wwPDB X-ray Structure Validation Summary Report (i)

Oct 28, 2024 – 04:26 pm GMT

PDB ID	:	1O95
Title	:	Ternary complex between trimethylamine dehydrogenase and electron transferring flavoprotein
Authors	:	Leys, D.; Basran, J.; Talfournier, F.; Sutcliffe, M.J.; Scrutton, N.S.
Deposited on	:	2002-12-11
Resolution	:	3.70 Å(reported)

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

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

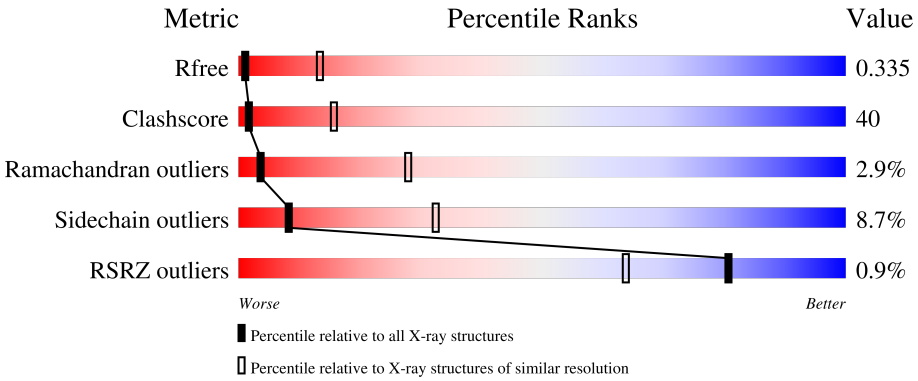
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 3.70 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}	164625	1017 (3.80-3.60)
Clashscore	180529	1074 (3.80-3.60)
Ramachandran outliers	177936	1055 (3.80-3.60)
Sidechain outliers	177891	1052 (3.80-3.60)
RSRZ outliers	164620	1017 (3.80-3.60)

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

Mol	Chain	Length	Quality of chain
1	A	729	36% 48% 14%
1	B	729	33% 53% 11%
2	C	264	42% 34% 11% 12%
2	E	264	39% 35% 14% 11%
3	D	320	27% 23% 7% 41%

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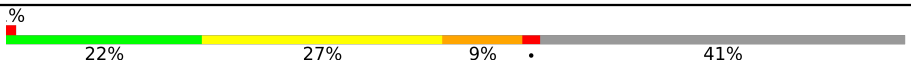
Mol	Chain	Length	Quality of chain
3	F	320	

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 17776 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 TRIMETHYLAMINE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	729	Total	C	N	O	S	0	0	0
			5692	3589	996	1079	28			
1	B	729	Total	C	N	O	S	0	0	0
			5676	3583	994	1071	28			

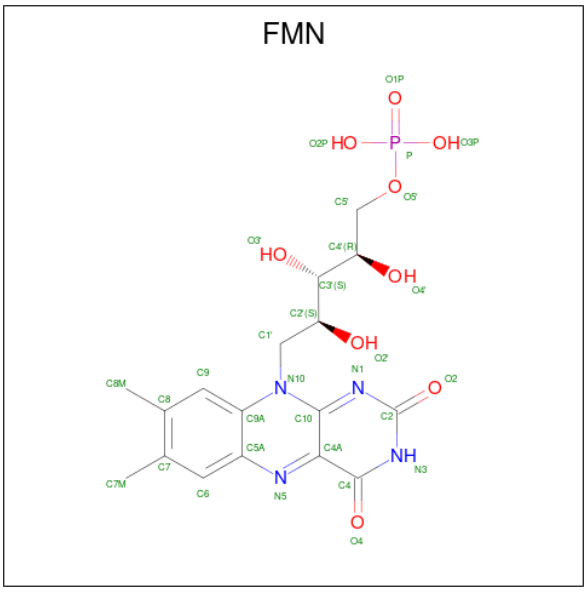
- Molecule 2 is a protein called ELECTRON TRANSFER FLAVOPROTEIN BETA-SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	233	Total	C	N	O	S	0	0	0
			1749	1097	301	341	10			
2	E	236	Total	C	N	O	S	0	0	0
			1751	1102	299	340	10			

- Molecule 3 is a protein called ELECTRON TRANSFER FLAVOPROTEIN ALPHA-SUBUNIT.

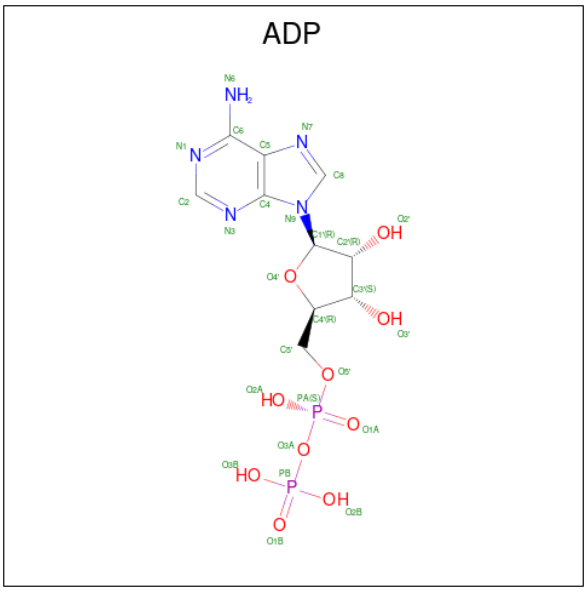
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	189	Total	C	N	O	0	0	0
			1354	857	230	267			
3	F	189	Total	C	N	O	0	0	0
			1376	870	232	274			

- Molecule 4 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



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

- Molecule 5 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

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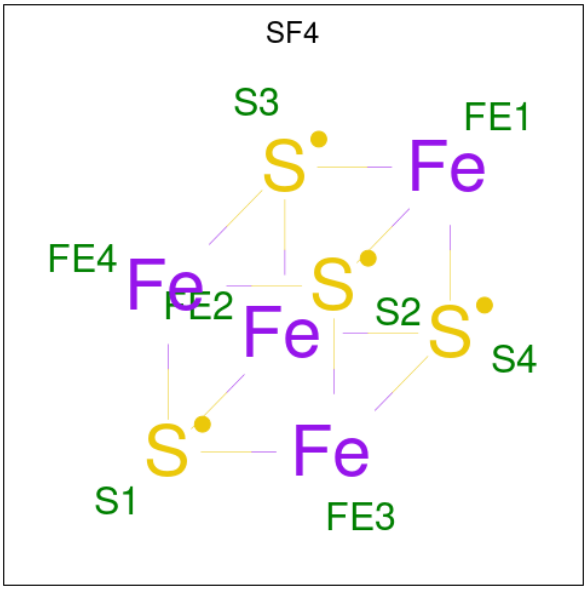
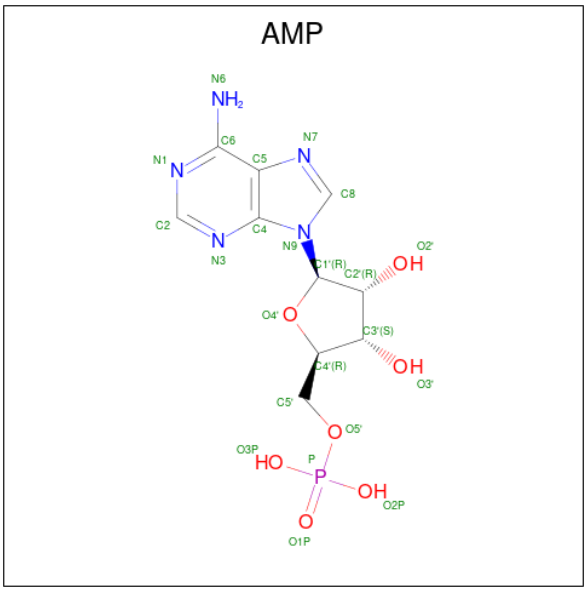
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 6 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



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

- Molecule 7 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: $C_{10}H_{14}N_5O_7P$).



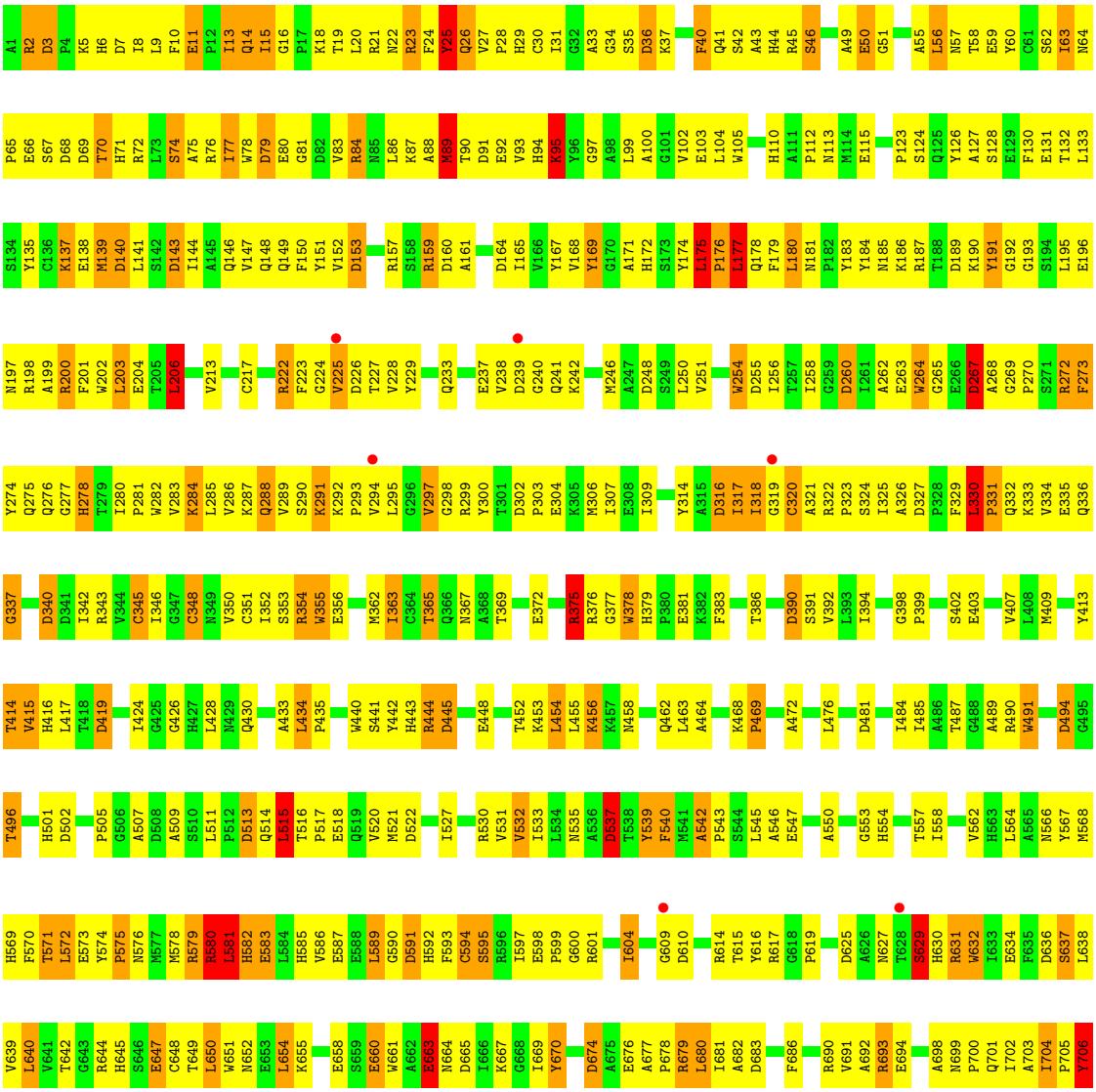
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	C	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
7	E	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

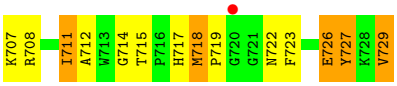
3 Residue-property plots (i)

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: TRIMETHYLAMINE DEHYDROGENASE

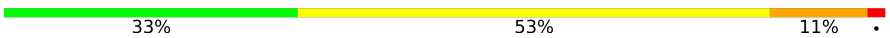
Chain A:

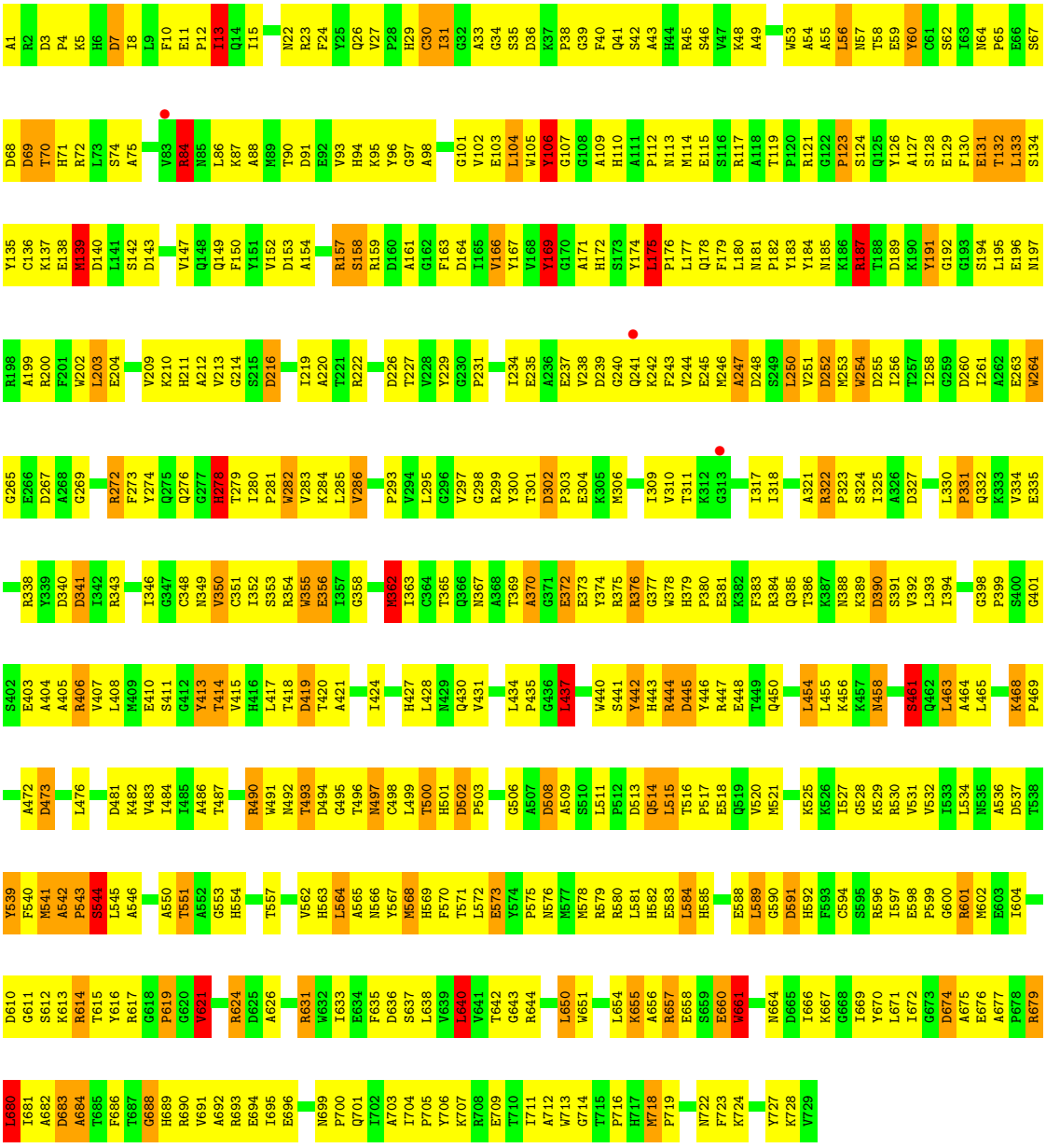




• Molecule 1: TRIMETHYLAMINE DEHYDROGENASE

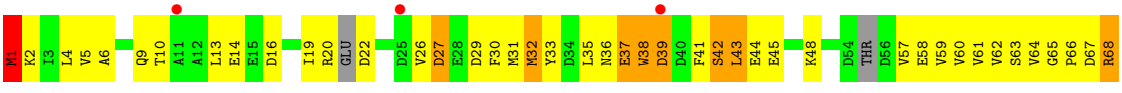
Chain B:

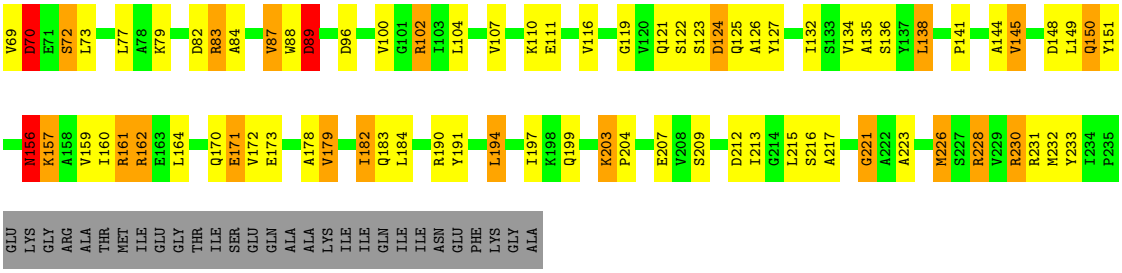




• Molecule 2: ELECTRON TRANSFER FLAVOPROTEIN BETA-SUBUNIT

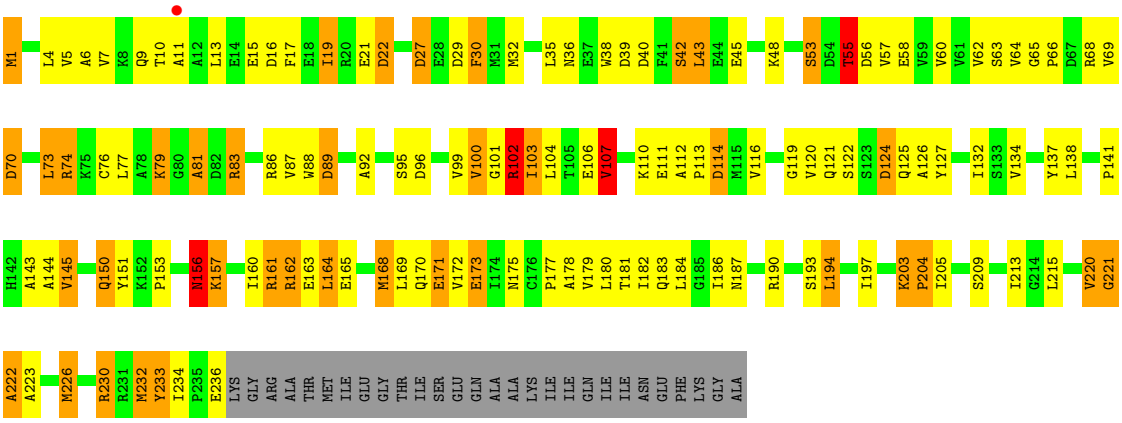
Chain C:





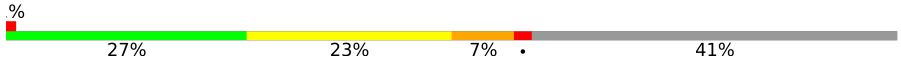
• Molecule 2: ELECTRON TRANSFER FLAVOPROTEIN BETA-SUBUNIT

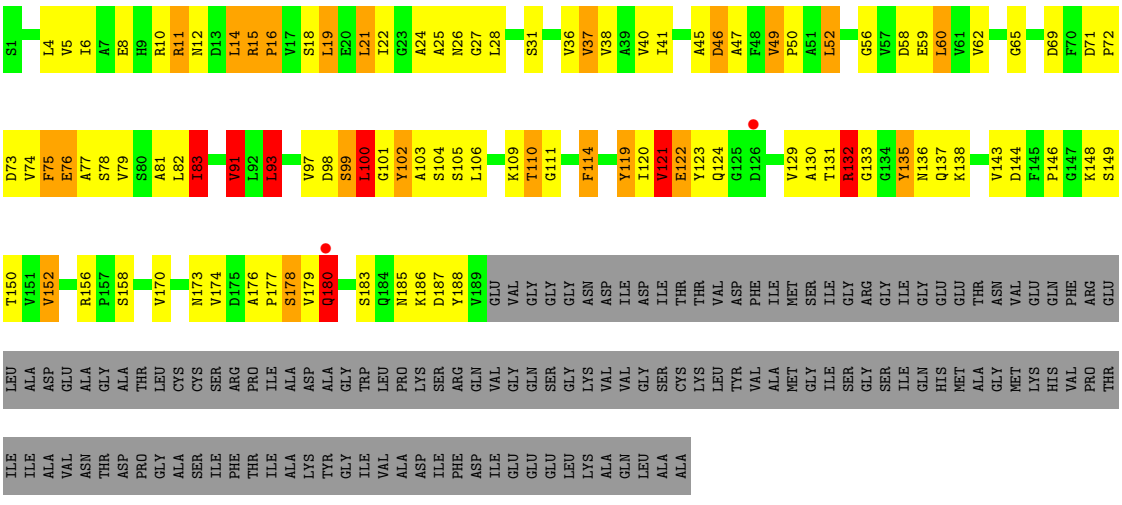
Chain E:



• Molecule 3: ELECTRON TRANSFER FLAVOPROTEIN ALPHA-SUBUNIT

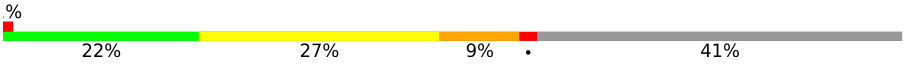
Chain D:

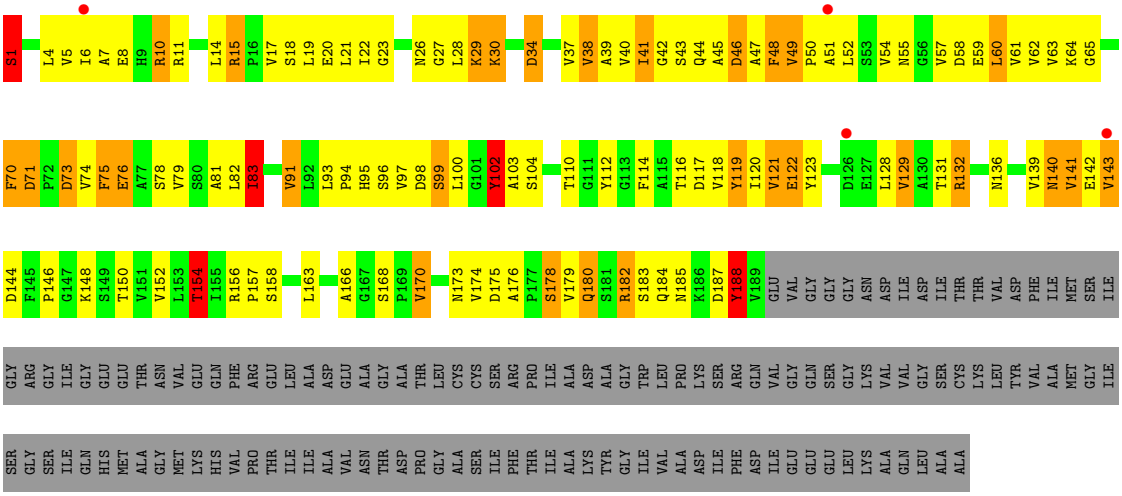




• Molecule 3: ELECTRON TRANSFER FLAVOPROTEIN ALPHA-SUBUNIT

Chain F:




S1 L4 V5 I6 A7 E8 H9 R10 R11 L14 R15 P16 V17 S18 L19 E20 L21 I22 G23 N26 G27 L28 K29 K30 D34 V37 V38 A39 V40 I41 G42 S43 Q44 A45 D46 A47 F48 V49 P50 A51 L52 S53 V54 N55 G56 V57 D58 E59 L60 V61 V62 V63 K64 G65
F70 D71 P72 D73 V74 F75 E76 A77 S78 V79 S80 A81 L82 I83 V91 L92 L93 P94 H95 S96 V97 D98 S99 L100 G101 V102 A103 S104 T110 G111 Y112 G113 F114 A115 T116 D117 V118 Y119 I120 V121 E122 Y123 D126 E127 L128 V129 A130 T131 R132 N136 V139 N140 V141 E142 V143
D144 F145 P146 G147 K148 S149 T150 V151 V152 L153 T154 T155 R156 P157 S158 L163 A166 G167 S168 P169 V170 N173 V174 D175 A176 P177 S178 V179 Q180 S181 R182 S183 Q184 N185 K186 D187 Y188 V189 GLU VAL GLY GLY GLY ASN ASP ILE ASP ILE THR THR VAL ASP PHE ILE MET SER ILE
GLY ARG GLY ILE GLY GLU GLU THR ASN VAL GLU GLN PHE ARG GLU LEU ALA ASP GLU ALA GLY ALA THR LEU CYS CYS SER ARG PRO ILE ALA ASP ALA GLY TRP LEU PRO LYS SER ARG GLN VAL GLY GLN SER GLY LYS VAL VAL GLY SER CYS LYS LEU TYR VAL ALA MET GLY ILE
SER GLY SER ILE GLN HIS MET ALA GLY MET LYS HIS VAL PRO THR ILE ILE ALA VAL ASN THR ASP PRO GLY ALA SER ILE PHE THR ILE ALA LYS TYR GLY ILE VAL ALA ASP ILE PHE ASP ILE GLU GLU GLU LEU LYS ALA GLN LEU ALA ALA

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	102.50Å 116.51Å 138.71Å 90.00° 95.35° 90.00°	Depositor
Resolution (Å)	20.00 – 3.70 20.00 – 3.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-3.70) 96.3 (20.00-3.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	1.77 (at 3.71Å)	Xtriage
Refinement program	REFMAC 5.1.08	Depositor
R, R_{free}	0.252 , 0.353 0.237 , 0.335	Depositor DCC
R_{free} test set	1679 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	77.0	Xtriage
Anisotropy	0.862	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.24 , 36.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	17776	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 35.02 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.2278e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: AMP, ADP, SF4, FMN

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	1.61	53/5834 (0.9%)	1.66	102/7918 (1.3%)
1	B	1.63	49/5818 (0.8%)	1.66	97/7902 (1.2%)
2	C	1.60	22/1771 (1.2%)	1.54	24/2399 (1.0%)
2	E	1.70	22/1775 (1.2%)	1.65	34/2408 (1.4%)
3	D	1.61	13/1378 (0.9%)	1.59	21/1884 (1.1%)
3	F	2.01	34/1400 (2.4%)	1.77	26/1913 (1.4%)
All	All	1.66	193/17976 (1.1%)	1.65	304/24424 (1.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	B	0	3
2	E	0	1
3	D	0	3
3	F	0	3
All	All	0	14

The worst 5 of 193 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	718	MET	SD-CE	12.45	2.47	1.77
3	F	188	TYR	CE1-CZ	9.02	1.50	1.38
1	B	254	TRP	CB-CG	-8.99	1.34	1.50
2	E	232	MET	C-O	8.98	1.40	1.23
3	D	180	GLN	CB-CG	8.94	1.76	1.52

The worst 5 of 304 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	69	ASP	CB-CG-OD2	13.04	130.03	118.30
1	B	272	ARG	NE-CZ-NH1	-12.16	114.22	120.30
3	F	15	ARG	NE-CZ-NH2	11.80	126.20	120.30
1	A	302	ASP	CB-CG-OD2	11.78	128.90	118.30
1	A	665	ASP	CB-CG-OD2	11.31	128.48	118.30

There are no chirality outliers.

5 of 14 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	139	MET	Peptide
1	A	320	CYS	Peptide
1	A	539	TYR	Peptide
1	A	66	GLU	Peptide
1	B	139	MET	Peptide

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	5692	0	5445	505	0
1	B	5676	0	5424	519	0
2	C	1749	0	1722	121	0
2	E	1751	0	1716	129	0
3	D	1354	0	1311	85	0
3	F	1376	0	1358	129	0
4	A	31	0	18	5	0
4	B	31	0	18	6	0
5	A	27	0	12	6	0
5	B	27	0	12	2	0
6	A	8	0	0	1	0
6	B	8	0	0	0	0
7	C	23	0	11	6	0
7	E	23	0	12	4	0
All	All	17776	0	17059	1402	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 40.

The worst 5 of 1402 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:B:346:ILE:CD1	1:B:346:ILE:CG1	1.75	1.63
1:B:500:THR:CA	1:B:500:THR:CB	1.75	1.57
3:D:180:GLN:CG	3:D:180:GLN:CB	1.76	1.56
3:D:16:PRO:CB	3:D:16:PRO:CG	1.74	1.48
1:A:718:MET:SD	1:A:718:MET:CE	2.04	1.46

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	727/729 (100%)	624 (86%)	83 (11%)	20 (3%)	4	28
1	B	727/729 (100%)	614 (84%)	98 (14%)	15 (2%)	5	33
2	C	227/264 (86%)	202 (89%)	21 (9%)	4 (2%)	7	35
2	E	234/264 (89%)	210 (90%)	14 (6%)	10 (4%)	2	20
3	D	187/320 (58%)	153 (82%)	24 (13%)	10 (5%)	1	18
3	F	187/320 (58%)	162 (87%)	18 (10%)	7 (4%)	2	24
All	All	2289/2626 (87%)	1965 (86%)	258 (11%)	66 (3%)	3	28

5 of 66 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	600	GLY
1	A	680	LEU
1	B	264	TRP
1	B	680	LEU
3	D	27	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	584/602 (97%)	537 (92%)	47 (8%)	10 35
1	B	578/602 (96%)	527 (91%)	51 (9%)	8 32
2	C	180/216 (83%)	167 (93%)	13 (7%)	12 38
2	E	177/216 (82%)	161 (91%)	16 (9%)	8 31
3	D	143/258 (55%)	123 (86%)	20 (14%)	3 17
3	F	150/258 (58%)	139 (93%)	11 (7%)	11 38
All	All	1812/2152 (84%)	1654 (91%)	158 (9%)	8 32

5 of 158 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	60	LEU
2	E	157	LYS
3	D	93	LEU
3	D	186	LYS
3	F	49	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 36 such sidechains are listed below:

Mol	Chain	Res	Type
3	D	180	GLN
3	F	137	GLN
2	E	150	GLN
2	E	183	GLN
1	B	429	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

8 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	$\#\|Z\| > 2$
6	SF4	A	1732	1	0,12,12	-	-	-		
7	AMP	C	1236	-	22,25,25	2.01	7 (31%)	25,38,38	3.15	14 (56%)
6	SF4	B	1732	1	0,12,12	-	-	-		
5	ADP	A	1731	-	24,29,29	1.83	7 (29%)	29,45,45	2.33	11 (37%)
7	AMP	E	1237	-	22,25,25	2.30	6 (27%)	25,38,38	2.92	11 (44%)
4	FMN	A	1730	1	33,33,33	1.67	6 (18%)	48,50,50	2.48	17 (35%)
5	ADP	B	1731	-	24,29,29	1.58	4 (16%)	29,45,45	2.43	9 (31%)
4	FMN	B	1730	1	33,33,33	1.68	4 (12%)	48,50,50	2.44	23 (47%)

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
6	SF4	A	1732	1	-	-	0/6/5/5
7	AMP	C	1236	-	-	3/6/26/26	0/3/3/3
6	SF4	B	1732	1	-	-	0/6/5/5
5	ADP	A	1731	-	-	4/12/32/32	0/3/3/3
7	AMP	E	1237	-	-	3/6/26/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FMN	A	1730	1	-	7/18/18/18	0/3/3/3
5	ADP	B	1731	-	-	3/12/32/32	0/3/3/3
4	FMN	B	1730	1	-	1/18/18/18	0/3/3/3

The worst 5 of 34 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	E	1237	AMP	C2-N3	5.37	1.40	1.32
4	B	1730	FMN	C4A-N5	5.24	1.40	1.30
7	E	1237	AMP	C2'-C1'	-5.04	1.46	1.53
4	A	1730	FMN	C4A-N5	5.01	1.40	1.30
7	E	1237	AMP	C4-N3	4.99	1.42	1.35

The worst 5 of 85 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1730	FMN	C8M-C8-C9	-8.08	104.55	119.49
7	E	1237	AMP	N3-C2-N1	-7.87	116.38	128.68
5	B	1731	ADP	N3-C2-N1	-7.01	117.73	128.68
7	C	1236	AMP	O3'-C3'-C2'	-7.00	89.16	111.82
5	A	1731	ADP	O2'-C2'-C1'	-6.37	87.33	110.85

There are no chirality outliers.

5 of 21 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1730	FMN	O3'-C3'-C4'-C5'
4	A	1730	FMN	C5'-O5'-P-O3P
5	A	1731	ADP	C5'-O5'-PA-O1A
7	C	1236	AMP	C5'-O5'-P-O3P
7	E	1237	AMP	C5'-O5'-P-O1P

There are no ring outliers.

7 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1732	SF4	1	0
7	C	1236	AMP	6	0
5	A	1731	ADP	6	0
7	E	1237	AMP	4	0

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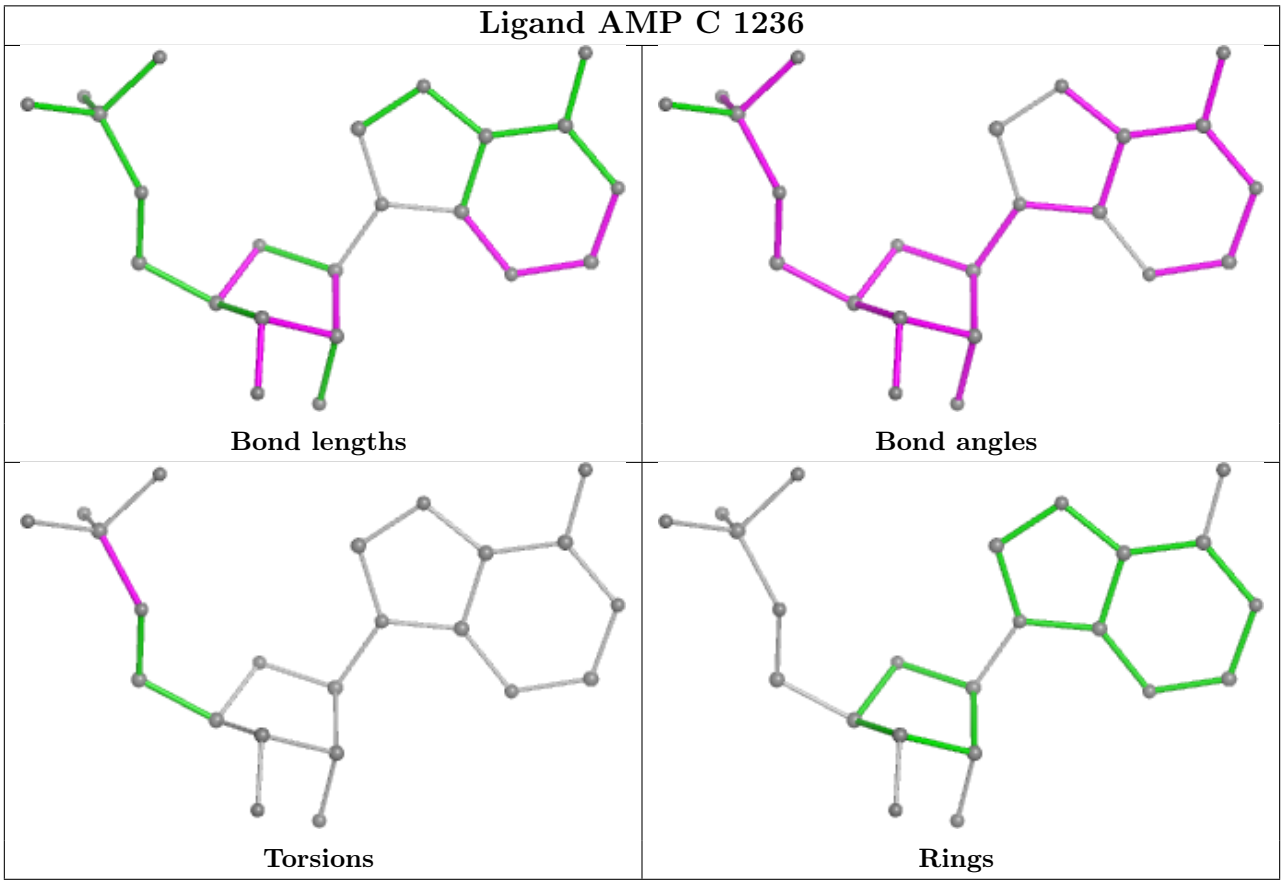
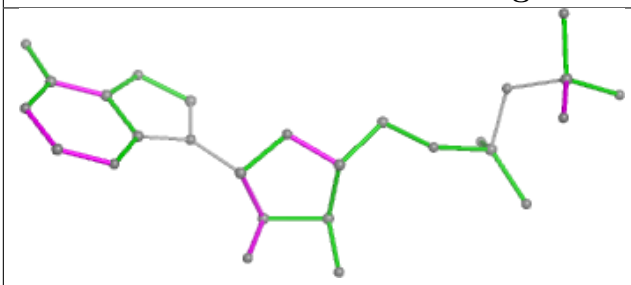
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1730	FMN	5	0
5	B	1731	ADP	2	0
4	B	1730	FMN	6	0

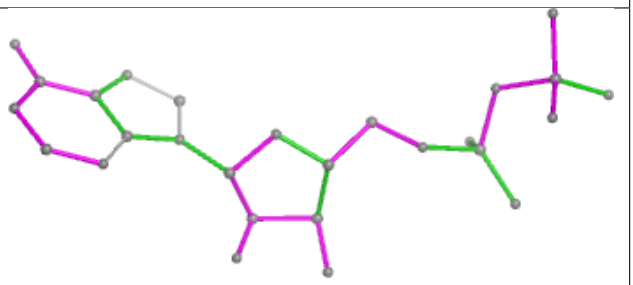
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



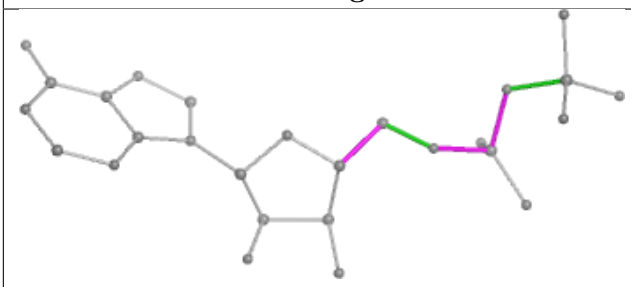
Ligand ADP A 1731



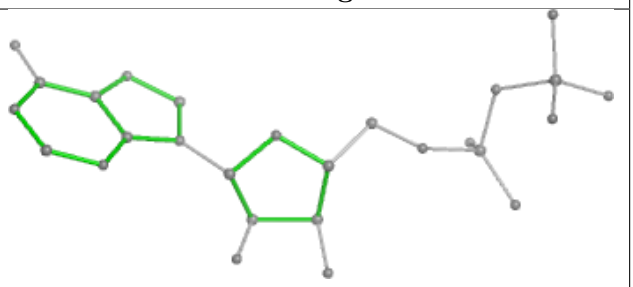
Bond lengths



Bond angles

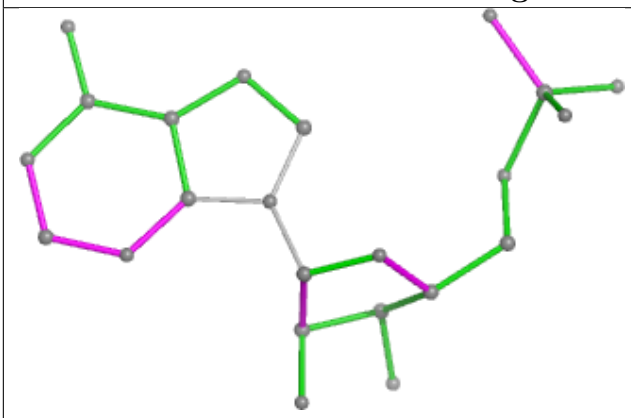


Torsions

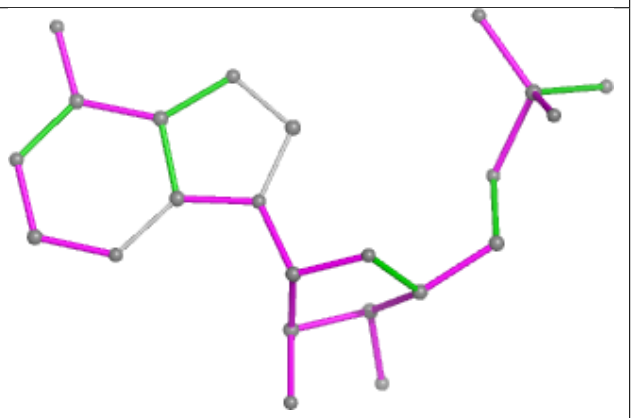


Rings

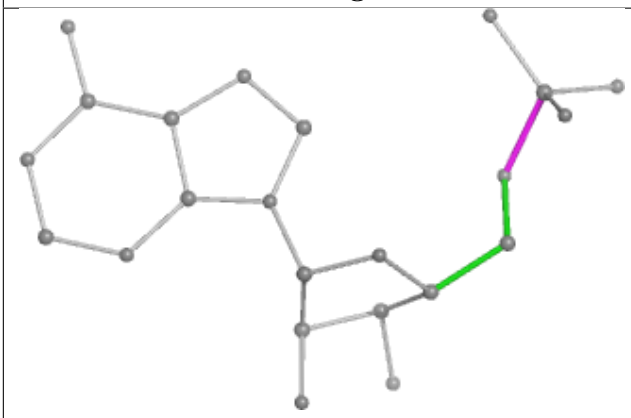
Ligand AMP E 1237



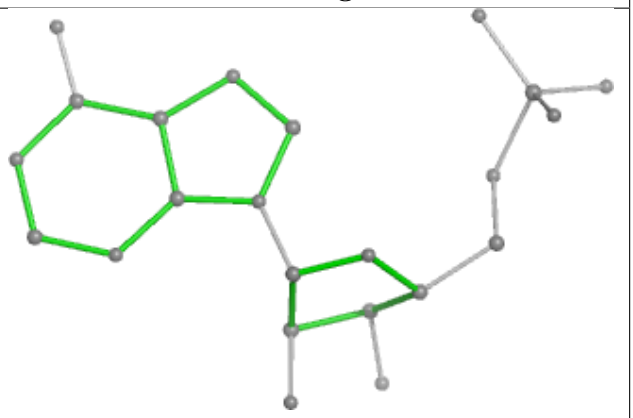
Bond lengths



Bond angles

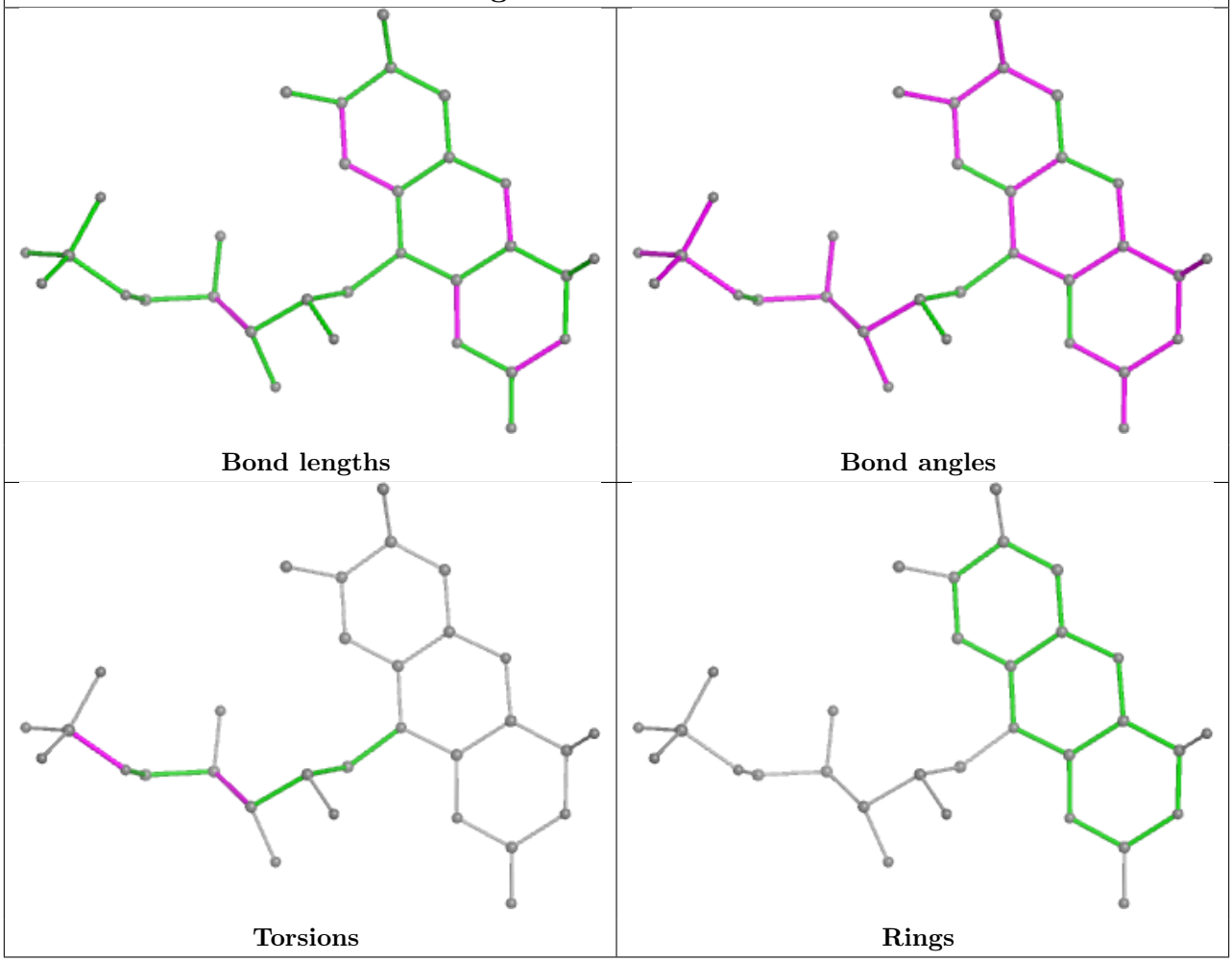


Torsions

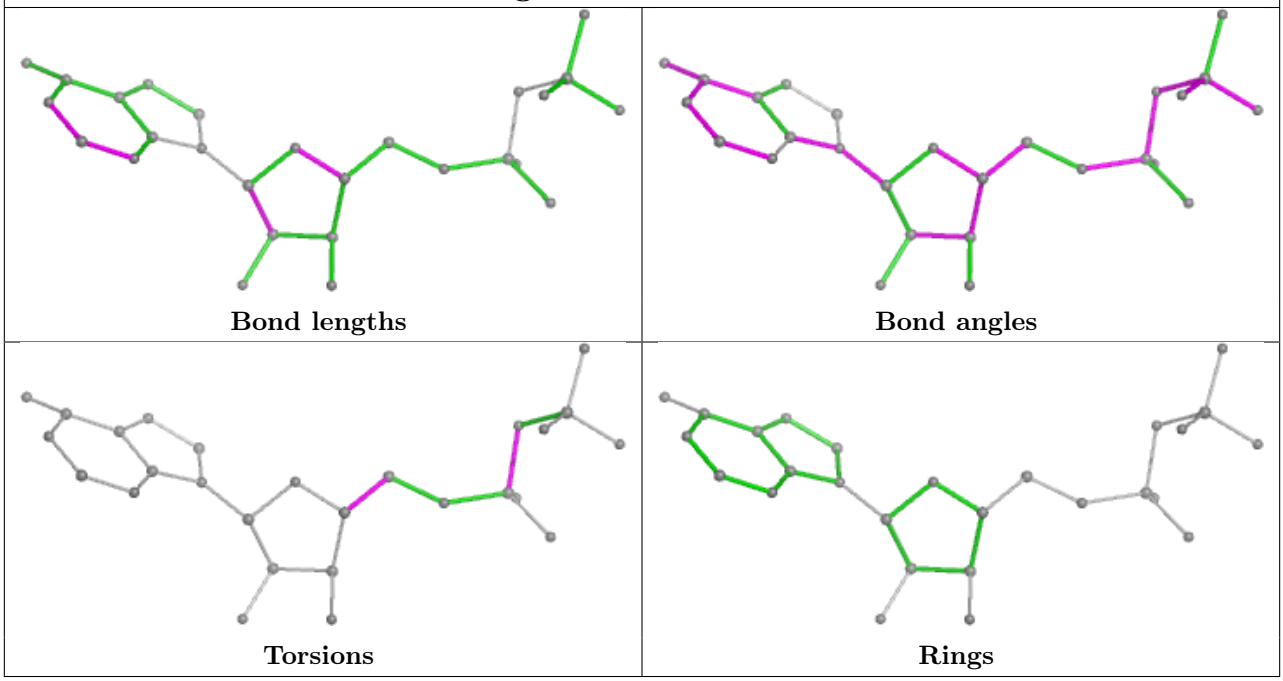


Rings

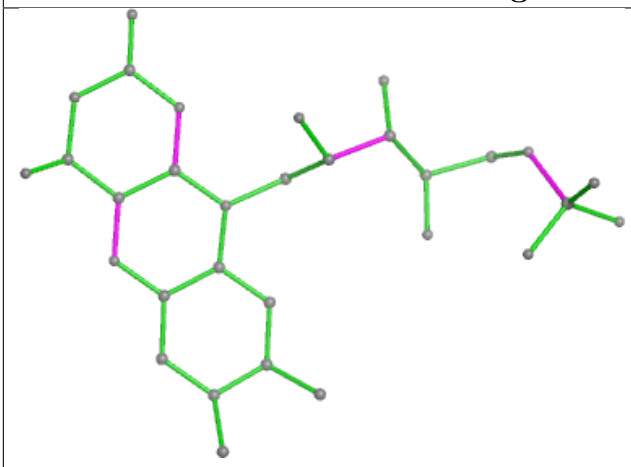
Ligand FMN A 1730



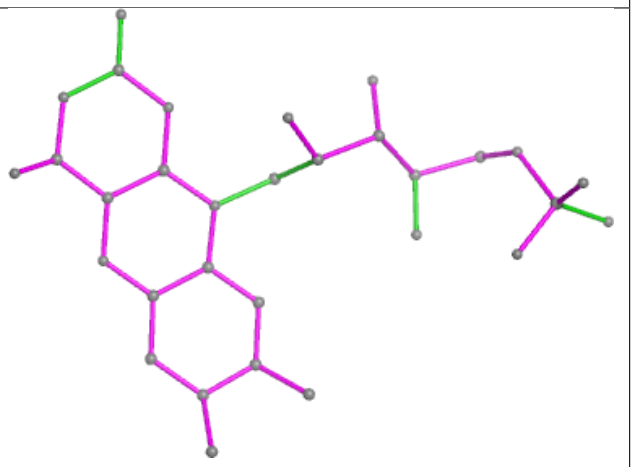
Ligand ADP B 1731



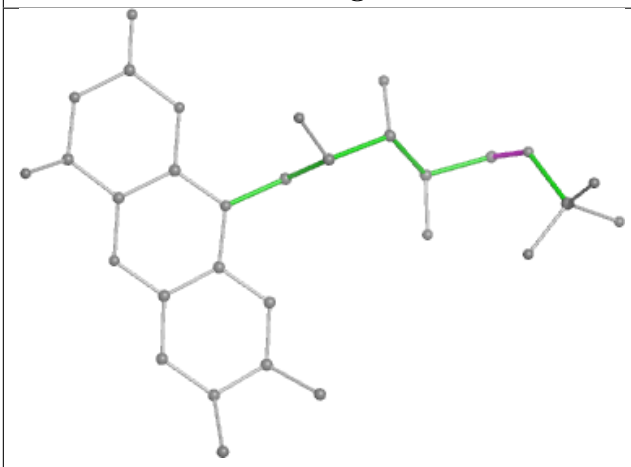
Ligand FMN B 1730



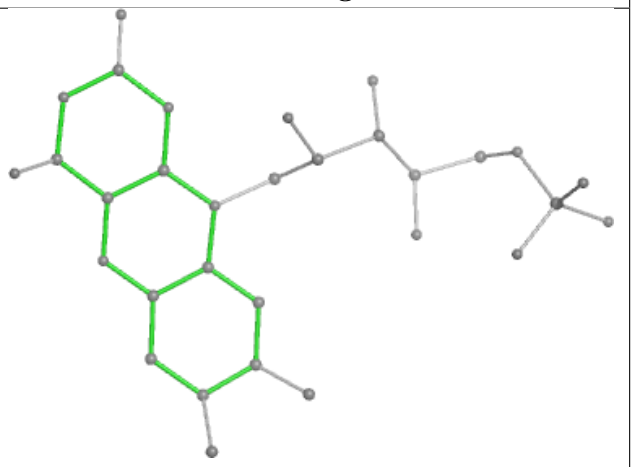
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	729/729 (100%)	-0.13	7 (0%)	79	61	39, 57, 67, 73	0
1	B	729/729 (100%)	-0.17	3 (0%)	89	76	38, 57, 67, 73	0
2	C	233/264 (88%)	-0.24	3 (1%)	74	55	49, 58, 65, 71	0
2	E	236/264 (89%)	-0.23	1 (0%)	89	76	50, 59, 65, 70	0
3	D	189/320 (59%)	-0.14	2 (1%)	77	59	55, 61, 69, 75	0
3	F	189/320 (59%)	0.22	4 (2%)	63	45	56, 62, 70, 76	0
All	All	2305/2626 (87%)	-0.14	20 (0%)	81	64	38, 59, 67, 76	0

The worst 5 of 20 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	6	ILE	3.2
1	B	241	GLN	2.8
1	B	83	VAL	2.5
2	E	11	ALA	2.5
3	D	180	GLN	2.5

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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands (i)

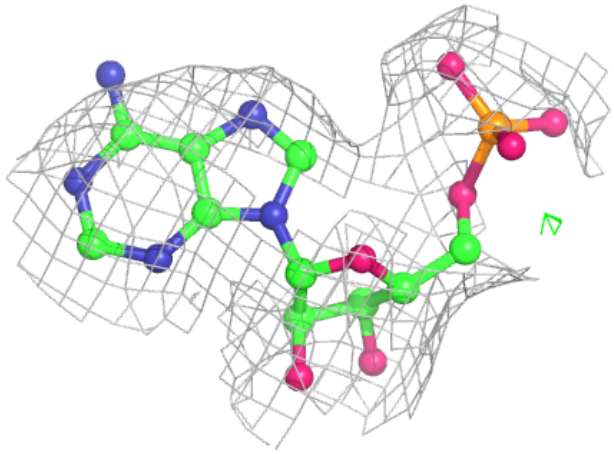
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

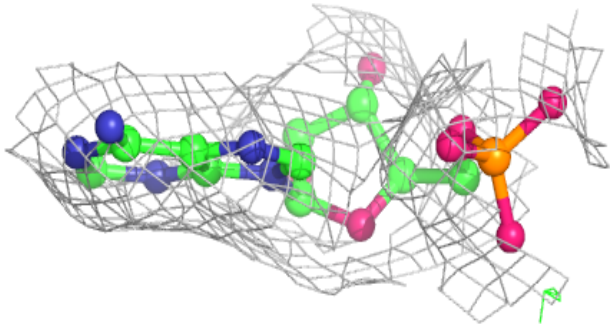
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	AMP	E	1237	23/23	0.92	0.10	33,52,63,66	0
4	FMN	B	1730	31/31	0.93	0.12	23,39,46,52	0
4	FMN	A	1730	31/31	0.93	0.10	35,47,60,61	0
5	ADP	B	1731	27/27	0.94	0.09	45,52,59,61	0
7	AMP	C	1236	23/23	0.94	0.09	34,50,56,60	0
5	ADP	A	1731	27/27	0.94	0.09	40,47,52,53	0
6	SF4	A	1732	8/8	1.00	0.02	31,36,40,41	0
6	SF4	B	1732	8/8	1.00	0.03	33,34,42,44	0

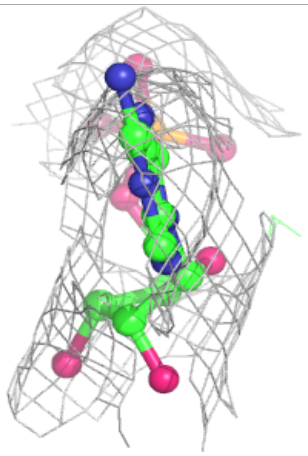
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around AMP E 1237:

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

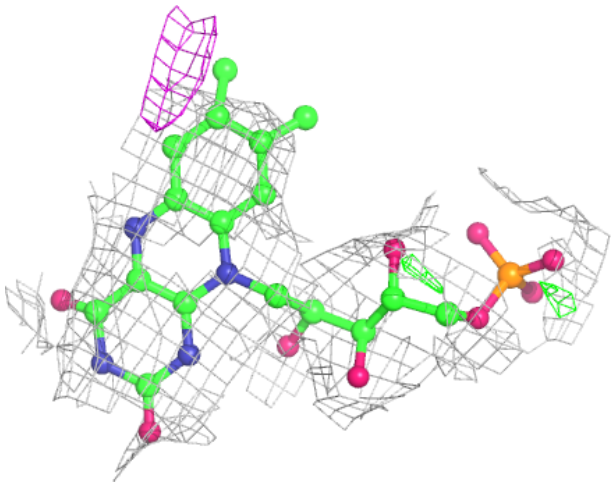


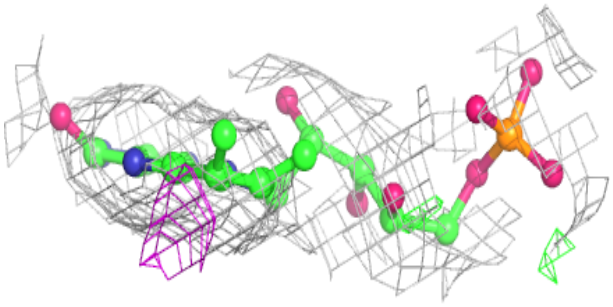


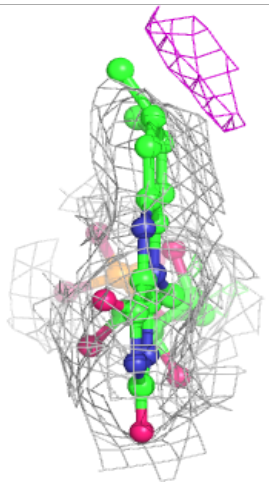


Electron density around FMN B 1730:

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

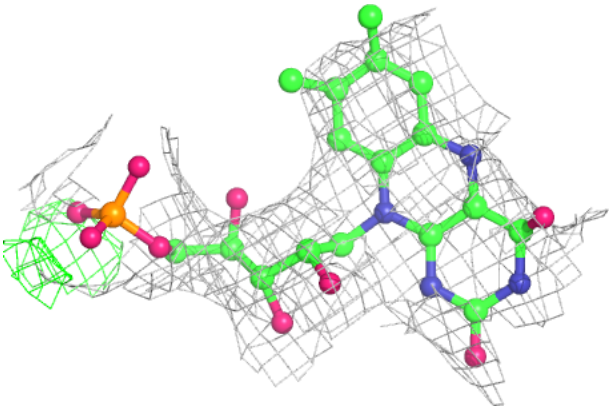


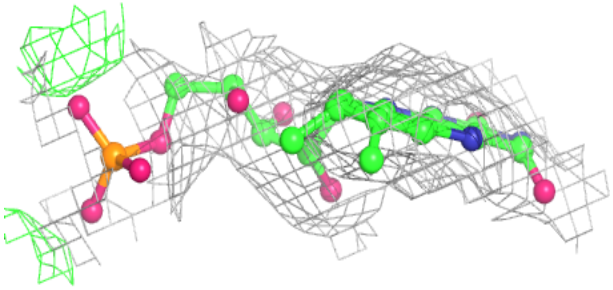


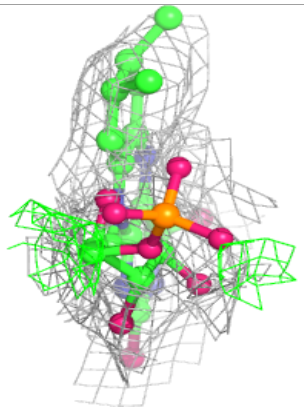


Electron density around FMN A 1730:

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

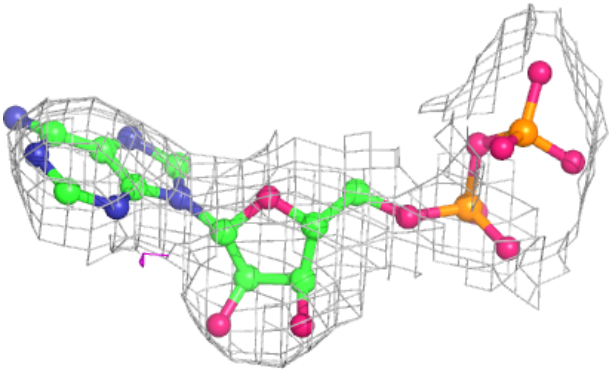


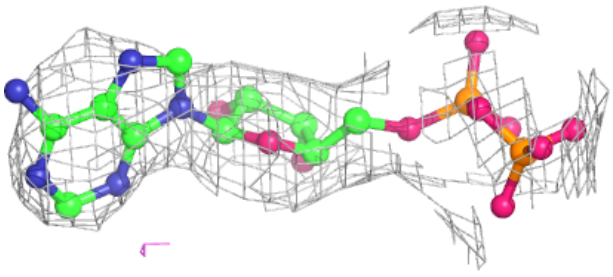


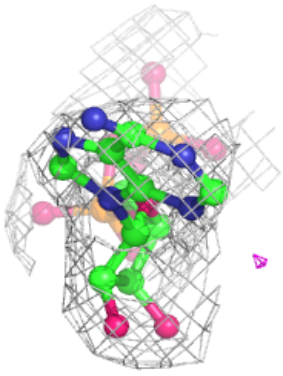


Electron density around ADP B 1731:

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







Electron density around AMP C 1236:

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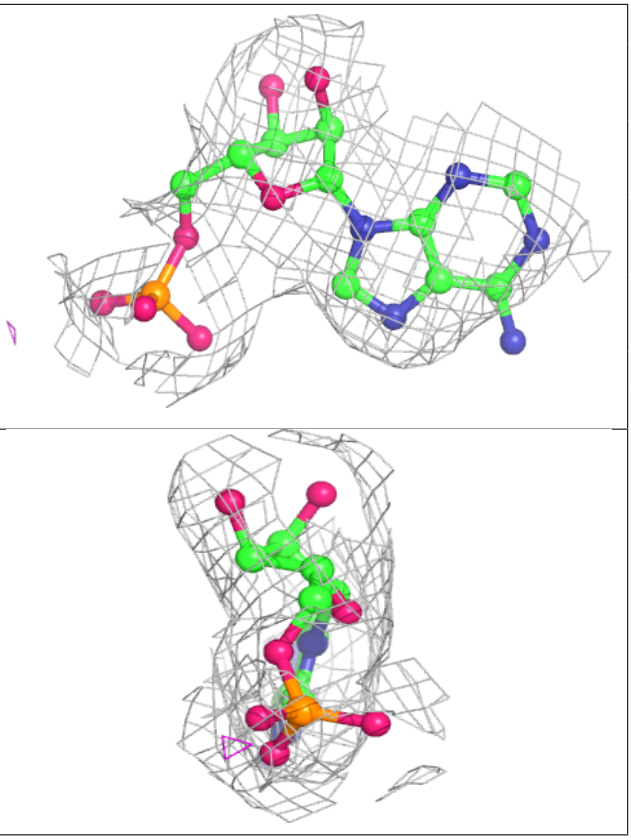
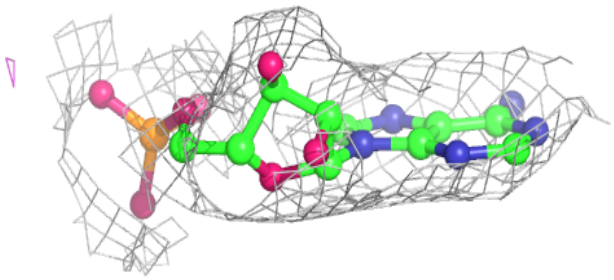
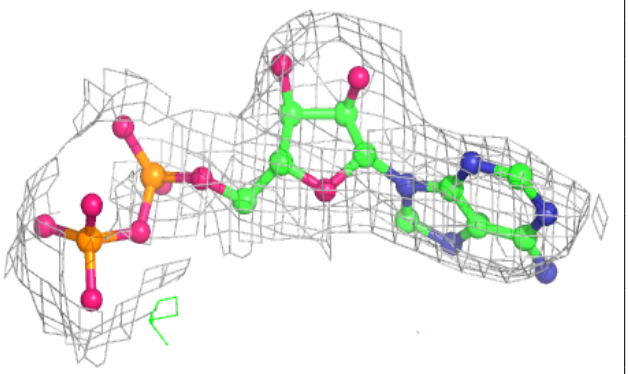
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

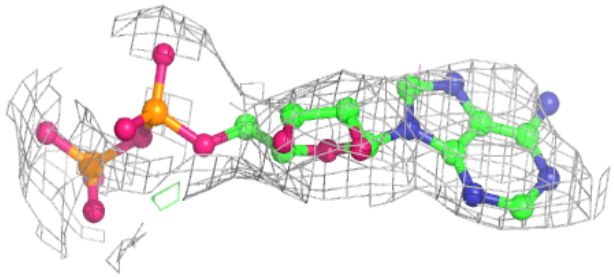


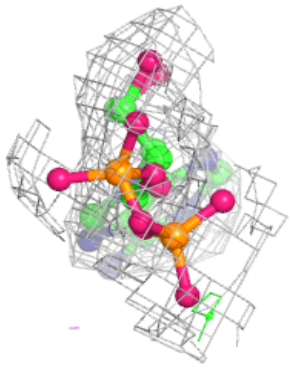


Electron density around ADP A 1731:

$2mF_o$-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.