Full wwPDB X-ray Structure Validation Report ⓘ

Jun 22, 2024 – 06:04 PM EDT

PDB ID	:	6SEK
Title	:	Crystal Structure of Ancestral Flavin-containing monooxygenase (FMO) 5
Authors	:	Nicoll, C.; Bailleul, G.; Fiorentini, F.; Mascotti, M.L.; Fraaije, M.; Mattevi, A.
Deposited on	:	2019-07-30
Resolution	:	2.70 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 ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

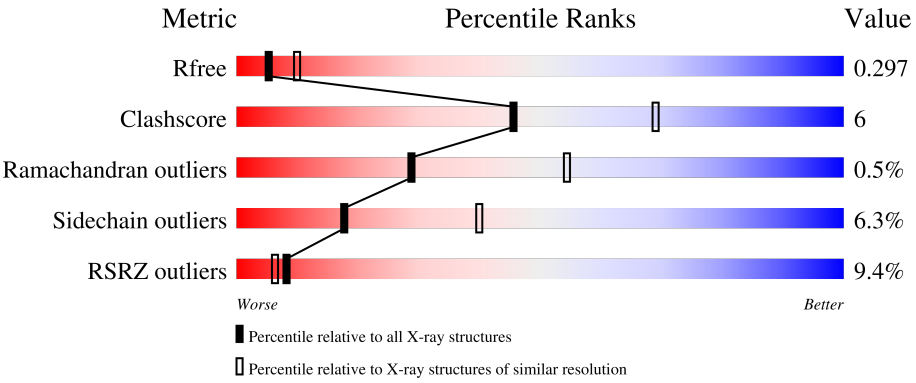
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.70 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}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	533	11% 79% 15% • 5%
1	B	533	6% 77% 16% • 5%

2 Entry composition (i)

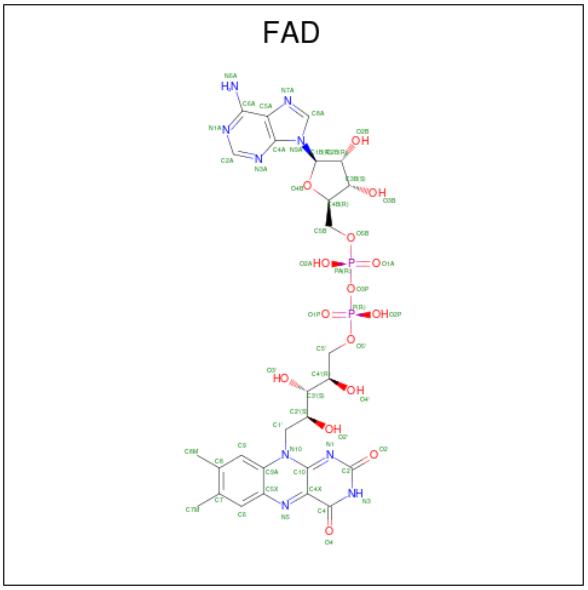
There are 7 unique types of molecules in this entry. The entry contains 8329 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Ancestral Flavin-containing monooxygenase 5.

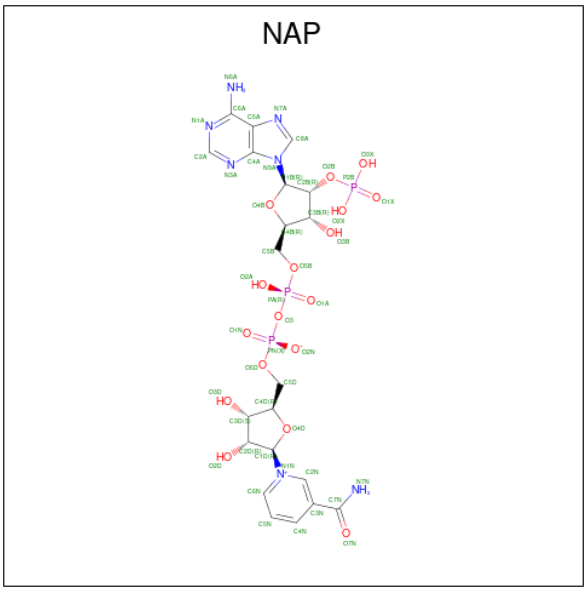
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	504	Total	C	N	O	S	0	0	0
			4010	2568	680	740	22			
1	B	504	Total	C	N	O	S	0	0	0
			4010	2568	680	740	22			

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



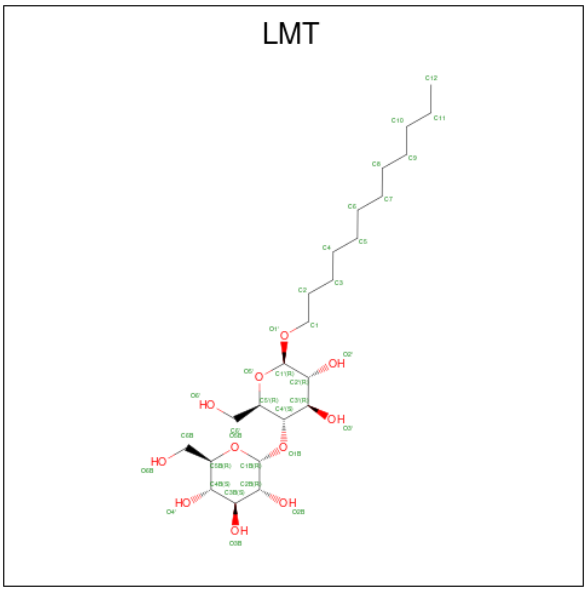
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



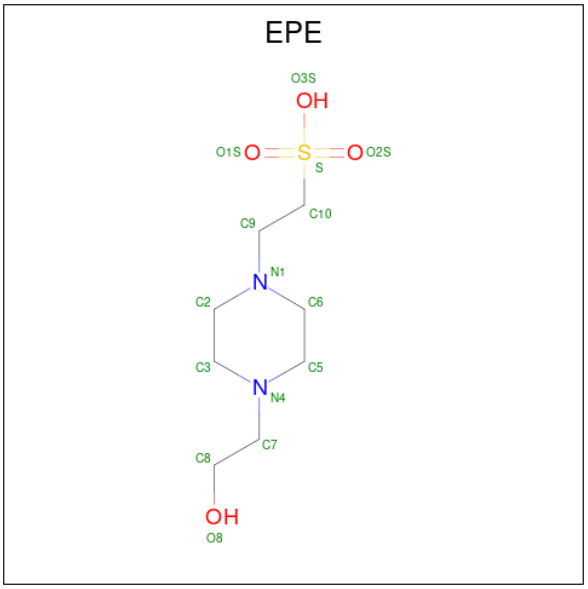
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 4 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



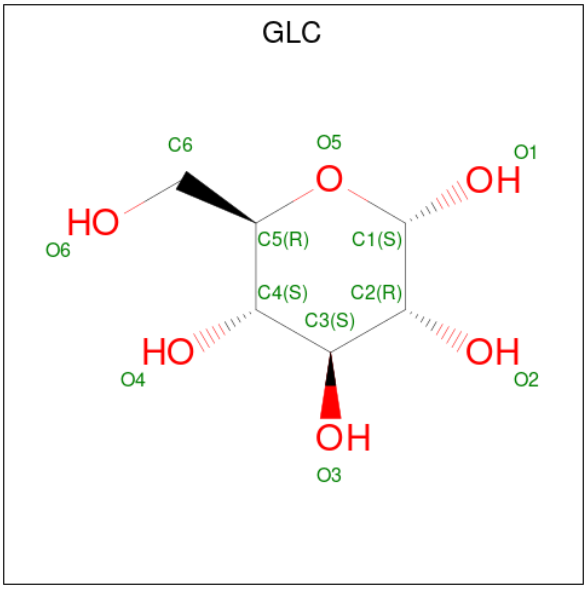
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			26	15	11		

- Molecule 5 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: $C_8H_{18}N_2O_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
5	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 6 is alpha-D-glucopyranose (three-letter code: GLC) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 12 6 6	0	0
6	A	1	Total C O 12 6 6	0	0

- Molecule 7 is water.

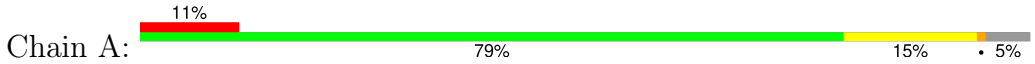
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	17	Total O 17 17	0	0
7	B	10	Total O 10 10	0	0

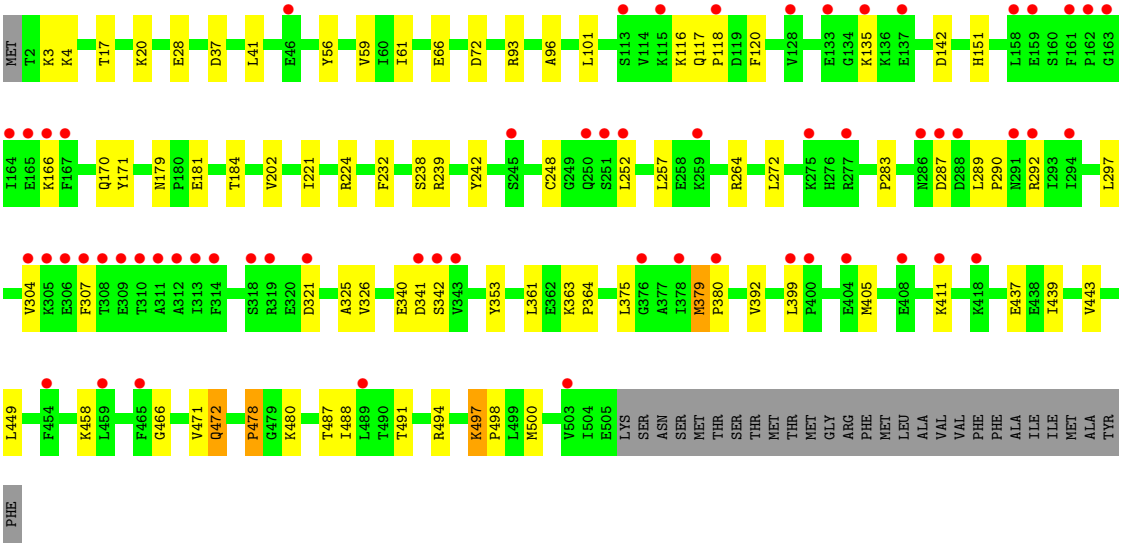
3 Residue-property plots (i)

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: Ancestral Flavin-containing monooxygenase 5

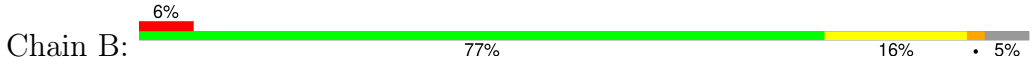
Chain A:

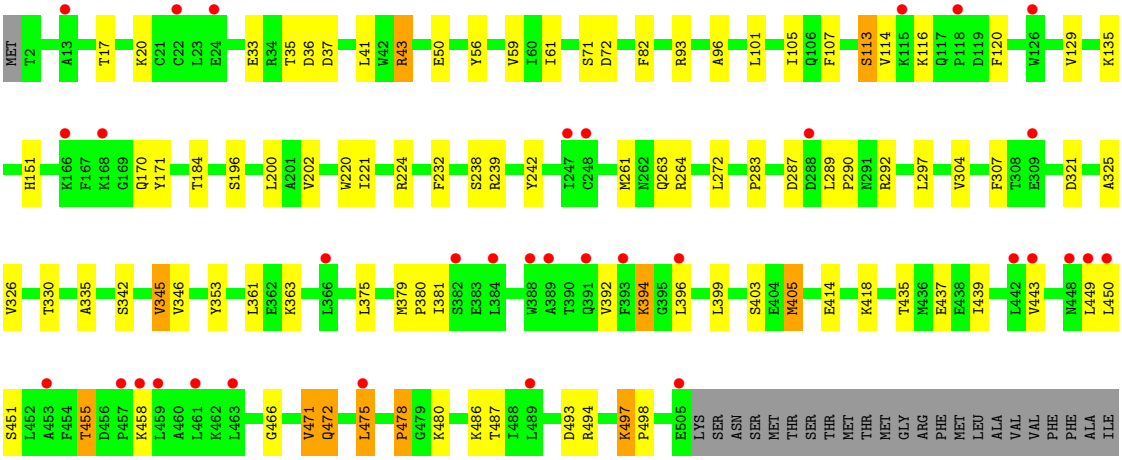




• Molecule 1: Ancestral Flavin-containing monooxygenase 5

Chain B:






ILE
MET
ALA
TYR
PHE

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α, β, γ	96.78Å 100.07Å 143.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.00 – 2.70 49.89 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.00-2.70) 99.8 (49.89-2.70)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.33 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, R_{free}	0.222 , 0.295 0.227 , 0.297	Depositor DCC
R_{free} test set	1964 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	74.0	Xtriage
Anisotropy	0.205	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 38.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.014 for k,h,-l	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	8329	wwPDB-VP
Average B, all atoms (Å^2)	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.51% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EPE, LMT, FAD, NAP, GLC

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	0.68	0/4104	0.84	0/5539
1	B	0.69	0/4104	0.86	0/5539
All	All	0.69	0/8208	0.85	0/11078

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4010	0	4007	44	0
1	B	4010	0	4007	57	0
2	A	53	0	31	7	0
2	B	53	0	31	10	0
3	A	48	0	25	3	0
3	B	48	0	25	5	0
4	A	26	0	25	0	0
5	A	15	0	18	1	0
5	B	15	0	18	0	0
6	A	24	0	24	0	0
7	A	17	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	10	0	0	0	0
All	All	8329	0	8211	106	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 6.

All (106) 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:A:488:ILE:O	1:A:491:THR:HG22	1.91	0.69
2:A:601:FAD:C6	3:A:602:NAP:C2N	2.74	0.66
1:B:151:HIS:CD2	2:B:601:FAD:H1'1	2.31	0.65
1:A:20:LYS:NZ	1:A:72:ASP:OD2	2.30	0.65
1:B:335:ALA:HA	1:B:345:VAL:HG21	1.78	0.64
1:B:399:LEU:HD13	1:B:405:MET:HE1	1.78	0.64
1:A:399:LEU:HD13	1:A:405:MET:HE1	1.77	0.64
1:B:221:ILE:HD12	1:B:272:LEU:HD13	1.79	0.64
1:B:394:LYS:HB2	1:B:396:LEU:HD23	1.80	0.63
1:B:239:ARG:HE	1:B:472:GLN:NE2	1.98	0.62
1:A:239:ARG:HE	1:A:472:GLN:NE2	1.98	0.61
2:B:601:FAD:C6	3:B:602:NAP:C2N	2.79	0.60
1:B:396:LEU:HD22	1:B:396:LEU:N	2.16	0.59
1:A:171:TYR:HA	1:A:326:VAL:O	2.03	0.59
1:B:20:LYS:NZ	1:B:72:ASP:OD2	2.35	0.59
1:B:41:LEU:HD11	2:B:601:FAD:C8M	2.33	0.58
1:A:399:LEU:HD13	1:A:405:MET:CE	2.33	0.58
1:B:33:GLU:OE1	2:B:601:FAD:O3B	2.20	0.58
1:B:71:SER:O	1:B:471:VAL:HG12	2.04	0.58
1:B:151:HIS:HD2	2:B:601:FAD:H1'1	1.67	0.57
1:B:171:TYR:HA	1:B:326:VAL:O	2.03	0.57
2:A:601:FAD:HM73	3:A:602:NAP:C5N	2.34	0.57
1:A:151:HIS:CD2	2:A:601:FAD:H1'1	2.40	0.56
1:B:399:LEU:HD13	1:B:405:MET:CE	2.36	0.56
1:A:487:THR:O	1:A:494:ARG:NH2	2.39	0.55
1:A:4:LYS:HG2	1:A:142:ASP:CB	2.37	0.54
1:A:221:ILE:HD12	1:A:272:LEU:HD13	1.88	0.54
1:A:239:ARG:HE	1:A:472:GLN:HE21	1.54	0.53
1:B:487:THR:O	1:B:494:ARG:NH2	2.42	0.53
1:A:116:LYS:HB2	1:A:120:PHE:CG	2.44	0.53
1:A:4:LYS:HG2	1:A:142:ASP:HB3	1.90	0.52
1:B:396:LEU:N	1:B:396:LEU:CD2	2.72	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:353:TYR:HB3	1:A:405:MET:HE2	1.91	0.52
1:B:239:ARG:HE	1:B:472:GLN:HE21	1.56	0.52
1:B:439:ILE:O	1:B:443:VAL:HG23	2.10	0.51
1:A:353:TYR:CG	1:A:405:MET:HG2	2.45	0.51
2:B:601:FAD:HM73	3:B:602:NAP:C5N	2.40	0.51
1:A:96:ALA:HA	1:A:101:LEU:HD12	1.92	0.50
1:A:283:PRO:HD3	1:A:375:LEU:HD22	1.94	0.50
1:B:304:VAL:HG11	1:B:307:PHE:CZ	2.47	0.49
1:B:116:LYS:HB2	1:B:120:PHE:CG	2.48	0.49
1:B:396:LEU:CD2	1:B:396:LEU:H	2.25	0.49
1:B:35:THR:HG22	1:B:36:ASP:H	1.77	0.49
1:A:439:ILE:O	1:A:443:VAL:HG23	2.14	0.48
1:B:105:ILE:HG21	1:B:107:PHE:CE1	2.47	0.48
1:B:239:ARG:HH12	1:B:437:GLU:CD	2.17	0.48
1:B:353:TYR:CG	1:B:405:MET:HG2	2.48	0.48
1:B:82:PHE:CD1	1:B:224:ARG:HD2	2.49	0.48
1:B:96:ALA:HA	1:B:101:LEU:HD12	1.96	0.48
1:A:283:PRO:CD	1:A:375:LEU:HD22	2.44	0.48
1:A:304:VAL:HG11	1:A:307:PHE:CZ	2.48	0.48
1:A:66:GLU:OE1	1:A:494:ARG:NH1	2.47	0.47
1:B:239:ARG:O	1:B:242:TYR:HB3	2.15	0.47
1:A:170:GLN:O	1:A:325:ALA:HA	2.14	0.47
1:A:151:HIS:HD2	2:A:601:FAD:H1'1	1.80	0.47
1:B:41:LEU:HD11	2:B:601:FAD:HM81	1.97	0.47
1:B:82:PHE:CZ	1:B:224:ARG:HB3	2.50	0.46
1:A:117:GLN:HB3	1:A:118:PRO:HD2	1.97	0.46
1:B:497:LYS:N	1:B:498:PRO:CD	2.78	0.46
1:A:41:LEU:HD11	2:A:601:FAD:C8M	2.45	0.46
1:A:497:LYS:N	1:A:498:PRO:CD	2.79	0.46
1:B:61:ILE:HG13	2:B:601:FAD:O4	2.15	0.46
1:B:353:TYR:HB3	1:B:405:MET:HE2	1.98	0.46
1:A:364:PRO:HB3	1:A:399:LEU:HD12	1.98	0.46
1:B:170:GLN:O	1:B:325:ALA:HA	2.16	0.45
1:A:379:MET:N	1:A:380:PRO:HD2	2.32	0.45
1:A:61:ILE:HG13	2:A:601:FAD:O4	2.16	0.45
1:B:379:MET:N	1:B:380:PRO:HD2	2.32	0.44
1:A:37:ASP:OD2	1:A:93:ARG:NH2	2.50	0.44
2:A:601:FAD:H6	3:A:602:NAP:C3N	2.48	0.44
1:A:257:LEU:HD11	5:A:604:EPE:H82	2.00	0.44
1:A:239:ARG:HH21	1:A:472:GLN:HE21	1.65	0.44
1:B:238:SER:HB2	1:B:466:GLY:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:113:SER:HB3	1:B:129:VAL:CG1	2.48	0.43
1:A:292:ARG:NH2	1:A:297:LEU:HD13	2.34	0.43
1:A:471:VAL:HG11	1:A:487:THR:OG1	2.19	0.43
1:B:239:ARG:HH21	1:B:472:GLN:HE21	1.66	0.43
1:B:82:PHE:CE2	1:B:224:ARG:HB3	2.54	0.43
1:B:283:PRO:HD3	1:B:375:LEU:HD22	2.00	0.43
1:A:353:TYR:CB	1:A:405:MET:HE2	2.48	0.43
1:B:56:TYR:CE2	1:B:59:VAL:HG22	2.54	0.43
1:B:330:THR:HA	3:B:602:NAP:O4B	2.19	0.43
1:A:248:CYS:HB3	1:A:252:LEU:HD23	1.99	0.42
1:B:381:ILE:HD12	1:B:435:THR:HG21	2.02	0.42
1:B:35:THR:HG21	1:B:43:ARG:HH12	1.83	0.42
1:A:135:LYS:O	1:A:135:LYS:CG	2.67	0.42
1:A:238:SER:HB2	1:A:466:GLY:O	2.19	0.42
1:B:41:LEU:HD13	2:B:601:FAD:H2'	2.02	0.42
1:B:61:ILE:CG1	2:B:601:FAD:O4	2.68	0.42
1:B:151:HIS:CE1	3:B:602:NAP:H4D	2.55	0.42
1:A:361:LEU:HB3	1:A:363:LYS:O	2.20	0.41
1:B:475:LEU:HD12	1:B:475:LEU:HA	1.87	0.41
1:A:239:ARG:HH12	1:A:437:GLU:CD	2.23	0.41
1:A:500:MET:O	1:A:500:MET:HG3	2.20	0.41
1:A:289:LEU:N	1:A:290:PRO:CD	2.82	0.41
1:A:239:ARG:O	1:A:242:TYR:HB3	2.21	0.41
1:B:379:MET:HB2	1:B:380:PRO:HD3	2.01	0.41
1:B:292:ARG:NH2	1:B:297:LEU:HD13	2.35	0.41
1:B:220:TRP:HB3	1:B:261:MET:CE	2.51	0.41
1:A:56:TYR:CE2	1:A:59:VAL:HG22	2.55	0.41
1:B:56:TYR:HH	3:B:602:NAP:H4N	1.86	0.41
1:B:361:LEU:HB3	1:B:363:LYS:O	2.20	0.41
1:B:196:SER:O	1:B:200:LEU:HG	2.21	0.40
1:B:289:LEU:N	1:B:290:PRO:CD	2.84	0.40
1:B:451:SER:O	1:B:455:THR:HG23	2.21	0.40
1:B:37:ASP:OD2	1:B:93:ARG:NH2	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	502/533 (94%)	477 (95%)	23 (5%)	2 (0%)	34	60
1	B	502/533 (94%)	478 (95%)	21 (4%)	3 (1%)	25	50
All	All	1004/1066 (94%)	955 (95%)	44 (4%)	5 (0%)	29	54

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	480	LYS
1	B	480	LYS
1	B	394	LYS
1	A	478	PRO
1	B	478	PRO

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	441/466 (95%)	417 (95%)	24 (5%)	22	47
1	B	441/466 (95%)	409 (93%)	32 (7%)	14	33
All	All	882/932 (95%)	826 (94%)	56 (6%)	18	40

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LYS

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Mol	Chain	Res	Type
1	A	17	THR
1	A	28	GLU
1	A	166	LYS
1	A	179	ASN
1	A	181	GLU
1	A	184	THR
1	A	202	VAL
1	A	224	ARG
1	A	232	PHE
1	A	264	ARG
1	A	287	ASP
1	A	321	ASP
1	A	340	GLU
1	A	341	ASP
1	A	342	SER
1	A	379	MET
1	A	392	VAL
1	A	411	LYS
1	A	449	LEU
1	A	458	LYS
1	A	472	GLN
1	A	478	PRO
1	A	497	LYS
1	B	17	THR
1	B	43	ARG
1	B	50	GLU
1	B	113	SER
1	B	114	VAL
1	B	135	LYS
1	B	184	THR
1	B	202	VAL
1	B	232	PHE
1	B	263	GLN
1	B	264	ARG
1	B	287	ASP
1	B	321	ASP
1	B	342	SER
1	B	345	VAL
1	B	346	VAL
1	B	392	VAL
1	B	403	SER
1	B	405	MET

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Mol	Chain	Res	Type
1	B	414	GLU
1	B	418	LYS
1	B	449	LEU
1	B	450	LEU
1	B	455	THR
1	B	458	LYS
1	B	471	VAL
1	B	472	GLN
1	B	475	LEU
1	B	478	PRO
1	B	486	LYS
1	B	493	ASP
1	B	497	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	117	GLN
1	A	151	HIS
1	A	153	ASN
1	A	179	ASN
1	A	424	GLN
1	A	429	GLN
1	A	472	GLN
1	B	117	GLN
1	B	151	HIS
1	B	424	GLN
1	B	429	GLN
1	B	472	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

9 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NAP	A	602	-	46,52,52	1.01	3 (6%)	61,80,80	1.39	8 (13%)
2	FAD	A	601	-	54,58,58	0.84	2 (3%)	71,89,89	0.86	3 (4%)
5	EPE	A	604	-	15,15,15	2.44	1 (6%)	19,20,20	1.53	5 (26%)
6	GLC	A	606	-	12,12,12	0.87	0	17,17,17	1.17	2 (11%)
5	EPE	B	603	-	15,15,15	2.18	1 (6%)	19,20,20	1.46	2 (10%)
4	LMT	A	603	-	27,27,36	1.15	1 (3%)	38,38,47	1.61	10 (26%)
2	FAD	B	601	-	54,58,58	0.70	1 (1%)	71,89,89	0.94	5 (7%)
3	NAP	B	602	-	46,52,52	1.45	4 (8%)	61,80,80	1.69	15 (24%)
6	GLC	A	605	-	12,12,12	1.28	1 (8%)	17,17,17	1.26	3 (17%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAP	A	602	-	-	11/31/67/67	0/5/5/5
2	FAD	A	601	-	-	10/30/50/50	0/6/6/6
5	EPE	A	604	-	-	2/9/19/19	0/1/1/1
6	GLC	A	606	-	-	2/2/22/22	0/1/1/1
5	EPE	B	603	-	-	6/9/19/19	0/1/1/1
4	LMT	A	603	-	-	9/12/52/61	0/2/2/2
2	FAD	B	601	-	-	5/30/50/50	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAP	B	602	-	-	4/31/67/67	0/5/5/5
6	GLC	A	605	-	-	2/2/22/22	0/1/1/1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	604	EPE	C10-S	-8.61	1.65	1.77
5	B	603	EPE	C10-S	-7.71	1.66	1.77
3	B	602	NAP	PA-O3	5.19	1.65	1.59
3	B	602	NAP	PN-O3	4.17	1.64	1.59
3	B	602	NAP	O4D-C1D	3.90	1.46	1.40
4	A	603	LMT	O1'-C1'	3.80	1.46	1.40
2	A	601	FAD	P-O3P	3.44	1.63	1.59
3	B	602	NAP	O4B-C1B	2.94	1.44	1.40
3	A	602	NAP	C2A-N3A	2.81	1.36	1.32
3	A	602	NAP	O4D-C1D	2.70	1.44	1.40
3	A	602	NAP	P2B-O2B	2.42	1.63	1.59
6	A	605	GLC	C1-C2	2.09	1.57	1.52
2	A	601	FAD	PA-O3P	2.07	1.61	1.59
2	B	601	FAD	P-O3P	2.05	1.61	1.59

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	602	NAP	N3A-C2A-N1A	-5.60	121.07	128.67
3	A	602	NAP	N3A-C2A-N1A	-4.00	123.24	128.67
5	A	604	EPE	C6-N1-C2	3.64	116.69	108.84
3	A	602	NAP	N6A-C6A-N1A	3.56	125.95	118.33
5	B	603	EPE	O1S-S-C10	3.21	111.58	106.73
3	B	602	NAP	C6N-N1N-C2N	-3.16	119.19	121.88
4	A	603	LMT	O1'-C1'-C2'	3.14	113.04	108.27
3	A	602	NAP	C5A-C6A-N6A	-3.12	115.55	120.31
5	B	603	EPE	C6-N1-C2	3.11	115.55	108.84
3	B	602	NAP	C5A-C6A-N6A	-3.07	115.63	120.31
3	B	602	NAP	C4B-O4B-C1B	-3.05	107.14	109.92
3	B	602	NAP	C4D-O4D-C1D	-3.05	107.14	109.92
3	A	602	NAP	C2D-C3D-C4D	3.03	108.47	102.61
3	B	602	NAP	O3-PA-O1A	-2.93	101.88	110.70
3	B	602	NAP	C5N-C4N-C3N	-2.86	117.55	120.36
4	A	603	LMT	O5B-C1B-C2B	2.85	116.23	110.37
4	A	603	LMT	C3'-C4'-C5'	2.83	117.20	110.93
5	A	604	EPE	O1S-S-C10	2.69	110.79	106.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	602	NAP	N6A-C6A-N1A	2.59	123.87	118.33
3	B	602	NAP	O5D-PN-O1N	2.52	118.94	108.94
3	A	602	NAP	O3-PA-O1A	-2.52	103.12	110.70
3	B	602	NAP	O4B-C1B-N9A	2.51	112.08	108.75
4	A	603	LMT	C2'-C3'-C4'	2.51	115.38	109.68
4	A	603	LMT	O5'-C1'-C2'	-2.51	105.21	110.37
4	A	603	LMT	O4'-C4B-C3B	-2.48	104.54	110.38
4	A	603	LMT	C1-O1'-C1'	2.42	117.81	113.68
3	A	602	NAP	O7N-C7N-C3N	-2.42	116.64	119.60
2	B	601	FAD	C4'-C3'-C2'	2.38	117.54	113.57
6	A	605	GLC	C1-C2-C3	2.36	115.17	110.36
3	B	602	NAP	C2N-C3N-C4N	2.36	121.00	118.26
2	A	601	FAD	O2P-P-O3P	2.30	113.50	107.27
4	A	603	LMT	O5B-C5B-C4B	2.29	113.82	109.70
2	B	601	FAD	C5A-C6A-N6A	2.29	123.80	120.31
3	B	602	NAP	C3N-C7N-N7N	2.27	120.53	117.74
2	B	601	FAD	O2P-P-O1P	2.27	122.99	112.44
2	B	601	FAD	C4-N3-C2	-2.23	121.68	125.64
6	A	606	GLC	O5-C5-C6	2.21	111.92	106.44
2	A	601	FAD	C5A-C6A-N6A	2.19	123.65	120.31
3	A	602	NAP	O2A-PA-O1A	2.15	122.46	112.44
4	A	603	LMT	C3B-C4B-C5B	2.14	114.11	110.23
3	B	602	NAP	O3D-C3D-C2D	-2.12	105.03	111.82
3	A	602	NAP	O2B-C2B-C1B	2.10	117.45	110.05
6	A	606	GLC	O5-C5-C4	-2.10	105.92	109.70
6	A	605	GLC	C1-O5-C5	2.10	117.71	113.65
2	A	601	FAD	C4-N3-C2	-2.09	121.93	125.64
5	A	604	EPE	C6-C5-N4	2.09	114.86	110.65
3	B	602	NAP	O2A-PA-O3	2.08	112.89	107.27
3	B	602	NAP	O3X-P2B-O2X	2.04	115.46	107.80
5	A	604	EPE	C8-C7-N4	2.03	120.55	113.44
5	A	604	EPE	O3S-S-C10	2.02	109.95	106.00
4	A	603	LMT	C4B-C3B-C2B	2.02	114.37	110.83
2	B	601	FAD	C4X-C4-N3	2.01	118.36	113.25
6	A	605	GLC	O5-C5-C6	2.01	111.41	106.44

There are no chirality outliers.

All (51) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	FAD	N10-C1'-C2'-O2'
2	A	601	FAD	N10-C1'-C2'-C3'

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Mol	Chain	Res	Type	Atoms
2	A	601	FAD	C2'-C3'-C4'-O4'
2	A	601	FAD	C2'-C3'-C4'-C5'
2	A	601	FAD	O3'-C3'-C4'-O4'
2	A	601	FAD	O3'-C3'-C4'-C5'
2	A	601	FAD	C5'-O5'-P-O2P
2	A	601	FAD	C5'-O5'-P-O3P
2	B	601	FAD	C5B-O5B-PA-O1A
3	A	602	NAP	C5B-O5B-PA-O1A
3	A	602	NAP	C5B-O5B-PA-O2A
3	A	602	NAP	C5B-O5B-PA-O3
3	A	602	NAP	C5D-O5D-PN-O3
3	A	602	NAP	C5D-O5D-PN-O1N
3	A	602	NAP	C5D-O5D-PN-O2N
5	A	604	EPE	C8-C7-N4-C3
5	A	604	EPE	N4-C7-C8-O8
5	B	603	EPE	C9-C10-S-O1S
5	B	603	EPE	C9-C10-S-O2S
4	A	603	LMT	O5B-C1B-O1B-C4'
4	A	603	LMT	O5'-C5'-C6'-O6'
6	A	606	GLC	C4-C5-C6-O6
3	A	602	NAP	O4D-C4D-C5D-O5D
4	A	603	LMT	O5'-C1'-O1'-C1
4	A	603	LMT	C4'-C5'-C6'-O6'
4	A	603	LMT	C2'-C1'-O1'-C1
6	A	606	GLC	O5-C5-C6-O6
4	A	603	LMT	C2B-C1B-O1B-C4'
3	A	602	NAP	O4B-C4B-C5B-O5B
4	A	603	LMT	O1'-C1-C2-C3
5	B	603	EPE	C9-C10-S-O3S
3	A	602	NAP	C3B-C4B-C5B-O5B
4	A	603	LMT	O5B-C5B-C6B-O6B
2	B	601	FAD	O4B-C4B-C5B-O5B
2	B	601	FAD	C3B-C4B-C5B-O5B
3	A	602	NAP	C3D-C4D-C5D-O5D
3	B	602	NAP	O4D-C4D-C5D-O5D
5	B	603	EPE	C10-C9-N1-C6
5	B	603	EPE	C8-C7-N4-C3
6	A	605	GLC	C4-C5-C6-O6
4	A	603	LMT	C4B-C5B-C6B-O6B
3	A	602	NAP	PN-O3-PA-O5B
3	B	602	NAP	C3D-C4D-C5D-O5D
2	A	601	FAD	C5'-O5'-P-O1P

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Mol	Chain	Res	Type	Atoms
2	B	601	FAD	C5B-O5B-PA-O2A
2	B	601	FAD	C5B-O5B-PA-O3P
5	B	603	EPE	C10-C9-N1-C2
6	A	605	GLC	O5-C5-C6-O6
2	A	601	FAD	O4B-C4B-C5B-O5B
3	B	602	NAP	C2B-O2B-P2B-O1X
3	B	602	NAP	C4N-C3N-C7N-N7N

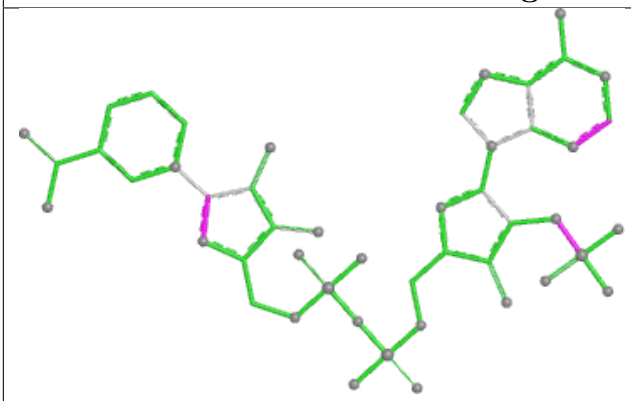
There are no ring outliers.

5 monomers are involved in 21 short contacts:

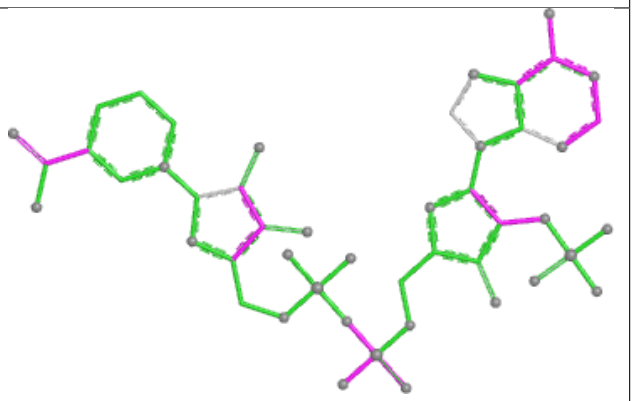
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	602	NAP	3	0
2	A	601	FAD	7	0
5	A	604	EPE	1	0
2	B	601	FAD	10	0
3	B	602	NAP	5	0

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.

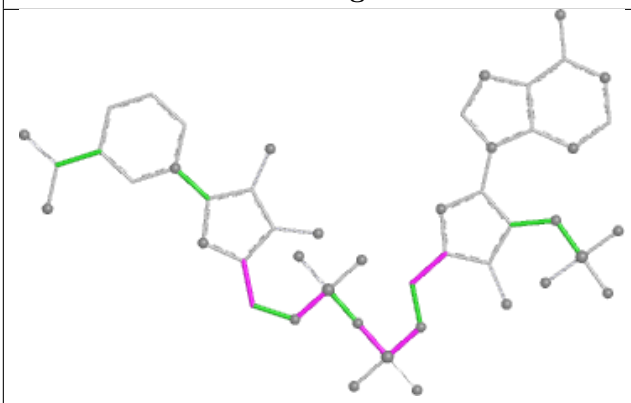
Ligand NAP A 602



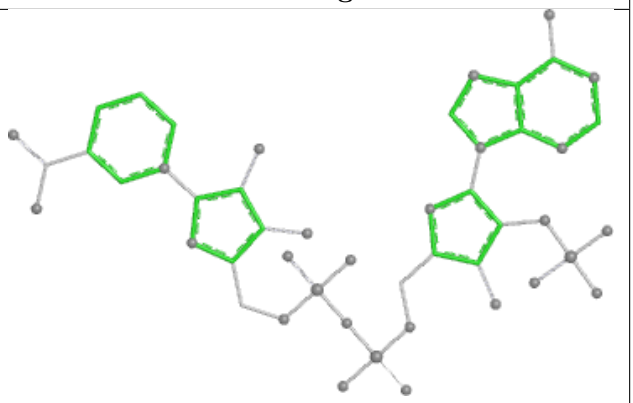
Bond lengths



Bond angles

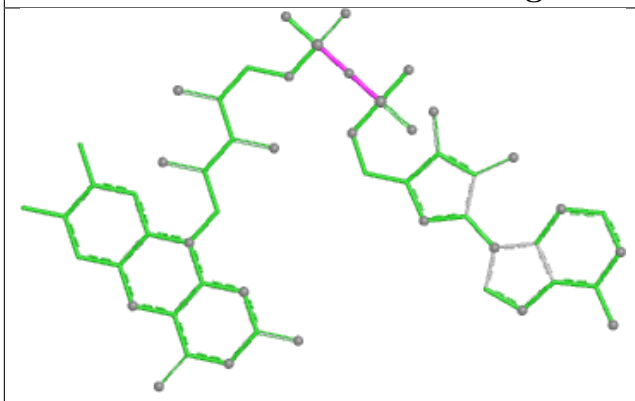


Torsions



Rings

Ligand FAD A 601



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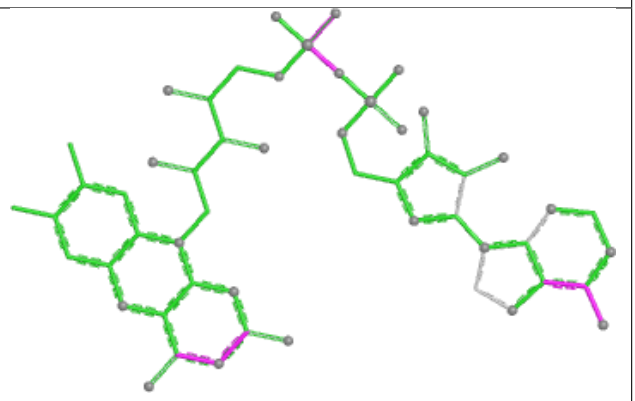
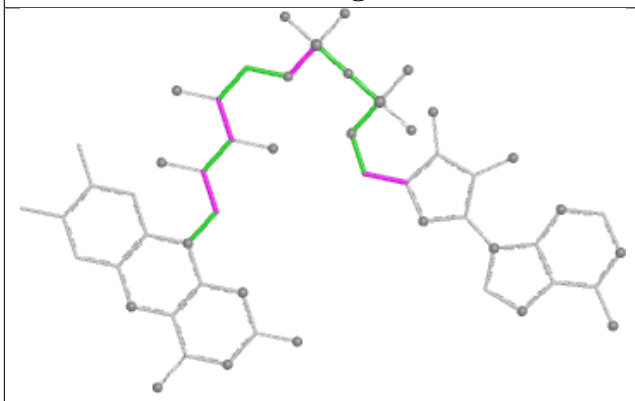


Bond angles



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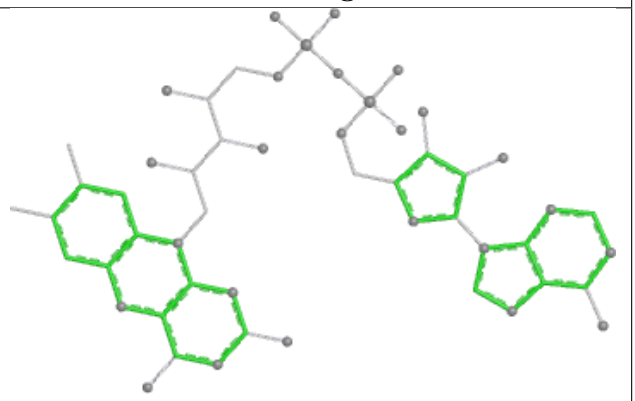
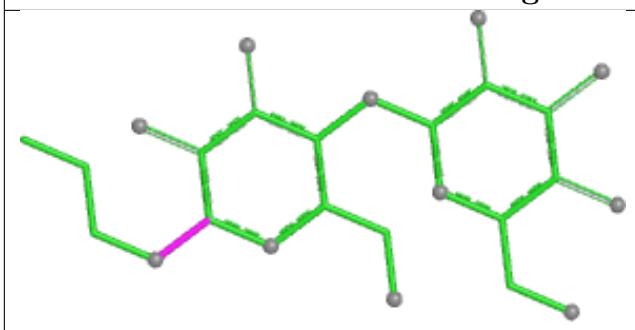
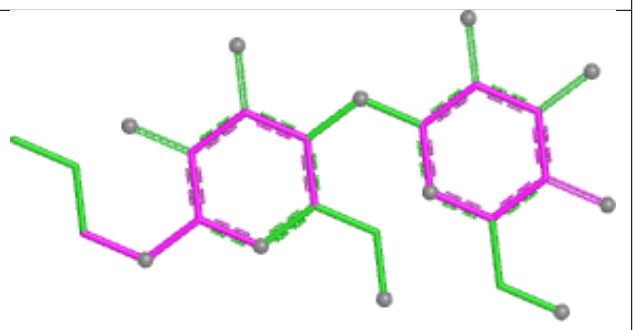


Rings

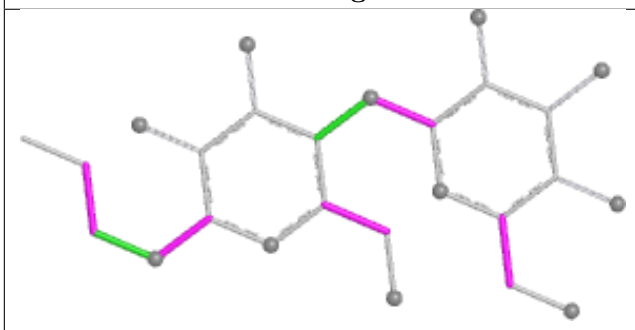
Ligand LMT A 603



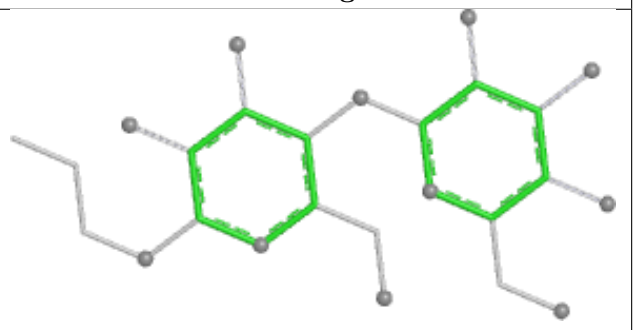
Bond lengths



Bond angles

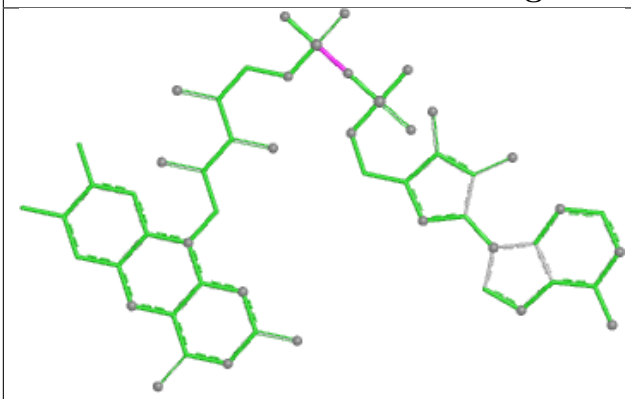


Torsions

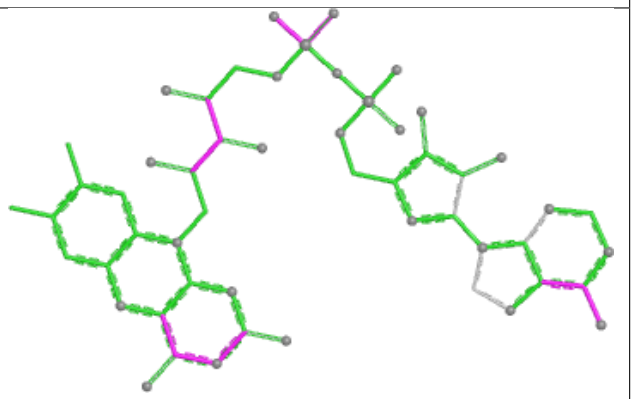


Rings

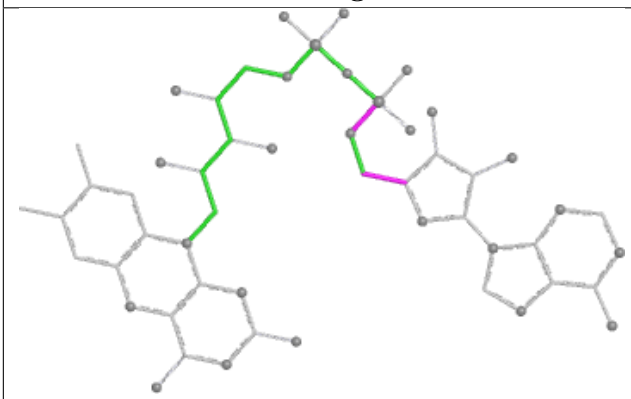
Ligand FAD B 601



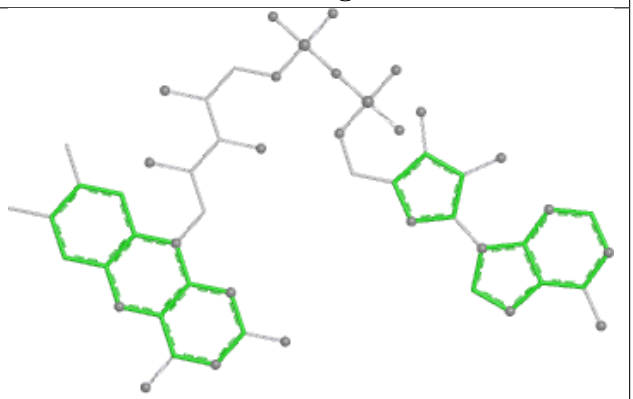
Bond lengths



Bond angles

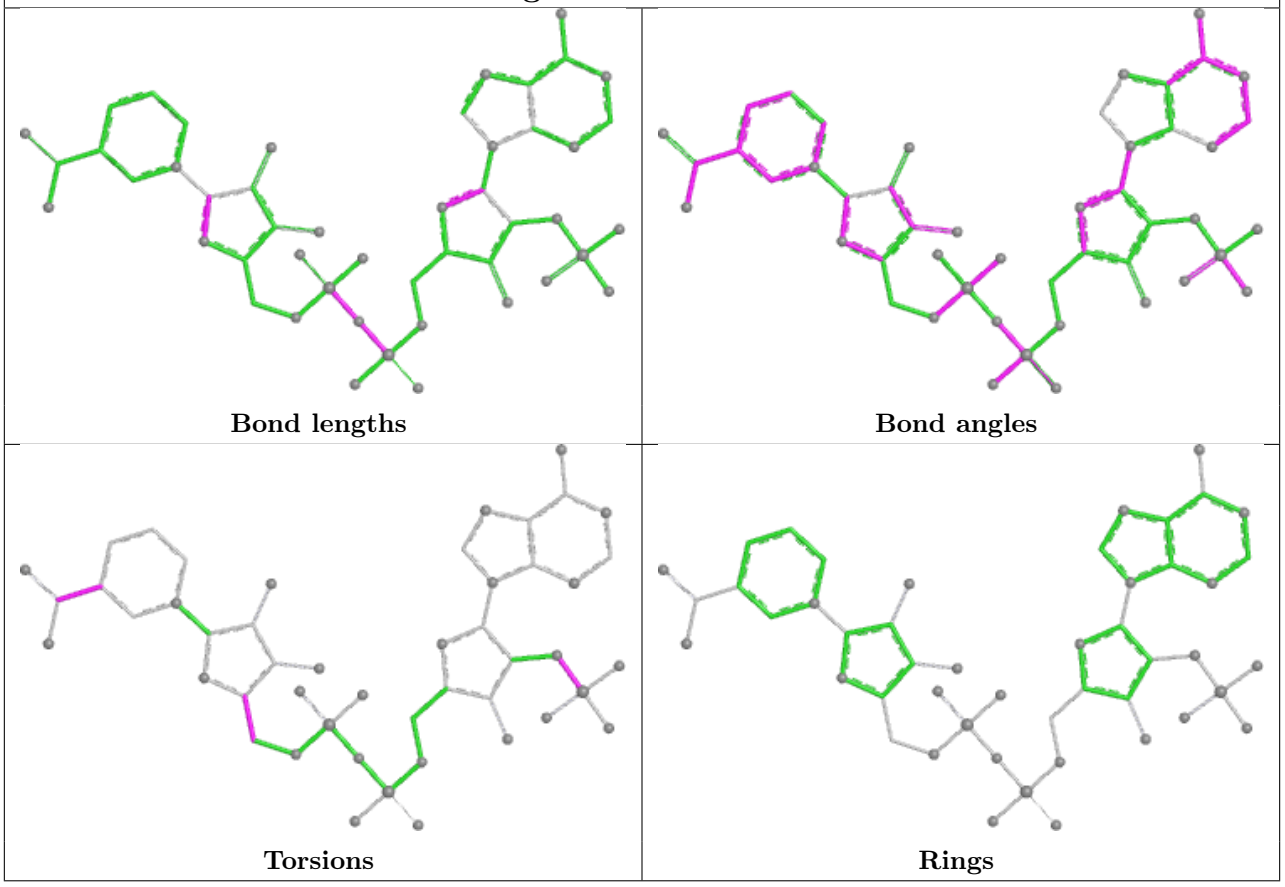


Torsions



Rings

Ligand NAP B 602



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{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	504/533 (94%)	0.54	61 (12%) 4 3	59, 83, 114, 132	0
1	B	504/533 (94%)	0.25	34 (6%) 17 16	61, 93, 122, 150	0
All	All	1008/1066 (94%)	0.39	95 (9%) 8 6	59, 87, 119, 150	0

All (95) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	505	GLU	8.2
1	A	307	PHE	8.1
1	A	312	ALA	7.4
1	A	164	ILE	6.3
1	B	449	LEU	6.0
1	A	400	PRO	6.0
1	A	311	ALA	5.5
1	A	399	LEU	5.3
1	A	308	THR	5.2
1	A	313	ILE	5.1
1	B	382	SER	5.0
1	A	163	GLY	5.0
1	B	166	LYS	4.9
1	B	248	CYS	4.6
1	A	133	GLU	4.4
1	B	247	ILE	4.4
1	A	319	ARG	4.3
1	B	391	GLN	4.3
1	A	306	GLU	4.2
1	B	458	LYS	4.0
1	B	384	LEU	3.9
1	A	287	ASP	3.9
1	B	489	LEU	3.8
1	A	286	ASN	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	393	PHE	3.7
1	A	162	PRO	3.6
1	A	166	LYS	3.5
1	A	251	SER	3.4
1	B	396	LEU	3.3
1	A	454	PHE	3.2
1	B	459	LEU	3.2
1	A	314	PHE	3.1
1	B	309	GLU	3.1
1	A	250	GLN	3.0
1	A	115	LYS	2.9
1	B	461	LEU	2.9
1	A	304	VAL	2.9
1	A	341	ASP	2.9
1	A	277	ARG	2.9
1	A	378	ILE	2.9
1	A	321	ASP	2.9
1	A	161	PHE	2.8
1	B	118	PRO	2.8
1	A	291	ASN	2.8
1	B	389	ALA	2.7
1	A	318	SER	2.7
1	B	24	GLU	2.7
1	A	288	ASP	2.7
1	B	288	ASP	2.7
1	A	275	LYS	2.6
1	A	309	GLU	2.6
1	A	408	GLU	2.5
1	B	475	LEU	2.5
1	A	465	PHE	2.5
1	A	418	LYS	2.5
1	A	459	LEU	2.5
1	A	259	LYS	2.5
1	B	115	LYS	2.5
1	A	411	LYS	2.4
1	A	503	VAL	2.4
1	B	450	LEU	2.4
1	A	128	VAL	2.4
1	A	165	GLU	2.4
1	B	126	TRP	2.4
1	B	168	LYS	2.3
1	B	13	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	388	TRP	2.3
1	A	113	SER	2.3
1	B	442	LEU	2.3
1	A	342	SER	2.3
1	A	380	PRO	2.3
1	B	457	PRO	2.3
1	A	292	ARG	2.3
1	A	376	GLY	2.3
1	A	158	LEU	2.3
1	B	448	ASN	2.3
1	A	135	LYS	2.3
1	A	137	GLU	2.2
1	A	118	PRO	2.2
1	B	453	ALA	2.2
1	A	294	ILE	2.2
1	A	252	LEU	2.2
1	A	245	SER	2.1
1	A	305	LYS	2.1
1	A	310	THR	2.1
1	A	343	VAL	2.1
1	B	463	LEU	2.1
1	A	159	GLU	2.1
1	A	489	LEU	2.1
1	A	46	GLU	2.1
1	A	167	PHE	2.1
1	B	443	VAL	2.0
1	B	366	LEU	2.0
1	B	22	CYS	2.0
1	A	404	GLU	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

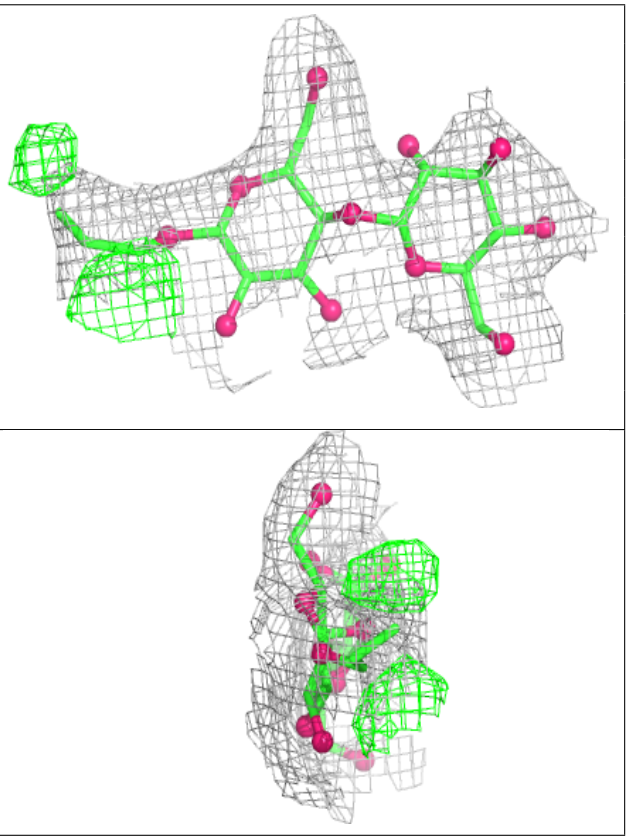
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
4	LMT	A	603	26/35	0.63	0.19	105,146,169,176	0
6	GLC	A	606	12/12	0.68	0.36	111,131,145,153	0
6	GLC	A	605	12/12	0.77	0.22	107,121,135,138	0
5	EPE	A	604	15/15	0.80	0.45	68,99,158,165	0
5	EPE	B	603	15/15	0.87	0.17	100,121,145,147	0
2	FAD	A	601	53/53	0.93	0.17	67,83,121,126	0
3	NAP	A	602	48/48	0.94	0.20	63,74,83,85	0
2	FAD	B	601	53/53	0.94	0.17	72,99,147,161	0
3	NAP	B	602	48/48	0.97	0.14	57,73,91,101	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.

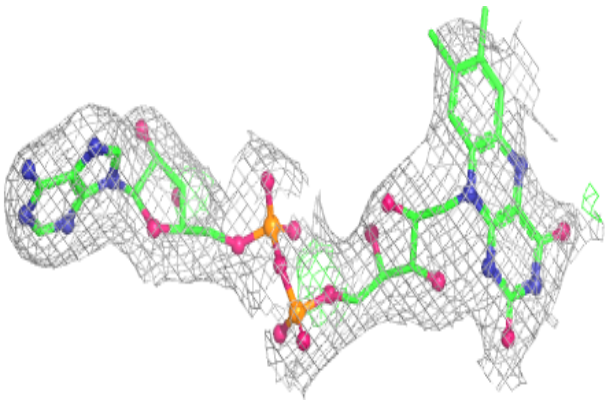
Electron density around LMT A 603:

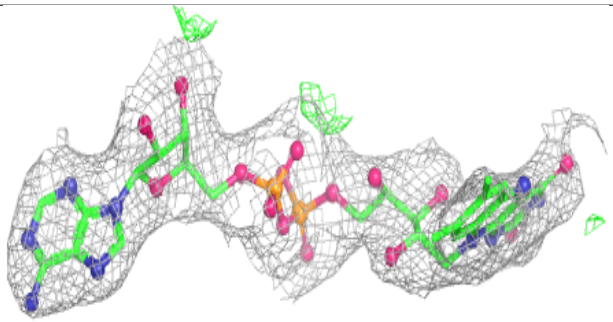
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

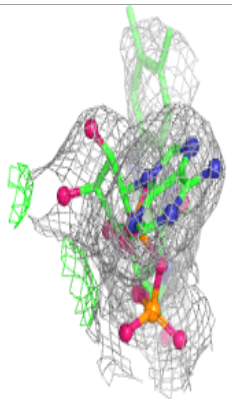


Electron density around FAD A 601:

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

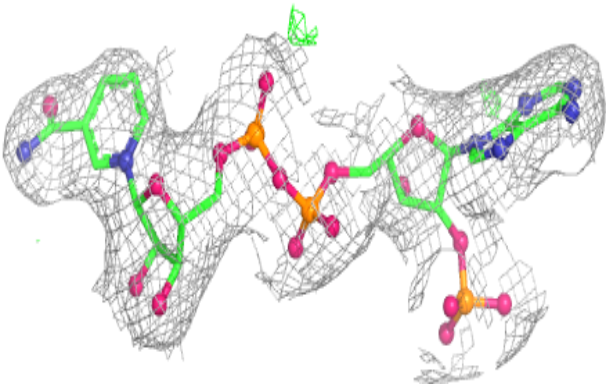


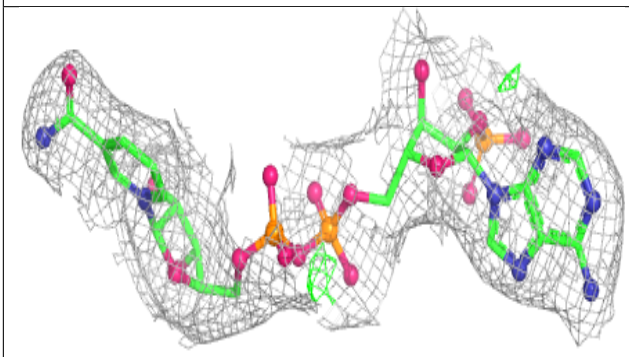


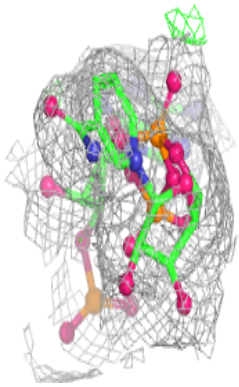


Electron density around NAP A 602:

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

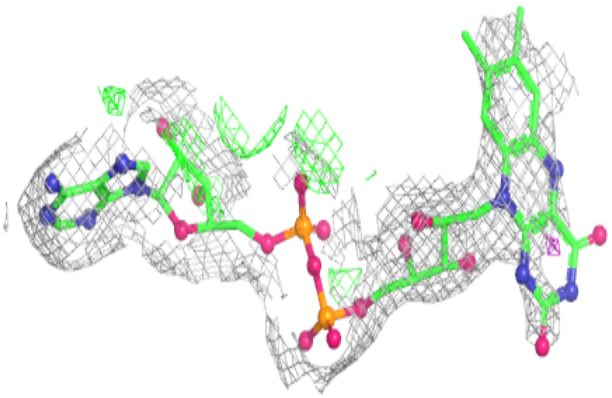


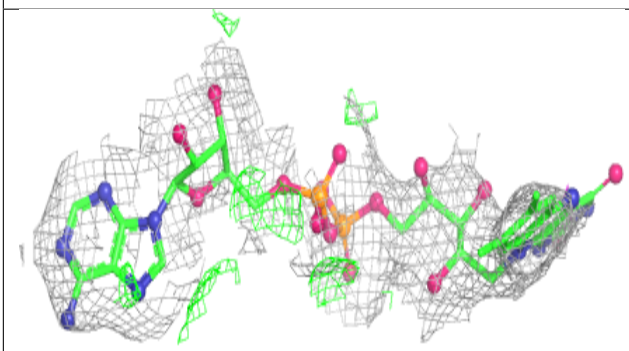


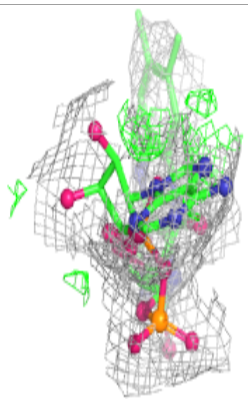


Electron density around FAD B 601:

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

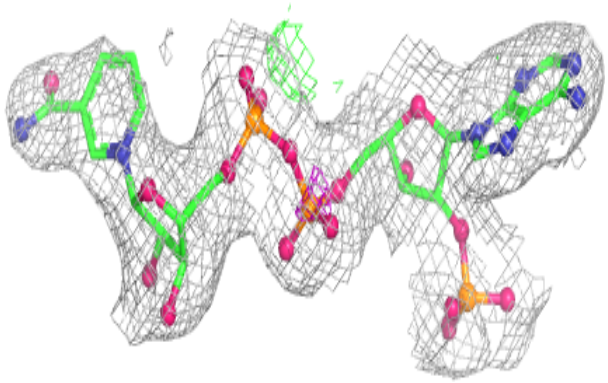


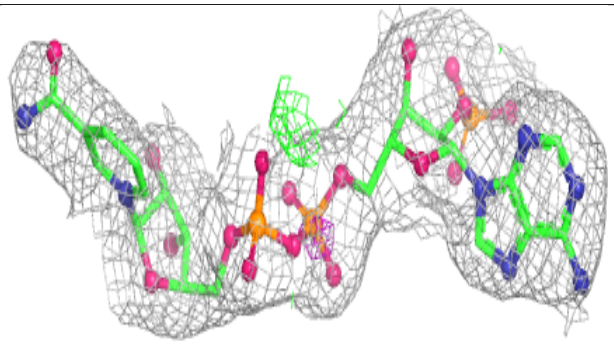


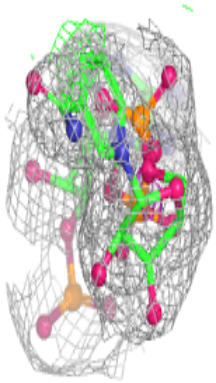


Electron density around NAP B 602:

$2mF_o$-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.