rings

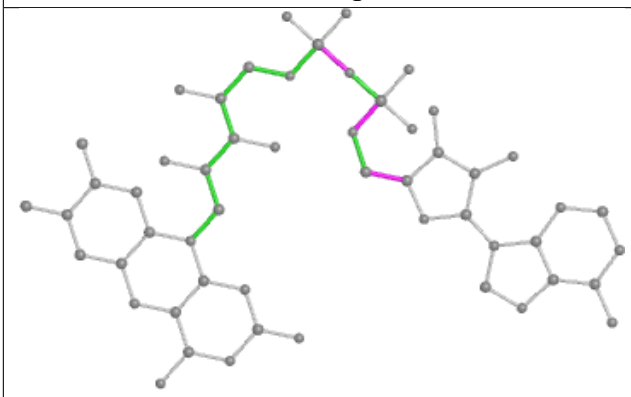
Ligand FAD C 1031



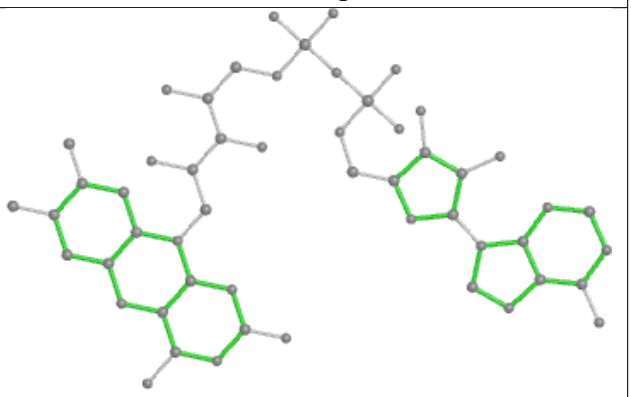
Bond lengths



Bond angles

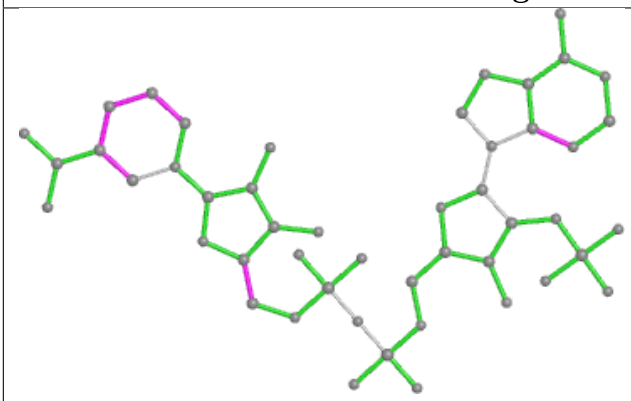


Torsions



Rings

Ligand NDP D 1032



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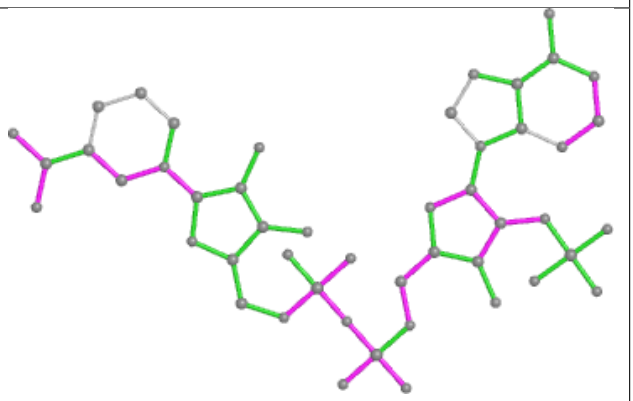
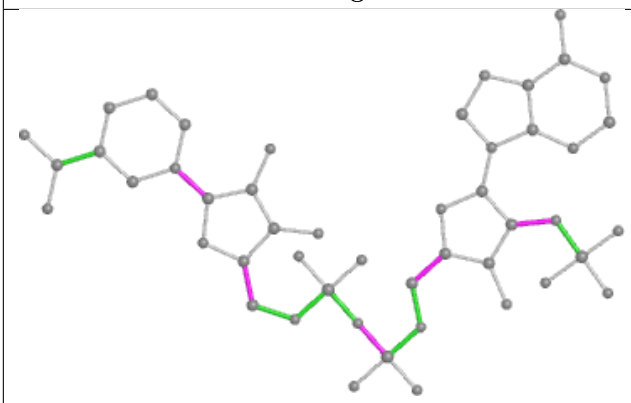


Bond angles



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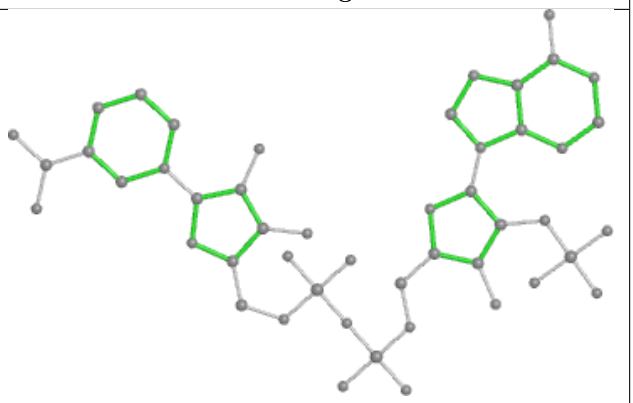
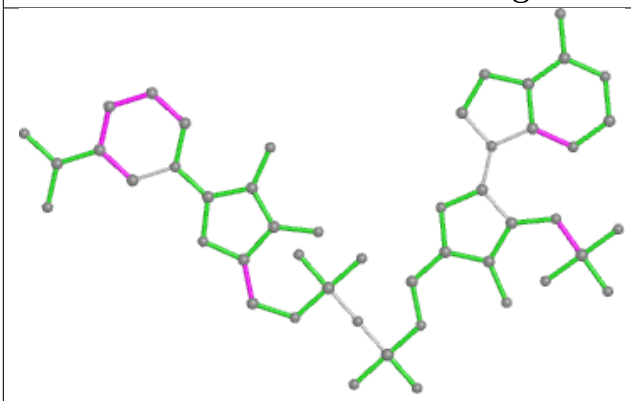
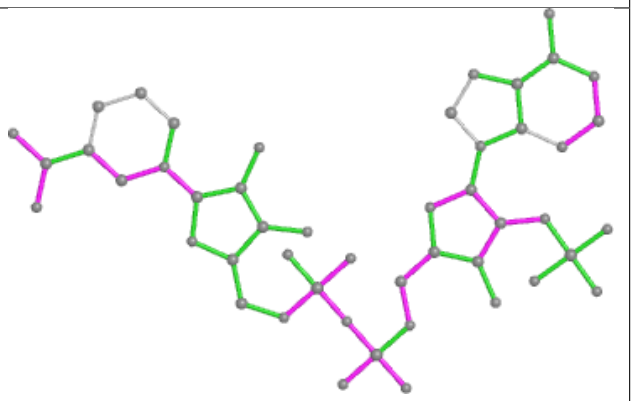


Rings

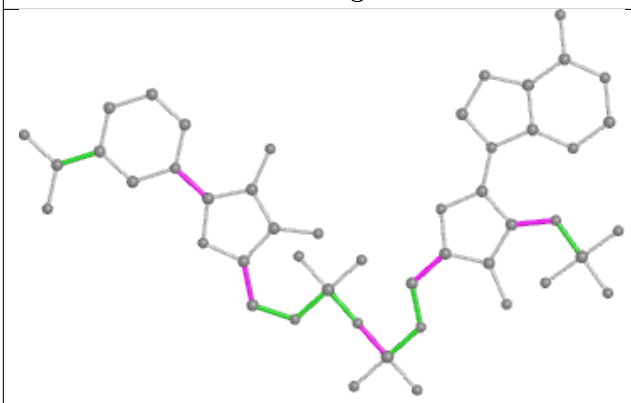
Ligand NDP A 1032



Bond lengths



Bond angles



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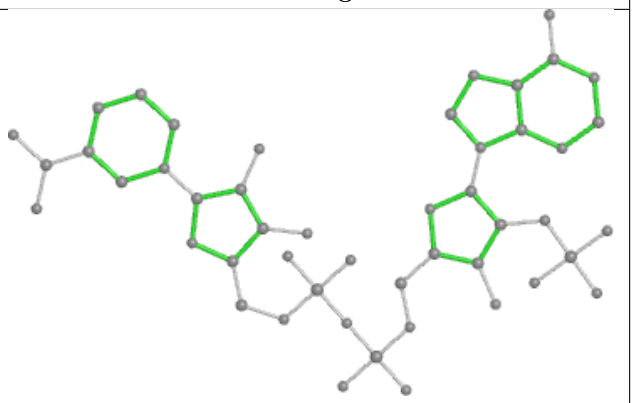
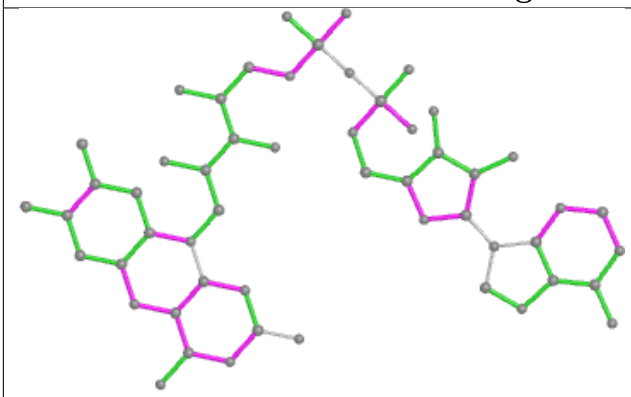


Rings

Ligand FAD D 1031



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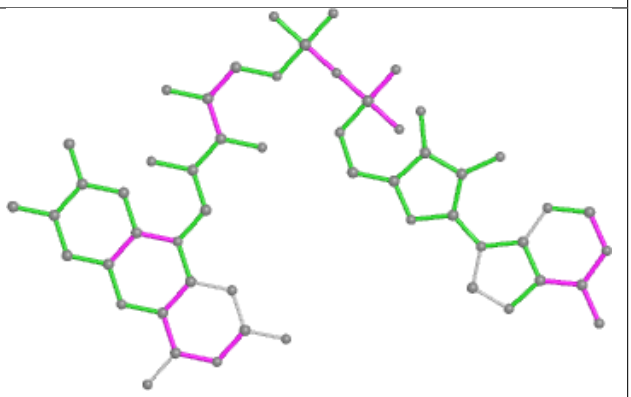
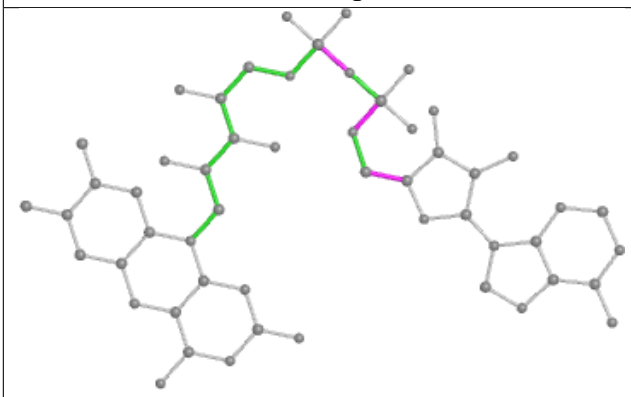
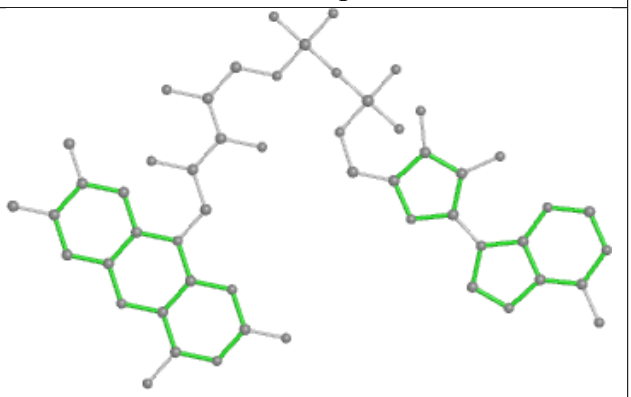


Bond angles

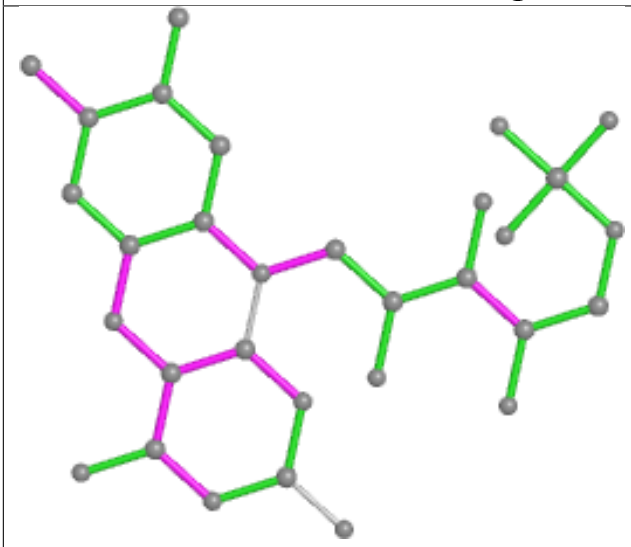


Torsions

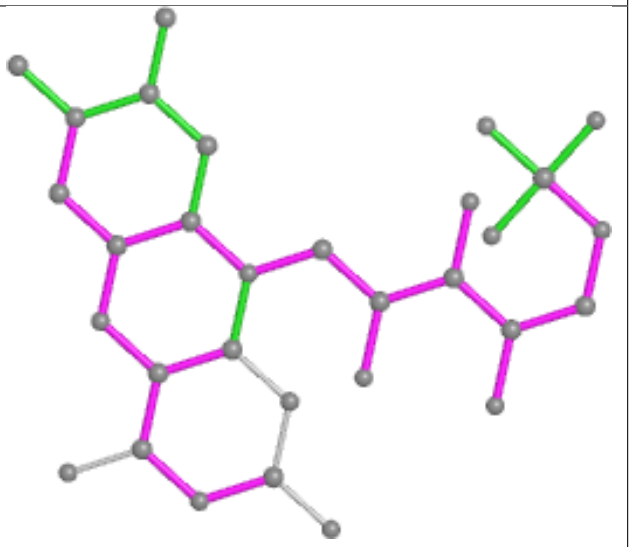


Rings

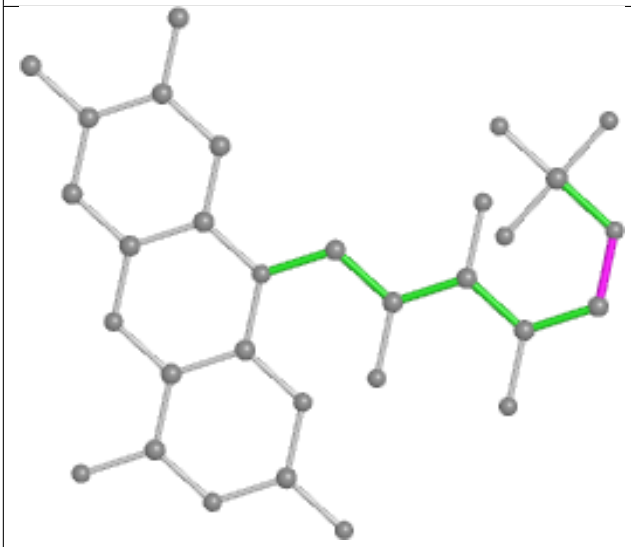
Ligand FMN D 1030



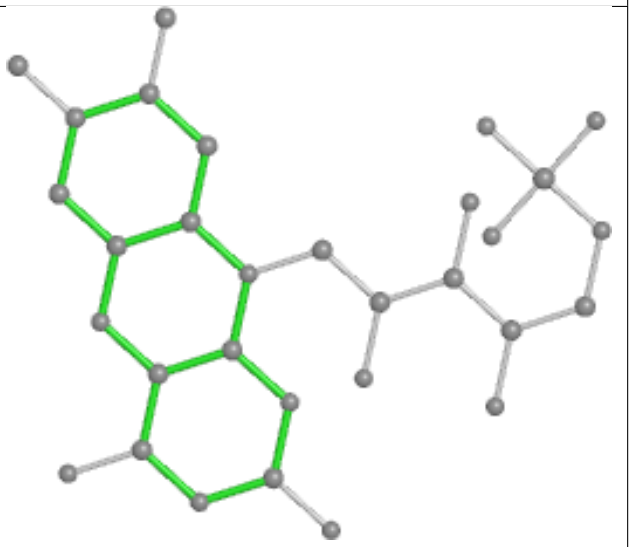
Bond lengths



Bond angles

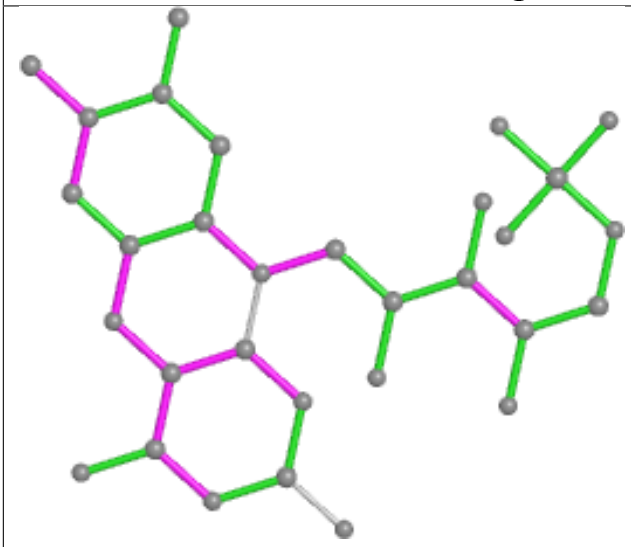


Torsions

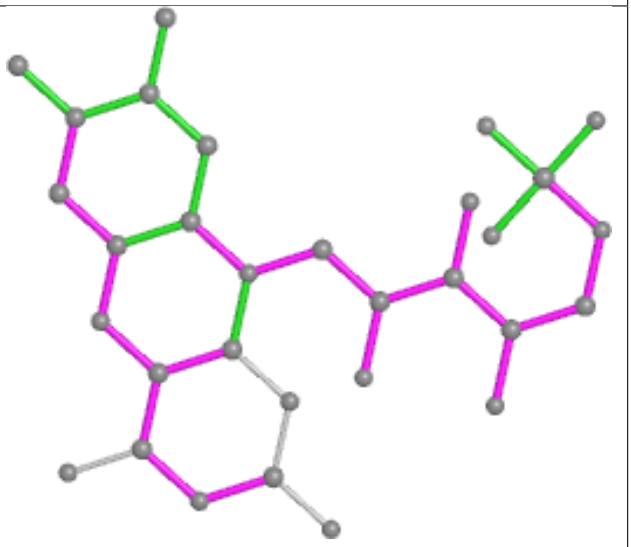


Rings

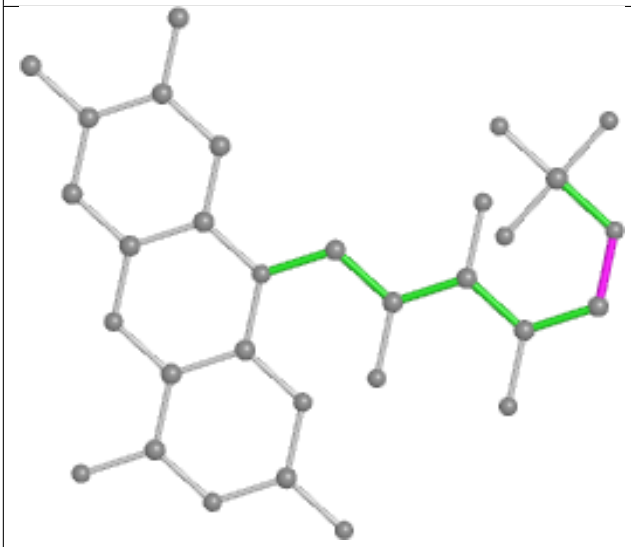
Ligand FMN C 1030



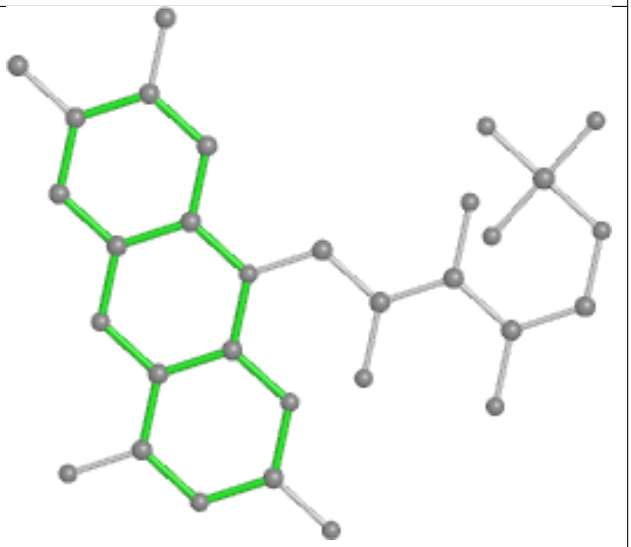
Bond lengths



Bond angles

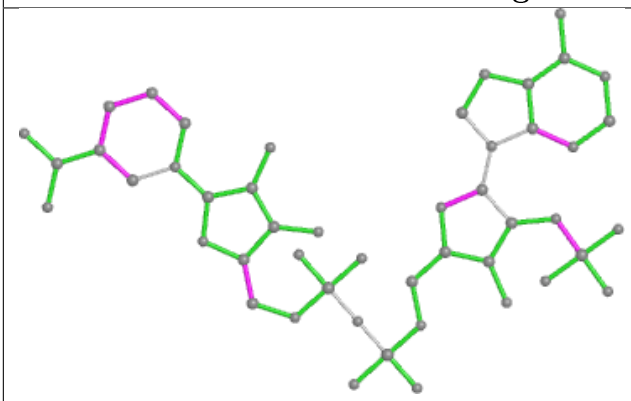


Torsions

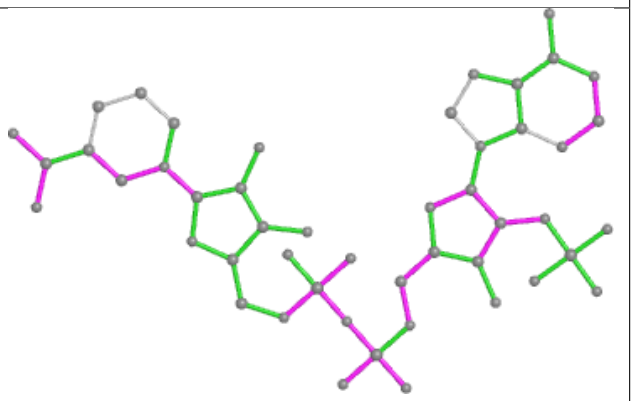


Rings

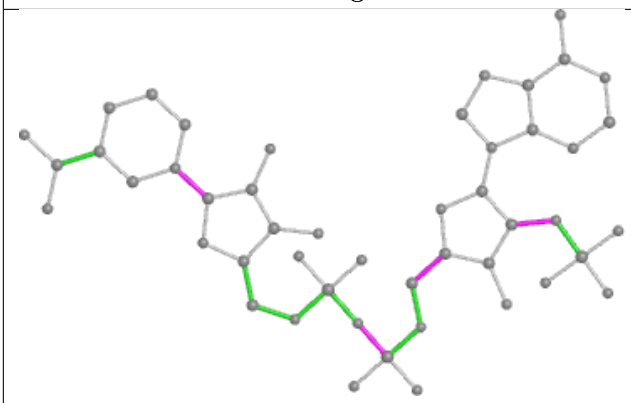
Ligand NDP C 1032



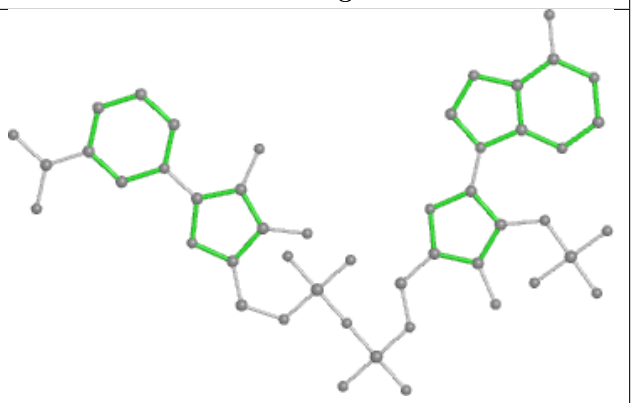
Bond lengths



Bond angles

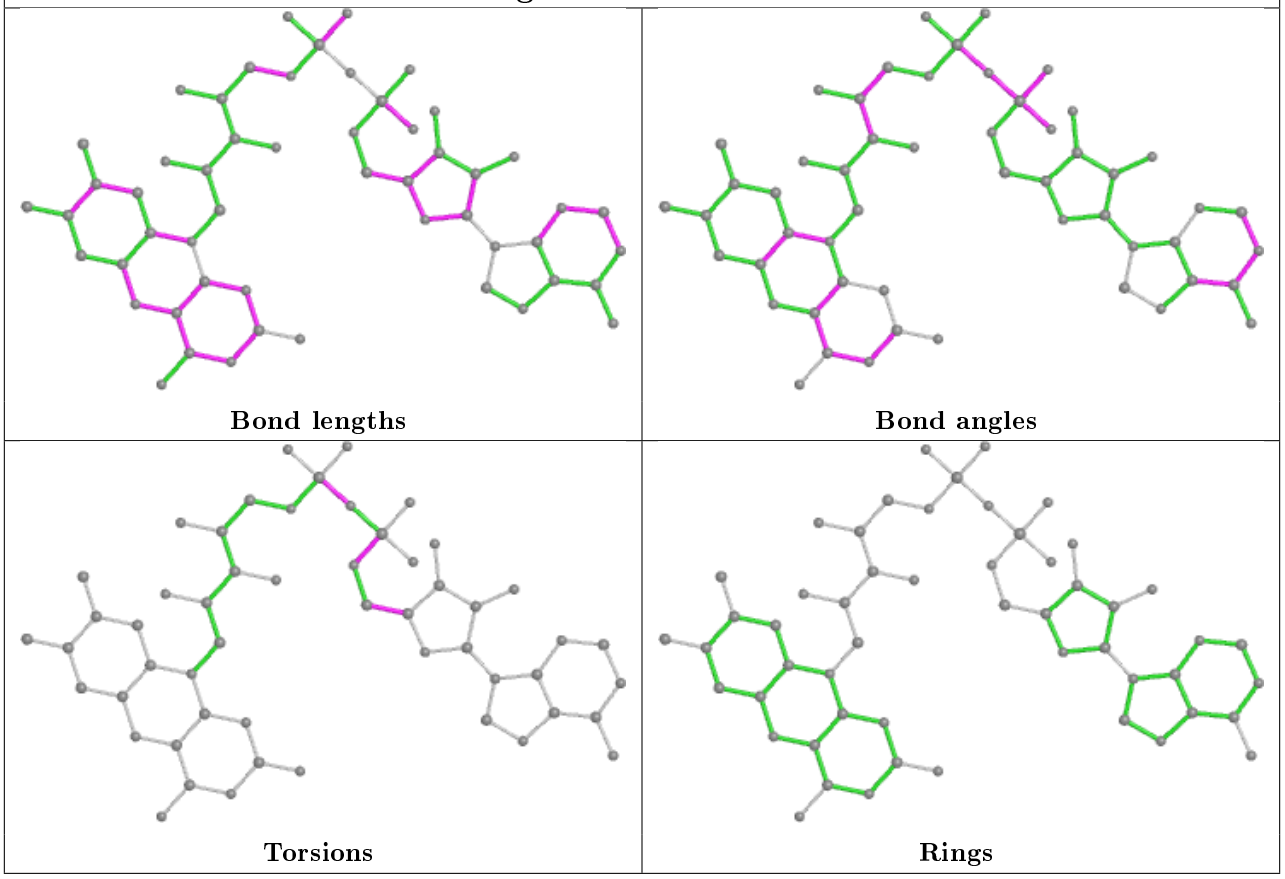


Torsions



Rings

Ligand FAD A 1031



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	1019/1025 (99%)	-0.01	50 (4%) 29 32	14, 27, 63, 83	0
1	B	1012/1025 (98%)	0.01	56 (5%) 25 27	15, 27, 61, 83	0
1	C	1015/1025 (99%)	0.07	74 (7%) 15 15	17, 29, 63, 85	0
1	D	1019/1025 (99%)	0.23	104 (10%) 6 6	17, 29, 67, 87	0
All	All	4065/4100 (99%)	0.08	284 (6%) 16 17	14, 28, 64, 87	0

All (284) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	2	ALA	10.8
1	D	2	ALA	10.6
1	D	904	PHE	10.3
1	D	682	LEU	10.0
1	C	679	GLY	9.9
1	D	1020	ALA	9.2
1	C	1020	ALA	9.0
1	B	2	ALA	8.8
1	D	905	PRO	8.8
1	C	907	LEU	8.2
1	A	682	LEU	8.1
1	C	682	LEU	7.8
1	D	1010	PRO	7.5
1	C	1018	PRO	7.1
1	A	2	ALA	6.9
1	A	52	CYS	6.7
1	B	682	LEU	6.6
1	C	51	HIS	6.6
1	B	51	HIS	6.2
1	D	52	CYS	6.1
1	D	324	CYS	6.1

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Mol	Chain	Res	Type	RSRZ
1	B	1020	ALA	6.1
1	D	907	LEU	6.1
1	D	423	GLU	6.0
1	C	1010	PRO	6.0
1	D	415	GLU	5.9
1	A	51	HIS	5.9
1	D	422	ASP	5.8
1	A	1020	ALA	5.6
1	A	904	PHE	5.6
1	C	902	ALA	5.6
1	C	901	ASN	5.6
1	C	415	GLU	5.6
1	D	676	GLY	5.6
1	D	906	PRO	5.4
1	D	1019	LEU	5.4
1	A	415	GLU	5.4
1	B	1010	PRO	5.4
1	D	296	GLY	5.4
1	C	1009	THR	5.3
1	C	52	CYS	5.3
1	A	50	PHE	5.2
1	D	416	THR	5.0
1	B	50	PHE	4.9
1	D	678	ARG	4.9
1	D	51	HIS	4.9
1	C	416	THR	4.8
1	A	902	ALA	4.8
1	A	901	ASN	4.8
1	A	903	ALA	4.7
1	C	899	GLU	4.7
1	C	872	MET	4.6
1	B	681	GLY	4.5
1	A	679	GLY	4.5
1	B	872	MET	4.4
1	D	424	ASP	4.4
1	D	50	PHE	4.4
1	B	418	LYS	4.4
1	B	458	ARG	4.4
1	C	908	GLU	4.4
1	C	50	PHE	4.4
1	D	458	ARG	4.4
1	B	415	GLU	4.4

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Mol	Chain	Res	Type	RSRZ
1	D	396	VAL	4.3
1	C	681	GLY	4.3
1	D	292	ASP	4.3
1	B	679	GLY	4.3
1	C	1019	LEU	4.3
1	C	423	GLU	4.3
1	D	872	MET	4.3
1	D	908	GLU	4.2
1	D	867	ARG	4.2
1	B	424	ASP	4.1
1	D	869	ALA	4.1
1	D	325	HIS	4.1
1	A	424	ASP	4.0
1	C	518	LYS	4.0
1	B	867	ARG	4.0
1	B	1019	LEU	4.0
1	B	428	HIS	3.9
1	D	517	ALA	3.9
1	B	899	GLU	3.9
1	D	414	ASP	3.9
1	B	417	GLY	3.8
1	D	428	HIS	3.8
1	B	410	ARG	3.8
1	D	49	CYS	3.8
1	D	179	GLN	3.8
1	A	325	HIS	3.8
1	C	324	CYS	3.8
1	A	899	GLU	3.7
1	C	867	ARG	3.7
1	B	52	CYS	3.7
1	B	676	GLY	3.7
1	D	425	GLN	3.7
1	D	323	ALA	3.7
1	B	1018	PRO	3.6
1	D	401	GLY	3.6
1	C	325	HIS	3.6
1	D	54	LYS	3.5
1	D	180	GLU	3.5
1	D	897	LEU	3.5
1	D	915	LYS	3.4
1	A	1010	PRO	3.4
1	D	332	ARG	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	847	GLN	3.4
1	A	872	MET	3.3
1	C	330	SER	3.3
1	C	180	GLU	3.3
1	C	418	LYS	3.3
1	D	430	LYS	3.3
1	D	175	CYS	3.3
1	C	424	ASP	3.2
1	D	300	ASP	3.2
1	D	426	ILE	3.2
1	B	423	GLU	3.2
1	D	398	VAL	3.2
1	D	892	GLU	3.2
1	A	1019	LEU	3.2
1	C	678	ARG	3.2
1	A	426	ILE	3.2
1	C	414	ASP	3.2
1	A	870	GLU	3.2
1	C	900	GLN	3.1
1	D	412	GLU	3.1
1	B	3	PRO	3.1
1	D	302	GLY	3.1
1	A	905	PRO	3.1
1	B	869	ALA	3.1
1	C	371	ARG	3.1
1	D	11	ASP	3.1
1	A	273	GLU	3.1
1	D	419	TRP	3.1
1	A	337	VAL	3.1
1	C	677	GLU	3.1
1	B	401	GLY	3.1
1	A	678	ARG	3.1
1	D	459	TRP	3.1
1	D	1009	THR	3.1
1	B	908	GLU	3.1
1	D	407	GLN	3.0
1	A	900	GLN	3.0
1	C	873	GLY	3.0
1	C	420	ASN	3.0
1	B	1009	THR	3.0
1	C	332	ARG	3.0
1	D	400	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	404	VAL	3.0
1	B	416	THR	3.0
1	B	426	ILE	3.0
1	C	426	ILE	3.0
1	C	459	TRP	3.0
1	D	677	GLU	2.9
1	A	1018	PRO	2.9
1	D	427	VAL	2.9
1	B	517	ALA	2.9
1	A	867	ARG	2.9
1	C	1008	THR	2.9
1	A	517	ALA	2.9
1	C	417	GLY	2.9
1	B	290	THR	2.8
1	A	908	GLU	2.8
1	B	49	CYS	2.8
1	D	681	GLY	2.8
1	D	873	GLY	2.8
1	D	903	ALA	2.8
1	B	900	GLN	2.8
1	C	869	ALA	2.8
1	D	371	ARG	2.8
1	B	325	HIS	2.8
1	A	676	GLY	2.7
1	B	296	GLY	2.7
1	C	874	LYS	2.7
1	B	443	ARG	2.7
1	C	422	ASP	2.7
1	D	679	GLY	2.7
1	D	402	ARG	2.7
1	D	443	ARG	2.7
1	D	1018	PRO	2.7
1	C	458	ARG	2.7
1	D	410	ARG	2.7
1	D	420	ASN	2.7
1	A	416	THR	2.7
1	D	330	SER	2.7
1	A	425	GLN	2.7
1	A	873	GLY	2.7
1	C	357	ARG	2.6
1	C	847	GLN	2.6
1	B	295	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	517	ALA	2.6
1	D	357	ARG	2.6
1	D	871	LEU	2.6
1	B	678	ARG	2.6
1	D	455	LYS	2.6
1	D	900	GLN	2.6
1	C	917	PRO	2.6
1	D	397	ILE	2.6
1	B	459	TRP	2.6
1	D	899	GLU	2.6
1	D	418	LYS	2.6
1	D	1012	GLU	2.5
1	B	915	LYS	2.5
1	D	320	GLY	2.5
1	C	367	PHE	2.5
1	B	181	LYS	2.5
1	A	179	GLN	2.5
1	C	516	SER	2.5
1	C	179	GLN	2.5
1	C	680	MET	2.5
1	A	458	ARG	2.5
1	C	402	ARG	2.5
1	D	518	LYS	2.4
1	C	870	GLU	2.4
1	B	910	LYS	2.4
1	B	425	GLN	2.4
1	C	1012	GLU	2.4
1	B	175	CYS	2.4
1	C	273	GLU	2.4
1	D	333	GLY	2.4
1	D	421	GLU	2.4
1	D	917	PRO	2.4
1	A	677	GLU	2.4
1	A	1009	THR	2.4
1	D	295	GLN	2.4
1	C	322	CYS	2.4
1	B	292	ASP	2.3
1	C	175	CYS	2.3
1	C	683	ALA	2.3
1	D	322	CYS	2.3
1	A	907	LEU	2.3
1	B	319	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	1014	LYS	2.3
1	C	455	LYS	2.3
1	C	53	GLU	2.3
1	A	430	LYS	2.3
1	D	294	PHE	2.3
1	A	414	ASP	2.3
1	C	174	PRO	2.3
1	C	675	MET	2.2
1	C	428	HIS	2.2
1	D	273	GLU	2.2
1	B	362	VAL	2.2
1	C	181	LYS	2.2
1	A	417	GLY	2.2
1	A	1008	THR	2.2
1	C	264	ASN	2.2
1	B	874	LYS	2.2
1	A	264	ASN	2.2
1	A	518	LYS	2.2
1	C	410	ARG	2.2
1	D	1011	TYR	2.2
1	A	906	PRO	2.2
1	A	410	ARG	2.1
1	B	892	GLU	2.1
1	D	53	GLU	2.1
1	D	181	LYS	2.1
1	B	683	ALA	2.1
1	D	756	ALA	2.1
1	D	868	ILE	2.1
1	B	338	LEU	2.1
1	D	901	ASN	2.1
1	D	675	MET	2.1
1	A	459	TRP	2.1
1	B	402	ARG	2.1
1	D	902	ALA	2.1
1	C	676	GLY	2.1
1	C	176	LEU	2.1
1	C	429	LEU	2.1
1	D	432	ASP	2.1
1	C	48	ASN	2.1
1	D	10	ALA	2.1
1	D	916	LYS	2.1
1	D	3	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	281	ILE	2.1
1	B	422	ASP	2.1
1	D	862	GLY	2.1
1	D	954	ILE	2.0
1	D	298	THR	2.0
1	B	339	GLY	2.0
1	B	337	VAL	2.0
1	C	430	LYS	2.0
1	A	180	GLU	2.0
1	C	397	ILE	2.0
1	D	221	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 carbohydrates in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	IDH	B	1034	9/9	0.90	0.25	39,42,45,52	1
5	NDP	D	1032	48/48	0.92	0.17	40,47,57,58	0
7	IUR	C	1034	9/9	0.93	0.13	27,28,32,38	1
6	IDH	A	1033	8/9	0.93	0.16	23,28,32,32	0
5	NDP	C	1032	48/48	0.93	0.15	39,46,56,57	0
5	NDP	A	1032	48/48	0.94	0.15	36,42,56,56	0
2	SF4	C	1026	8/8	0.94	0.13	26,28,29,29	0
5	NDP	B	1032	48/48	0.94	0.15	36,44,56,57	0
2	SF4	A	1026	8/8	0.95	0.12	21,23,23,24	0
4	FAD	D	1031	53/53	0.95	0.13	25,28,35,37	0
2	SF4	A	1027	8/8	0.95	0.12	17,20,20,21	0
8	URA	D	1034	8/8	0.95	0.14	28,30,31,32	0

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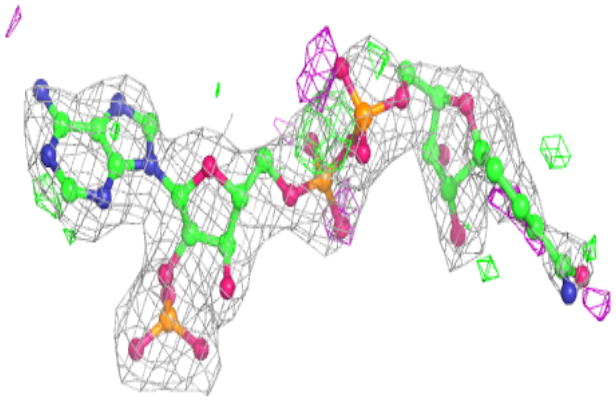
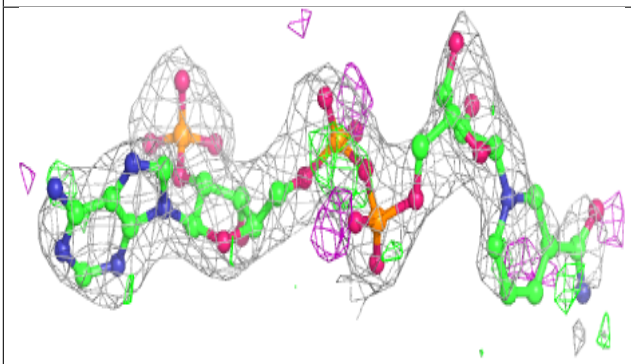
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	FAD	C	1031	53/53	0.95	0.13	26,31,33,34	0
2	SF4	B	1029	8/8	0.96	0.11	22,23,24,24	0
2	SF4	D	1028	8/8	0.96	0.11	28,29,30,31	0
2	SF4	C	1027	8/8	0.96	0.13	24,26,26,26	0
2	SF4	D	1026	8/8	0.96	0.12	26,28,28,28	0
2	SF4	B	1028	8/8	0.96	0.11	20,22,23,23	0
2	SF4	B	1027	8/8	0.96	0.13	18,19,21,21	0
3	FMN	B	1030	31/31	0.97	0.12	17,19,21,22	0
2	SF4	D	1029	8/8	0.97	0.11	29,30,31,31	0
2	SF4	A	1029	8/8	0.97	0.12	21,22,23,23	0
3	FMN	C	1030	31/31	0.97	0.10	16,20,22,22	0
2	SF4	B	1026	8/8	0.97	0.11	19,23,24,24	0
2	SF4	D	1027	8/8	0.97	0.13	22,23,24,24	0
2	SF4	C	1028	8/8	0.97	0.10	23,25,26,26	0
2	SF4	A	1028	8/8	0.97	0.12	21,23,24,24	0
4	FAD	B	1031	53/53	0.97	0.12	22,26,32,34	0
4	FAD	A	1031	53/53	0.97	0.11	21,26,32,33	0
2	SF4	C	1029	8/8	0.98	0.10	24,25,27,27	0
3	FMN	A	1030	31/31	0.98	0.11	16,19,21,22	0
3	FMN	D	1030	31/31	0.98	0.08	16,20,22,23	0

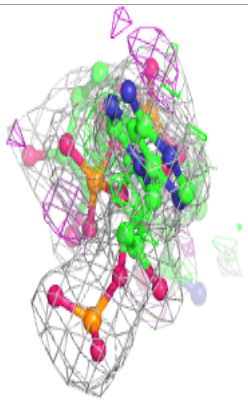
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NDP 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)

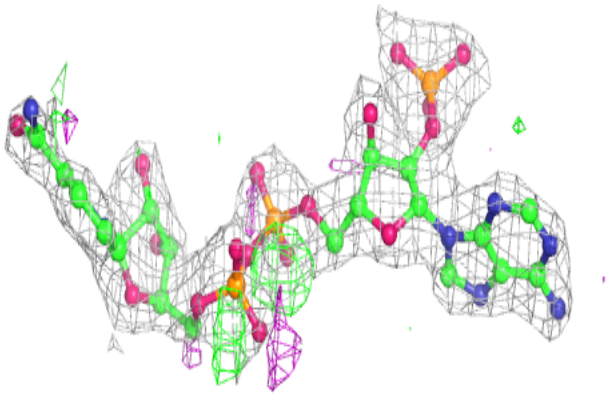


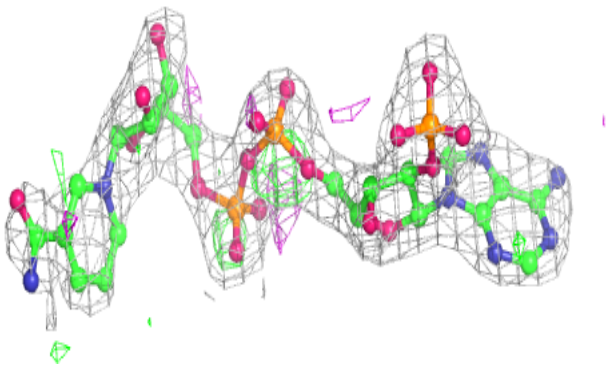


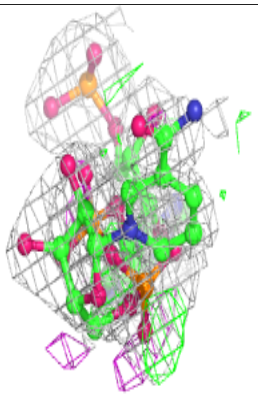


Electron density around NDP C 1032:

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

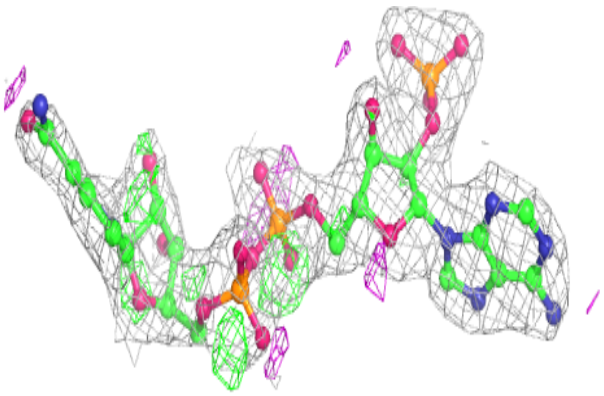


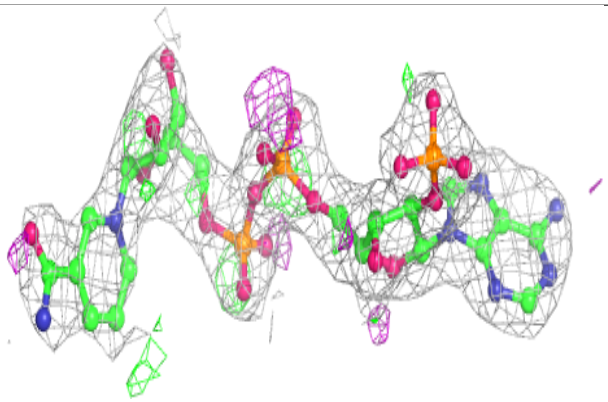




Electron density around NDP A 1032:

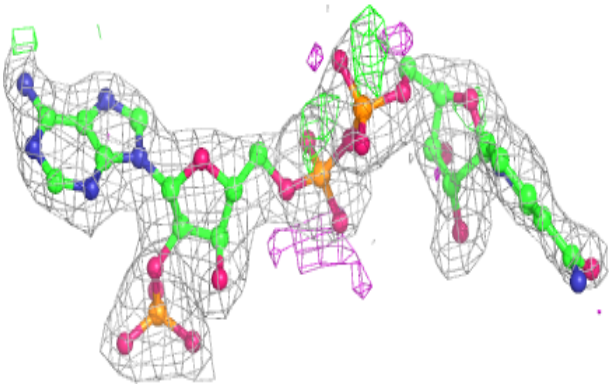
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

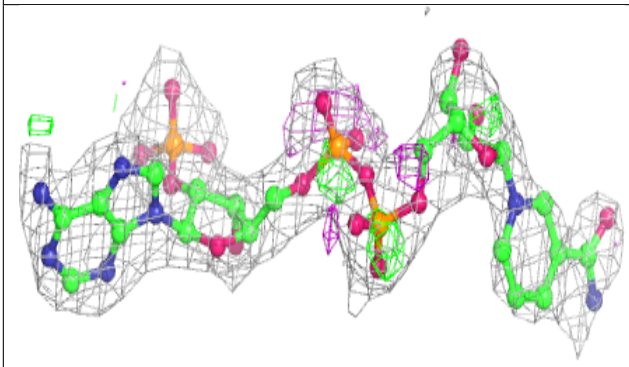


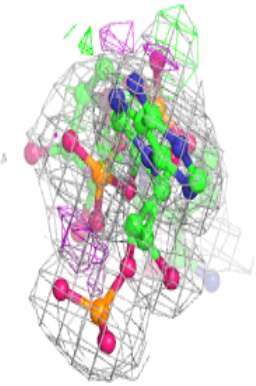


Electron density around NDP B 1032:

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

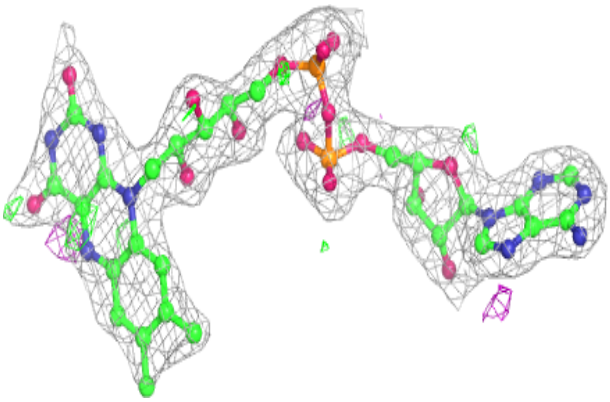


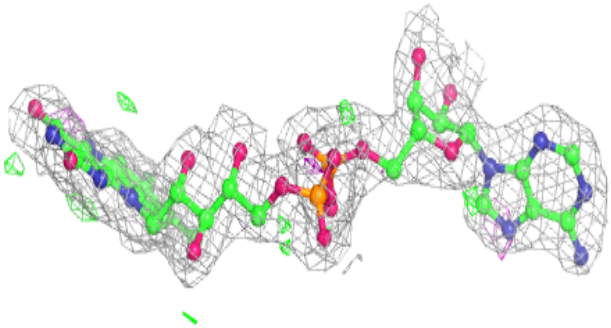


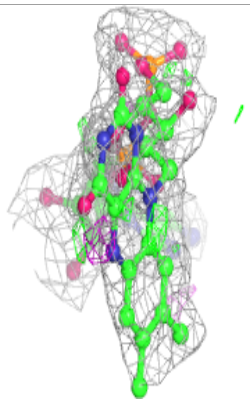


Electron density around FAD D 1031:

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

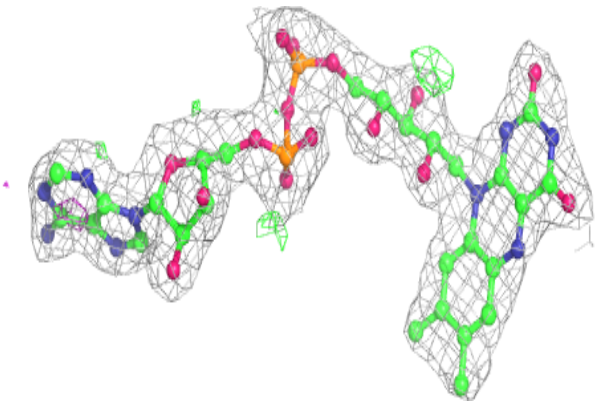


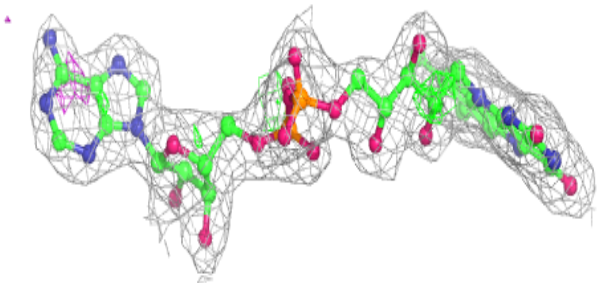


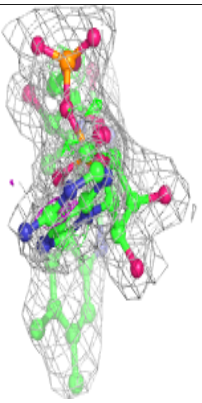


Electron density around FAD C 1031:

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

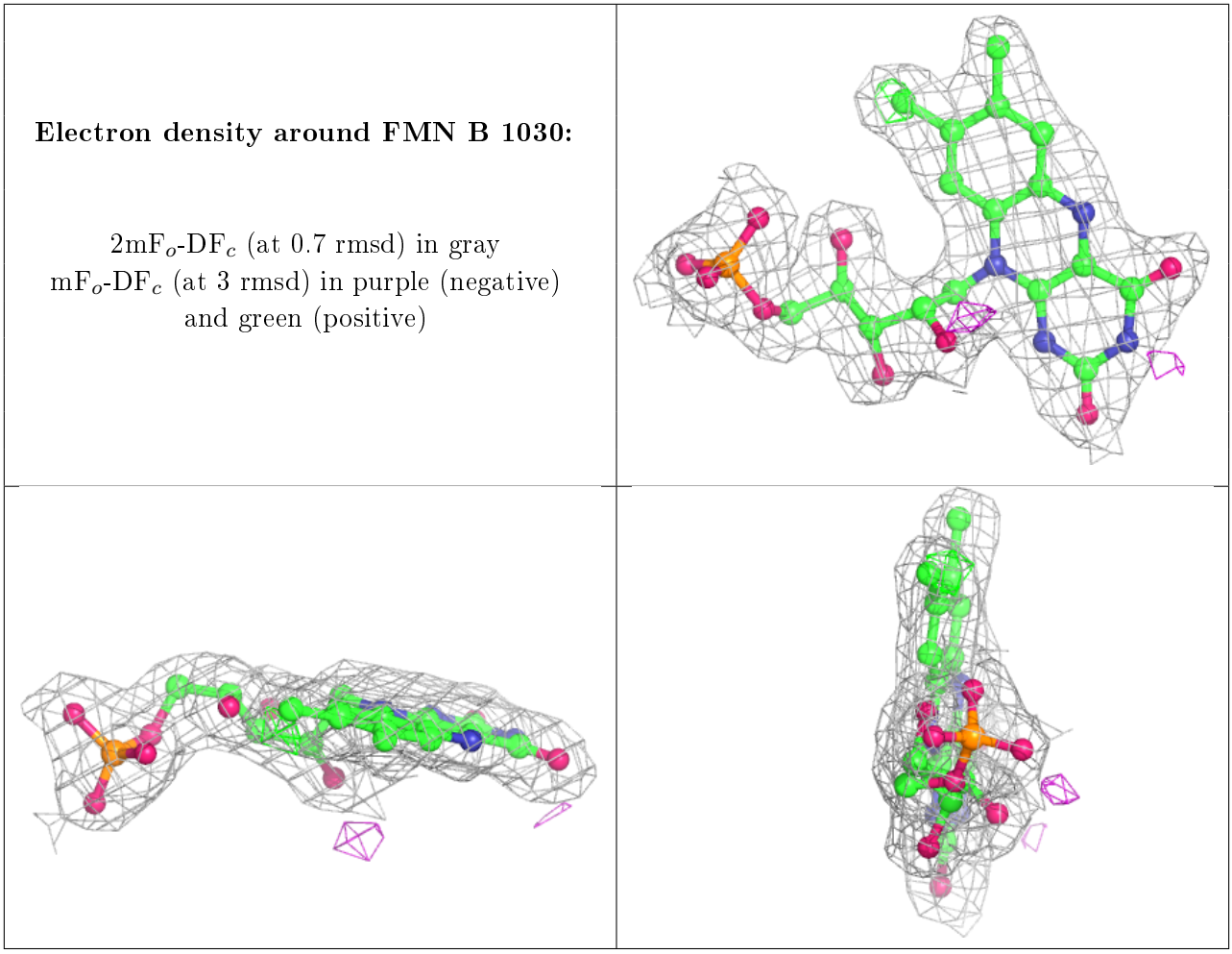






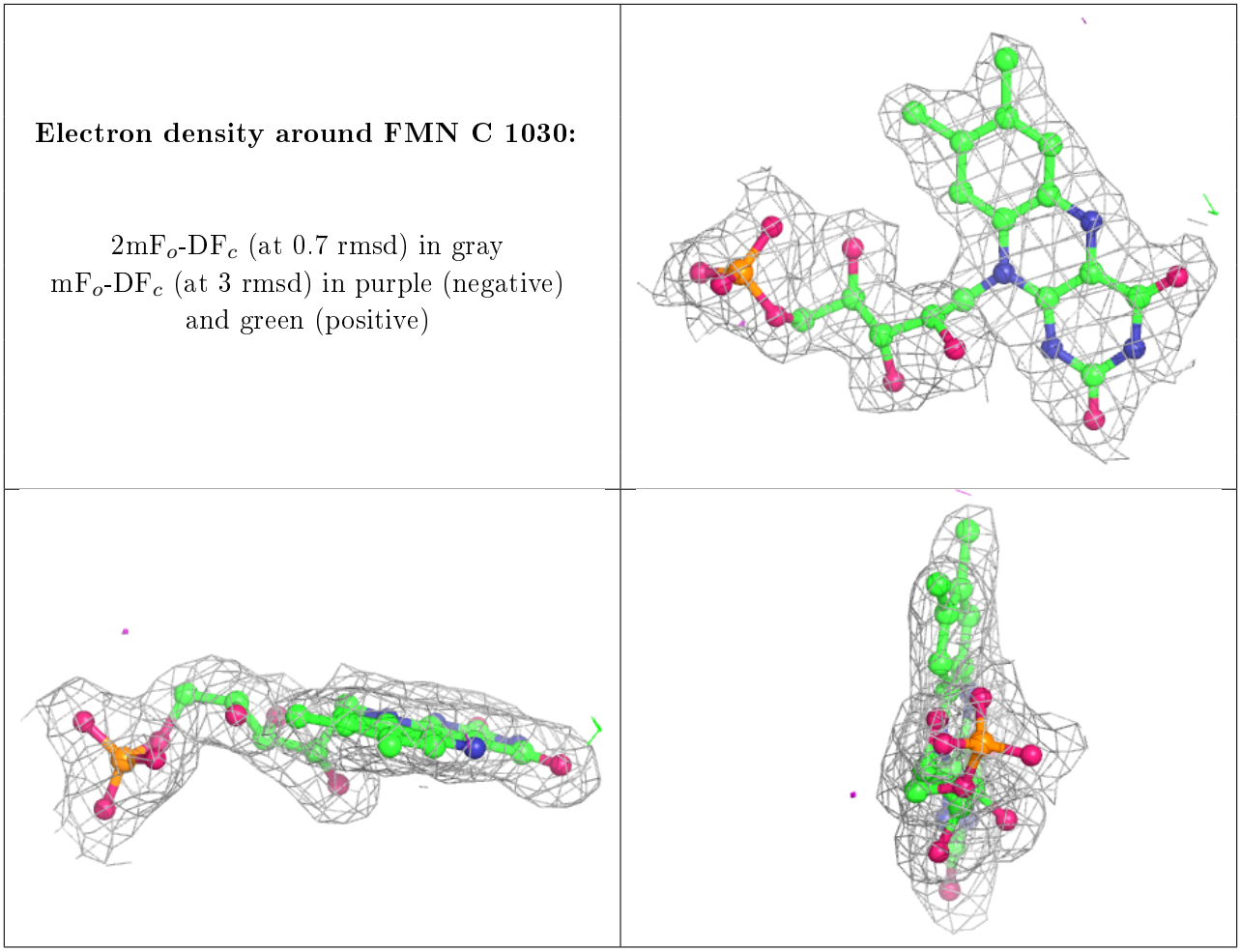
Electron density around FMN B 1030:

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



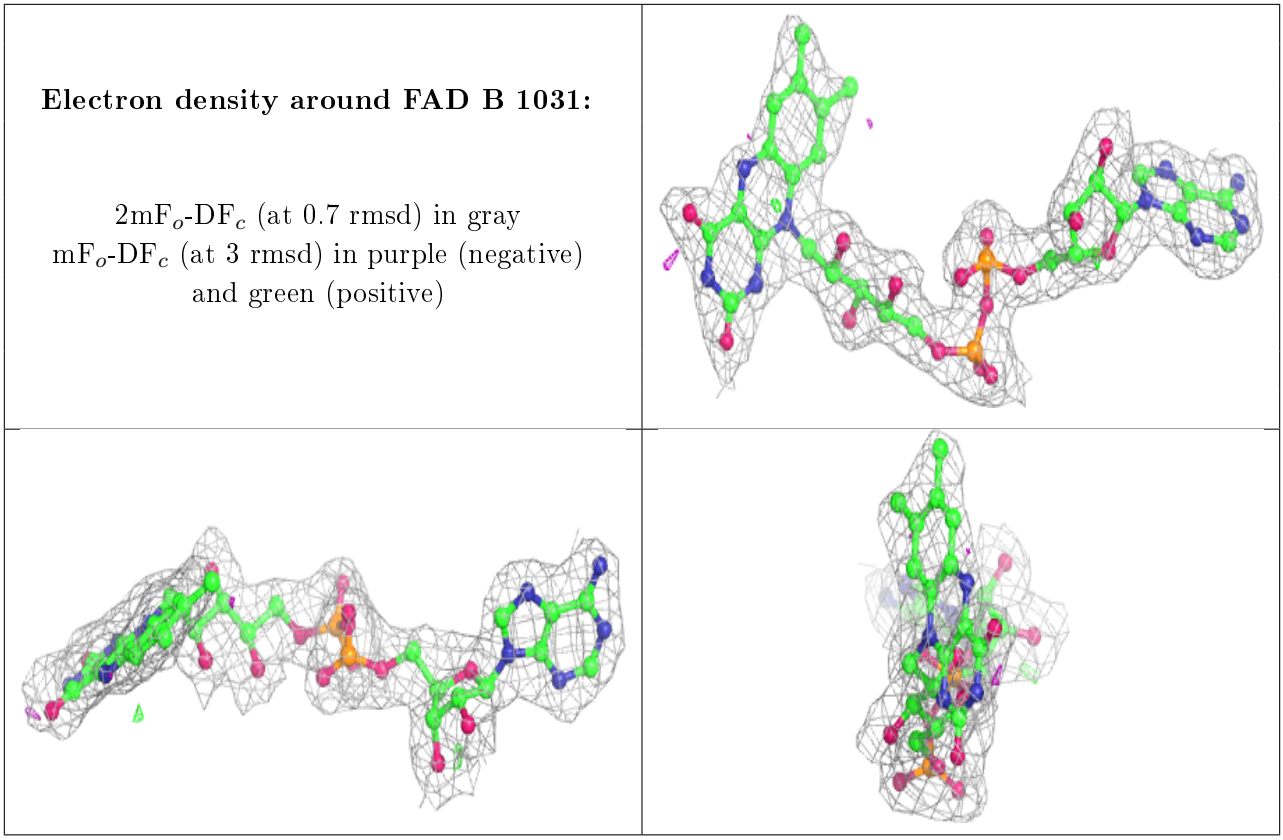
Electron density around FMN C 1030:

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



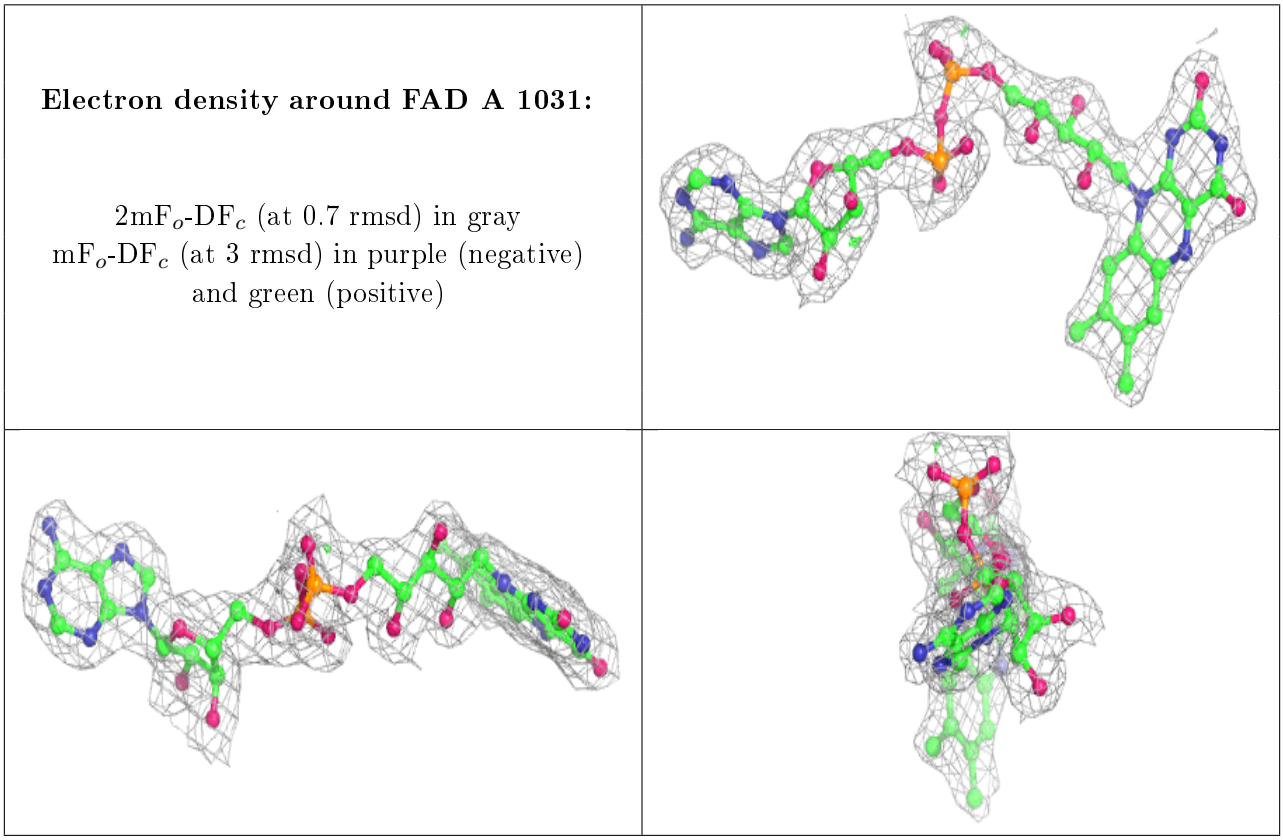
Electron density around FAD B 1031:

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



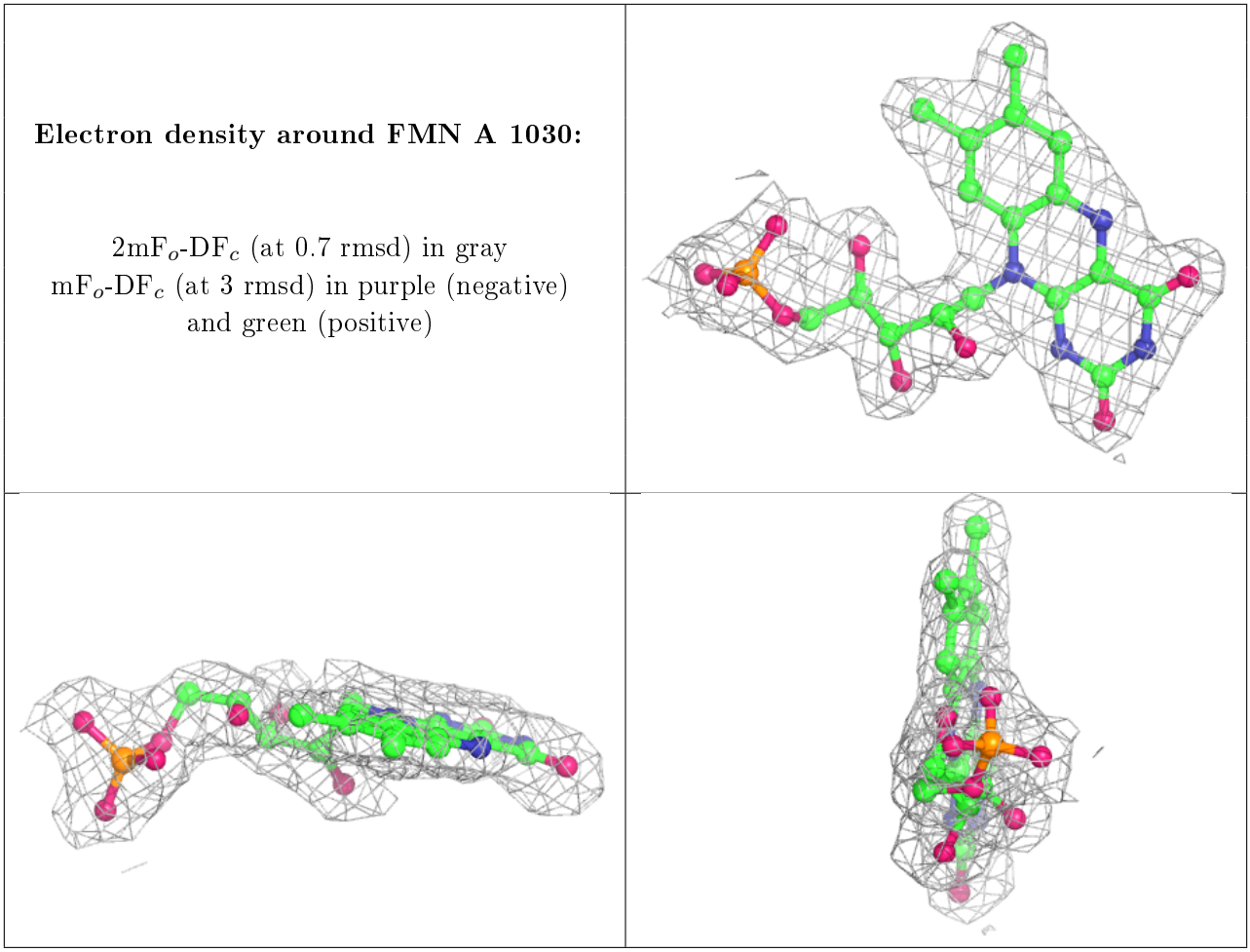
Electron density around FAD A 1031:

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



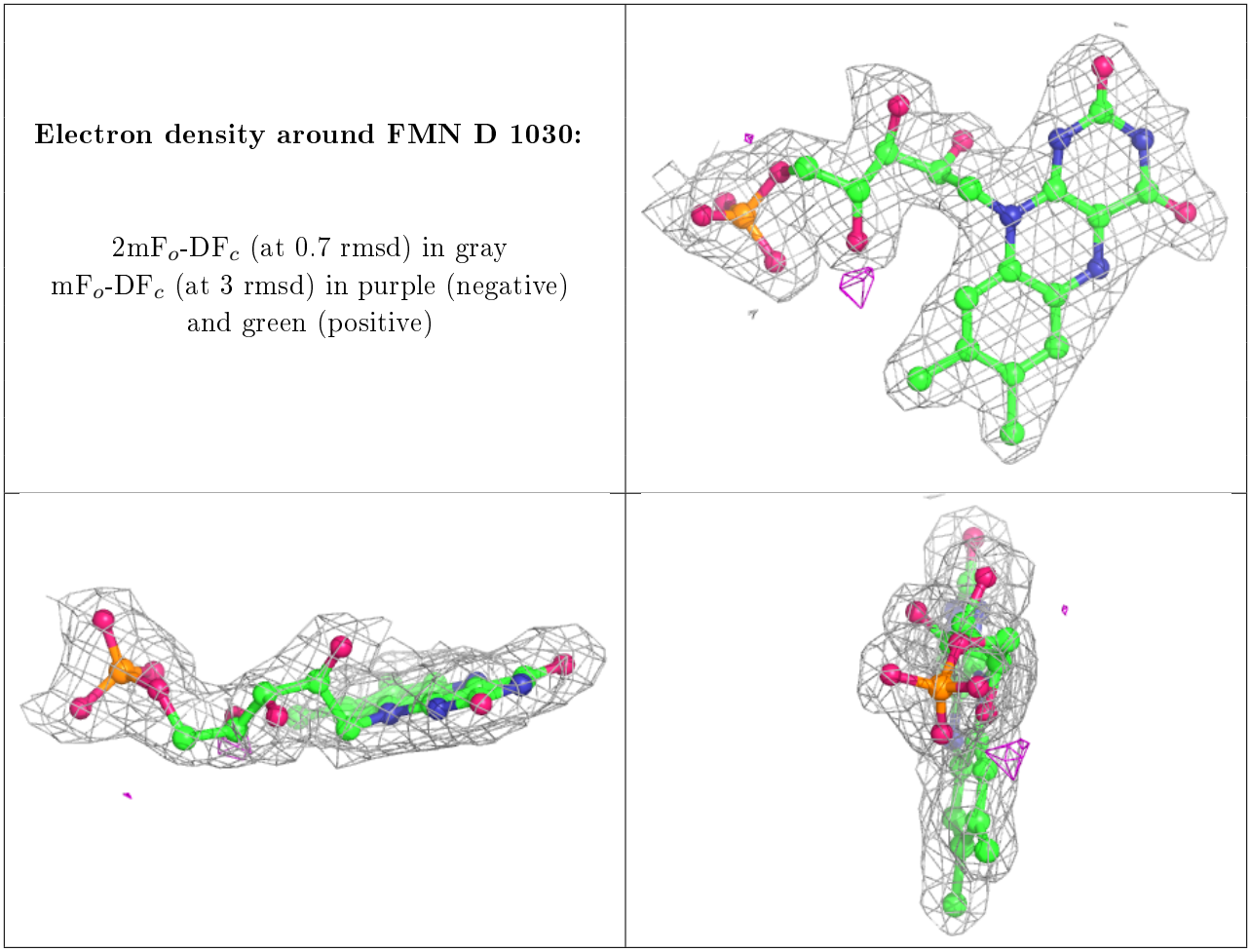
Electron density around FMN A 1030:

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



Electron density around FMN D 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.