Full wwPDB X-ray Structure Validation Report (i)

Apr 21, 2024 – 03:47 am BST

PDB ID	:	1H7X
Title	:	Dihydropyrimidine dehydrogenase (DPD) from pig, ternary complex of a mutant enzyme (C671A), NADPH and 5-fluorouracil
Authors	:	Dobritzsch, D.; Schneider, G.; Schnackerz, K.D.; Lindqvist, Y.
Deposited on	:	2001-01-19
Resolution	:	2.01 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

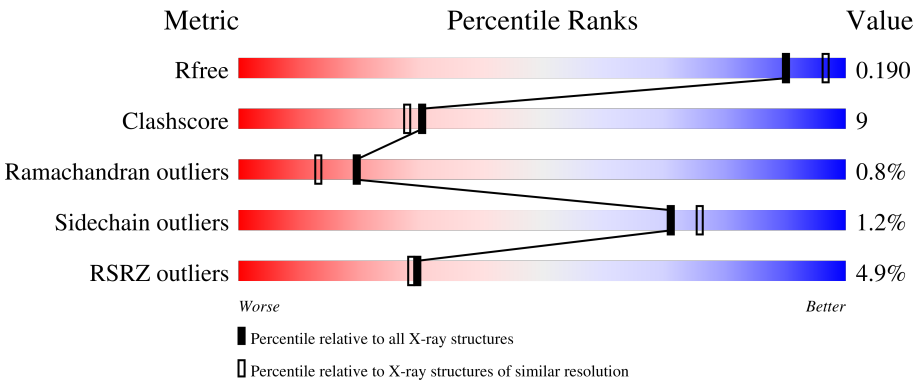
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.01 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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

Mol	Chain	Length	Quality of chain
1	A	1025	5% 83% 16% ••
1	B	1025	5% 83% 16% ••
1	C	1025	5% 82% 16% ••
1	D	1025	4% 83% 16% ••

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	B	1027	-	-	X	-
2	SF4	D	1027	-	-	X	-
5	NDP	A	1032	X	-	-	-
5	NDP	B	1032	X	-	-	-
5	NDP	C	1032	X	-	-	-
5	NDP	D	1032	X	-	-	-
6	URF	A	1033	-	X	-	-
6	URF	B	1033	-	X	-	-
6	URF	C	1033	-	X	-	-
6	URF	D	1033	-	X	-	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 36037 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.

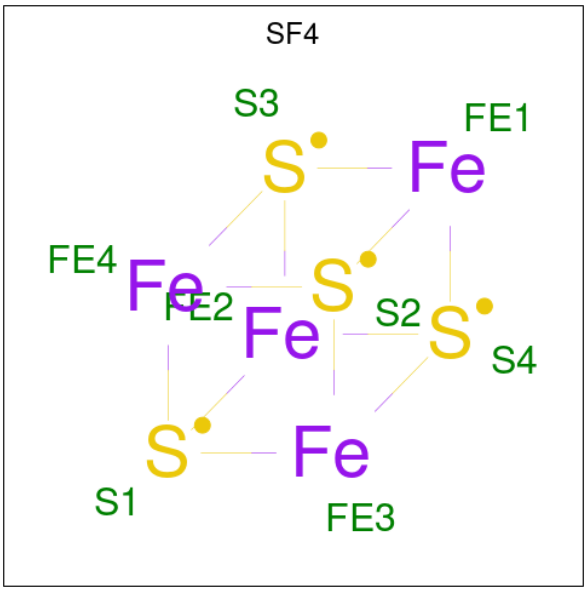
- Molecule 1 is a protein called DIHYDROPYRIMIDINE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1016	7749	4913	1314	1467	55	124	0	0
1	B	1019	7769	4927	1317	1470	55	95	0	0
1	C	1019	7769	4927	1317	1470	55	44	0	0
1	D	1019	7769	4927	1317	1470	55	110	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	60	ASP	GLY	conflict	UNP Q28943
A	671	ALA	CYS	engineered mutation	UNP Q28943
B	60	ASP	GLY	conflict	UNP Q28943
B	671	ALA	CYS	engineered mutation	UNP Q28943
C	60	ASP	GLY	conflict	UNP Q28943
C	671	ALA	CYS	engineered mutation	UNP Q28943
D	60	ASP	GLY	conflict	UNP Q28943
D	671	ALA	CYS	engineered mutation	UNP Q28943

- Molecule 2 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



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

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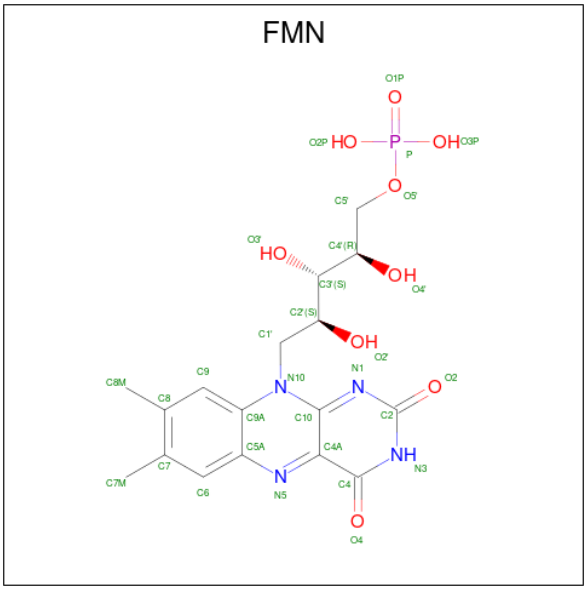
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	Fe	S			
2	D	1	8	4	4		0	0
			Total	Fe	S			
2	D	1	8	4	4		0	0

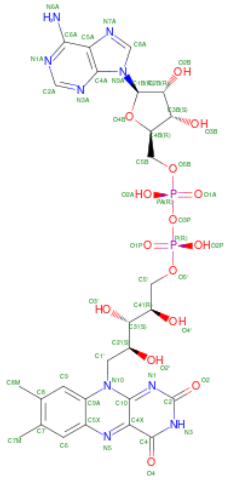
- Molecule 3 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



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

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

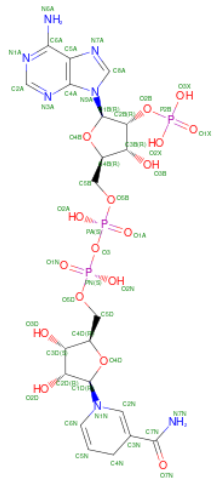
FAD



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

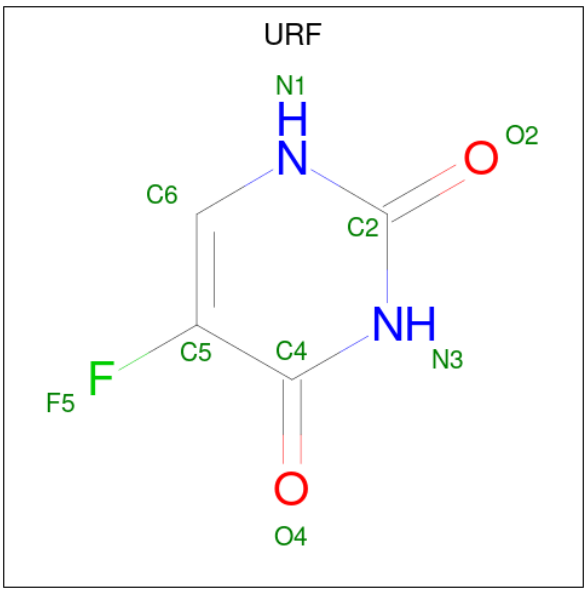
- Molecule 5 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).

NDP



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
5	A	1	48	21	7	17	3	9	0
5	B	1	48	21	7	17	3	0	0
5	C	1	48	21	7	17	3	9	0
5	D	1	48	21	7	17	3	0	0

- Molecule 6 is 5-FLUOROURACIL (three-letter code: URF) (formula: $C_4H_3FN_2O_2$).



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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	1052	1052	1052	0	0
7	B	1048	1048	1048	0	0

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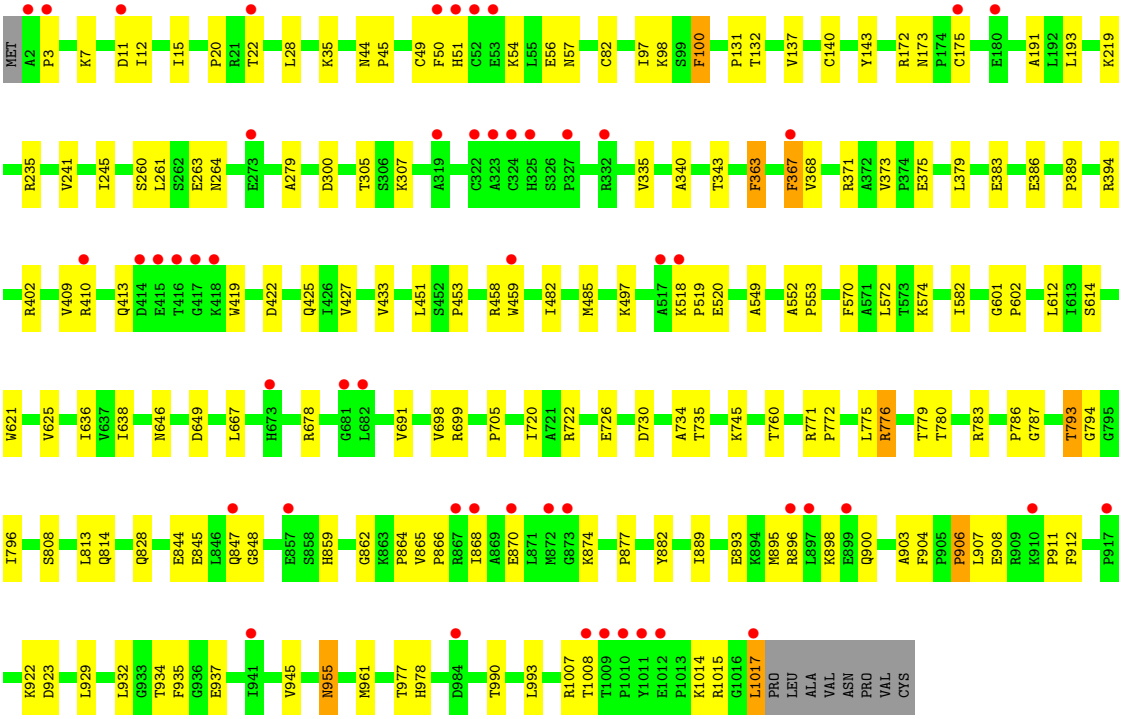
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	C	1096	1096	1096	0	0
			Total	O		
7	D	1093	1093	1093	0	0

3 Residue-property plots (i)

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

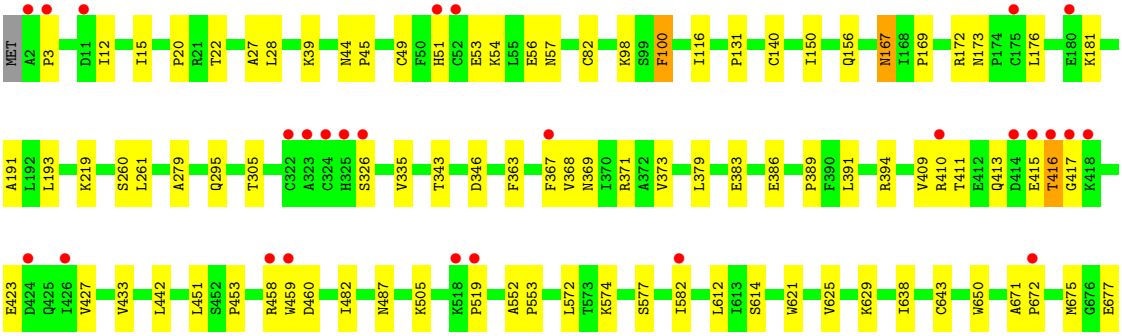
• Molecule 1: DIHYDROPYRIMIDINE DEHYDROGENASE

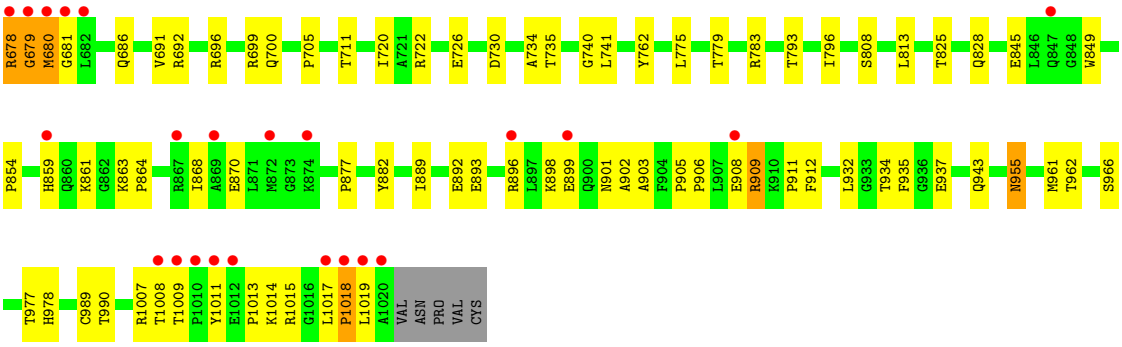
Chain A:



• Molecule 1: DIHYDROPYRIMIDINE DEHYDROGENASE

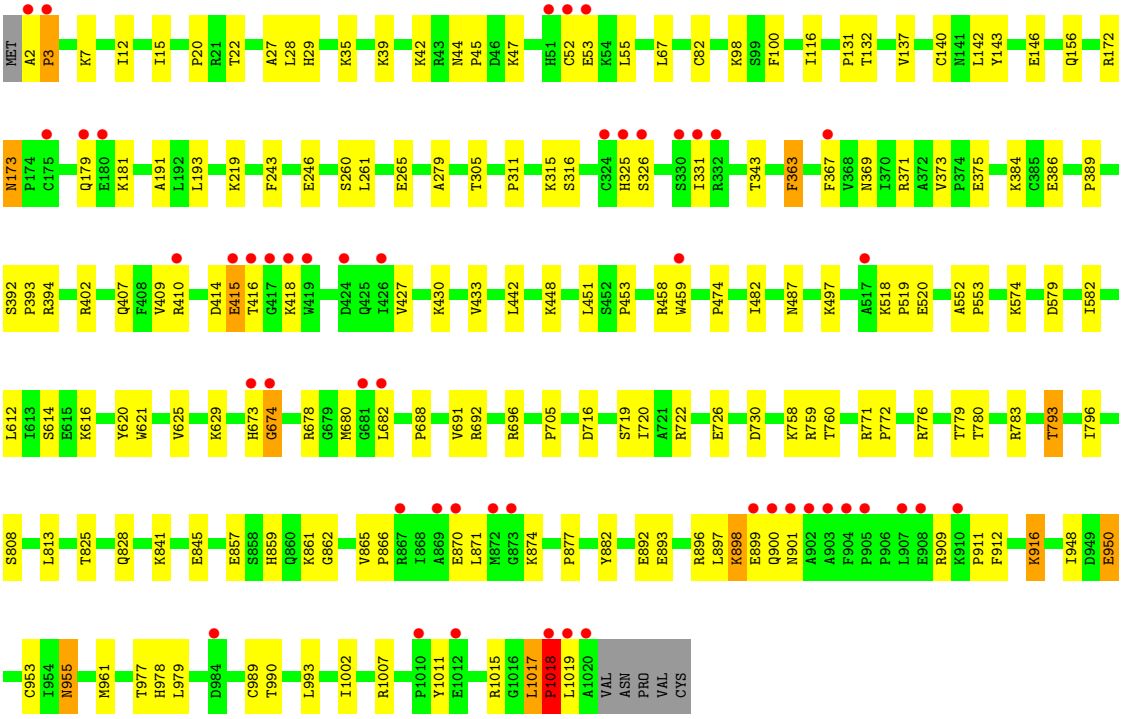
Chain B:





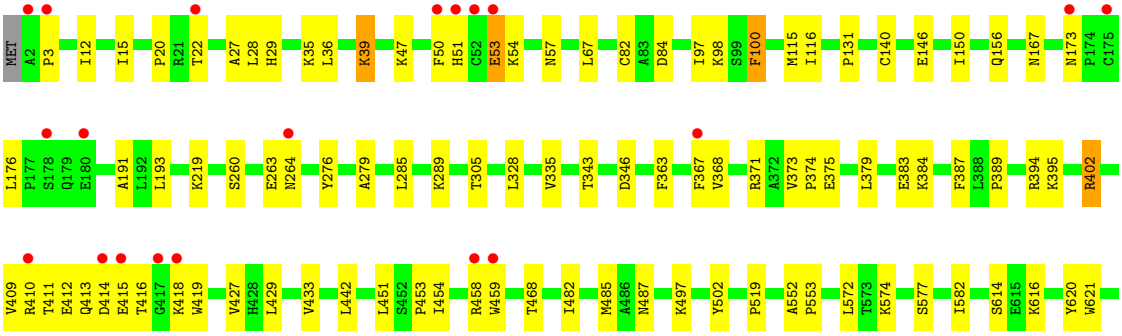
- Molecule 1: DIHYDROPYRIMIDINE DEHYDROGENASE

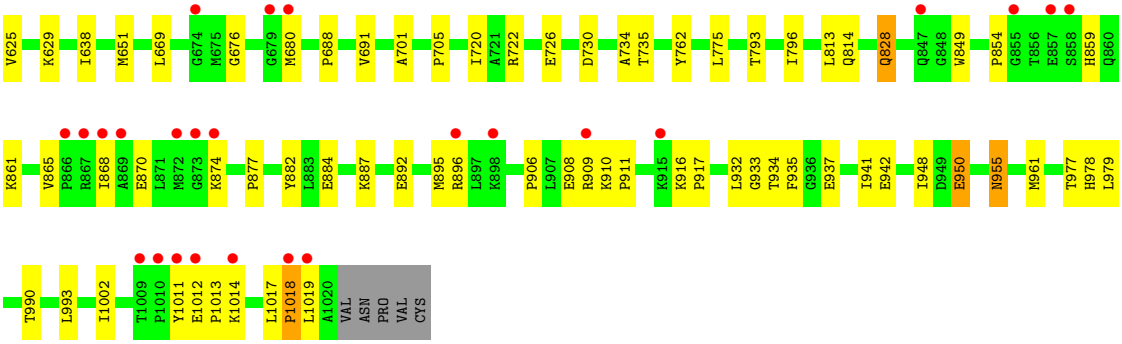
Chain C:



- Molecule 1: DIHYDROPYRIMIDINE DEHYDROGENASE

Chain D:




V625
K629
I638
M651
L669
G674
M675
G676
G679
M680
P688
V691
A701
P705
I720
A721
R722
E726
D730
A734
T735
Y762
L775
T793
I796
L813
Q814
Q828
Q847
G848
W849
P854
G855
T856
E857
S858
H859
Q860
K861
V865
P866
R867
I868
A869
E870
L871
M872
G873
K874
P877
Y882
L883
E884
K887
E892
M895
R896
L897
K898
P906
L907
E908
R909
K910
P911
K915
K916
P917
L932
G933
T934
F935
G936
E937
I941
E942
I948
D949
E950
N955
M961
T977
H978
L979
T990
L993
I1002
T1009
P1010
Y1011
E1012
P1013
K1014
L1017
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	81.95Å 159.29Å 163.57Å 90.00° 96.04° 90.00°	Depositor
Resolution (Å)	25.08 – 2.01 25.08 – 2.01	Depositor EDS
% Data completeness (in resolution range)	98.6 (25.08-2.01) 98.7 (25.08-2.01)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	4.07 (at 2.01Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.171 , 0.192 0.168 , 0.190	Depositor DCC
R_{free} test set	5418 reflections (1.98%)	wwPDB-VP
Wilson B-factor (Å^2)	15.5	Xtriage
Anisotropy	0.360	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 58.4	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	36037	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.61% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: FMN, SF4, URF, NDP, 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	0.31	0/7910	0.60	3/10720 (0.0%)
1	B	0.31	0/7931	0.59	1/10750 (0.0%)
1	C	0.33	0/7931	0.60	1/10750 (0.0%)
1	D	0.31	0/7931	0.60	1/10750 (0.0%)
All	All	0.32	0/31703	0.60	6/42970 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1017	LEU	CA-CB-CG	-5.88	101.77	115.30
1	C	305	THR	N-CA-C	-5.28	96.74	111.00
1	D	305	THR	N-CA-C	-5.13	97.15	111.00
1	B	305	THR	N-CA-C	-5.08	97.28	111.00
1	A	1017	LEU	N-CA-C	5.02	124.56	111.00
1	A	305	THR	N-CA-C	-5.01	97.48	111.00

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	7749	0	7775	160	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	7769	0	7798	157	1
1	C	7769	0	7798	164	0
1	D	7769	0	7798	175	1
2	A	32	0	0	2	0
2	B	32	0	0	2	0
2	C	32	0	0	1	0
2	D	32	0	0	3	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	3	0
4	B	53	0	31	3	0
4	C	53	0	31	1	0
4	D	53	0	31	2	0
5	A	48	0	26	1	0
5	B	48	0	26	3	0
5	C	48	0	26	1	0
5	D	48	0	26	7	0
6	A	9	0	3	0	0
6	B	9	0	3	0	0
6	C	9	0	3	0	0
6	D	9	0	3	0	0
7	A	1052	0	0	36	0
7	B	1048	0	0	31	0
7	C	1096	0	0	26	0
7	D	1093	0	0	28	0
All	All	36037	0	31485	579	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (579) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:22:THR:HG22	7:D:2056:HOH:O	1.62	0.96
1:A:410:ARG:HH21	1:B:427:VAL:HG21	1.30	0.96
1:A:410:ARG:NH2	1:B:427:VAL:HG21	1.81	0.95
1:A:923:ASP:OD1	1:D:937:GLU:HG2	1.67	0.93
1:A:1017:LEU:O	1:A:1017:LEU:HD12	1.68	0.93
1:C:487:ASN:HD21	1:D:35:LYS:HZ1	1.22	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1015:ARG:C	1:A:1017:LEU:H	1.78	0.87
1:A:50:PHE:HE2	1:B:369:ASN:HA	1.40	0.85
1:A:410:ARG:HH21	1:B:427:VAL:CG2	1.90	0.85
1:A:173:ASN:HB2	7:A:2315:HOH:O	1.77	0.84
1:D:487:ASN:O	5:D:1032:NDP:H2N	1.77	0.82
1:D:22:THR:HG23	7:D:2057:HOH:O	1.79	0.81
1:D:402:ARG:HH11	1:D:402:ARG:HB3	1.45	0.81
1:A:427:VAL:HG13	1:B:410:ARG:NH1	1.94	0.81
1:A:427:VAL:HG13	1:B:410:ARG:CZ	2.10	0.80
1:D:264:ASN:HB2	7:D:2412:HOH:O	1.79	0.80
1:A:22:THR:HB	7:A:2049:HOH:O	1.81	0.78
1:C:1017:LEU:HD23	1:C:1018:PRO:HD2	1.65	0.78
1:D:51:HIS:HA	1:D:384:LYS:HG3	1.66	0.77
1:C:487:ASN:HD21	1:D:35:LYS:NZ	1.82	0.76
1:C:776:ARG:O	1:C:780:THR:HG23	1.86	0.76
1:B:458:ARG:HG2	1:B:459:TRP:CE3	2.21	0.75
1:B:896:ARG:HH11	1:B:896:ARG:HG2	1.51	0.75
7:A:2049:HOH:O	1:B:825:THR:HB	1.87	0.74
1:C:53:GLU:OE2	1:C:55:LEU:HD21	1.88	0.74
1:C:579:ASP:O	1:C:582:ILE:HG12	1.86	0.74
1:C:369:ASN:HA	1:D:50:PHE:HE1	1.51	0.73
1:C:427:VAL:HG13	1:D:410:ARG:CZ	2.18	0.73
1:C:260:SER:HB2	1:C:265:GLU:OE1	1.88	0.73
1:A:410:ARG:HE	1:B:427:VAL:HG22	1.52	0.73
1:D:487:ASN:HB3	5:D:1032:NDP:C7N	2.18	0.73
1:D:1018:PRO:HD3	7:D:3069:HOH:O	1.88	0.73
1:A:371:ARG:HD3	7:A:3046:HOH:O	1.89	0.72
1:C:859:HIS:HD2	1:C:862:GLY:H	1.35	0.72
1:C:316:SER:HA	1:C:325:HIS:CD2	2.25	0.72
1:A:386:GLU:OE2	1:B:368:VAL:HG22	1.89	0.72
1:C:1017:LEU:CD2	1:C:1018:PRO:HD2	2.20	0.72
1:A:22:THR:HG22	7:A:2050:HOH:O	1.88	0.72
1:D:1011:TYR:CE2	1:D:1013:PRO:HG3	2.25	0.71
1:B:678:ARG:O	1:B:680:MET:N	2.23	0.70
1:A:50:PHE:CE2	1:B:369:ASN:HA	2.25	0.70
1:C:458:ARG:HH21	1:C:459:TRP:HH2	1.39	0.70
1:C:427:VAL:HG13	1:D:410:ARG:NH1	2.06	0.70
1:A:371:ARG:HH11	1:A:371:ARG:HG2	1.57	0.69
1:A:54:LYS:HE3	7:A:2115:HOH:O	1.93	0.68
1:D:909:ARG:HG3	7:D:2272:HOH:O	1.92	0.68
5:D:1032:NDP:O2N	5:D:1032:NDP:C4D	2.42	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:487:ASN:ND2	1:D:35:LYS:NZ	2.41	0.67
1:C:487:ASN:ND2	1:D:35:LYS:HZ1	1.90	0.67
1:A:776:ARG:O	1:A:780:THR:HG23	1.94	0.67
1:A:1017:LEU:O	1:A:1017:LEU:CD1	2.43	0.67
1:C:1019:LEU:HD21	1:D:582:ILE:CD1	2.25	0.67
1:A:868:ILE:HD12	1:A:893:GLU:HB2	1.77	0.66
1:C:950:GLU:HG3	1:C:979:LEU:HD22	1.76	0.66
1:C:870:GLU:O	1:C:874:LYS:HD2	1.96	0.66
1:A:410:ARG:NH1	7:A:2542:HOH:O	2.20	0.66
1:A:458:ARG:HG2	1:A:459:TRP:CE3	2.31	0.66
1:D:36:LEU:HA	1:D:39:LYS:HE2	1.78	0.66
1:A:7:LYS:HE2	7:A:2009:HOH:O	1.95	0.65
1:C:371:ARG:HG2	1:C:371:ARG:HH11	1.61	0.65
1:D:1014:LYS:NZ	7:D:3061:HOH:O	2.27	0.65
1:A:410:ARG:NH2	1:B:427:VAL:CG2	2.54	0.65
1:D:458:ARG:HH21	1:D:459:TRP:HH2	1.43	0.65
1:A:787:GLY:HA3	1:D:942:GLU:OE2	1.97	0.65
1:D:487:ASN:HB3	5:D:1032:NDP:C3N	2.26	0.65
1:A:458:ARG:HD3	7:A:2577:HOH:O	1.95	0.65
1:B:893:GLU:OE1	1:B:896:ARG:NH2	2.30	0.65
1:D:328:LEU:HD12	7:D:2119:HOH:O	1.97	0.65
1:A:722:ARG:O	1:A:726:GLU:HG3	1.97	0.64
1:A:870:GLU:O	1:A:874:LYS:HD3	1.98	0.64
1:C:52:CYS:HB2	1:C:384:LYS:HB2	1.79	0.64
1:A:54:LYS:NZ	1:A:895:MET:HG3	2.13	0.63
1:A:699:ARG:O	1:A:699:ARG:HD3	1.98	0.63
1:C:448:LYS:HD3	7:C:2589:HOH:O	1.97	0.63
1:D:394:ARG:HG3	1:D:409:VAL:HG13	1.79	0.63
1:D:722:ARG:O	1:D:726:GLU:HG3	1.98	0.63
1:B:722:ARG:O	1:B:726:GLU:HG3	1.99	0.63
1:C:780:THR:HG22	1:D:762:TYR:CZ	2.33	0.62
1:C:990:THR:O	1:C:990:THR:HG22	1.99	0.62
7:C:2879:HOH:O	1:D:22:THR:CG2	2.46	0.62
1:C:2:ALA:HB3	7:D:2747:HOH:O	1.99	0.62
1:C:369:ASN:HA	1:D:50:PHE:CE1	2.33	0.61
1:D:414:ASP:O	1:D:416:THR:N	2.32	0.61
1:D:379:LEU:O	1:D:383:GLU:HG3	2.01	0.61
1:D:402:ARG:HB3	1:D:402:ARG:NH1	2.14	0.61
1:D:285:LEU:HD12	7:D:3081:HOH:O	2.00	0.61
1:B:394:ARG:HG3	1:B:409:VAL:HG13	1.82	0.61
1:A:582:ILE:HD11	1:B:1015:ARG:CZ	2.31	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	2.01	0.60
1:C:179:GLN:HG3	7:C:2274:HOH:O	2.01	0.60
1:B:678:ARG:O	1:B:680:MET:HE3	2.01	0.60
1:C:1007:ARG:CD	1:C:1011:TYR:HB2	2.31	0.60
1:A:896:ARG:HD2	7:A:2923:HOH:O	2.00	0.60
1:A:868:ILE:HG12	1:A:870:GLU:H	1.67	0.60
1:B:678:ARG:O	1:B:679:GLY:C	2.38	0.60
1:C:219:LYS:HG3	1:C:260:SER:OG	2.01	0.60
1:B:990:THR:HG22	1:B:990:THR:O	2.02	0.60
1:C:410:ARG:CZ	1:D:427:VAL:HG13	2.32	0.60
1:A:859:HIS:HD2	1:A:862:GLY:H	1.47	0.59
1:D:343:THR:HA	4:D:1031:FAD:HM73	1.84	0.59
1:D:51:HIS:HD2	1:D:384:LYS:HB2	1.66	0.59
1:D:990:THR:HG22	1:D:990:THR:O	2.01	0.59
1:D:950:GLU:HG3	1:D:979:LEU:HD22	1.85	0.59
1:B:845:GLU:HG3	1:B:912:PHE:CD1	2.38	0.59
1:B:696:ARG:HD2	7:B:2763:HOH:O	2.02	0.59
1:C:845:GLU:HG3	1:C:912:PHE:CD1	2.37	0.59
1:A:410:ARG:NE	1:B:427:VAL:HG22	2.16	0.59
1:B:859:HIS:HE1	1:B:864:PRO:HG3	1.67	0.59
1:C:371:ARG:HG2	1:C:371:ARG:NH1	2.18	0.59
1:A:1007:ARG:NH2	7:A:3025:HOH:O	2.36	0.59
1:C:367:PHE:CZ	1:D:367:PHE:CE1	2.91	0.58
1:C:1015:ARG:CZ	1:D:582:ILE:HD11	2.33	0.58
1:D:289:LYS:HD2	7:D:2583:HOH:O	2.03	0.58
1:B:413:GLN:HE21	1:B:417:GLY:HA2	1.68	0.58
1:A:845:GLU:HG3	1:A:912:PHE:CE1	2.39	0.58
1:A:54:LYS:HZ1	1:A:895:MET:HG3	1.69	0.58
1:C:243:PHE:HD1	1:C:909:ARG:NH1	2.02	0.58
1:B:896:ARG:NH2	7:B:2915:HOH:O	2.36	0.58
1:A:219:LYS:HG3	1:A:260:SER:OG	2.02	0.57
1:A:12:ILE:O	1:A:15:ILE:HG22	2.04	0.57
1:A:57:ASN:HB2	7:A:2120:HOH:O	2.03	0.57
4:B:1031:FAD:H1'1	5:B:1032:NDP:H3D	1.86	0.57
1:C:722:ARG:O	1:C:726:GLU:HG3	2.05	0.57
1:A:363:PHE:HE1	1:A:389:PRO:HB3	1.70	0.57
1:A:485:MET:HE3	7:A:2266:HOH:O	2.04	0.57
1:C:582:ILE:CD1	7:C:2719:HOH:O	2.53	0.57
1:A:745:LYS:HD2	7:A:2801:HOH:O	2.05	0.57
1:C:780:THR:HG22	1:D:762:TYR:CE2	2.39	0.56
1:C:861:LYS:HE3	7:C:2922:HOH:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:870:GLU:OE1	1:A:889:ILE:HG23	2.05	0.56
1:A:877:PRO:HD2	1:A:882:TYR:CG	2.40	0.56
1:B:877:PRO:HD2	1:B:882:TYR:CG	2.41	0.56
1:B:343:THR:HA	4:B:1031:FAD:HM73	1.87	0.56
1:C:783:ARG:HD3	7:C:2852:HOH:O	2.05	0.56
1:A:371:ARG:HG2	1:A:371:ARG:NH1	2.20	0.56
1:C:246:GLU:HG3	1:C:909:ARG:HG2	1.87	0.56
1:A:828:GLN:HG2	7:A:2853:HOH:O	2.06	0.56
1:B:326:SER:HB3	7:B:2437:HOH:O	2.05	0.56
1:C:386:GLU:OE1	1:D:368:VAL:HG22	2.06	0.56
1:D:167:ASN:ND2	1:D:910:LYS:O	2.38	0.56
1:D:367:PHE:HZ	1:D:387:PHE:HB2	1.70	0.56
1:A:1014:LYS:HB3	7:A:3032:HOH:O	2.06	0.56
1:B:505:LYS:HE2	7:B:2602:HOH:O	2.06	0.56
1:C:367:PHE:CZ	1:D:367:PHE:CZ	2.94	0.56
1:A:775:LEU:O	1:A:779:THR:HG23	2.06	0.55
1:A:143:TYR:O	1:B:861:LYS:HE2	2.06	0.55
1:A:779:THR:HG22	1:A:808:SER:HB3	1.88	0.55
1:A:845:GLU:HG3	1:A:912:PHE:CD1	2.42	0.55
1:B:415:GLU:O	1:B:416:THR:OG1	2.20	0.55
1:C:978:HIS:HE1	1:D:84:ASP:OD2	1.88	0.55
1:B:783:ARG:HD3	7:B:2825:HOH:O	2.05	0.55
7:C:2879:HOH:O	1:D:22:THR:HG21	2.07	0.55
1:A:911:PRO:HG2	7:A:2379:HOH:O	2.06	0.55
1:C:172:ARG:HG3	7:C:2303:HOH:O	2.06	0.55
1:C:442:LEU:HD22	1:C:482:ILE:HD11	1.87	0.55
1:A:870:GLU:OE2	1:A:896:ARG:NH2	2.28	0.55
1:A:1014:LYS:HE3	7:A:2976:HOH:O	2.07	0.55
1:A:780:THR:HG22	1:B:762:TYR:CZ	2.42	0.55
1:A:1015:ARG:C	1:A:1017:LEU:N	2.54	0.55
1:C:343:THR:HA	4:C:1031:FAD:HM73	1.87	0.55
1:A:340:ALA:HB3	7:A:3050:HOH:O	2.06	0.55
1:B:413:GLN:HG3	1:B:417:GLY:O	2.06	0.55
1:C:845:GLU:HG3	1:C:912:PHE:CE1	2.42	0.55
1:A:379:LEU:O	1:A:383:GLU:HG3	2.07	0.54
1:B:131:PRO:HB2	1:B:373:VAL:HG11	1.89	0.54
1:B:582:ILE:HG13	7:B:2701:HOH:O	2.05	0.54
1:B:12:ILE:O	1:B:15:ILE:HG22	2.07	0.54
1:C:682:LEU:HD23	7:C:2777:HOH:O	2.06	0.54
1:C:410:ARG:HH22	1:D:429:LEU:HD13	1.73	0.54
1:D:193:LEU:N	1:D:193:LEU:HD22	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:582:ILE:HG13	7:D:2737:HOH:O	2.06	0.54
1:C:900:GLN:HG2	1:C:901:ASN:N	2.22	0.54
1:D:877:PRO:HD2	1:D:882:TYR:CG	2.43	0.54
1:D:574:LYS:HG3	1:D:614:SER:HB2	1.90	0.54
1:D:934:THR:OG1	1:D:937:GLU:HG3	2.07	0.54
1:C:582:ILE:HD11	1:D:1019:LEU:CD1	2.36	0.54
1:A:263:GLU:O	1:A:264:ASN:HB2	2.08	0.54
1:B:261:LEU:HD21	1:B:451:LEU:HD21	1.90	0.54
1:C:691:VAL:HG21	1:C:720:ILE:HG23	1.90	0.54
1:A:343:THR:HA	4:A:1031:FAD:HM73	1.89	0.53
1:B:1011:TYR:HE2	1:B:1013:PRO:HG3	1.73	0.53
1:A:367:PHE:CE1	1:B:367:PHE:CZ	2.96	0.53
1:C:27:ALA:O	1:D:497:LYS:HE2	2.09	0.53
1:D:911:PRO:HG2	7:D:2390:HOH:O	2.07	0.53
1:C:474:PRO:HG2	7:C:2277:HOH:O	2.07	0.53
1:C:582:ILE:HG13	1:D:1019:LEU:HD21	1.90	0.53
7:C:3092:HOH:O	1:D:35:LYS:HE3	2.08	0.53
1:D:793:THR:HG21	3:D:1030:FMN:O3'	2.09	0.53
1:A:552:ALA:HB3	1:A:553:PRO:HD3	1.91	0.53
1:B:552:ALA:HB3	1:B:553:PRO:HD3	1.91	0.53
1:C:780:THR:HG22	1:D:762:TYR:OH	2.09	0.53
1:B:877:PRO:CG	1:B:977:THR:HB	2.39	0.53
1:C:131:PRO:HB2	1:C:373:VAL:HG11	1.91	0.53
1:A:955:ASN:HB3	1:A:978:HIS:HB3	1.89	0.53
1:B:572:LEU:HD13	1:B:638:ILE:HB	1.90	0.53
1:B:691:VAL:HG21	1:B:720:ILE:HG23	1.90	0.53
1:C:331:ILE:HG23	1:C:433:VAL:HG21	1.91	0.53
1:B:896:ARG:HG2	1:B:896:ARG:NH1	2.21	0.53
7:A:2937:HOH:O	1:D:941:ILE:HD11	2.08	0.52
1:C:955:ASN:HB3	1:C:978:HIS:HB3	1.90	0.52
1:A:848:GLY:HA3	7:A:2866:HOH:O	2.09	0.52
1:C:143:TYR:O	1:D:861:LYS:HE2	2.09	0.52
1:B:442:LEU:HD22	1:B:482:ILE:HD11	1.91	0.52
1:C:12:ILE:O	1:C:15:ILE:HG22	2.10	0.52
1:C:793:THR:HG21	7:C:2871:HOH:O	2.10	0.52
1:D:54:LYS:NZ	1:D:895:MET:HG3	2.24	0.52
5:D:1032:NDP:O2N	5:D:1032:NDP:H4D	2.09	0.52
1:B:877:PRO:HG2	1:B:977:THR:HB	1.92	0.52
1:D:1011:TYR:CZ	1:D:1013:PRO:HG3	2.44	0.52
1:B:861:LYS:HE3	7:B:2040:HOH:O	2.09	0.52
1:C:497:LYS:HE2	1:D:27:ALA:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:53:GLU:HG3	1:D:887:LYS:HB3	1.92	0.52
1:D:219:LYS:HG3	1:D:260:SER:OG	2.08	0.52
1:B:779:THR:HG22	1:B:808:SER:HB3	1.92	0.52
1:B:1008:THR:HG23	7:B:3014:HOH:O	2.08	0.52
1:A:859:HIS:HA	1:A:865:VAL:HG23	1.90	0.52
1:A:131:PRO:HB2	1:A:373:VAL:HG11	1.91	0.52
1:B:692:ARG:O	1:B:696:ARG:HD3	2.10	0.51
1:D:552:ALA:HB3	1:D:553:PRO:HD3	1.92	0.51
1:A:497:LYS:HE2	1:B:27:ALA:O	2.10	0.51
1:B:870:GLU:N	1:B:870:GLU:OE1	2.43	0.51
1:B:845:GLU:HG3	1:B:912:PHE:CE1	2.46	0.51
1:C:181:LYS:HD2	7:C:2272:HOH:O	2.10	0.51
1:A:235:ARG:NH2	4:A:1031:FAD:O4	2.34	0.51
1:A:307:LYS:HE3	7:A:2516:HOH:O	2.11	0.51
1:A:410:ARG:NH2	1:B:391:LEU:HD21	2.25	0.51
1:B:219:LYS:HG3	1:B:260:SER:OG	2.09	0.51
1:B:1017:LEU:HB3	7:B:3030:HOH:O	2.10	0.51
1:C:877:PRO:HG2	1:C:977:THR:HB	1.93	0.51
1:C:7:LYS:HE3	7:D:2753:HOH:O	2.10	0.51
1:C:900:GLN:HG2	1:C:901:ASN:H	1.76	0.51
1:D:892:GLU:HG3	7:D:2958:HOH:O	2.10	0.51
1:A:793:THR:HG21	7:A:2773:HOH:O	2.11	0.51
1:B:577:SER:HB2	7:B:2667:HOH:O	2.11	0.51
1:A:934:THR:OG1	1:A:937:GLU:HG3	2.09	0.51
1:C:993:LEU:HD23	1:C:993:LEU:C	2.32	0.50
1:A:612:LEU:HD11	1:B:935:PHE:CE2	2.46	0.50
1:A:646:ASN:HD22	1:A:649:ASP:CG	2.14	0.50
1:A:896:ARG:NH2	7:A:2921:HOH:O	2.43	0.50
1:C:82:CYS:O	1:C:98:LYS:HD2	2.11	0.50
1:C:373:VAL:HG12	1:D:47:LYS:HD3	1.94	0.50
1:A:870:GLU:HG3	7:A:2902:HOH:O	2.11	0.50
1:A:945:VAL:HG13	1:A:1007:ARG:HG2	1.94	0.50
1:B:363:PHE:CE2	1:B:389:PRO:HB3	2.47	0.50
1:B:574:LYS:CG	1:B:614:SER:HB2	2.41	0.50
1:C:796:ILE:HD13	1:C:813:LEU:HB3	1.94	0.50
1:C:877:PRO:HD2	1:C:882:TYR:CG	2.46	0.50
1:B:696:ARG:O	1:B:700:GLN:HG3	2.11	0.50
1:A:1015:ARG:O	1:A:1017:LEU:N	2.39	0.50
1:D:263:GLU:O	1:D:264:ASN:HB3	2.12	0.50
1:A:582:ILE:HG13	7:A:2702:HOH:O	2.11	0.49
1:C:410:ARG:NH2	1:D:429:LEU:HD13	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:552:ALA:HB3	1:C:553:PRO:HD3	1.94	0.49
1:A:20:PRO:HG2	1:A:961:MET:SD	2.52	0.49
1:C:897:LEU:C	1:C:899:GLU:H	2.15	0.49
1:C:953:CYS:HB3	7:C:3015:HOH:O	2.10	0.49
1:C:430:LYS:HE3	7:D:2564:HOH:O	2.11	0.49
1:D:793:THR:OG1	1:D:814:GLN:HB2	2.12	0.49
1:A:937:GLU:OE1	1:D:1012:GLU:OE2	2.31	0.49
1:B:621:TRP:O	1:B:625:VAL:HG23	2.12	0.49
1:B:720:ILE:HG21	7:B:2758:HOH:O	2.12	0.49
1:C:371:ARG:HD3	5:C:1032:NDP:O1A	2.12	0.49
1:B:629:LYS:HE2	1:B:629:LYS:HA	1.95	0.49
1:A:1015:ARG:CZ	1:B:582:ILE:HD11	2.42	0.49
1:B:295:GLN:HG3	7:B:2415:HOH:O	2.13	0.49
1:C:841:LYS:O	1:C:916:LYS:HE2	2.12	0.49
1:B:796:ILE:HD13	1:B:813:LEU:HB3	1.95	0.49
1:B:908:GLU:O	1:B:909:ARG:C	2.52	0.49
1:C:39:LYS:HG3	7:C:2074:HOH:O	2.11	0.49
1:C:410:ARG:NH1	1:D:427:VAL:HG13	2.28	0.49
1:C:416:THR:HG22	1:C:416:THR:O	2.12	0.49
1:C:574:LYS:CG	1:C:614:SER:HB2	2.42	0.49
1:A:932:LEU:HD11	1:B:741:LEU:HD11	1.94	0.49
1:A:935:PHE:CE2	1:B:612:LEU:HD11	2.48	0.49
1:D:115:MET:HE1	1:D:828:GLN:NE2	2.28	0.49
1:D:442:LEU:HD22	1:D:482:ILE:HD11	1.95	0.49
1:D:688:PRO:HG3	1:D:720:ILE:HD13	1.94	0.49
1:A:844:GLU:O	1:A:847:GLN:HG3	2.13	0.48
1:B:699:ARG:HA	1:B:699:ARG:NE	2.27	0.48
1:B:783:ARG:NH1	7:B:2825:HOH:O	2.36	0.48
1:C:978:HIS:HD2	7:D:2242:HOH:O	1.95	0.48
1:A:193:LEU:HD22	1:A:193:LEU:N	2.27	0.48
1:B:705:PRO:HA	1:B:730:ASP:OD2	2.13	0.48
1:D:54:LYS:HZ1	1:D:895:MET:HG3	1.77	0.48
1:B:1009:THR:HG21	7:B:2994:HOH:O	2.12	0.48
1:C:47:LYS:HD3	1:D:373:VAL:HG12	1.95	0.48
1:C:243:PHE:CD1	1:C:909:ARG:NH1	2.81	0.48
1:D:173:ASN:HB3	1:D:176:LEU:HD12	1.95	0.48
1:D:413:GLN:HG3	1:D:419:TRP:CD2	2.49	0.48
1:D:651:MET:HG2	1:D:701:ALA:HB2	1.95	0.48
1:D:680:MET:CE	1:D:688:PRO:HD3	2.43	0.48
1:A:864:PRO:HG3	7:A:2449:HOH:O	2.13	0.48
1:B:363:PHE:HE2	1:B:389:PRO:HB3	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:909:ARG:HD2	7:C:2360:HOH:O	2.12	0.48
1:C:116:ILE:HD13	1:C:156:GLN:HG3	1.95	0.48
1:C:427:VAL:CG1	1:D:410:ARG:CZ	2.89	0.48
1:D:82:CYS:O	1:D:98:LYS:HD2	2.12	0.48
1:B:458:ARG:HG2	1:B:459:TRP:CZ3	2.49	0.48
1:A:574:LYS:CG	1:A:614:SER:HB2	2.43	0.48
1:B:1007:ARG:HD3	1:B:1009:THR:O	2.13	0.48
1:C:758:LYS:HD3	7:C:2837:HOH:O	2.14	0.48
1:A:866:PRO:HG3	7:A:2127:HOH:O	2.14	0.48
1:B:1011:TYR:CE2	1:B:1013:PRO:HG3	2.48	0.48
1:C:418:LYS:HD2	7:C:2549:HOH:O	2.12	0.48
1:B:172:ARG:HG3	7:B:2294:HOH:O	2.13	0.48
1:B:775:LEU:O	1:B:779:THR:HG23	2.14	0.48
1:D:577:SER:HB2	7:D:2703:HOH:O	2.14	0.48
1:A:877:PRO:CG	1:A:977:THR:HB	2.45	0.47
1:B:487:ASN:ND2	7:B:2590:HOH:O	2.47	0.47
1:B:1009:THR:HB	7:B:2996:HOH:O	2.13	0.47
1:B:1014:LYS:HG3	7:B:3023:HOH:O	2.13	0.47
1:C:673:HIS:O	1:C:674:GLY:O	2.32	0.47
1:D:955:ASN:HB3	1:D:978:HIS:HB3	1.95	0.47
1:A:518:LYS:O	1:A:520:GLU:HG3	2.15	0.47
1:D:796:ILE:HD13	1:D:813:LEU:HB3	1.97	0.47
1:C:877:PRO:CG	1:C:977:THR:HB	2.45	0.47
1:D:375:GLU:H	1:D:375:GLU:CD	2.18	0.47
1:C:692:ARG:O	1:C:696:ARG:HG3	2.15	0.47
1:D:468:THR:HA	1:D:502:TYR:CD2	2.49	0.47
1:A:44:ASN:HB2	1:A:45:PRO:CD	2.45	0.47
1:A:132:THR:HB	1:A:137:VAL:HG23	1.97	0.47
1:A:300:ASP:O	1:A:402:ARG:NH1	2.47	0.47
1:A:410:ARG:HG3	1:A:425:GLN:HB3	1.97	0.47
1:A:582:ILE:HG13	7:A:2673:HOH:O	2.13	0.47
1:A:691:VAL:HG21	1:A:720:ILE:HG23	1.97	0.47
1:A:922:LYS:HE3	1:D:937:GLU:OE1	2.14	0.47
1:C:779:THR:HG22	1:C:808:SER:HB3	1.96	0.47
1:D:115:MET:CE	1:D:828:GLN:NE2	2.78	0.47
1:A:868:ILE:CD1	1:A:870:GLU:HB2	2.45	0.47
1:D:97:ILE:HD11	2:D:1026:SF4:S4	2.54	0.47
1:C:407:GLN:NE2	7:C:2543:HOH:O	2.48	0.47
7:C:2721:HOH:O	1:D:1014:LYS:HD3	2.15	0.47
1:D:1017:LEU:HD22	1:D:1018:PRO:HD2	1.97	0.47
1:B:193:LEU:N	1:B:193:LEU:HD22	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:363:PHE:HE2	1:C:389:PRO:HB3	1.80	0.47
1:D:12:ILE:O	1:D:15:ILE:HG22	2.15	0.47
1:B:955:ASN:HB3	1:B:978:HIS:HB3	1.96	0.46
1:A:49:CYS:SG	1:A:51:HIS:CE1	3.08	0.46
1:A:572:LEU:HD13	1:A:638:ILE:HB	1.95	0.46
1:D:22:THR:HA	7:D:2056:HOH:O	2.15	0.46
1:D:849:TRP:CH2	1:D:854:PRO:HG3	2.50	0.46
1:B:173:ASN:HB3	1:B:176:LEU:HG	1.97	0.46
1:D:705:PRO:HA	1:D:730:ASP:OD2	2.15	0.46
1:D:948:ILE:HG12	1:D:1002:ILE:HG12	1.97	0.46
1:C:146:GLU:HG2	1:D:67:LEU:HD23	1.98	0.46
1:C:909:ARG:O	1:C:911:PRO:HD3	2.14	0.46
1:A:82:CYS:O	1:A:98:LYS:HD2	2.15	0.46
1:A:699:ARG:NH2	1:A:730:ASP:OD2	2.49	0.46
1:A:780:THR:HG22	1:B:762:TYR:OH	2.16	0.46
1:B:828:GLN:HG2	7:B:2848:HOH:O	2.14	0.46
1:C:518:LYS:O	1:C:520:GLU:HG3	2.15	0.46
1:C:191:ALA:O	1:C:279:ALA:HA	2.16	0.46
1:B:1007:ARG:NH1	7:B:2993:HOH:O	2.44	0.46
1:C:688:PRO:HG3	1:C:720:ILE:HD13	1.98	0.46
1:A:375:GLU:H	1:A:375:GLU:CD	2.19	0.46
1:A:582:ILE:HD12	1:B:1019:LEU:HD22	1.97	0.46
1:C:1019:LEU:HD21	1:D:582:ILE:HD13	1.98	0.46
1:D:20:PRO:HG2	1:D:961:MET:SD	2.56	0.46
1:D:410:ARG:HG2	1:D:411:THR:N	2.30	0.46
1:D:574:LYS:CG	1:D:614:SER:HB2	2.45	0.46
1:D:859:HIS:HA	1:D:865:VAL:HG13	1.97	0.46
1:A:175:CYS:HB3	7:A:2277:HOH:O	2.16	0.46
1:A:241:VAL:O	1:A:245:ILE:HG12	2.17	0.46
1:C:2:ALA:HB1	1:C:3:PRO:HD2	1.96	0.46
1:C:582:ILE:HD11	1:D:1019:LEU:HD13	1.98	0.46
1:D:374:PRO:HG3	7:D:2231:HOH:O	2.16	0.46
1:D:868:ILE:HG22	1:D:870:GLU:H	1.80	0.46
1:A:870:GLU:HB3	1:A:889:ILE:CG2	2.46	0.45
1:C:582:ILE:HD11	1:D:1019:LEU:HD11	1.97	0.45
1:D:884:GLU:HB3	7:D:2112:HOH:O	2.16	0.45
1:A:845:GLU:CD	1:A:845:GLU:H	2.20	0.45
1:B:82:CYS:O	1:B:98:LYS:HD2	2.16	0.45
1:B:191:ALA:O	1:B:279:ALA:HA	2.17	0.45
1:B:1014:LYS:HE3	7:B:3027:HOH:O	2.16	0.45
1:B:335:VAL:HG22	1:B:433:VAL:HB	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:711:THR:HG22	7:B:2774:HOH:O	2.15	0.45
1:D:367:PHE:CZ	1:D:387:PHE:CB	3.00	0.45
1:B:169:PRO:HD3	1:B:911:PRO:HB3	1.97	0.45
1:B:943:GLN:HG3	1:B:1011:TYR:CB	2.47	0.45
1:C:948:ILE:HG12	1:C:1002:ILE:HG12	1.97	0.45
1:A:56:GLU:OE2	1:A:898:LYS:NZ	2.48	0.45
1:A:877:PRO:HG2	1:A:977:THR:HB	1.97	0.45
1:B:681:GLY:HA3	1:B:686:GLN:OE1	2.16	0.45
1:D:572:LEU:HD13	1:D:638:ILE:HB	1.98	0.45
1:A:100:PHE:CD1	1:A:100:PHE:C	2.90	0.45
1:C:616:LYS:HD3	1:C:620:TYR:CE2	2.51	0.45
1:A:868:ILE:CD1	1:A:893:GLU:HB2	2.46	0.45
1:D:263:GLU:O	1:D:264:ASN:CB	2.65	0.45
1:D:896:ARG:HD2	7:D:2960:HOH:O	2.15	0.45
1:C:705:PRO:HA	1:C:730:ASP:OD2	2.16	0.45
1:D:54:LYS:HZ1	1:D:895:MET:CG	2.29	0.45
1:A:413:GLN:HG3	1:A:419:TRP:CE2	2.52	0.45
1:A:796:ILE:HD13	1:A:813:LEU:HB3	1.99	0.45
1:B:49:CYS:SG	1:B:51:HIS:CE1	3.10	0.45
1:B:574:LYS:HG3	1:B:614:SER:HB2	1.98	0.45
1:B:870:GLU:O	1:B:889:ILE:HD13	2.17	0.45
1:C:67:LEU:HD23	1:D:146:GLU:HG2	1.99	0.45
1:D:451:LEU:O	1:D:454:ILE:HG12	2.17	0.45
4:A:1031:FAD:H1'1	5:A:1032:NDP:H3D	1.98	0.45
7:A:2197:HOH:O	1:B:22:THR:HG22	2.17	0.45
1:D:335:VAL:HG22	1:D:433:VAL:HB	1.99	0.45
1:B:346:ASP:OD2	4:B:1031:FAD:H6	2.17	0.44
1:D:367:PHE:HZ	1:D:387:PHE:CB	2.29	0.44
1:D:371:ARG:HH21	5:D:1032:NDP:H5N	1.82	0.44
1:A:261:LEU:HD21	1:A:451:LEU:HD21	1.99	0.44
1:A:786:PRO:CB	1:D:942:GLU:HA	2.47	0.44
1:B:696:ARG:NH2	7:B:2765:HOH:O	2.51	0.44
5:B:1032:NDP:H4D	5:B:1032:NDP:O2N	2.17	0.44
1:C:53:GLU:O	1:C:55:LEU:HG	2.17	0.44
1:D:131:PRO:HB2	1:D:373:VAL:HG11	2.00	0.44
1:B:849:TRP:CH2	1:B:854:PRO:HG3	2.52	0.44
1:C:367:PHE:CE1	1:D:367:PHE:CZ	3.05	0.44
7:C:2174:HOH:O	1:D:29:HIS:HB2	2.17	0.44
1:A:191:ALA:O	1:A:279:ALA:HA	2.17	0.44
1:A:993:LEU:C	1:A:993:LEU:HD23	2.38	0.44
1:B:845:GLU:HG3	1:B:912:PHE:CG	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1008:THR:HG23	7:A:3024:HOH:O	2.16	0.44
1:C:574:LYS:HG3	1:C:614:SER:HB2	2.00	0.44
1:C:1007:ARG:HD3	1:C:1011:TYR:HB2	2.00	0.44
1:D:116:ILE:HD13	1:D:156:GLN:HG3	1.99	0.44
1:B:845:GLU:CD	1:B:845:GLU:H	2.21	0.44
1:C:311:PRO:O	1:C:315:LYS:HG3	2.18	0.44
1:C:414:ASP:C	1:C:416:THR:H	2.21	0.44
1:D:346:ASP:OD2	4:D:1031:FAD:H6	2.18	0.44
1:D:485:MET:O	1:D:487:ASN:OD1	2.35	0.44
1:B:22:THR:CG2	7:B:2053:HOH:O	2.66	0.44
1:B:54:LYS:HD3	7:B:2050:HOH:O	2.18	0.44
1:D:870:GLU:OE1	1:D:870:GLU:N	2.45	0.43
1:A:97:ILE:HD11	2:A:1026:SF4:S4	2.58	0.43
1:A:786:PRO:C	1:D:942:GLU:HG2	2.39	0.43
1:B:39:LYS:HG3	7:B:2079:HOH:O	2.18	0.43
1:B:394:ARG:NH2	1:B:423:GLU:OE2	2.51	0.43
1:C:44:ASN:HB2	1:C:45:PRO:CD	2.47	0.43
1:C:893:GLU:OE1	1:C:896:ARG:NH2	2.44	0.43
1:D:412:GLU:O	1:D:419:TRP:HA	2.18	0.43
1:D:680:MET:HE1	1:D:688:PRO:CD	2.47	0.43
1:B:116:ILE:HD13	1:B:156:GLN:HG3	1.99	0.43
1:B:678:ARG:C	1:B:680:MET:N	2.71	0.43
1:B:896:ARG:NH1	1:B:896:ARG:CG	2.80	0.43
1:C:1017:LEU:O	1:C:1018:PRO:C	2.56	0.43
1:D:54:LYS:NZ	1:D:895:MET:CG	2.81	0.43
1:D:57:ASN:HB2	7:D:2119:HOH:O	2.18	0.43
1:A:870:GLU:HB3	1:A:889:ILE:HG23	2.00	0.43
1:B:167:ASN:HD22	1:B:911:PRO:HA	1.83	0.43
1:A:368:VAL:HG23	1:B:386:GLU:OE1	2.17	0.43
1:A:776:ARG:HB2	1:B:740:GLY:HA2	2.00	0.43
1:B:20:PRO:HG2	1:B:961:MET:SD	2.58	0.43
1:B:181:LYS:HD2	7:B:2263:HOH:O	2.19	0.43
1:D:629:LYS:CE	1:D:629:LYS:HA	2.49	0.43
1:D:877:PRO:CG	1:D:977:THR:HB	2.49	0.43
1:A:870:GLU:O	1:A:874:LYS:CD	2.65	0.43
1:C:22:THR:HG22	7:D:2204:HOH:O	2.18	0.43
1:C:859:HIS:HE1	7:C:3051:HOH:O	2.02	0.43
1:C:1017:LEU:HD22	1:C:1018:PRO:HD2	2.00	0.43
7:C:2820:HOH:O	1:D:775:LEU:HD12	2.18	0.43
1:A:667:LEU:HD21	1:A:698:VAL:HG21	2.00	0.43
1:A:929:LEU:HB2	1:D:941:ILE:CD1	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:150:ILE:HB	2:B:1027:SF4:S4	2.59	0.43
1:B:868:ILE:HG22	1:B:870:GLU:H	1.84	0.43
1:C:193:LEU:N	1:C:193:LEU:HD22	2.34	0.43
1:D:140:CYS:HA	2:D:1027:SF4:S3	2.59	0.43
1:B:44:ASN:HB2	1:B:45:PRO:CD	2.49	0.43
1:B:140:CYS:HA	2:B:1027:SF4:S3	2.58	0.43
1:C:142:LEU:HD23	1:C:142:LEU:HA	1.85	0.43
1:C:369:ASN:ND2	1:D:50:PHE:CD1	2.87	0.43
1:C:1019:LEU:HD11	1:D:582:ILE:HD12	2.01	0.43
1:B:100:PHE:CD1	1:B:100:PHE:C	2.92	0.43
1:C:20:PRO:HG2	1:C:961:MET:SD	2.59	0.43
1:D:97:ILE:HA	1:D:100:PHE:CD2	2.54	0.43
1:A:621:TRP:O	1:A:625:VAL:HG23	2.19	0.43
1:B:379:LEU:O	1:B:383:GLU:HG3	2.19	0.43
1:B:892:GLU:HG3	7:B:2908:HOH:O	2.19	0.43
1:C:759:ARG:HH21	1:D:933:GLY:HA3	1.84	0.43
1:D:264:ASN:ND2	7:D:2411:HOH:O	2.51	0.43
1:D:487:ASN:HB3	5:D:1032:NDP:C2N	2.48	0.43
1:D:621:TRP:O	1:D:625:VAL:HG23	2.19	0.43
1:A:263:GLU:O	1:A:264:ASN:CB	2.67	0.42
1:A:570:PHE:HB3	1:A:636:ILE:HB	2.01	0.42
1:A:574:LYS:HG3	1:A:614:SER:HB2	2.01	0.42
1:B:1017:LEU:O	1:B:1018:PRO:C	2.57	0.42
1:C:871:LEU:HD12	1:C:871:LEU:HA	1.90	0.42
1:D:115:MET:HE1	1:D:828:GLN:HE21	1.82	0.42
1:B:173:ASN:HB3	1:B:176:LEU:CD1	2.49	0.42
1:C:845:GLU:HG3	1:C:912:PHE:CG	2.54	0.42
1:C:990:THR:O	1:C:990:THR:CG2	2.68	0.42
1:A:427:VAL:CG1	1:B:410:ARG:CZ	2.92	0.42
1:A:582:ILE:CD1	1:B:1019:LEU:HD22	2.49	0.42
1:B:394:ARG:NH1	1:B:409:VAL:HG21	2.34	0.42
1:A:705:PRO:HA	1:A:730:ASP:OD2	2.19	0.42
1:C:2:ALA:HB1	1:C:3:PRO:CD	2.50	0.42
1:C:427:VAL:CG1	1:D:410:ARG:NH1	2.80	0.42
1:C:612:LEU:HD11	1:D:935:PHE:CE2	2.55	0.42
1:C:783:ARG:NH1	7:C:2852:HOH:O	2.50	0.42
1:D:870:GLU:O	1:D:874:LYS:HG3	2.19	0.42
1:D:877:PRO:HG2	1:D:977:THR:HB	2.00	0.42
1:A:760:THR:HG23	1:B:932:LEU:HD23	2.01	0.42
1:D:167:ASN:ND2	1:D:911:PRO:HA	2.34	0.42
1:B:371:ARG:HG2	1:B:371:ARG:HH11	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:859:HIS:HA	1:C:865:VAL:HG23	2.02	0.42
1:D:868:ILE:HG22	1:D:870:GLU:OE1	2.19	0.42
1:A:519:PRO:HB3	1:B:28:LEU:HD22	2.00	0.42
1:B:989:CYS:O	1:B:990:THR:HB	2.20	0.42
1:C:394:ARG:HG3	1:C:409:VAL:HG13	2.01	0.42
1:D:916:LYS:HB2	1:D:917:PRO:HD2	2.01	0.42
1:A:335:VAL:HG22	1:A:433:VAL:HB	2.02	0.42
1:A:868:ILE:HG12	1:A:870:GLU:HB2	2.00	0.42
1:C:825:THR:HA	7:C:2879:HOH:O	2.19	0.42
1:B:680:MET:HE2	1:B:680:MET:HA	2.02	0.42
1:C:132:THR:HB	1:C:137:VAL:HG23	2.01	0.42
1:C:771:ARG:N	1:C:772:PRO:CD	2.83	0.42
1:C:989:CYS:O	1:C:990:THR:HB	2.20	0.42
1:D:50:PHE:O	1:D:384:LYS:HD2	2.20	0.42
1:B:56:GLU:OE2	1:B:898:LYS:NZ	2.53	0.42
1:B:173:ASN:HB3	1:B:176:LEU:HD12	2.02	0.42
1:B:734:ALA:HA	1:B:735:THR:HA	1.69	0.42
1:B:899:GLU:HB2	7:B:2913:HOH:O	2.18	0.42
1:C:760:THR:CG2	1:D:932:LEU:HD23	2.50	0.42
1:C:845:GLU:CD	1:C:845:GLU:H	2.23	0.42
1:D:993:LEU:C	1:D:993:LEU:HD23	2.41	0.42
1:A:132:THR:HB	1:A:137:VAL:CG2	2.50	0.41
1:C:173:ASN:OD1	1:C:173:ASN:N	2.49	0.41
1:C:375:GLU:CD	1:C:375:GLU:H	2.23	0.41
1:D:367:PHE:HE1	1:D:389:PRO:HD3	1.85	0.41
1:A:54:LYS:NZ	1:A:895:MET:CG	2.82	0.41
1:C:29:HIS:HB2	7:D:2191:HOH:O	2.20	0.41
1:A:172:ARG:HG3	7:A:2312:HOH:O	2.20	0.41
1:A:783:ARG:NE	7:A:2825:HOH:O	2.52	0.41
1:A:898:LYS:HD2	7:A:2120:HOH:O	2.19	0.41
1:C:140:CYS:HA	2:C:1027:SF4:S3	2.60	0.41
1:D:669:LEU:HD13	1:D:691:VAL:HG22	2.02	0.41
1:D:734:ALA:HA	1:D:735:THR:HA	1.66	0.41
1:B:57:ASN:ND2	1:B:898:LYS:HB2	2.35	0.41
1:B:410:ARG:HG2	1:B:411:THR:N	2.34	0.41
1:A:410:ARG:HB2	1:A:422:ASP:HB2	2.03	0.41
1:C:897:LEU:C	1:C:899:GLU:N	2.74	0.41
1:D:191:ALA:HB2	1:D:276:TYR:CD2	2.56	0.41
1:A:549:ALA:HB2	1:A:814:GLN:HB3	2.03	0.41
1:A:771:ARG:N	1:A:772:PRO:CD	2.84	0.41
1:B:629:LYS:HA	1:B:629:LYS:CE	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:261:LEU:HD21	1:C:451:LEU:HD21	2.02	0.41
1:C:629:LYS:HA	1:C:629:LYS:HE2	2.03	0.41
1:C:892:GLU:HG3	7:C:2950:HOH:O	2.19	0.41
1:D:150:ILE:HB	2:D:1027:SF4:S4	2.60	0.41
1:A:28:LEU:HD22	1:B:519:PRO:HB3	2.03	0.41
1:C:42:LYS:HE3	1:C:44:ASN:O	2.20	0.41
1:A:394:ARG:HG3	1:A:409:VAL:HG13	2.02	0.41
1:A:582:ILE:HD11	1:B:1015:ARG:NE	2.36	0.41
1:B:458:ARG:NE	1:B:459:TRP:CZ3	2.88	0.41
1:B:671:ALA:HA	1:B:672:PRO:HD3	1.88	0.41
1:C:716:ASP:OD2	1:C:719:SER:HB3	2.21	0.41
1:A:35:LYS:NZ	1:B:487:ASN:ND2	2.69	0.41
1:A:601:GLY:HA3	1:A:602:PRO:HD2	1.97	0.41
1:B:53:GLU:HB2	7:B:2907:HOH:O	2.20	0.41
1:C:392:SER:HA	1:C:393:PRO:HD3	1.93	0.41
1:C:415:GLU:HA	1:C:415:GLU:OE1	2.21	0.41
1:D:191:ALA:O	1:D:279:ALA:HA	2.21	0.41
1:B:934:THR:OG1	1:B:937:GLU:HG3	2.21	0.41
1:C:28:LEU:HD22	1:D:519:PRO:HB3	2.02	0.41
1:C:35:LYS:HE2	7:D:2627:HOH:O	2.19	0.41
1:C:621:TRP:O	1:C:625:VAL:HG23	2.21	0.41
1:D:413:GLN:HG3	1:D:419:TRP:CE2	2.55	0.41
7:A:2757:HOH:O	1:B:722:ARG:HD2	2.20	0.40
1:C:1007:ARG:NE	1:C:1011:TYR:HB2	2.35	0.40
1:D:413:GLN:HA	1:D:418:LYS:O	2.20	0.40
1:A:140:CYS:HA	2:A:1027:SF4:S3	2.62	0.40
1:A:929:LEU:HB2	1:D:941:ILE:HD12	2.02	0.40
1:B:863:LYS:HA	1:B:864:PRO:HD3	1.95	0.40
1:C:779:THR:O	1:C:783:ARG:HG3	2.21	0.40
1:C:898:LYS:O	1:C:898:LYS:HG2	2.21	0.40
1:D:54:LYS:HE2	7:D:2118:HOH:O	2.21	0.40
1:D:363:PHE:HE2	1:D:389:PRO:HB3	1.86	0.40
1:A:734:ALA:HA	1:A:735:THR:HA	1.67	0.40
1:C:865:VAL:HA	1:C:866:PRO:HD3	1.94	0.40
1:B:643:CYS:HB2	1:B:650:TRP:CE2	2.56	0.40
1:C:519:PRO:HB3	1:D:28:LEU:HD22	2.04	0.40
1:D:616:LYS:HD3	1:D:620:TYR:CE1	2.56	0.40
1:D:911:PRO:HG3	7:D:2122:HOH:O	2.21	0.40
1:B:962:THR:O	1:B:966:SER:HB2	2.22	0.40
5:B:1032:NDP:H8A	7:B:2546:HOH:O	2.19	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:460:ASP:OD1	1:D:395:LYS:NZ[1_656]	2.18	0.02

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	1014/1025 (99%)	972 (96%)	34 (3%)	8 (1%)	19	13
1	B	1017/1025 (99%)	966 (95%)	39 (4%)	12 (1%)	13	7
1	C	1017/1025 (99%)	973 (96%)	37 (4%)	7 (1%)	22	16
1	D	1017/1025 (99%)	974 (96%)	36 (4%)	7 (1%)	22	16
All	All	4065/4100 (99%)	3885 (96%)	146 (4%)	34 (1%)	19	13

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	678	ARG
1	A	903	ALA
1	A	904	PHE
1	A	908	GLU
1	B	416	THR
1	B	675	MET
1	B	678	ARG
1	B	901	ASN
1	B	902	ALA
1	B	903	ALA
1	C	678	ARG
1	D	415	GLU
1	D	906	PRO
1	D	908	GLU
1	B	677	GLU
1	B	679	GLY

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Mol	Chain	Res	Type
1	C	3	PRO
1	C	674	GLY
1	C	680	MET
1	C	1018	PRO
1	D	676	GLY
1	A	907	LEU
1	B	909	ARG
1	B	1018	PRO
1	C	898	LYS
1	D	3	PRO
1	D	1018	PRO
1	A	3	PRO
1	A	906	PRO
1	C	415	GLU
1	B	3	PRO
1	D	53	GLU
1	B	905	PRO
1	A	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	845/853 (99%)	834 (99%)	11 (1%)	69 74
1	B	847/853 (99%)	840 (99%)	7 (1%)	81 86
1	C	847/853 (99%)	833 (98%)	14 (2%)	60 65
1	D	847/853 (99%)	840 (99%)	7 (1%)	81 86
All	All	3386/3412 (99%)	3347 (99%)	39 (1%)	71 76

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	ASP
1	A	100	PHE
1	A	363	PHE

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Mol	Chain	Res	Type
1	A	367	PHE
1	A	453	PRO
1	A	482	ILE
1	A	776	ARG
1	A	793	THR
1	A	900	GLN
1	A	906	PRO
1	A	955	ASN
1	B	100	PHE
1	B	167	ASN
1	B	453	PRO
1	B	680	MET
1	B	793	THR
1	B	906	PRO
1	B	955	ASN
1	C	100	PHE
1	C	173	ASN
1	C	326	SER
1	C	363	PHE
1	C	402	ARG
1	C	453	PRO
1	C	793	THR
1	C	828	GLN
1	C	857	GLU
1	C	916	LYS
1	C	950	GLU
1	C	955	ASN
1	C	1017	LEU
1	C	1018	PRO
1	D	39	LYS
1	D	100	PHE
1	D	402	ARG
1	D	453	PRO
1	D	828	GLN
1	D	950	GLU
1	D	955	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	HIS
1	A	295	GLN

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Mol	Chain	Res	Type
1	A	828	GLN
1	A	859	HIS
1	B	51	HIS
1	B	167	ASN
1	B	295	GLN
1	B	413	GLN
1	B	487	ASN
1	B	700	GLN
1	C	295	GLN
1	C	407	GLN
1	C	487	ASN
1	C	859	HIS
1	C	978	HIS
1	D	51	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	1028	-	0,12,12	-	-	-		
2	SF4	C	1027	-	0,12,12	-	-	-		
3	FMN	C	1030	-	33,33,33	1.91	8 (24%)	48,50,50	1.96	14 (29%)
2	SF4	D	1026	-	0,12,12	-	-	-		
6	URF	D	1033	-	9,9,9	2.28	4 (44%)	12,12,12	2.13	5 (41%)
3	FMN	D	1030	-	33,33,33	1.87	8 (24%)	48,50,50	1.95	13 (27%)
2	SF4	C	1028	-	0,12,12	-	-	-		
4	FAD	D	1031	-	53,58,58	1.99	23 (43%)	68,89,89	1.22	8 (11%)
6	URF	C	1033	-	9,9,9	2.32	4 (44%)	12,12,12	2.16	5 (41%)
5	NDP	D	1032	-	45,52,52	2.04	13 (28%)	53,80,80	1.98	14 (26%)
2	SF4	D	1027	1	0,12,12	-	-	-		
2	SF4	D	1028	1	0,12,12	-	-	-		
2	SF4	C	1029	-	0,12,12	-	-	-		
2	SF4	A	1029	-	0,12,12	-	-	-		
2	SF4	B	1027	-	0,12,12	-	-	-		
3	FMN	A	1030	-	33,33,33	1.89	8 (24%)	48,50,50	1.98	13 (27%)
2	SF4	A	1028	-	0,12,12	-	-	-		
5	NDP	B	1032	-	45,52,52	1.94	10 (22%)	53,80,80	1.87	11 (20%)
4	FAD	A	1031	-	53,58,58	1.96	21 (39%)	68,89,89	1.25	10 (14%)
5	NDP	A	1032	-	45,52,52	1.93	10 (22%)	53,80,80	1.85	10 (18%)
2	SF4	A	1027	-	0,12,12	-	-	-		
2	SF4	B	1026	-	0,12,12	-	-	-		
2	SF4	D	1029	1	0,12,12	-	-	-		
2	SF4	A	1026	-	0,12,12	-	-	-		
2	SF4	C	1026	-	0,12,12	-	-	-		
3	FMN	B	1030	-	33,33,33	1.91	8 (24%)	48,50,50	1.97	14 (29%)
4	FAD	B	1031	-	53,58,58	1.99	20 (37%)	68,89,89	1.24	8 (11%)
5	NDP	C	1032	-	45,52,52	1.98	13 (28%)	53,80,80	1.97	11 (20%)
6	URF	A	1033	-	9,9,9	2.26	4 (44%)	12,12,12	2.17	5 (41%)
6	URF	B	1033	-	9,9,9	2.30	5 (55%)	12,12,12	2.16	5 (41%)
2	SF4	B	1029	-	0,12,12	-	-	-		
4	FAD	C	1031	-	53,58,58	1.98	24 (45%)	68,89,89	1.24	9 (13%)

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	1028	-	-	-	0/6/5/5
2	SF4	C	1027	-	-	-	0/6/5/5
3	FMN	C	1030	-	-	1/18/18/18	0/3/3/3
2	SF4	D	1026	-	-	-	0/6/5/5
6	URF	D	1033	-	-	-	0/1/1/1
3	FMN	D	1030	-	-	1/18/18/18	0/3/3/3
2	SF4	C	1028	-	-	-	0/6/5/5
4	FAD	D	1031	-	-	3/30/50/50	0/6/6/6
6	URF	C	1033	-	-	-	0/1/1/1
5	NDP	D	1032	-	3/3/14/17	11/30/77/77	0/5/5/5
2	SF4	D	1027	1	-	-	0/6/5/5
2	SF4	D	1028	1	-	-	0/6/5/5
2	SF4	C	1029	-	-	-	0/6/5/5
2	SF4	A	1029	-	-	-	0/6/5/5
2	SF4	B	1027	-	-	-	0/6/5/5
3	FMN	A	1030	-	-	1/18/18/18	0/3/3/3
2	SF4	A	1028	-	-	-	0/6/5/5
5	NDP	B	1032	-	3/3/14/17	12/30/77/77	0/5/5/5
4	FAD	A	1031	-	-	3/30/50/50	0/6/6/6
5	NDP	A	1032	-	3/3/14/17	12/30/77/77	0/5/5/5
2	SF4	A	1027	-	-	-	0/6/5/5
2	SF4	B	1026	-	-	-	0/6/5/5
2	SF4	D	1029	1	-	-	0/6/5/5
3	FMN	B	1030	-	-	1/18/18/18	0/3/3/3
2	SF4	A	1026	-	-	-	0/6/5/5
4	FAD	B	1031	-	-	3/30/50/50	0/6/6/6
5	NDP	C	1032	-	3/3/14/17	7/30/77/77	0/5/5/5
2	SF4	C	1026	-	-	-	0/6/5/5
6	URF	A	1033	-	-	-	0/1/1/1
6	URF	B	1033	-	-	-	0/1/1/1
2	SF4	B	1029	-	-	-	0/6/5/5
4	FAD	C	1031	-	-	3/30/50/50	0/6/6/6

All (183) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	1032	NDP	C4N-C3N	-6.04	1.38	1.49
5	B	1032	NDP	C4N-C5N	-5.29	1.35	1.48
5	B	1032	NDP	C4N-C3N	-5.22	1.39	1.49
5	A	1032	NDP	C4N-C3N	-5.08	1.39	1.49
5	A	1032	NDP	C4N-C5N	-5.04	1.35	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1030	FMN	C4A-N5	4.98	1.40	1.30
3	B	1030	FMN	C4A-N5	4.98	1.40	1.30
5	A	1032	NDP	C5B-C4B	-4.86	1.36	1.51
3	C	1030	FMN	C4A-N5	4.84	1.40	1.30
3	D	1030	FMN	C4A-N5	4.83	1.40	1.30
5	B	1032	NDP	C5B-C4B	-4.75	1.36	1.51
5	C	1032	NDP	O4B-C1B	4.61	1.47	1.41
5	D	1032	NDP	C6N-C5N	4.58	1.41	1.33
5	B	1032	NDP	C2N-C3N	4.36	1.47	1.34
4	B	1031	FAD	O4B-C1B	4.25	1.47	1.41
4	C	1031	FAD	O4B-C1B	4.21	1.46	1.41
4	B	1031	FAD	PA-O2A	-4.14	1.35	1.55
5	A	1032	NDP	C2N-C3N	4.12	1.46	1.34
4	D	1031	FAD	PA-O2A	-4.11	1.36	1.55
3	B	1030	FMN	C7M-C7	4.09	1.59	1.51
4	C	1031	FAD	PA-O2A	-3.98	1.36	1.55
4	A	1031	FAD	O4B-C1B	3.97	1.46	1.41
4	A	1031	FAD	PA-O2A	-3.95	1.36	1.55
5	C	1032	NDP	C2D-C3D	-3.94	1.42	1.53
5	D	1032	NDP	C2N-C3N	3.94	1.46	1.34
4	D	1031	FAD	O4B-C1B	3.92	1.46	1.41
5	C	1032	NDP	PN-O5D	3.88	1.75	1.59
5	C	1032	NDP	C4N-C3N	-3.84	1.42	1.49
6	C	1033	URF	C2-N1	3.81	1.41	1.36
5	D	1032	NDP	C4N-C5N	-3.81	1.38	1.48
3	C	1030	FMN	C7M-C7	3.80	1.58	1.51
6	B	1033	URF	C2-N1	3.80	1.41	1.36
3	A	1030	FMN	C7M-C7	3.77	1.58	1.51
4	C	1031	FAD	C4X-N5	3.77	1.38	1.30
3	D	1030	FMN	C7M-C7	3.76	1.58	1.51
4	B	1031	FAD	C4X-N5	3.75	1.38	1.30
4	D	1031	FAD	C5'-C4'	3.74	1.57	1.51
5	C	1032	NDP	O2D-C2D	3.73	1.51	1.43
6	A	1033	URF	C2-N1	3.73	1.41	1.36
6	D	1033	URF	C2-N1	3.70	1.41	1.36
3	B	1030	FMN	C1'-N10	-3.65	1.38	1.48
6	D	1033	URF	C6-N1	3.64	1.42	1.36
3	C	1030	FMN	C1'-N10	-3.64	1.38	1.48
4	D	1031	FAD	C4X-N5	3.63	1.37	1.30
6	C	1033	URF	C6-N1	3.61	1.42	1.36
5	C	1032	NDP	C4N-C5N	-3.54	1.39	1.48
6	B	1033	URF	C6-N1	3.54	1.42	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	1032	NDP	C5B-C4B	-3.53	1.40	1.51
3	D	1030	FMN	C1'-N10	-3.51	1.39	1.48
3	A	1030	FMN	C1'-N10	-3.50	1.39	1.48
4	B	1031	FAD	C5'-C4'	3.49	1.56	1.51
4	A	1031	FAD	C4X-N5	3.49	1.37	1.30
4	A	1031	FAD	C9A-N10	3.41	1.47	1.41
4	C	1031	FAD	C9A-N10	3.40	1.47	1.41
4	B	1031	FAD	C9A-N10	3.38	1.47	1.41
5	D	1032	NDP	C2D-C1D	3.38	1.64	1.53
4	D	1031	FAD	P-O2P	-3.38	1.39	1.55
4	A	1031	FAD	P-O2P	-3.37	1.39	1.55
6	A	1033	URF	C6-N1	3.34	1.41	1.36
3	C	1030	FMN	C9A-C5A	3.28	1.46	1.41
4	C	1031	FAD	P-O2P	-3.27	1.40	1.55
4	D	1031	FAD	C9A-N10	3.23	1.46	1.41
5	C	1032	NDP	C2N-C3N	3.20	1.43	1.34
4	B	1031	FAD	P-O2P	-3.20	1.40	1.55
5	A	1032	NDP	C2D-C1D	3.16	1.63	1.53
3	A	1030	FMN	C9A-C5A	3.16	1.46	1.41
4	C	1031	FAD	C5'-C4'	3.14	1.56	1.51
5	A	1032	NDP	C1D-N1N	3.13	1.55	1.46
3	C	1030	FMN	C4'-C3'	3.11	1.59	1.53
3	A	1030	FMN	C4'-C3'	3.09	1.59	1.53
4	A	1031	FAD	C5'-C4'	3.08	1.56	1.51
5	D	1032	NDP	O4D-C1D	3.08	1.49	1.42
3	B	1030	FMN	C9A-N10	3.06	1.46	1.41
6	A	1033	URF	F5-C5	-3.05	1.30	1.35
3	D	1030	FMN	C4'-C3'	3.05	1.59	1.53
5	B	1032	NDP	C2D-C1D	3.05	1.63	1.53
3	C	1030	FMN	C1'-C2'	3.04	1.56	1.52
3	B	1030	FMN	C9A-C5A	3.00	1.46	1.41
3	A	1030	FMN	C1'-C2'	2.98	1.56	1.52
3	D	1030	FMN	C1'-C2'	2.98	1.56	1.52
4	D	1031	FAD	C9A-C5X	2.98	1.46	1.41
6	B	1033	URF	F5-C5	-2.93	1.30	1.35
4	C	1031	FAD	C9A-C5X	2.91	1.46	1.41
4	B	1031	FAD	C9A-C5X	2.91	1.46	1.41
4	C	1031	FAD	C8-C7	2.91	1.48	1.40
3	D	1030	FMN	C9A-C5A	2.89	1.46	1.41
4	A	1031	FAD	C8-C7	2.88	1.48	1.40
3	D	1030	FMN	C9A-N10	2.88	1.46	1.41
3	C	1030	FMN	C9A-N10	2.87	1.46	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	1032	NDP	C6N-N1N	2.86	1.44	1.37
6	D	1033	URF	F5-C5	-2.86	1.31	1.35
5	D	1032	NDP	O5D-C5D	2.85	1.55	1.44
5	A	1032	NDP	C5D-C4D	2.85	1.60	1.51
3	A	1030	FMN	C9A-N10	2.84	1.46	1.41
4	D	1031	FAD	C8-C7	2.83	1.48	1.40
4	A	1031	FAD	C9A-C5X	2.83	1.45	1.41
3	B	1030	FMN	C1'-C2'	2.83	1.56	1.52
4	B	1031	FAD	C2A-N3A	2.83	1.36	1.32
4	A	1031	FAD	C2B-C1B	-2.82	1.49	1.53
5	C	1032	NDP	PA-O5B	2.81	1.70	1.59
4	D	1031	FAD	C2A-N3A	2.80	1.36	1.32
6	C	1033	URF	C6-C5	2.76	1.36	1.33
4	B	1031	FAD	O5'-C5'	2.76	1.55	1.44
3	B	1030	FMN	C4'-C3'	2.74	1.58	1.53
5	C	1032	NDP	C6N-C5N	2.73	1.38	1.33
4	B	1031	FAD	C8-C7	2.73	1.47	1.40
4	D	1031	FAD	C4A-N3A	2.69	1.39	1.35
5	C	1032	NDP	C2D-C1D	2.68	1.62	1.53
5	B	1032	NDP	C5D-C4D	2.66	1.59	1.51
4	D	1031	FAD	C1'-C2'	2.66	1.56	1.52
6	C	1033	URF	F5-C5	-2.66	1.31	1.35
5	A	1032	NDP	C6N-C5N	2.65	1.38	1.33
4	B	1031	FAD	C6-C5X	2.64	1.44	1.40
4	B	1031	FAD	C2B-C1B	-2.62	1.49	1.53
4	A	1031	FAD	O5'-C5'	2.60	1.54	1.44
5	B	1032	NDP	C1D-N1N	2.59	1.53	1.46
4	A	1031	FAD	C1'-C2'	2.58	1.56	1.52
4	C	1031	FAD	O5'-C5'	2.55	1.54	1.44
4	A	1031	FAD	C6-C5X	2.55	1.44	1.40
5	D	1032	NDP	O4B-C1B	2.55	1.44	1.41
5	C	1032	NDP	C5B-C4B	-2.54	1.43	1.51
4	D	1031	FAD	O5'-C5'	2.53	1.54	1.44
4	A	1031	FAD	C4A-N3A	2.53	1.39	1.35
4	D	1031	FAD	C2B-C1B	-2.53	1.49	1.53
5	D	1032	NDP	O3D-C3D	-2.52	1.37	1.43
4	B	1031	FAD	O4B-C4B	2.49	1.50	1.45
4	A	1031	FAD	C9-C9A	2.48	1.43	1.39
4	C	1031	FAD	C1'-C2'	2.48	1.56	1.52
4	C	1031	FAD	C4A-N3A	2.47	1.39	1.35
4	C	1031	FAD	C2A-N3A	2.46	1.36	1.32
4	C	1031	FAD	O4B-C4B	2.46	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1031	FAD	C2B-C1B	-2.46	1.50	1.53
4	C	1031	FAD	C6-C5X	2.45	1.43	1.40
4	D	1031	FAD	C10-N1	2.44	1.38	1.33
4	A	1031	FAD	O4B-C4B	2.43	1.50	1.45
4	D	1031	FAD	O4B-C4B	2.43	1.50	1.45
4	C	1031	FAD	C9-C9A	2.42	1.43	1.39
6	A	1033	URF	C6-C5	2.41	1.36	1.33
4	C	1031	FAD	C10-N1	2.41	1.38	1.33
4	D	1031	FAD	C2A-N1A	2.39	1.38	1.33
6	D	1033	URF	C6-C5	2.38	1.36	1.33
4	A	1031	FAD	C10-N1	2.35	1.38	1.33
4	B	1031	FAD	C2A-N1A	2.34	1.38	1.33
3	B	1030	FMN	C10-N1	2.34	1.38	1.33
4	B	1031	FAD	C10-N1	2.32	1.37	1.33
5	B	1032	NDP	PA-O2A	-2.31	1.44	1.55
4	B	1031	FAD	C4A-N3A	2.28	1.38	1.35
6	B	1033	URF	C6-C5	2.27	1.35	1.33
3	D	1030	FMN	C10-N1	2.27	1.37	1.33
5	B	1032	NDP	C6N-C5N	2.26	1.37	1.33
4	B	1031	FAD	C9-C9A	2.25	1.43	1.39
4	D	1031	FAD	C9-C9A	2.23	1.43	1.39
4	A	1031	FAD	C2A-N3A	2.22	1.35	1.32
3	C	1030	FMN	C10-N1	2.22	1.37	1.33
4	C	1031	FAD	C2A-N1A	2.21	1.38	1.33
4	D	1031	FAD	C6-C5X	2.21	1.43	1.40
3	A	1030	FMN	C10-N1	2.20	1.37	1.33
4	A	1031	FAD	C5B-C4B	2.20	1.58	1.51
4	D	1031	FAD	C5B-C4B	2.20	1.58	1.51
4	B	1031	FAD	P-O5'	-2.20	1.50	1.59
4	C	1031	FAD	P-O5'	-2.19	1.50	1.59
5	A	1032	NDP	P2B-O2B	-2.18	1.55	1.59
4	A	1031	FAD	P-O5'	-2.18	1.50	1.59
4	C	1031	FAD	C4-N3	2.15	1.42	1.38
4	C	1031	FAD	C9-C8	2.14	1.42	1.39
4	C	1031	FAD	C3B-C4B	2.13	1.58	1.53
5	D	1032	NDP	C1D-N1N	2.13	1.52	1.46
4	D	1031	FAD	C9-C8	2.12	1.42	1.39
6	B	1033	URF	C4-C5	2.11	1.46	1.44
4	C	1031	FAD	C5B-C4B	2.11	1.58	1.51
4	A	1031	FAD	C2A-N1A	2.10	1.37	1.33
5	A	1032	NDP	C4A-N3A	2.09	1.38	1.35
5	B	1032	NDP	C4A-N3A	2.08	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1031	FAD	C4-N3	2.07	1.42	1.38
5	C	1032	NDP	C4A-N3A	2.07	1.38	1.35
4	D	1031	FAD	P-O5'	-2.07	1.50	1.59
4	D	1031	FAD	C2-N3	2.07	1.43	1.39
4	A	1031	FAD	C4-N3	2.06	1.42	1.38
4	B	1031	FAD	C5B-C4B	2.05	1.58	1.51
5	C	1032	NDP	O3B-C3B	2.05	1.47	1.43
4	B	1031	FAD	C2-N3	2.04	1.43	1.39
4	C	1031	FAD	C2-N3	2.04	1.43	1.39
5	D	1032	NDP	C4A-N3A	2.02	1.38	1.35

All (155) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	1032	NDP	C1D-N1N-C2N	-7.57	108.52	121.11
5	D	1032	NDP	O5D-PN-O1N	-7.17	81.04	109.07
5	B	1032	NDP	O2N-PN-O5D	-6.41	77.97	107.75
5	A	1032	NDP	O2N-PN-O5D	-6.25	78.73	107.75
5	C	1032	NDP	PN-O3-PA	5.80	152.73	132.83
5	B	1032	NDP	O5D-PN-O1N	-5.27	88.50	109.07
5	A	1032	NDP	O5D-PN-O1N	-5.20	88.76	109.07
3	C	1030	FMN	C10-N1-C2	5.18	127.25	116.90
3	A	1030	FMN	C10-N1-C2	5.10	127.10	116.90
3	D	1030	FMN	C10-N1-C2	5.10	127.09	116.90
3	B	1030	FMN	C10-N1-C2	4.96	126.82	116.90
5	D	1032	NDP	C1D-N1N-C2N	-4.93	112.91	121.11
5	B	1032	NDP	C3N-C2N-N1N	-4.91	116.08	123.10
5	B	1032	NDP	O2N-PN-O1N	4.49	134.43	112.24
5	A	1032	NDP	O2N-PN-O1N	4.46	134.28	112.24
6	B	1033	URF	F5-C5-C4	4.43	120.50	116.40
6	C	1033	URF	F5-C5-C4	4.38	120.46	116.40
3	C	1030	FMN	C4A-C10-N1	-4.38	114.56	124.73
6	A	1033	URF	F5-C5-C4	4.36	120.44	116.40
3	A	1030	FMN	C4A-C10-N1	-4.36	114.61	124.73
3	D	1030	FMN	C4A-C10-N1	-4.31	114.73	124.73
3	B	1030	FMN	C4A-C10-N1	-4.30	114.76	124.73
6	D	1033	URF	F5-C5-C4	4.27	120.36	116.40
3	B	1030	FMN	C4-C4A-C10	4.25	123.93	116.79
5	A	1032	NDP	C3N-C2N-N1N	-4.21	117.09	123.10
3	A	1030	FMN	C4-C4A-C10	4.19	123.83	116.79
3	D	1030	FMN	C4-C4A-C10	4.04	123.59	116.79
3	C	1030	FMN	C4-C4A-C10	4.04	123.57	116.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1030	FMN	O4'-C4'-C3'	3.88	118.54	109.10
3	C	1030	FMN	O4'-C4'-C3'	3.88	118.54	109.10
3	D	1030	FMN	O4'-C4'-C3'	3.80	118.34	109.10
3	B	1030	FMN	O4'-C4'-C3'	3.80	118.33	109.10
3	D	1030	FMN	O3'-C3'-C2'	-3.67	99.95	108.81
5	D	1032	NDP	O2N-PN-O1N	3.56	129.85	112.24
5	C	1032	NDP	C3N-C2N-N1N	-3.54	118.04	123.10
3	A	1030	FMN	O3'-C3'-C2'	-3.54	100.27	108.81
4	B	1031	FAD	O2A-PA-O1A	3.53	129.68	112.24
4	D	1031	FAD	O2A-PA-O1A	3.52	129.62	112.24
3	B	1030	FMN	O3'-C3'-C2'	-3.50	100.36	108.81
6	C	1033	URF	C5-C6-N1	3.49	122.38	119.40
6	A	1033	URF	C5-C6-N1	3.47	122.36	119.40
3	B	1030	FMN	O2'-C2'-C1'	3.47	118.19	109.80
4	A	1031	FAD	O2A-PA-O1A	3.46	129.36	112.24
4	C	1031	FAD	O2A-PA-O1A	3.44	129.25	112.24
3	A	1030	FMN	O2'-C2'-C1'	3.38	117.97	109.80
6	D	1033	URF	C5-C6-N1	3.38	122.28	119.40
3	D	1030	FMN	O2'-C2'-C1'	3.37	117.95	109.80
3	C	1030	FMN	O3'-C3'-C2'	-3.37	100.67	108.81
3	C	1030	FMN	O2'-C2'-C1'	3.37	117.94	109.80
6	B	1033	URF	C5-C6-N1	3.34	122.24	119.40
3	C	1030	FMN	P-O5'-C5'	3.27	127.30	118.30
3	D	1030	FMN	P-O5'-C5'	3.21	127.14	118.30
3	B	1030	FMN	P-O5'-C5'	3.19	127.08	118.30
3	A	1030	FMN	P-O5'-C5'	3.16	127.01	118.30
3	C	1030	FMN	C5'-C4'-C3'	-3.16	106.10	112.20
3	A	1030	FMN	C5'-C4'-C3'	-3.14	106.14	112.20
5	D	1032	NDP	O2N-PN-O5D	-3.12	93.26	107.75
5	D	1032	NDP	C3D-C2D-C1D	3.11	107.33	101.43
5	D	1032	NDP	O4D-C1D-C2D	-3.10	99.89	106.64
3	B	1030	FMN	C5'-C4'-C3'	-3.08	106.26	112.20
6	D	1033	URF	C5-C4-N3	3.02	115.53	112.56
5	D	1032	NDP	O7N-C7N-N7N	-2.97	115.93	122.88
3	D	1030	FMN	C5'-C4'-C3'	-2.95	106.51	112.20
6	A	1033	URF	C5-C4-N3	2.92	115.43	112.56
5	D	1032	NDP	C3N-C2N-N1N	-2.91	118.94	123.10
5	D	1032	NDP	O5D-C5D-C4D	-2.90	99.01	108.99
6	C	1033	URF	C5-C4-N3	2.87	115.38	112.56
5	C	1032	NDP	O7N-C7N-N7N	-2.84	116.23	122.88
6	B	1033	URF	C5-C4-N3	2.81	115.32	112.56
5	A	1032	NDP	O7N-C7N-N7N	-2.77	116.41	122.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	1032	NDP	C1D-N1N-C6N	2.76	126.77	120.83
5	C	1032	NDP	O2B-C2B-C3B	2.73	121.57	111.68
5	B	1032	NDP	O7N-C7N-N7N	-2.65	116.68	122.88
3	A	1030	FMN	C4A-C10-N10	2.65	120.35	116.48
6	B	1033	URF	C6-C5-C4	-2.65	119.33	122.12
6	D	1033	URF	C6-C5-C4	-2.64	119.34	122.12
5	D	1032	NDP	O4B-C1B-C2B	2.60	111.09	106.59
3	D	1030	FMN	C4A-C10-N10	2.59	120.27	116.48
6	C	1033	URF	C6-C5-C4	-2.58	119.40	122.12
6	A	1033	URF	C6-C5-C4	-2.58	119.40	122.12
3	B	1030	FMN	C4A-C10-N10	2.58	120.25	116.48
3	C	1030	FMN	C4A-C10-N10	2.57	120.23	116.48
5	C	1032	NDP	O2N-PN-O5D	2.52	119.45	107.75
4	A	1031	FAD	C5'-C4'-C3'	-2.52	107.34	112.20
5	D	1032	NDP	C1D-N1N-C6N	2.50	126.21	120.83
4	C	1031	FAD	C5'-C4'-C3'	-2.49	107.40	112.20
3	B	1030	FMN	O3'-C3'-C4'	2.46	114.76	108.81
4	A	1031	FAD	C2A-N1A-C6A	2.45	122.94	118.75
5	D	1032	NDP	O2B-C2B-C3B	2.44	120.52	111.68
5	B	1032	NDP	O4D-C1D-C2D	-2.43	101.35	106.64
3	A	1030	FMN	O3'-C3'-C4'	2.42	114.65	108.81
5	B	1032	NDP	C3D-C2D-C1D	2.41	106.01	101.43
4	B	1031	FAD	C5'-C4'-C3'	-2.39	107.58	112.20
3	C	1030	FMN	N10-C10-N1	2.38	125.20	118.35
4	C	1031	FAD	C2A-N1A-C6A	2.38	122.82	118.75
4	D	1031	FAD	C5'-C4'-C3'	-2.38	107.61	112.20
5	D	1032	NDP	N3A-C2A-N1A	-2.37	124.97	128.68
4	B	1031	FAD	C2A-N1A-C6A	2.37	122.81	118.75
3	D	1030	FMN	O3'-C3'-C4'	2.35	114.50	108.81
4	A	1031	FAD	C5A-C6A-N1A	-2.35	115.02	120.35
4	D	1031	FAD	C2A-N1A-C6A	2.34	122.76	118.75
5	D	1032	NDP	O3D-C3D-C4D	-2.34	104.27	111.05
3	A	1030	FMN	N10-C10-N1	2.33	125.04	118.35
3	B	1030	FMN	N10-C10-N1	2.31	124.99	118.35
3	D	1030	FMN	N10-C10-N1	2.31	124.98	118.35
4	C	1031	FAD	C5A-C6A-N1A	-2.31	115.12	120.35
4	B	1031	FAD	C5A-C6A-N1A	-2.31	115.13	120.35
5	A	1032	NDP	O2B-C2B-C3B	2.30	120.03	111.68
5	B	1032	NDP	O2B-C2B-C3B	2.28	119.96	111.68
4	D	1031	FAD	C5A-C6A-N1A	-2.27	115.20	120.35
5	B	1032	NDP	N3A-C2A-N1A	-2.27	125.13	128.68
4	C	1031	FAD	C4-N3-C2	-2.26	121.46	125.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	1030	FMN	O3'-C3'-C4'	2.26	114.27	108.81
4	A	1031	FAD	C4-N3-C2	-2.26	121.47	125.64
6	C	1033	URF	F5-C5-C6	-2.24	120.14	121.73
4	C	1031	FAD	C10-N1-C2	2.23	121.36	116.90
4	B	1031	FAD	C4-N3-C2	-2.23	121.53	125.64
5	C	1032	NDP	N3A-C2A-N1A	-2.22	125.20	128.68
4	A	1031	FAD	C10-N1-C2	2.22	121.34	116.90
5	A	1032	NDP	O5B-C5B-C4B	-2.22	101.34	108.99
3	D	1030	FMN	N3-C2-N1	-2.22	115.03	119.38
5	C	1032	NDP	O5D-C5D-C4D	-2.22	101.36	108.99
6	A	1033	URF	F5-C5-C6	-2.22	120.16	121.73
6	B	1033	URF	F5-C5-C6	-2.21	120.16	121.73
3	B	1030	FMN	C4-C4A-N5	-2.20	115.10	118.23
5	B	1032	NDP	O5B-C5B-C4B	-2.19	101.47	108.99
4	A	1031	FAD	C5X-C9A-N10	-2.18	115.70	117.95
5	A	1032	NDP	O4B-C1B-C2B	2.18	110.36	106.59
5	C	1032	NDP	O4B-C1B-C2B	2.17	110.35	106.59
3	C	1030	FMN	N3-C2-N1	-2.17	115.14	119.38
4	B	1031	FAD	C10-N1-C2	2.16	121.22	116.90
3	A	1030	FMN	N3-C2-N1	-2.16	115.15	119.38
5	A	1032	NDP	N3A-C2A-N1A	-2.16	125.31	128.68
3	B	1030	FMN	N3-C2-N1	-2.15	115.16	119.38
4	D	1031	FAD	C4-N3-C2	-2.13	121.70	125.64
4	C	1031	FAD	P-O3P-PA	2.11	140.06	132.83
3	A	1030	FMN	C4-C4A-N5	-2.10	115.24	118.23
4	A	1031	FAD	O4B-C1B-C2B	-2.10	103.86	106.93
4	C	1031	FAD	C5X-C9A-N10	-2.10	115.79	117.95
4	A	1031	FAD	C5A-C6A-N6A	2.09	123.53	120.35
4	D	1031	FAD	C10-N1-C2	2.08	121.07	116.90
3	B	1030	FMN	C6-C5A-C9A	2.08	121.88	118.94
5	A	1032	NDP	O4D-C1D-C2D	-2.07	102.14	106.64
4	B	1031	FAD	C5A-C6A-N6A	2.06	123.49	120.35
5	C	1032	NDP	O2N-PN-O1N	2.06	122.42	112.24
5	B	1032	NDP	O4B-C1B-C2B	2.05	110.15	106.59
4	C	1031	FAD	O4B-C1B-C2B	-2.05	103.93	106.93
4	D	1031	FAD	C5X-C9A-N10	-2.05	115.84	117.95
4	B	1031	FAD	C5X-C9A-N10	-2.04	115.84	117.95
4	A	1031	FAD	P-O3P-PA	2.02	139.76	132.83
3	D	1030	FMN	C6-C5A-C9A	2.02	121.79	118.94
6	D	1033	URF	F5-C5-C6	-2.01	120.30	121.73
4	D	1031	FAD	C4A-C5A-N7A	2.01	111.50	109.40
3	C	1030	FMN	C6-C5A-C9A	2.01	121.78	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	1030	FMN	C4-C4A-N5	-2.01	115.38	118.23

All (12) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	1032	NDP	C2D
5	A	1032	NDP	C3D
5	A	1032	NDP	C4D
5	B	1032	NDP	C2D
5	B	1032	NDP	C3D
5	B	1032	NDP	C4D
5	C	1032	NDP	C2D
5	C	1032	NDP	C3D
5	C	1032	NDP	C4D
5	D	1032	NDP	C2D
5	D	1032	NDP	C3D
5	D	1032	NDP	C4D

All (58) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1031	FAD	C5B-O5B-PA-O1A
4	A	1031	FAD	PA-O3P-P-O5'
4	B	1031	FAD	C5B-O5B-PA-O1A
4	B	1031	FAD	PA-O3P-P-O5'
4	C	1031	FAD	C5B-O5B-PA-O1A
4	C	1031	FAD	PA-O3P-P-O5'
4	D	1031	FAD	C5B-O5B-PA-O1A
4	D	1031	FAD	PA-O3P-P-O5'
5	A	1032	NDP	C5D-O5D-PN-O1N
5	A	1032	NDP	C5D-O5D-PN-O2N
5	A	1032	NDP	C4D-C5D-O5D-PN
5	B	1032	NDP	C5D-O5D-PN-O1N
5	B	1032	NDP	C5D-O5D-PN-O2N
5	B	1032	NDP	C4D-C5D-O5D-PN
5	C	1032	NDP	C3B-C2B-O2B-P2B
5	D	1032	NDP	C5D-O5D-PN-O1N
5	D	1032	NDP	C5D-O5D-PN-O2N
5	D	1032	NDP	C4D-C5D-O5D-PN
5	D	1032	NDP	O4D-C4D-C5D-O5D
5	D	1032	NDP	C3D-C4D-C5D-O5D
5	B	1032	NDP	O4D-C1D-N1N-C2N

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Mol	Chain	Res	Type	Atoms
5	C	1032	NDP	O4D-C1D-N1N-C2N
5	A	1032	NDP	C3B-C2B-O2B-P2B
5	A	1032	NDP	C2D-C1D-N1N-C2N
5	A	1032	NDP	C2D-C1D-N1N-C6N
5	A	1032	NDP	O4D-C1D-N1N-C2N
5	A	1032	NDP	C1B-C2B-O2B-P2B
5	B	1032	NDP	C1B-C2B-O2B-P2B
5	C	1032	NDP	C1B-C2B-O2B-P2B
5	D	1032	NDP	C1B-C2B-O2B-P2B
5	B	1032	NDP	C3B-C2B-O2B-P2B
5	D	1032	NDP	C3B-C2B-O2B-P2B
5	B	1032	NDP	C3D-C4D-C5D-O5D
5	A	1032	NDP	C3D-C4D-C5D-O5D
5	C	1032	NDP	PN-O3-PA-O5B
5	D	1032	NDP	O4D-C1D-N1N-C2N
3	B	1030	FMN	C4'-C5'-O5'-P
3	C	1030	FMN	C4'-C5'-O5'-P
3	D	1030	FMN	C4'-C5'-O5'-P
5	C	1032	NDP	C4D-C5D-O5D-PN
3	A	1030	FMN	C4'-C5'-O5'-P
5	B	1032	NDP	PN-O3-PA-O2A
5	B	1032	NDP	O4B-C4B-C5B-O5B
5	B	1032	NDP	C2D-C1D-N1N-C6N
5	C	1032	NDP	O4D-C4D-C5D-O5D
5	A	1032	NDP	O4B-C4B-C5B-O5B
5	A	1032	NDP	C5D-O5D-PN-O3
5	B	1032	NDP	C5D-O5D-PN-O3
5	D	1032	NDP	C5D-O5D-PN-O3
5	D	1032	NDP	O4B-C4B-C5B-O5B
5	A	1032	NDP	PN-O3-PA-O1A
5	D	1032	NDP	PA-O3-PN-O1N
5	B	1032	NDP	C2N-C3N-C7N-N7N
4	A	1031	FAD	O4B-C4B-C5B-O5B
4	B	1031	FAD	O4B-C4B-C5B-O5B
4	C	1031	FAD	O4B-C4B-C5B-O5B
4	D	1031	FAD	O4B-C4B-C5B-O5B
5	C	1032	NDP	O4B-C4B-C5B-O5B

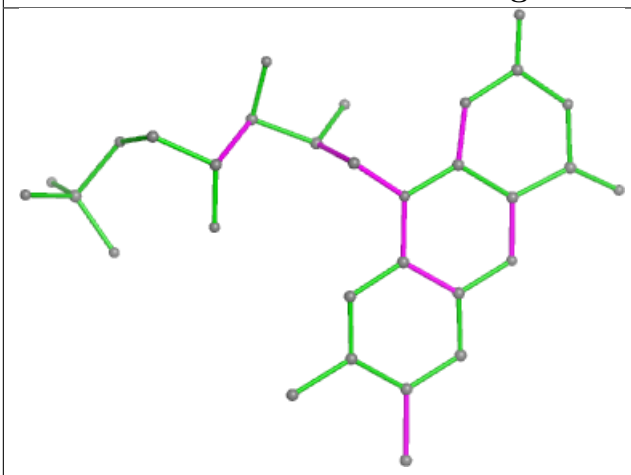
There are no ring outliers.

15 monomers are involved in 28 short contacts:

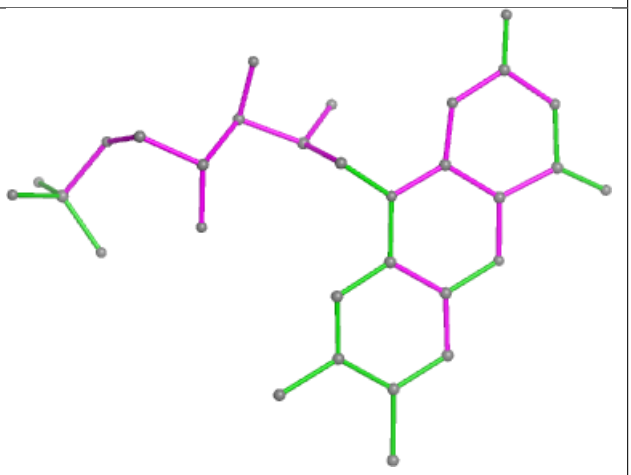
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1027	SF4	1	0
2	D	1026	SF4	1	0
3	D	1030	FMN	1	0
4	D	1031	FAD	2	0
5	D	1032	NDP	7	0
2	D	1027	SF4	2	0
2	B	1027	SF4	2	0
5	B	1032	NDP	3	0
4	A	1031	FAD	3	0
5	A	1032	NDP	1	0
2	A	1027	SF4	1	0
2	A	1026	SF4	1	0
4	B	1031	FAD	3	0
5	C	1032	NDP	1	0
4	C	1031	FAD	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

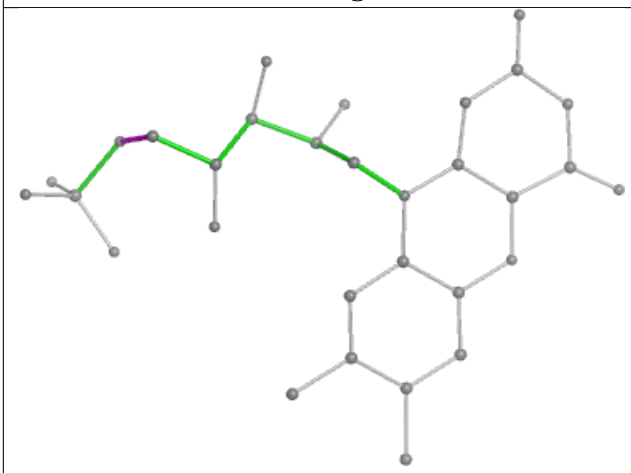
Ligand FMN C 1030



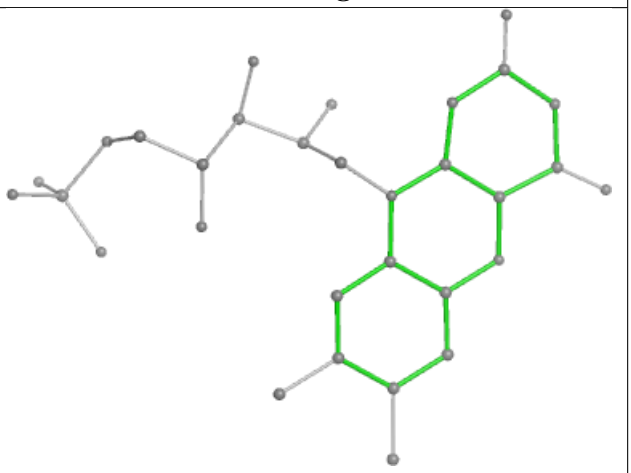
Bond lengths



Bond angles

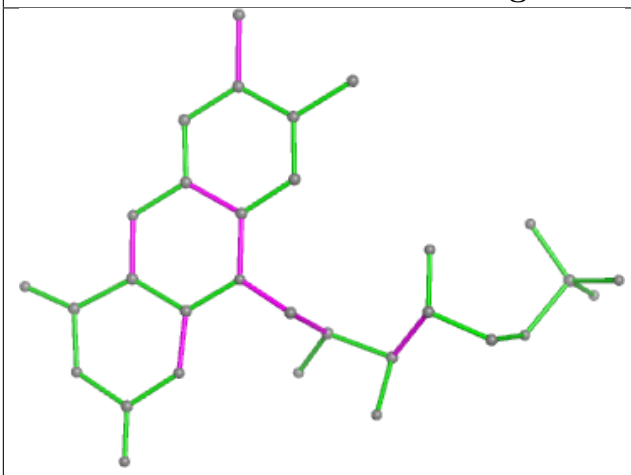


Torsions



Rings

Ligand FMN D 1030



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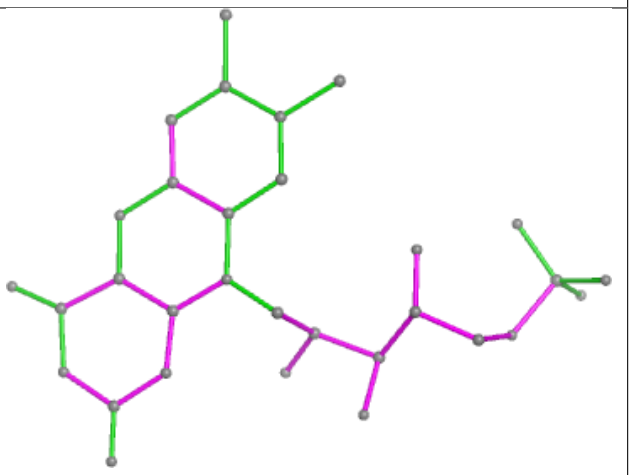
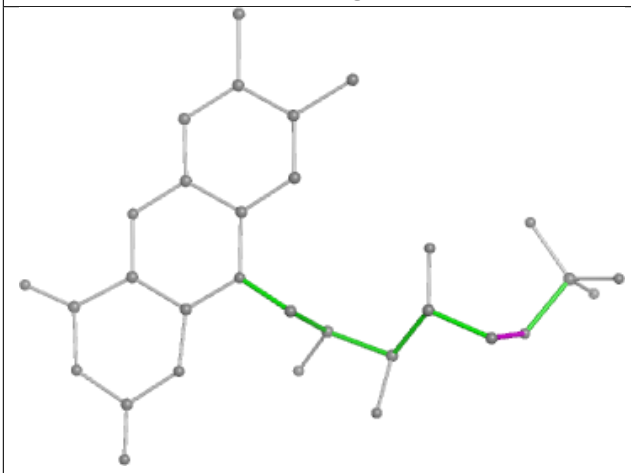
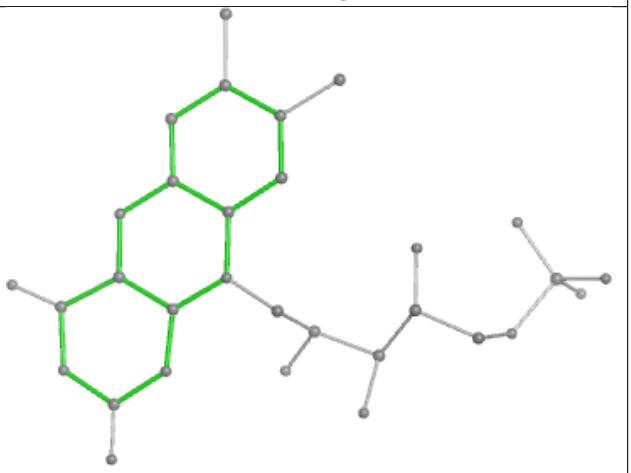


Bond angles

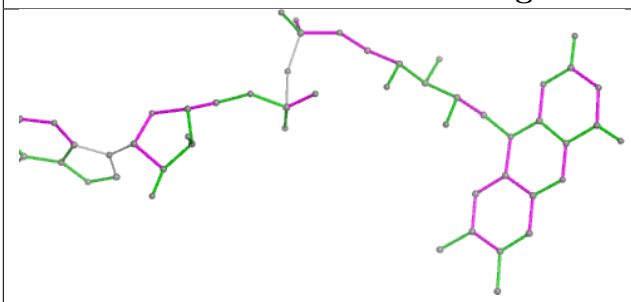


Torsions

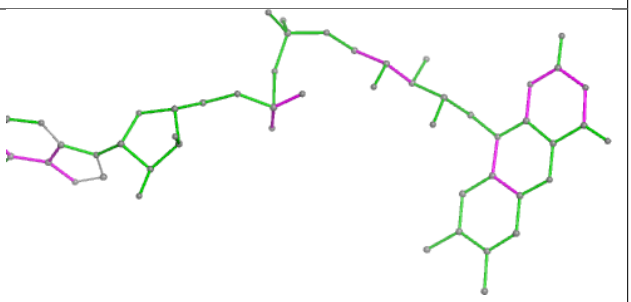


Rings

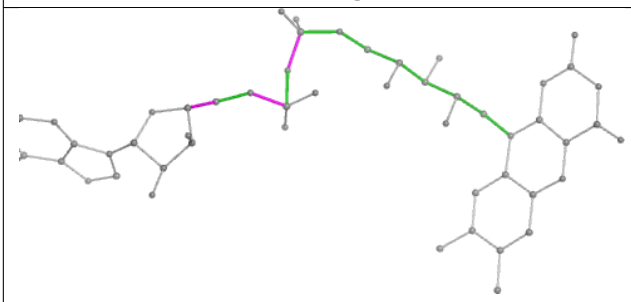
Ligand FAD D 1031



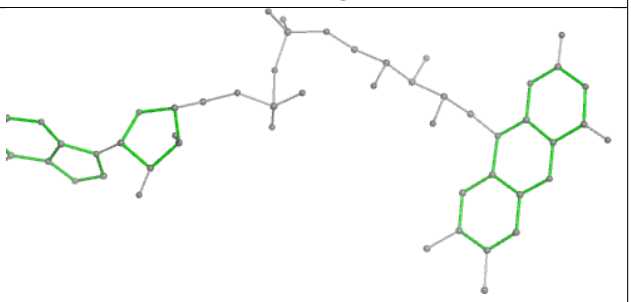
Bond lengths



Bond angles



Torsions



Rings

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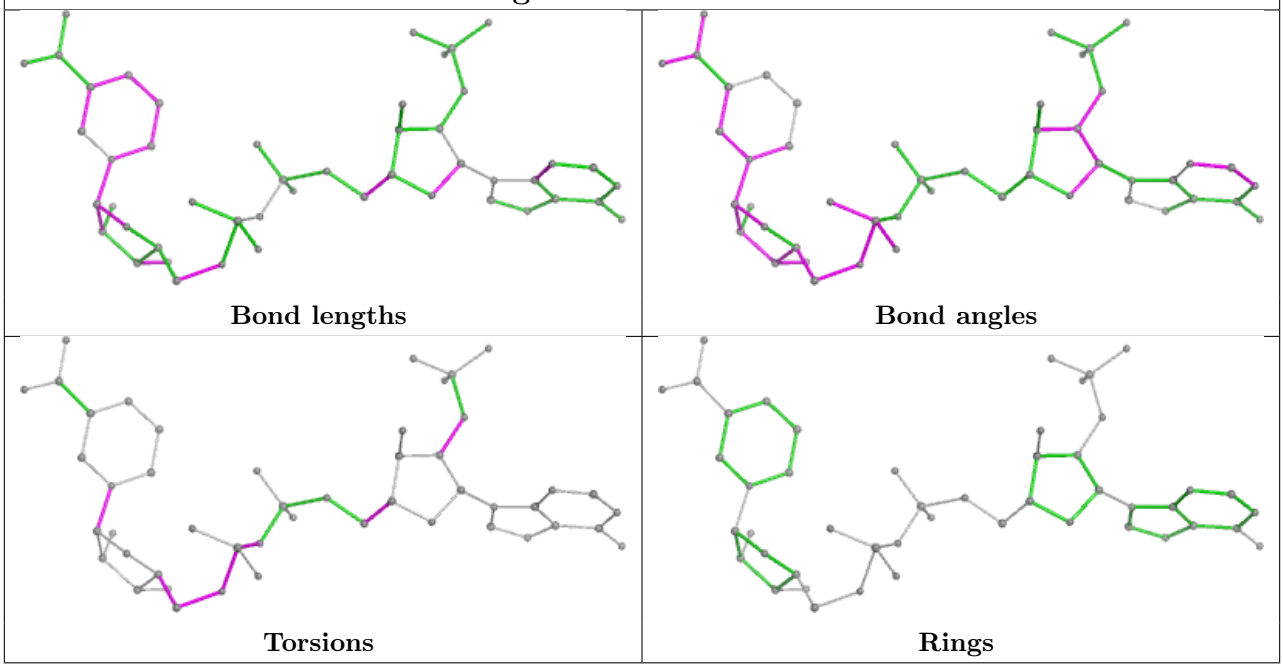
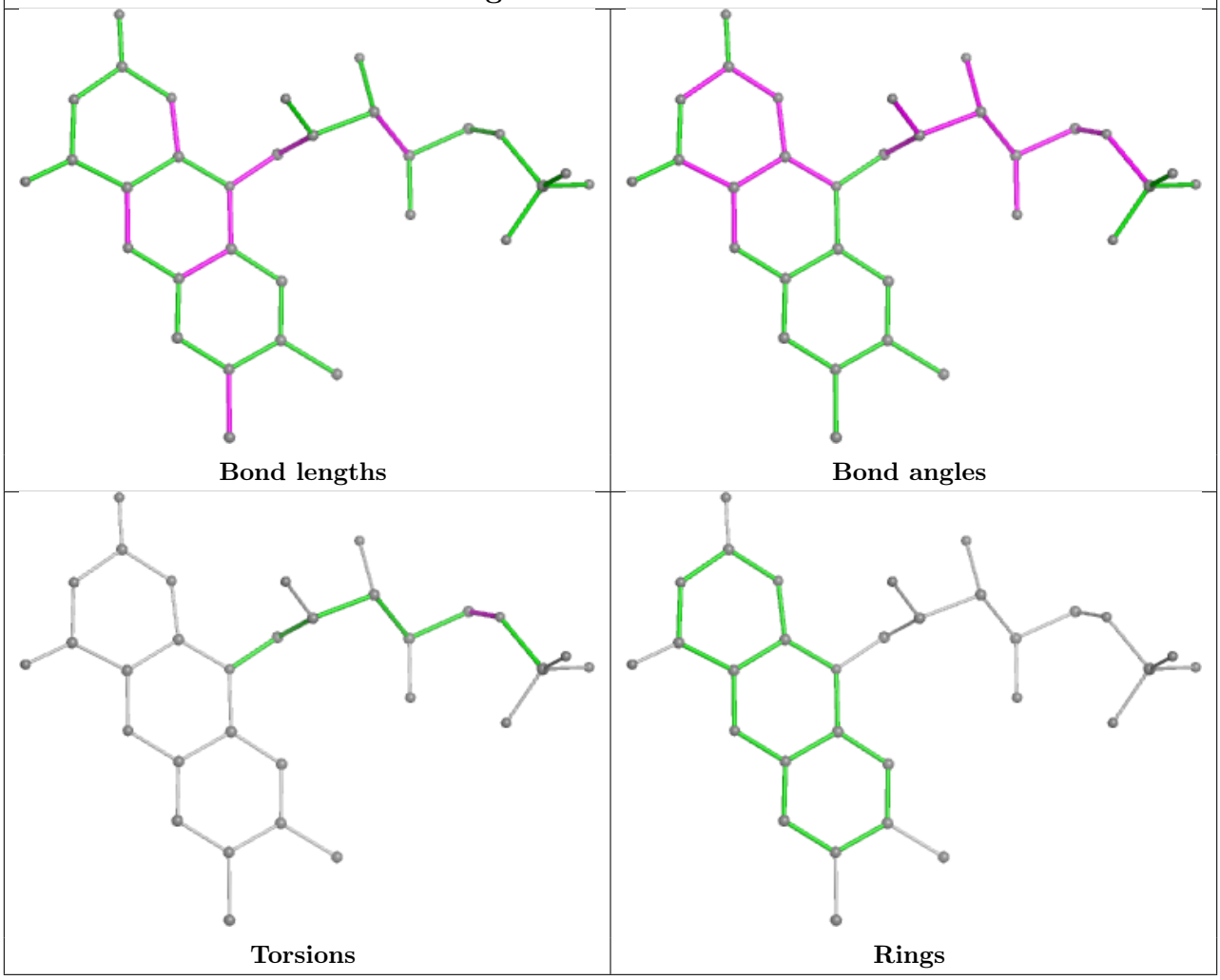
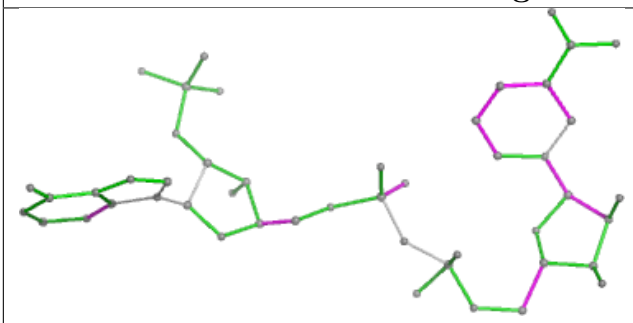


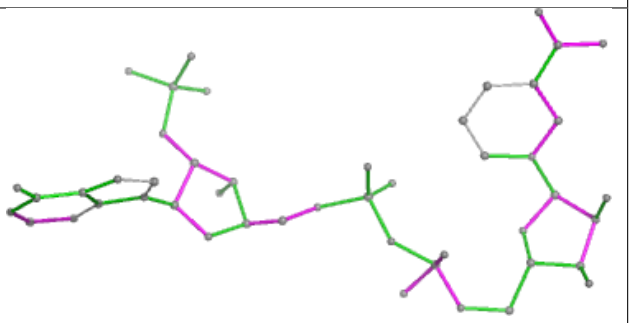
Ligand FMN A 1030



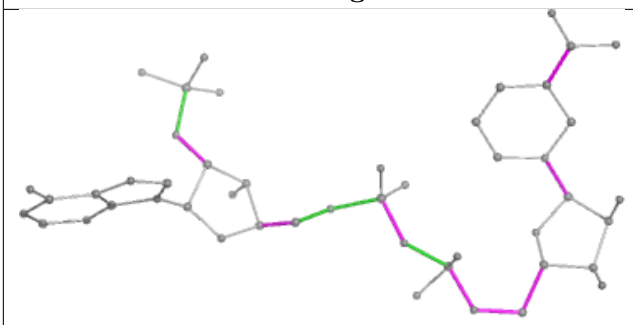
Ligand NDP B 1032



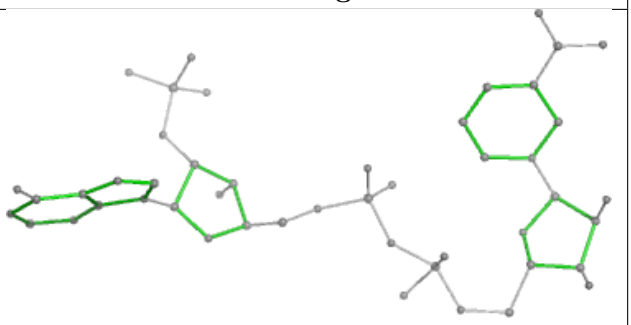
Bond lengths



Bond angles

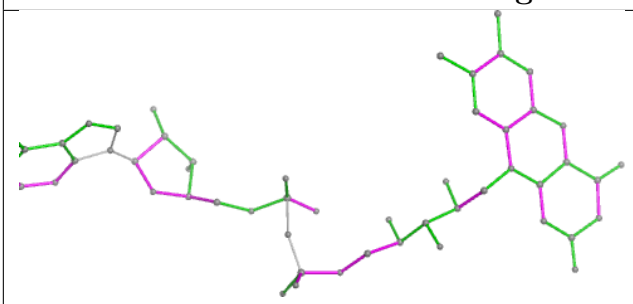


Torsions



Rings

Ligand FAD A 1031



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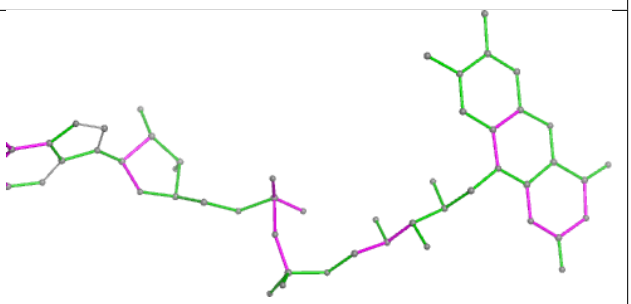
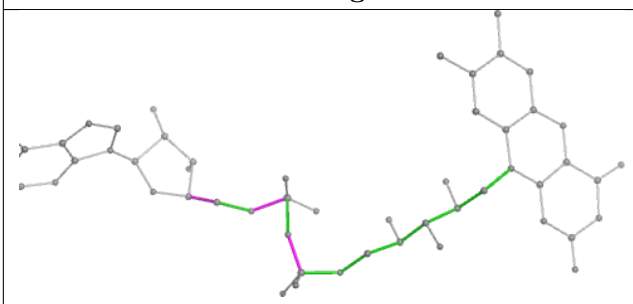


Bond angles



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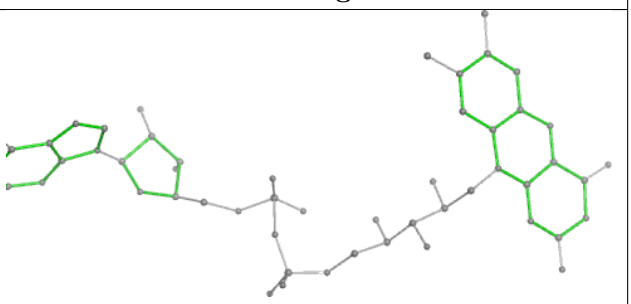

Rings

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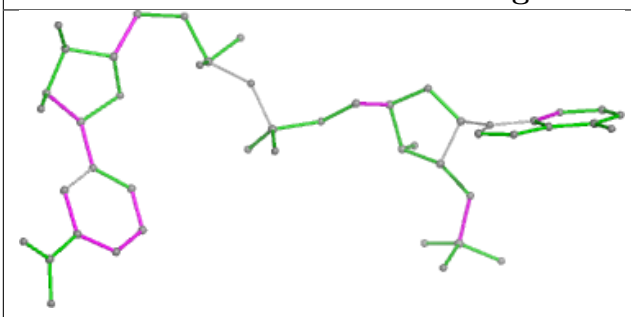
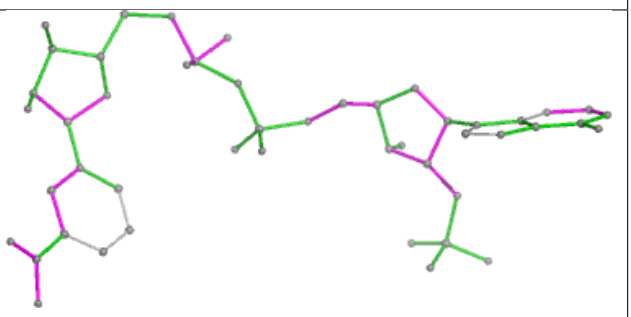
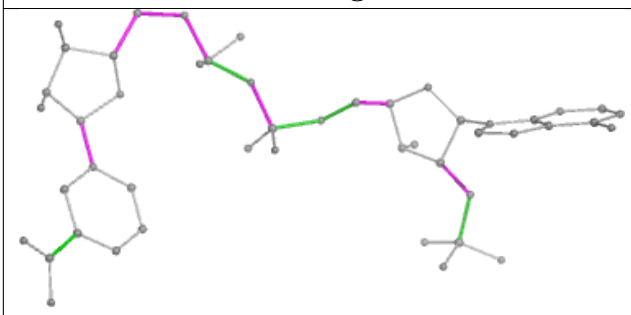
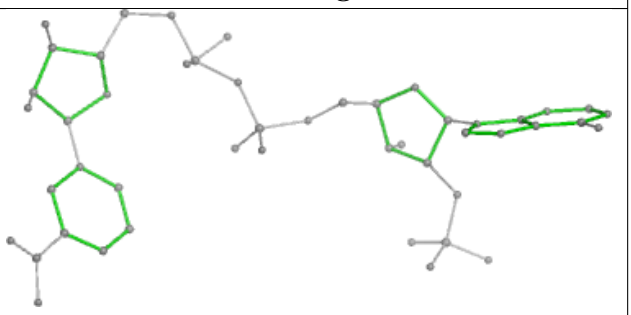
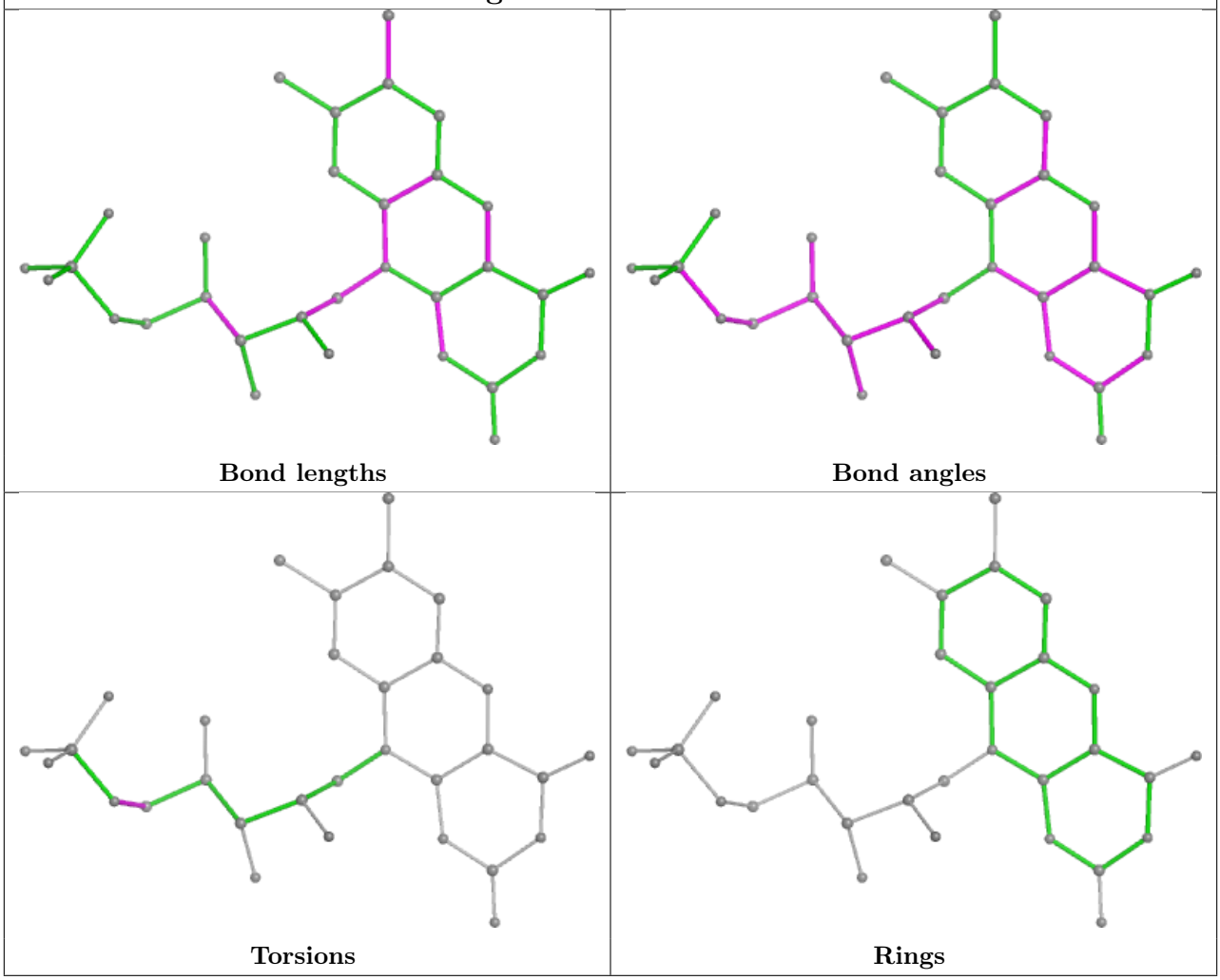
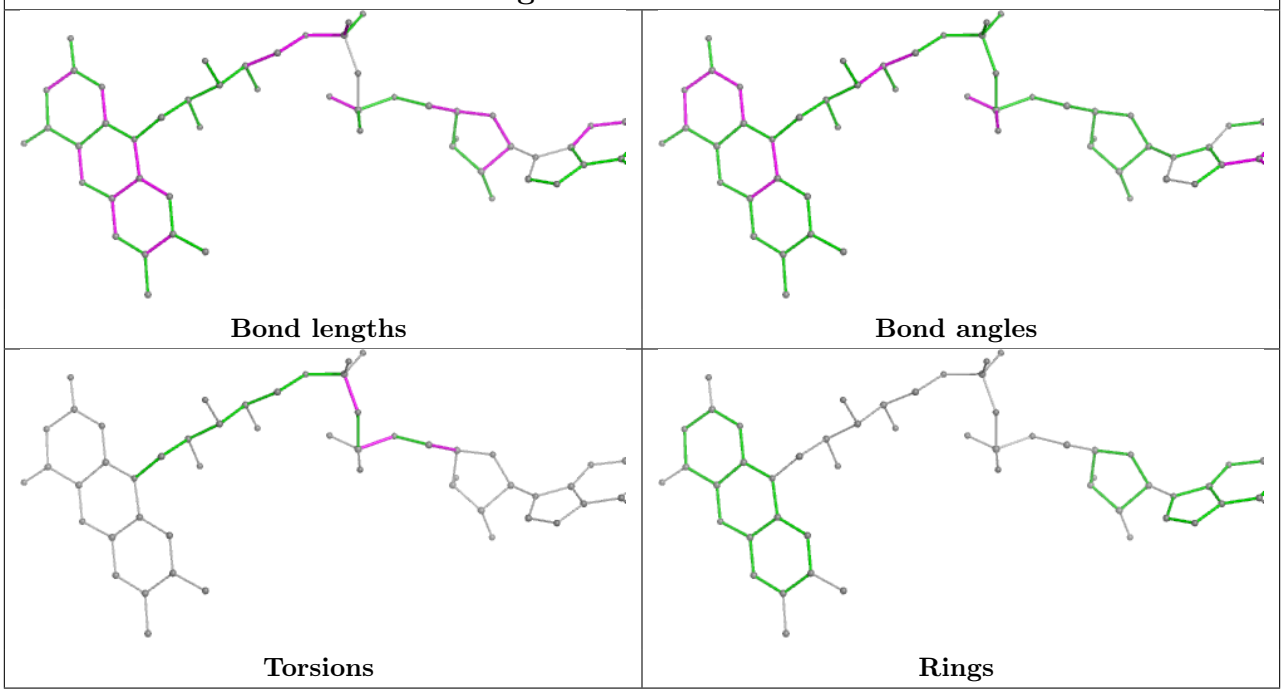
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand FMN B 1030



Ligand FAD B 1031



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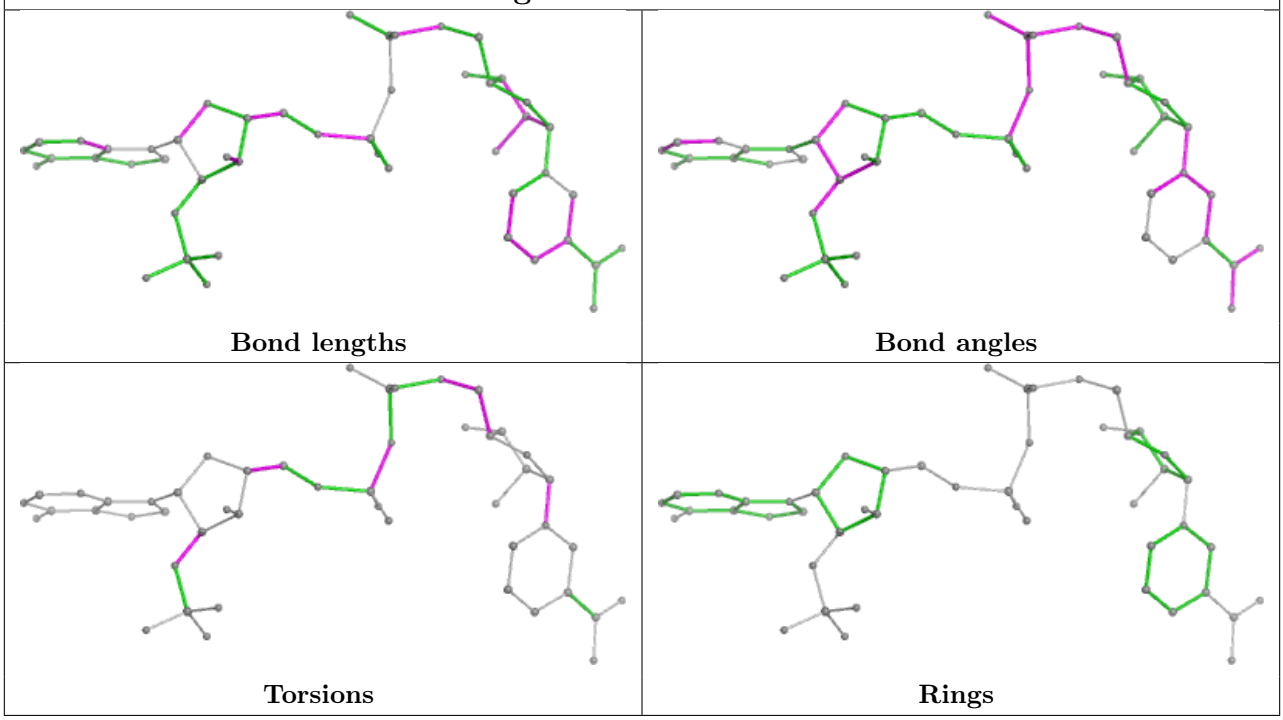

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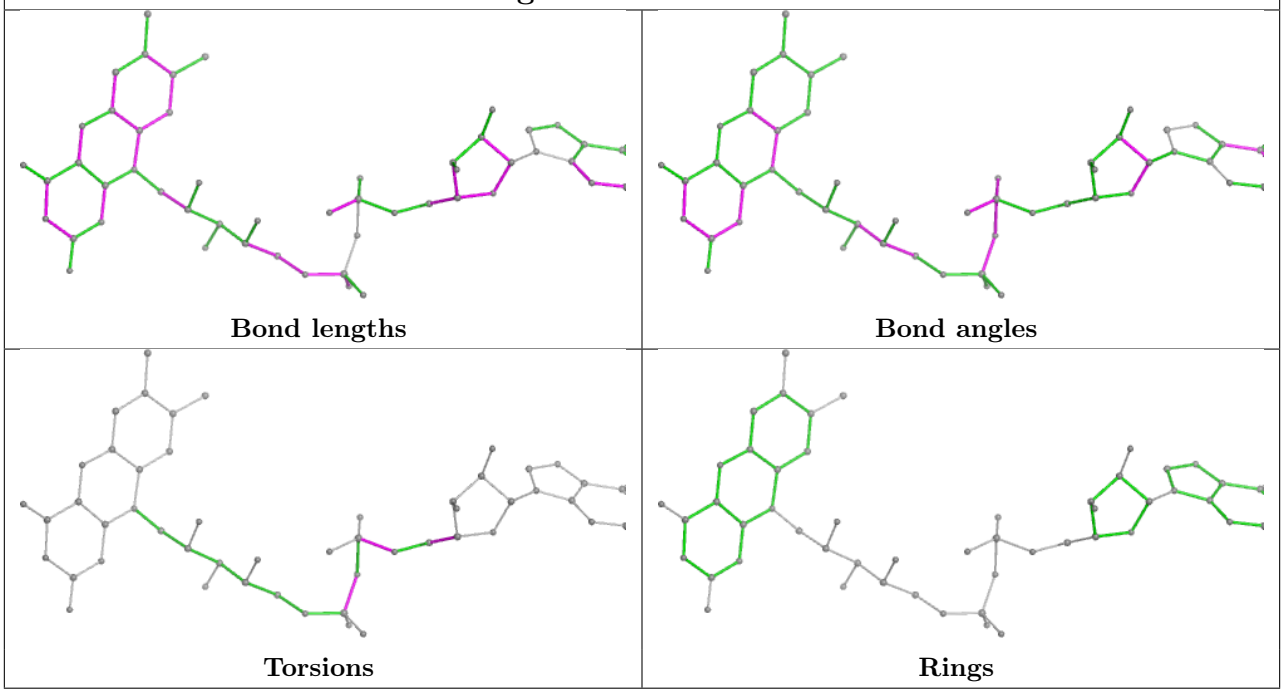

5.7 Other polymers (i)

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	1000/1025 (97%)	-0.15	51 (5%)	28	27	7, 16, 39, 59	0
1	B	1006/1025 (98%)	-0.08	50 (4%)	28	28	9, 17, 41, 64	0
1	C	1013/1025 (98%)	-0.12	50 (4%)	29	28	8, 16, 41, 59	0
1	D	1005/1025 (98%)	-0.16	45 (4%)	33	32	8, 16, 40, 60	0
All	All	4024/4100 (98%)	-0.13	196 (4%)	29	28	7, 16, 40, 64	0

All (196) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2	ALA	16.4
1	A	2	ALA	14.5
1	C	2	ALA	13.4
1	D	2	ALA	13.3
1	B	678	ARG	9.4
1	D	52	CYS	9.4
1	B	680	MET	7.9
1	A	1017	LEU	7.8
1	C	674	GLY	7.5
1	C	1019	LEU	7.5
1	B	679	GLY	7.3
1	A	175	CYS	7.2
1	B	908	GLU	7.1
1	A	1010	PRO	6.6
1	B	52	CYS	6.6
1	B	1020	ALA	6.2
1	C	415	GLU	5.9
1	A	324	CYS	5.9
1	D	50	PHE	5.9
1	C	1020	ALA	5.8
1	B	1018	PRO	5.7

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Mol	Chain	Res	Type	RSRZ
1	B	899	GLU	5.7
1	A	325	HIS	5.7
1	A	682	LEU	5.6
1	B	1019	LEU	5.6
1	B	415	GLU	5.6
1	D	459	TRP	5.5
1	D	51	HIS	5.5
1	A	52	CYS	5.5
1	B	682	LEU	5.4
1	C	51	HIS	5.4
1	C	1018	PRO	5.4
1	C	53	GLU	5.4
1	A	416	THR	5.3
1	C	52	CYS	5.3
1	C	459	TRP	5.1
1	B	867	ARG	5.1
1	C	682	LEU	5.1
1	B	872	MET	5.0
1	A	867	ARG	4.9
1	A	1009	THR	4.7
1	B	459	TRP	4.7
1	C	867	ARG	4.7
1	B	323	ALA	4.7
1	A	322	CYS	4.7
1	D	1010	PRO	4.7
1	B	416	THR	4.6
1	C	908	GLU	4.5
1	B	869	ALA	4.5
1	D	867	ARG	4.4
1	B	681	GLY	4.3
1	D	415	GLU	4.3
1	B	175	CYS	4.3
1	D	175	CYS	4.3
1	A	517	ALA	4.3
1	D	418	LYS	4.2
1	A	410	ARG	4.2
1	D	414	ASP	4.1
1	C	873	GLY	4.0
1	C	872	MET	4.0
1	C	681	GLY	4.0
1	B	180	GLU	3.9
1	C	175	CYS	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	1010	PRO	3.9
1	C	410	ARG	3.9
1	D	679	GLY	3.9
1	B	51	HIS	3.9
1	D	674	GLY	3.9
1	C	332	ARG	3.8
1	C	416	THR	3.8
1	A	415	GLU	3.8
1	C	326	SER	3.8
1	B	417	GLY	3.8
1	B	410	ARG	3.8
1	C	899	GLU	3.7
1	D	869	ALA	3.7
1	D	53	GLU	3.7
1	A	681	GLY	3.7
1	A	418	LYS	3.6
1	A	872	MET	3.6
1	C	417	GLY	3.6
1	B	1009	THR	3.5
1	D	22	THR	3.5
1	A	870	GLU	3.5
1	C	673	HIS	3.4
1	A	459	TRP	3.4
1	D	680	MET	3.3
1	B	424	ASP	3.3
1	A	51	HIS	3.3
1	C	330	SER	3.3
1	B	458	ARG	3.3
1	B	1011	TYR	3.2
1	A	673	HIS	3.2
1	B	1008	THR	3.2
1	D	872	MET	3.1
1	C	900	GLN	3.1
1	A	899	GLU	3.1
1	D	3	PRO	3.1
1	B	322	CYS	3.1
1	B	582	ILE	3.1
1	D	410	ARG	3.1
1	C	1010	PRO	3.0
1	A	22	THR	3.0
1	C	907	LEU	3.0
1	A	910	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	1019	LEU	3.0
1	A	868	ILE	3.0
1	C	418	LYS	3.0
1	C	904	PHE	3.0
1	D	180	GLU	2.9
1	A	873	GLY	2.9
1	C	517	ALA	2.9
1	A	50	PHE	2.9
1	A	53	GLU	2.9
1	A	1012	GLU	2.9
1	D	264	ASN	2.8
1	D	1018	PRO	2.8
1	C	870	GLU	2.8
1	D	1009	THR	2.8
1	B	3	PRO	2.8
1	D	868	ILE	2.8
1	C	424	ASP	2.8
1	A	518	LYS	2.8
1	C	179	GLN	2.7
1	D	915	LYS	2.7
1	D	857	GLU	2.7
1	A	1011	TYR	2.7
1	B	325	HIS	2.7
1	C	367	PHE	2.7
1	D	896	ARG	2.7
1	A	1008	THR	2.7
1	B	418	LYS	2.6
1	C	426	ILE	2.6
1	D	1012	GLU	2.6
1	B	426	ILE	2.6
1	C	331	ILE	2.6
1	D	855	GLY	2.6
1	A	319	ALA	2.5
1	A	417	GLY	2.5
1	D	874	LYS	2.5
1	D	1011	TYR	2.5
1	C	325	HIS	2.5
1	A	896	ARG	2.5
1	B	1012	GLU	2.5
1	B	326	SER	2.5
1	D	873	GLY	2.5
1	B	672	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	1012	GLU	2.5
1	A	323	ALA	2.5
1	D	458	ARG	2.4
1	C	910	LYS	2.4
1	A	857	GLU	2.4
1	B	896	ARG	2.4
1	B	414	ASP	2.4
1	D	847	GLN	2.4
1	B	1017	LEU	2.4
1	B	874	LYS	2.3
1	C	905	PRO	2.3
1	C	180	GLU	2.3
1	D	178	SER	2.3
1	B	518	LYS	2.3
1	C	869	ALA	2.3
1	A	11	ASP	2.3
1	A	327	PRO	2.3
1	B	324	CYS	2.3
1	C	324	CYS	2.3
1	B	11	ASP	2.3
1	D	1014	LYS	2.3
1	B	519	PRO	2.3
1	C	902	ALA	2.3
1	B	847	GLN	2.2
1	C	901	ASN	2.2
1	A	3	PRO	2.2
1	A	332	ARG	2.2
1	C	903	ALA	2.2
1	D	909	ARG	2.2
1	B	367	PHE	2.2
1	A	273	GLU	2.2
1	D	173	ASN	2.2
1	D	898	LYS	2.2
1	A	180	GLU	2.2
1	C	984	ASP	2.2
1	A	847	GLN	2.1
1	C	3	PRO	2.1
1	A	367	PHE	2.1
1	C	419	TRP	2.1
1	A	917	PRO	2.1
1	A	984	ASP	2.1
1	D	417	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	414	ASP	2.1
1	A	897	LEU	2.1
1	B	859	HIS	2.0
1	D	858	SER	2.0
1	D	866	PRO	2.0
1	A	941	ILE	2.0
1	D	367	PHE	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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(Å^2)	Q<0.9
5	NDP	A	1032	48/48	0.86	0.17	30,34,48,48	9
5	NDP	D	1032	48/48	0.86	0.21	21,26,52,56	0
5	NDP	C	1032	48/48	0.87	0.21	30,33,50,52	9
5	NDP	B	1032	48/48	0.89	0.17	19,24,42,46	0
6	URF	A	1033	9/9	0.93	0.10	22,23,24,26	0
6	URF	C	1033	9/9	0.94	0.11	19,20,22,23	0
6	URF	D	1033	9/9	0.94	0.09	17,19,20,25	0
2	SF4	C	1026	8/8	0.95	0.10	13,14,15,15	0
6	URF	B	1033	9/9	0.95	0.11	19,20,21,23	0
2	SF4	B	1029	8/8	0.96	0.09	16,16,17,18	0
2	SF4	A	1026	8/8	0.96	0.09	14,14,15,15	0
2	SF4	C	1027	8/8	0.96	0.11	11,13,14,15	0
4	FAD	B	1031	53/53	0.96	0.10	8,13,15,15	0
2	SF4	A	1029	8/8	0.96	0.09	16,17,18,19	0
2	SF4	B	1028	8/8	0.96	0.08	15,16,17,17	0
2	SF4	D	1029	8/8	0.97	0.08	15,16,17,18	0

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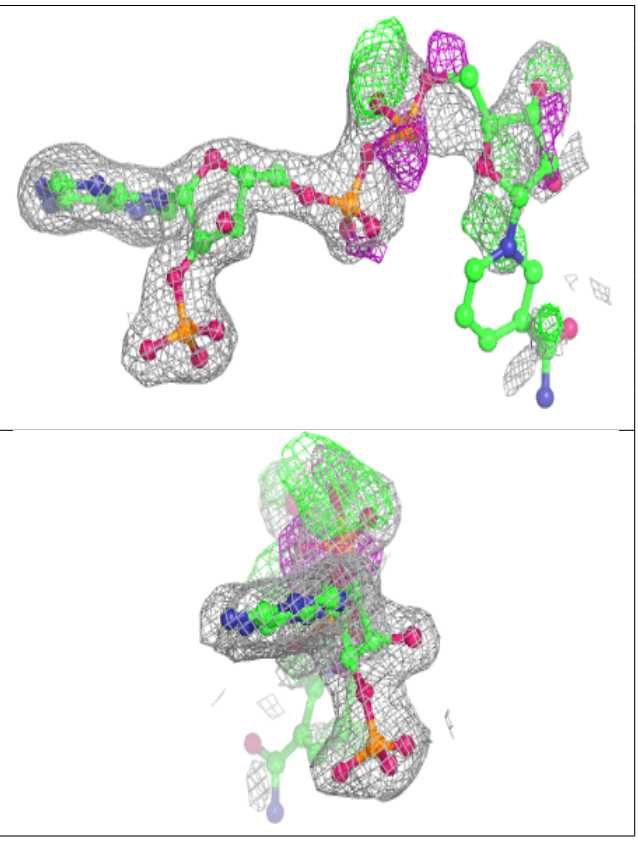
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	FMN	A	1030	31/31	0.97	0.08	10,13,14,15	0
3	FMN	B	1030	31/31	0.97	0.09	10,14,15,16	0
3	FMN	C	1030	31/31	0.97	0.08	8,12,14,17	0
3	FMN	D	1030	31/31	0.97	0.09	10,12,13,14	0
4	FAD	A	1031	53/53	0.97	0.11	9,12,14,14	0
2	SF4	A	1028	8/8	0.97	0.08	15,15,16,17	0
4	FAD	C	1031	53/53	0.97	0.08	10,13,15,16	0
4	FAD	D	1031	53/53	0.97	0.09	9,12,14,15	0
2	SF4	A	1027	8/8	0.97	0.09	12,14,15,15	0
2	SF4	B	1026	8/8	0.97	0.10	13,14,15,16	0
2	SF4	B	1027	8/8	0.97	0.09	12,14,15,16	0
2	SF4	C	1028	8/8	0.97	0.08	13,14,15,15	0
2	SF4	C	1029	8/8	0.97	0.10	13,14,16,16	0
2	SF4	D	1026	8/8	0.97	0.09	13,13,14,14	0
2	SF4	D	1027	8/8	0.97	0.11	11,12,13,13	0
2	SF4	D	1028	8/8	0.97	0.09	15,16,16,17	0

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

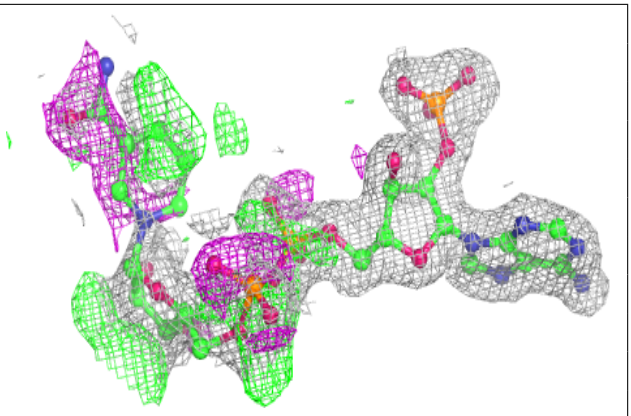
Electron density around NDP A 1032:

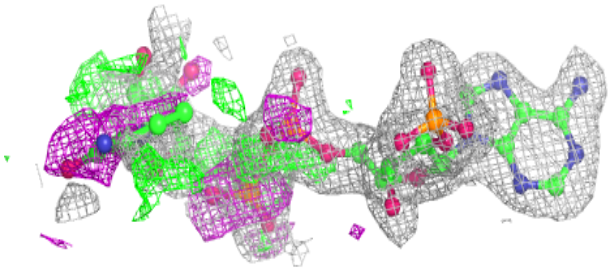
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

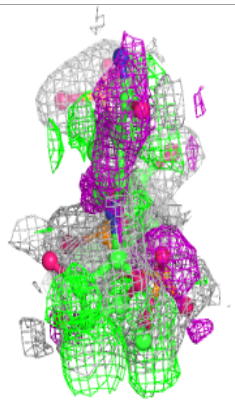


Electron density around NDP D 1032:

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

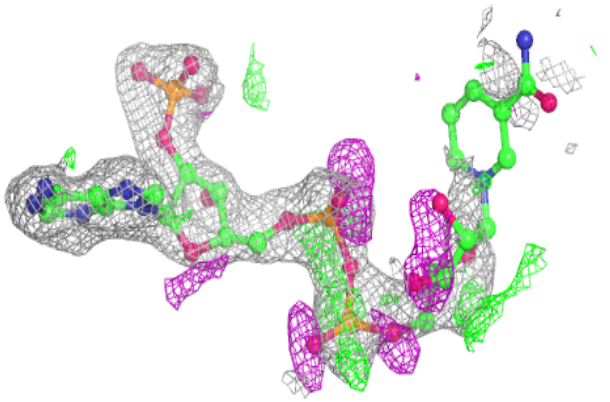


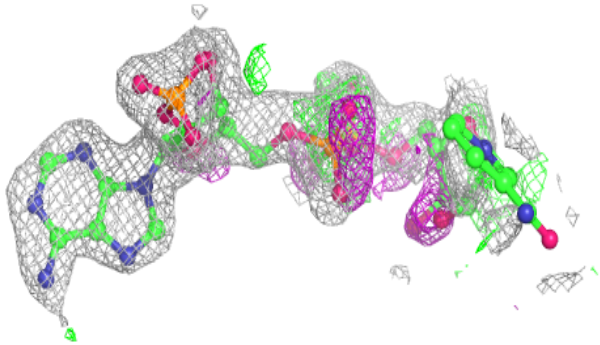


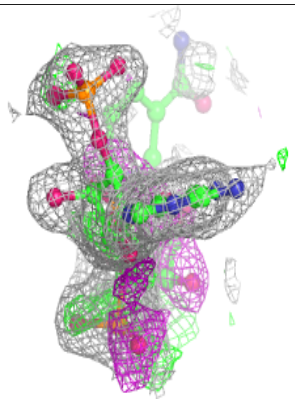


Electron density around NDP C 1032:

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

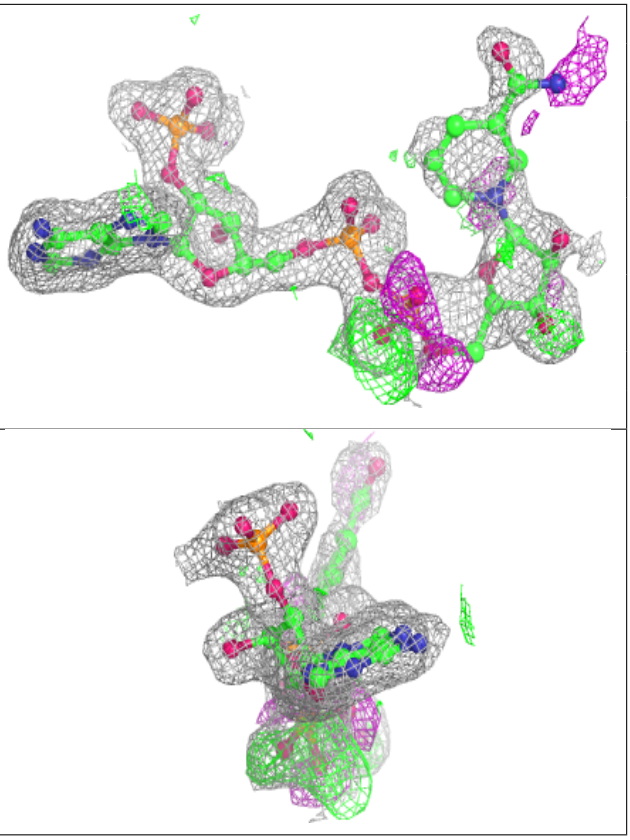


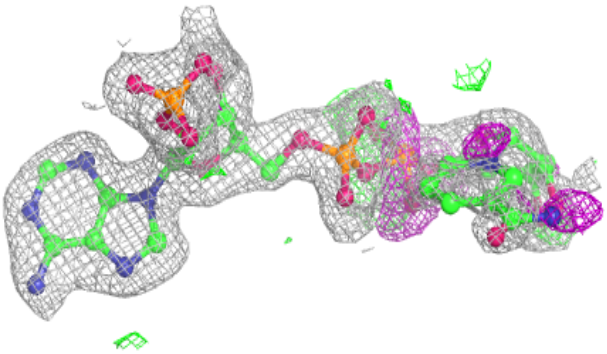




Electron density around NDP B 1032:

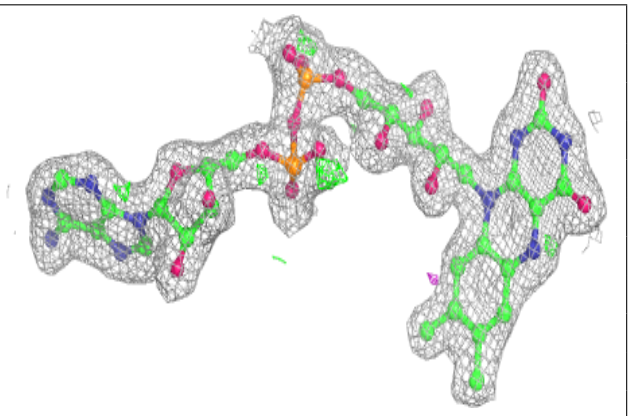
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

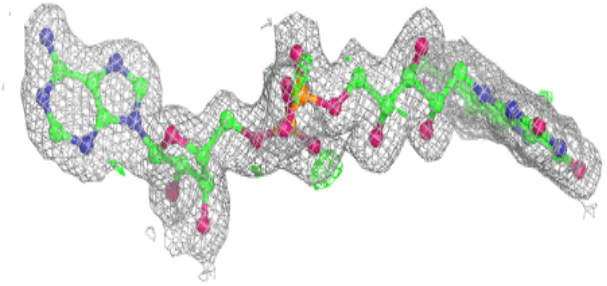


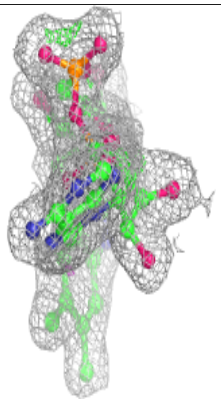


Electron density around FAD B 1031:

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

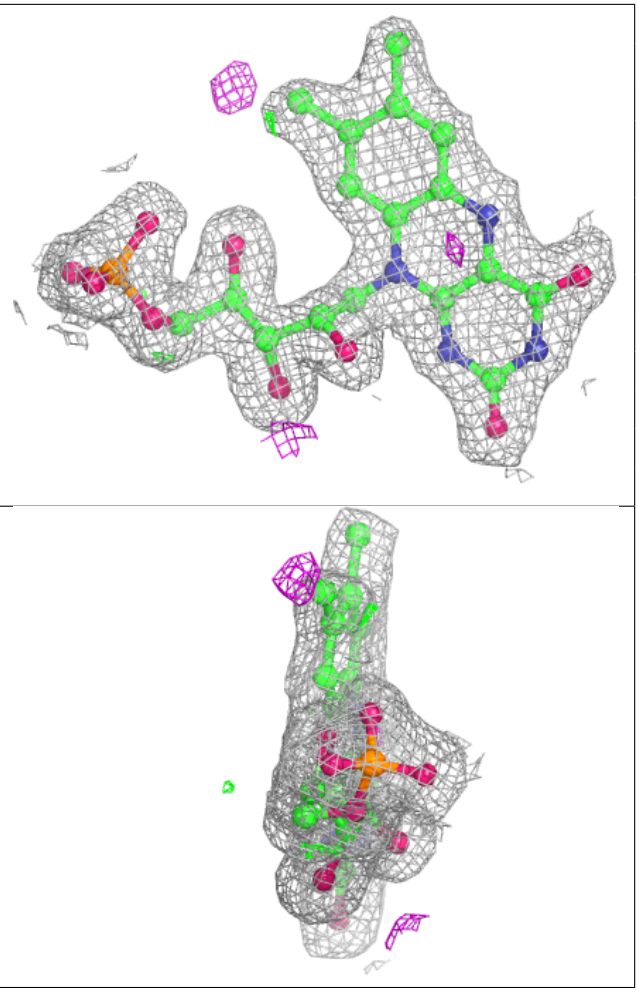






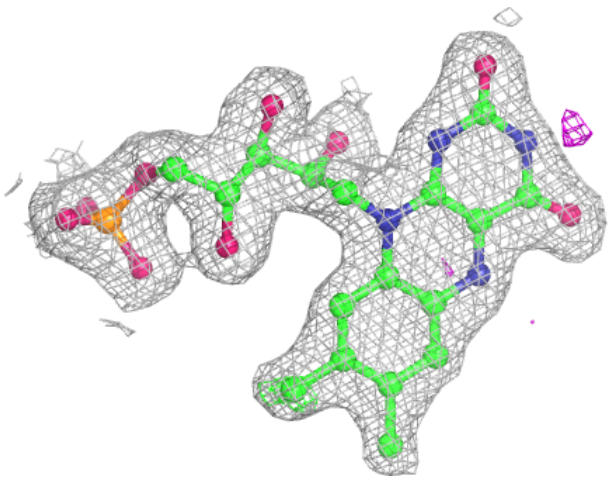
Electron density around FMN A 1030:

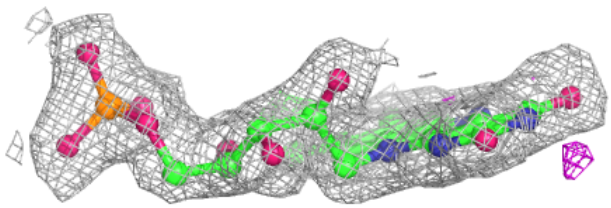
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

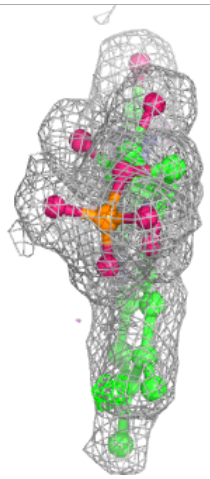


Electron density around FMN B 1030:

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

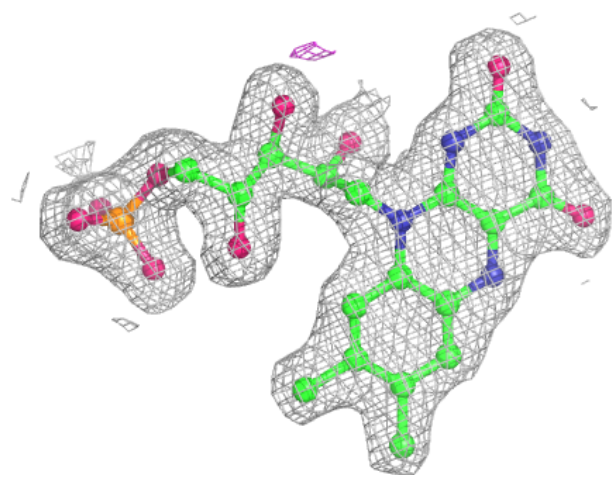


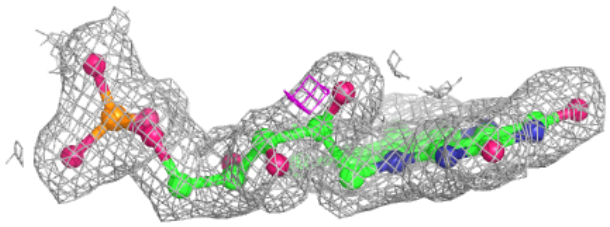


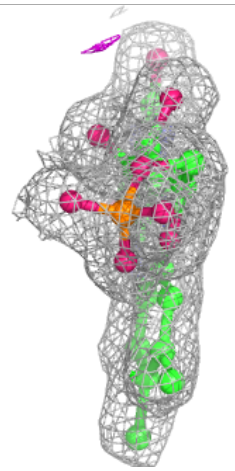


Electron density around FMN C 1030:

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

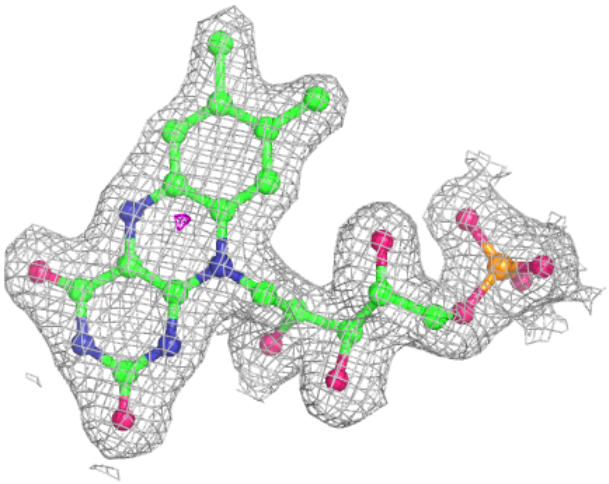


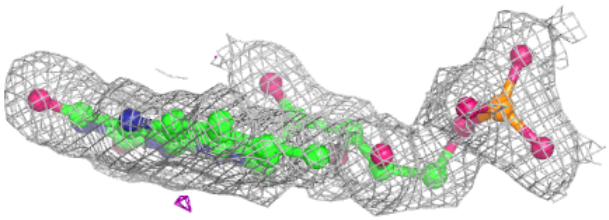


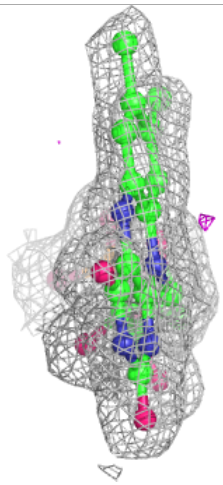


Electron density around FMN D 1030:

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

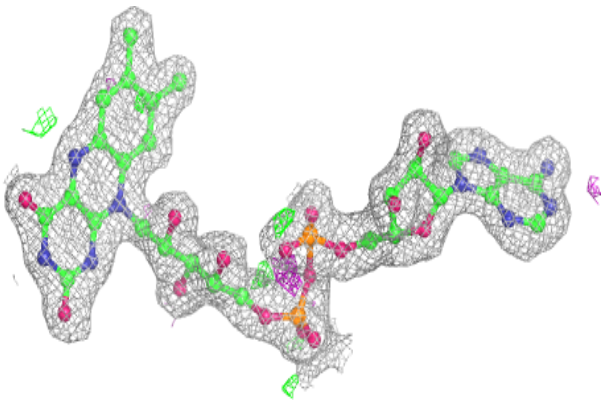


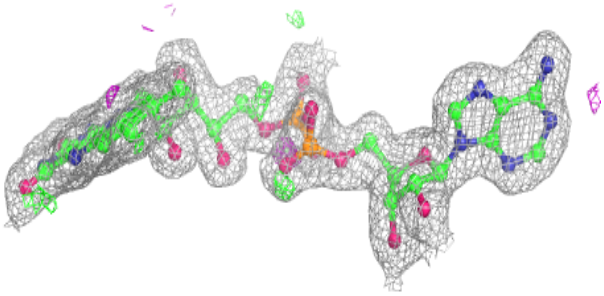


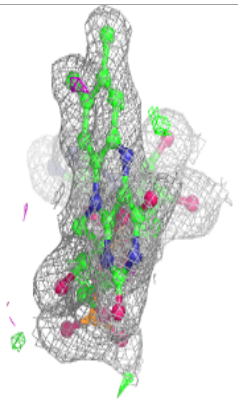


Electron density around FAD A 1031:

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

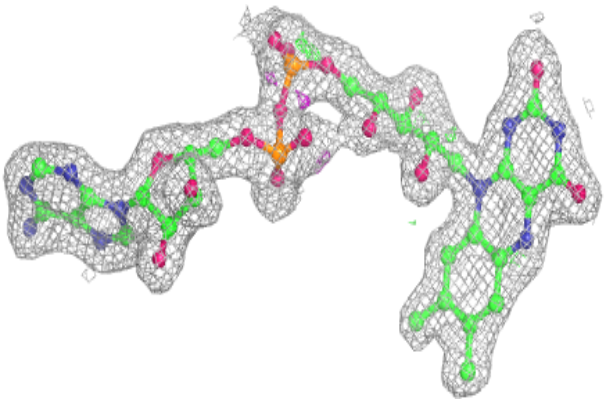


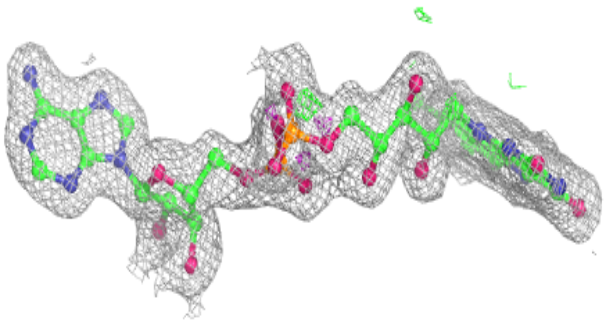


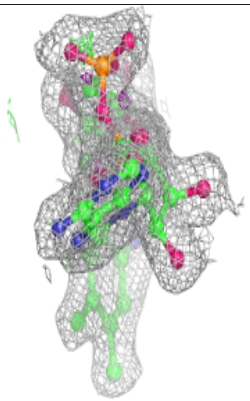


Electron density around FAD C 1031:

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

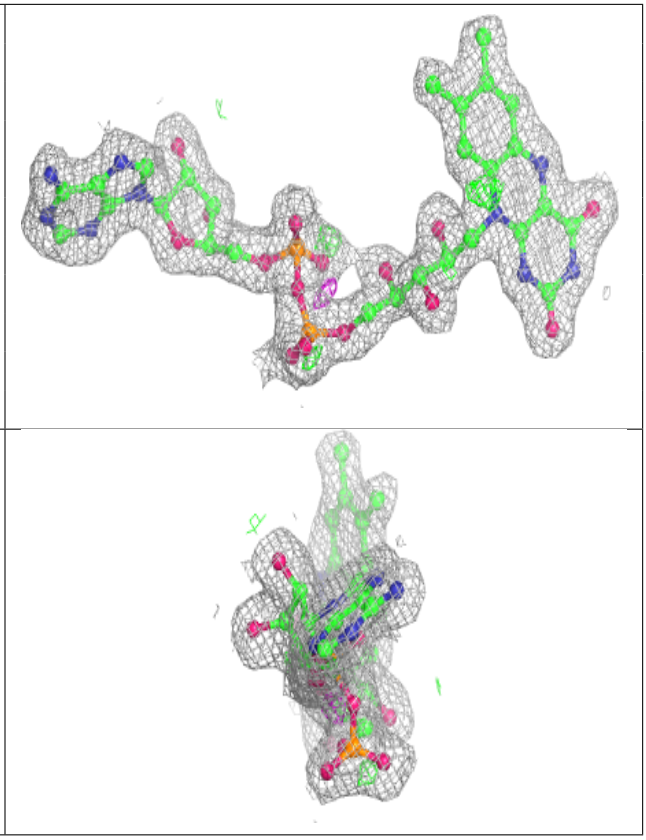






Electron density around FAD D 1031:

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



6.5 Other polymers (i)

There are no such residues in this entry.