



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 5, 2021 – 10:09 AM JST

PDB ID : 7D4K
Title : Crystal structure of Tmm from Pelagibacter sp. strain HTCC7211
Authors : Li, C.Y.; Zhang, Y.Z.
Deposited on : 2020-09-24
Resolution : 1.80 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.23.1
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) : 2.23.1

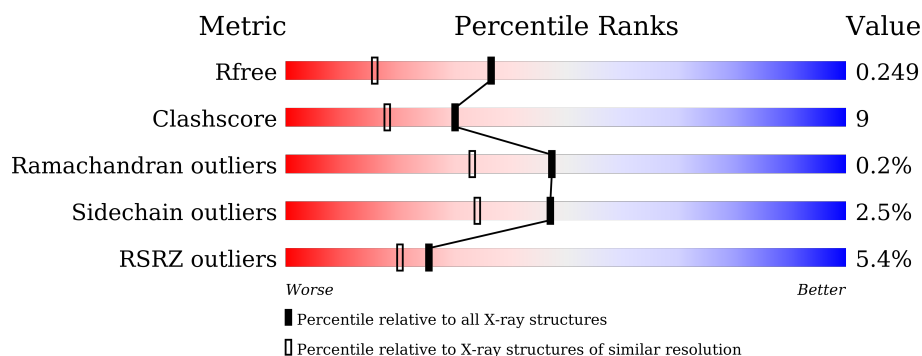
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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

Mol	Chain	Length	Quality of chain
1	A	464	<div> <div>5%</div> <div> <div></div> <div>79%</div> <div>15%</div> <div>• •</div> </div> </div>
1	B	464	<div> <div>5%</div> <div> <div></div> <div>77%</div> <div>17%</div> <div>• 5%</div> </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8384 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 Flavin-containing monooxygenase FMO.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	444	Total	C	N	O	S	0	3	0
			3682	2365	620	677	20			
1	B	440	Total	C	N	O	S	0	3	0
			3650	2344	612	675	19			

There are 40 discrepancies between the modelled and reference sequences:

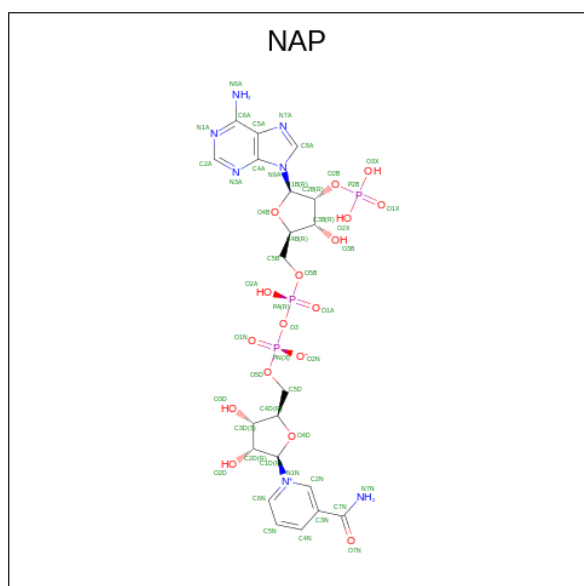
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP B6BQB2
A	-18	GLY	-	expression tag	UNP B6BQB2
A	-17	SER	-	expression tag	UNP B6BQB2
A	-16	SER	-	expression tag	UNP B6BQB2
A	-15	HIS	-	expression tag	UNP B6BQB2
A	-14	HIS	-	expression tag	UNP B6BQB2
A	-13	HIS	-	expression tag	UNP B6BQB2
A	-12	HIS	-	expression tag	UNP B6BQB2
A	-11	HIS	-	expression tag	UNP B6BQB2
A	-10	HIS	-	expression tag	UNP B6BQB2
A	-9	SER	-	expression tag	UNP B6BQB2
A	-8	SER	-	expression tag	UNP B6BQB2
A	-7	GLY	-	expression tag	UNP B6BQB2
A	-6	LEU	-	expression tag	UNP B6BQB2
A	-5	VAL	-	expression tag	UNP B6BQB2
A	-4	PRO	-	expression tag	UNP B6BQB2
A	-3	ARG	-	expression tag	UNP B6BQB2
A	-2	GLY	-	expression tag	UNP B6BQB2
A	-1	SER	-	expression tag	UNP B6BQB2
A	0	HIS	-	expression tag	UNP B6BQB2
B	-19	MET	-	expression tag	UNP B6BQB2
B	-18	GLY	-	expression tag	UNP B6BQB2
B	-17	SER	-	expression tag	UNP B6BQB2
B	-16	SER	-	expression tag	UNP B6BQB2
B	-15	HIS	-	expression tag	UNP B6BQB2

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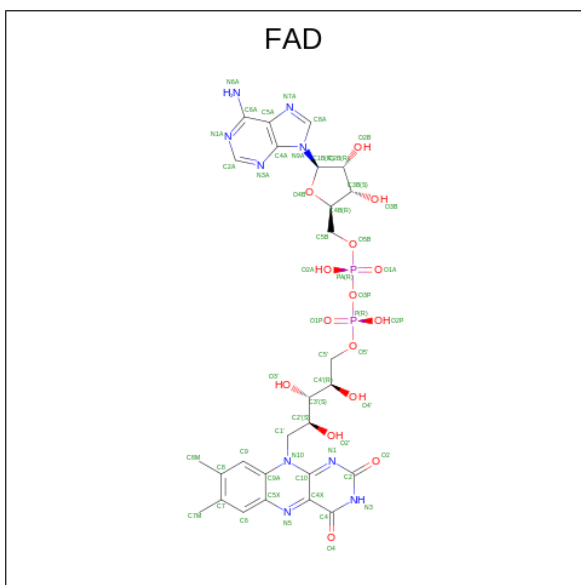
Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	HIS	-	expression tag	UNP B6BQB2
B	-13	HIS	-	expression tag	UNP B6BQB2
B	-12	HIS	-	expression tag	UNP B6BQB2
B	-11	HIS	-	expression tag	UNP B6BQB2
B	-10	HIS	-	expression tag	UNP B6BQB2
B	-9	SER	-	expression tag	UNP B6BQB2
B	-8	SER	-	expression tag	UNP B6BQB2
B	-7	GLY	-	expression tag	UNP B6BQB2
B	-6	LEU	-	expression tag	UNP B6BQB2
B	-5	VAL	-	expression tag	UNP B6BQB2
B	-4	PRO	-	expression tag	UNP B6BQB2
B	-3	ARG	-	expression tag	UNP B6BQB2
B	-2	GLY	-	expression tag	UNP B6BQB2
B	-1	SER	-	expression tag	UNP B6BQB2
B	0	HIS	-	expression tag	UNP B6BQB2

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$) (labeled as "Ligand of Interest" by depositor).



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

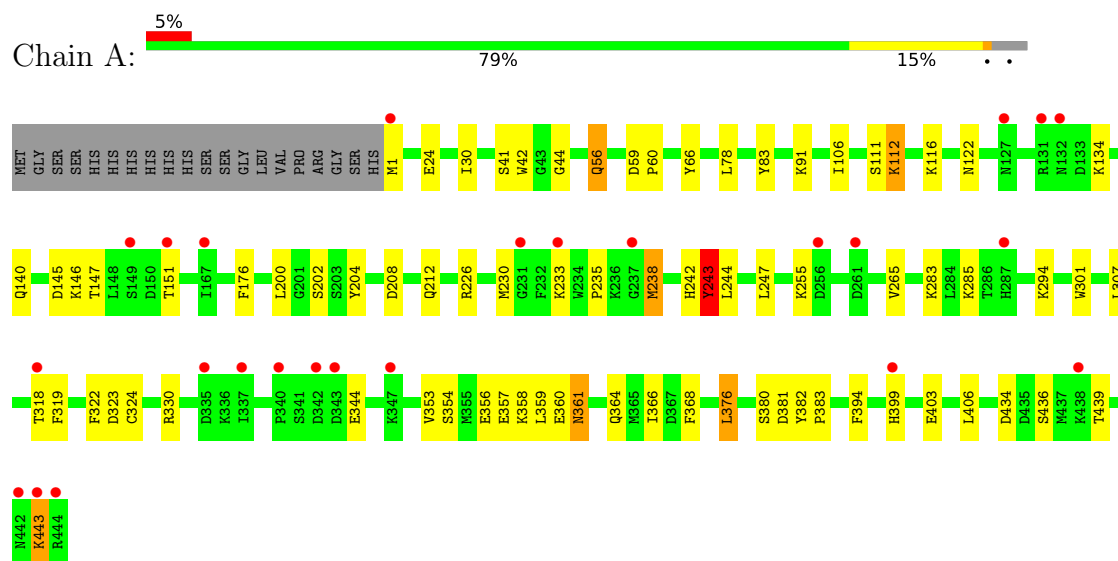
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	444	Total O 444 444	0	0
4	B	406	Total O 406 406	0	0

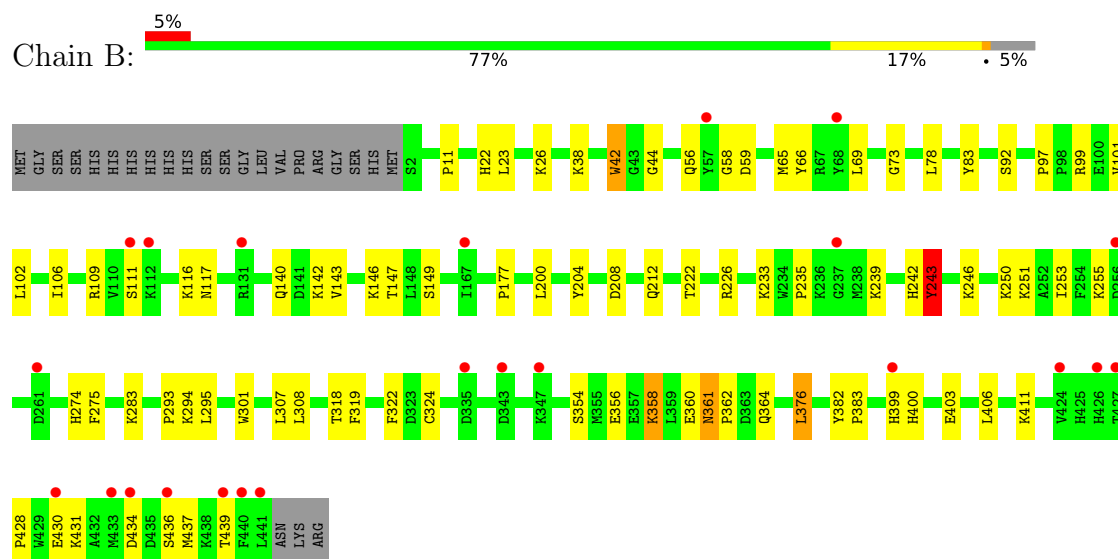
3 Residue-property plots [i](#)

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: Flavin-containing monooxygenase FMO



• Molecule 1: Flavin-containing monooxygenase FMO



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	69.42Å 82.08Å 97.91Å 90.00° 98.13° 90.00°	Depositor
Resolution (Å)	48.55 – 1.80 48.55 – 1.80	Depositor EDS
% Data completeness (in resolution range)	92.1 (48.55-1.80) 97.3 (48.55-1.80)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.03 (at 1.79Å)	Xtriage
Refinement program	PHENIX 1.6.4_486	Depositor
R, R_{free}	0.217 , 0.250 0.216 , 0.249	Depositor DCC
R_{free} test set	4919 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	27.1	Xtriage
Anisotropy	0.598	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 45.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8384	wwPDB-VP
Average B, all atoms (Å ²)	30.0	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 26.46 % 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 2.6260e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.35	0/3793	0.52	0/5121
1	B	0.35	0/3758	0.51	0/5076
All	All	0.35	0/7551	0.52	0/10197

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	3682	0	3562	63	0
1	B	3650	0	3512	73	0
2	A	48	0	24	2	0
2	B	48	0	24	3	0
3	A	53	0	31	1	0
3	B	53	0	31	3	0
4	A	444	0	0	21	0
4	B	406	0	0	17	0
All	All	8384	0	7184	137	0

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

All (137) 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:295:LEU:HD23	4:B:602:HOH:O	1.56	1.05
1:B:65:MET:HE2	1:B:99:ARG:HD3	1.43	0.99
1:B:65:MET:HE3	1:B:69:LEU:HD13	1.41	0.98
1:B:146:LYS:HD2	1:B:147:THR:H	1.26	0.98
1:B:301:TRP:HA	4:B:602:HOH:O	1.66	0.96
1:A:56:GLN:HE21	1:A:56:GLN:H	0.98	0.94
1:A:230:MET:SD	4:A:611:HOH:O	2.32	0.87
1:B:146:LYS:HD2	1:B:147:THR:N	1.90	0.87
1:B:65:MET:HE1	1:B:69:LEU:HD22	1.57	0.85
1:B:101:VAL:HA	1:B:437:MET:HE3	1.64	0.80
1:A:434:ASP:OD2	1:A:439:THR:HG21	1.83	0.78
1:A:56:GLN:H	1:A:56:GLN:NE2	1.81	0.76
1:A:83:TYR:CE1	4:A:610:HOH:O	2.35	0.76
1:B:101:VAL:HA	1:B:437:MET:CE	2.15	0.76
1:B:22:HIS:O	1:B:26:LYS:HD3	1.89	0.72
1:B:235:PRO:HG3	1:B:406:LEU:HD21	1.71	0.72
1:A:1:MET:N	4:A:605:HOH:O	2.23	0.70
1:A:66:TYR:OH	2:A:501:NAP:H4N	1.93	0.69
1:A:353:VAL:HG12	4:A:602:HOH:O	1.93	0.69
1:A:436:SER:OG	1:A:439:THR:HG23	1.92	0.69
1:A:1:MET:HA	4:A:605:HOH:O	1.93	0.68
1:A:91:LYS:NZ	4:A:607:HOH:O	2.27	0.66
1:B:65:MET:CE	1:B:69:LEU:HD22	2.26	0.66
1:A:1:MET:CA	4:A:605:HOH:O	2.44	0.65
1:B:23:LEU:HD23	1:B:26:LYS:NZ	2.10	0.65
1:B:149:SER:OG	4:B:601:HOH:O	2.14	0.65
1:A:204:TYR:HB2	2:A:501:NAP:H2D	1.77	0.65
1:B:399:HIS:O	1:B:403:GLU:HG3	1.97	0.64
1:A:41:SER:OG	4:A:601:HOH:O	2.15	0.63
1:B:354:SER:O	1:B:358:LYS:HD3	1.99	0.63
1:B:294:LYS:O	4:B:602:HOH:O	2.16	0.61
1:A:146:LYS:HE3	1:A:147:THR:O	2.01	0.61
1:B:66:TYR:OH	2:B:501:NAP:H4N	2.01	0.61
1:A:112:LYS:NZ	4:A:610:HOH:O	2.32	0.60
1:B:177:PRO:HG2	1:B:250:LYS:HG2	1.83	0.60
1:A:357:GLU:CD	4:A:602:HOH:O	2.40	0.60
1:B:204:TYR:HB2	2:B:501:NAP:H2D	1.83	0.59
1:B:253:ILE:N	1:B:253:ILE:HD12	2.18	0.59
1:A:235:PRO:HG3	1:A:406:LEU:HD21	1.85	0.59
1:A:354:SER:O	1:A:358:LYS:HD3	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:78:LEU:HD13	1:B:319:PHE:CD2	2.39	0.58
1:B:73:GLY:HA3	4:B:922:HOH:O	2.04	0.57
1:A:283:LYS:HD2	1:A:285:LYS:HE3	1.87	0.56
1:B:56:GLN:HG3	4:B:610:HOH:O	2.06	0.56
1:B:255:LYS:NZ	4:B:611:HOH:O	2.39	0.56
1:B:428:PRO:HG2	1:B:431:LYS:HE2	1.87	0.56
1:A:56:GLN:HE21	1:A:56:GLN:N	1.84	0.56
1:B:251:LYS:HD2	1:B:253:ILE:HD11	1.88	0.56
1:A:226:ARG:O	1:A:242:HIS:HE1	1.89	0.55
1:A:399:HIS:O	1:A:403:GLU:HG3	2.07	0.55
1:B:140:GLN:NE2	4:B:603:HOH:O	2.39	0.54
1:B:246:LYS:HE2	4:B:966:HOH:O	2.07	0.54
1:B:23:LEU:HD23	1:B:26:LYS:HZ3	1.72	0.54
1:B:92:SER:HB2	4:B:651:HOH:O	2.07	0.54
1:B:42:TRP:CE2	1:B:116:LYS:HE2	2.42	0.54
1:B:436:SER:OG	1:B:439:THR:HG23	2.08	0.53
1:B:243:TYR:HB3	1:B:255:LYS:HG3	1.90	0.53
1:B:65:MET:HE3	1:B:69:LEU:CD1	2.27	0.53
1:A:380:SER:OG	1:A:381:ASP:N	2.38	0.53
1:B:243:TYR:HB3	1:B:255:LYS:CG	2.39	0.53
1:A:176:PHE:CD1	1:A:247[B]:LEU:HD23	2.45	0.52
1:B:44:GLY:HA2	3:B:502:FAD:O3B	2.10	0.52
1:B:101:VAL:HA	1:B:437:MET:HE2	1.92	0.52
1:A:106:ILE:HD11	1:A:319:PHE:CZ	2.45	0.52
1:A:360:GLU:H	1:A:364:GLN:NE2	2.08	0.52
1:B:58:GLY:HA2	4:B:650:HOH:O	2.09	0.52
1:B:233:LYS:HD2	1:B:403:GLU:O	2.09	0.52
1:A:243:TYR:HB3	1:A:255:LYS:HG3	1.91	0.51
1:B:208:ASP:O	1:B:212:GLN:HG2	2.11	0.51
1:B:226:ARG:O	1:B:242:HIS:HE1	1.94	0.51
1:A:122:ASN:HA	4:A:612:HOH:O	2.10	0.50
1:A:361:ASN:HD21	1:A:364:GLN:HG3	1.77	0.50
1:A:78:LEU:HD13	1:A:319:PHE:CD2	2.46	0.50
1:A:44:GLY:HA2	3:A:502:FAD:O3B	2.12	0.50
1:A:202:SER:C	4:A:611:HOH:O	2.50	0.49
1:A:208:ASP:O	1:A:212:GLN:HG2	2.11	0.49
1:B:434:ASP:OD2	1:B:439:THR:HG21	2.12	0.49
1:A:357:GLU:OE2	4:A:602:HOH:O	2.19	0.49
1:B:106:ILE:HD11	1:B:319:PHE:CZ	2.47	0.49
1:B:140:GLN:HG3	4:B:603:HOH:O	2.13	0.49
1:B:11:PRO:HG2	3:B:502:FAD:H4'	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:318:THR:O	1:B:322:PHE:CG	2.66	0.48
1:B:324:CYS:HB3	1:B:376:LEU:HB3	1.94	0.48
1:B:275:PHE:O	1:B:283:LYS:HE2	2.14	0.48
1:A:24:GLU:HB2	1:A:30:ILE:HD13	1.95	0.48
1:A:145:ASP:OD1	4:A:603:HOH:O	2.20	0.48
1:B:143:VAL:HG13	4:B:663:HOH:O	2.13	0.48
1:A:140:GLN:HG3	4:A:603:HOH:O	2.13	0.47
1:A:59:ASP:OD1	1:A:60:PRO:HD2	2.15	0.47
1:A:361:ASN:ND2	1:A:364:GLN:H	2.13	0.47
1:B:65:MET:CE	1:B:99:ARG:HD3	2.30	0.47
1:B:361:ASN:ND2	1:B:364:GLN:H	2.13	0.46
1:A:323:ASP:HB3	1:A:382:TYR:CE1	2.50	0.46
1:B:361:ASN:HB2	1:B:362:PRO:HD2	1.96	0.46
1:B:65:MET:HE1	1:B:99:ARG:HB2	1.98	0.46
1:B:295:LEU:HA	4:B:602:HOH:O	2.15	0.46
1:A:111:SER:C	4:A:604:HOH:O	2.53	0.46
1:B:97:PRO:HB2	1:B:101:VAL:HB	1.98	0.45
1:B:360:GLU:H	1:B:364:GLN:NE2	2.15	0.45
4:A:728:HOH:O	1:B:274:HIS:HE1	2.00	0.45
1:B:430:GLU:HG3	4:B:835:HOH:O	2.17	0.45
1:B:97:PRO:HG2	1:B:102:LEU:HG	1.98	0.44
1:B:400:HIS:ND1	1:B:411:LYS:HG3	2.33	0.44
1:A:247[B]:LEU:HD21	1:A:265:VAL:HG21	1.98	0.44
1:A:324:CYS:HB3	1:A:376:LEU:HB3	1.99	0.44
1:A:359:LEU:HD11	1:A:368:PHE:CG	2.53	0.44
1:B:308:LEU:HD12	1:B:308:LEU:N	2.32	0.44
2:B:501:NAP:C2N	3:B:502:FAD:C6	2.96	0.43
1:A:140:GLN:NE2	4:A:603:HOH:O	2.47	0.43
1:A:353:VAL:CG1	4:A:602:HOH:O	2.60	0.43
1:A:361:ASN:ND2	1:A:364:GLN:HG3	2.34	0.43
1:B:38:LYS:HE2	1:B:59:ASP:OD2	2.17	0.43
1:A:443:LYS:H	1:A:443:LYS:HG2	1.54	0.43
1:B:142:LYS:HE3	4:B:628:HOH:O	2.18	0.43
1:A:116:LYS:NZ	4:A:601:HOH:O	2.44	0.42
1:B:293:PRO:O	1:B:294:LYS:HB2	2.20	0.42
1:B:382:TYR:HA	1:B:383:PRO:HD3	1.90	0.42
1:B:78:LEU:O	1:B:319:PHE:HB2	2.19	0.42
1:A:78:LEU:O	1:A:319:PHE:HB2	2.20	0.42
1:A:344:GLU:CG	4:A:928:HOH:O	2.66	0.42
1:A:294:LYS:HE3	1:A:301:TRP:CH2	2.54	0.42
1:B:222:THR:HG23	1:B:239:LYS:HG3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:318:THR:O	1:A:322:PHE:CG	2.73	0.42
1:B:239:LYS:NZ	4:B:620:HOH:O	2.50	0.42
1:A:134:LYS:HG2	1:A:151:THR:OG1	2.20	0.42
1:B:83:TYR:CD2	1:B:109:ARG:HB2	2.55	0.41
1:A:353:VAL:O	1:A:357:GLU:HG3	2.21	0.41
1:A:233:LYS:HD2	1:A:403:GLU:O	2.21	0.41
1:A:235:PRO:HD2	1:A:238:MET:HE3	2.03	0.41
1:A:330:ARG:HH22	1:A:381:ASP:HB2	1.85	0.41
1:B:235:PRO:HG3	1:B:406:LEU:HD11	2.02	0.41
1:A:366:ILE:HD13	1:A:394:PHE:HB3	2.03	0.40
1:B:117:ASN:HD22	1:B:117:ASN:HA	1.68	0.40
1:A:382:TYR:HA	1:A:383:PRO:HD3	1.96	0.40
1:B:65:MET:HE2	1:B:99:ARG:CD	2.31	0.40
1:A:244:LEU:HD21	1:A:247[B]:LEU:HD11	2.04	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	445/464 (96%)	427 (96%)	17 (4%)	1 (0%)	47	33
1	B	441/464 (95%)	422 (96%)	18 (4%)	1 (0%)	47	33
All	All	886/928 (96%)	849 (96%)	35 (4%)	2 (0%)	47	33

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	243	TYR
1	B	243	TYR

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	406/420 (97%)	395 (97%)	11 (3%)	44	31
1	B	402/420 (96%)	393 (98%)	9 (2%)	52	39
All	All	808/840 (96%)	788 (98%)	20 (2%)	47	34

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	TRP
1	A	56	GLN
1	A	112	LYS
1	A	200	LEU
1	A	238	MET
1	A	243	TYR
1	A	307	LEU
1	A	356	GLU
1	A	361	ASN
1	A	376	LEU
1	A	443	LYS
1	B	42	TRP
1	B	111	SER
1	B	200	LEU
1	B	243	TYR
1	B	307	LEU
1	B	356	GLU
1	B	358	LYS
1	B	361	ASN
1	B	376	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	GLN
1	A	117	ASN

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Mol	Chain	Res	Type
1	A	212	GLN
1	A	242	HIS
1	A	361	ASN
1	A	364	GLN
1	B	117	ASN
1	B	132	ASN
1	B	212	GLN
1	B	242	HIS
1	B	274	HIS
1	B	361	ASN
1	B	364	GLN
1	B	399	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](#)

4 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	FAD	A	502	-	51,58,58	1.80	6 (11%)	60,89,89	2.00	11 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAP	A	501	-	45,52,52	2.74	14 (31%)	56,80,80	1.48	6 (10%)
3	FAD	B	502	-	51,58,58	1.80	6 (11%)	60,89,89	1.96	11 (18%)
2	NAP	B	501	-	45,52,52	2.74	15 (33%)	56,80,80	1.46	6 (10%)

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	FAD	A	502	-	-	3/30/50/50	0/6/6/6
2	NAP	A	501	-	-	4/31/67/67	0/5/5/5
3	FAD	B	502	-	-	3/30/50/50	0/6/6/6
2	NAP	B	501	-	-	2/31/67/67	0/5/5/5

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	502	FAD	C4X-C10	9.31	1.48	1.38
3	A	502	FAD	C4X-C10	9.27	1.48	1.38
2	A	501	NAP	C7N-N7N	7.69	1.47	1.33
2	B	501	NAP	C7N-N7N	7.20	1.46	1.33
2	B	501	NAP	C2N-N1N	6.83	1.43	1.35
2	A	501	NAP	C2N-N1N	6.67	1.43	1.35
2	A	501	NAP	C4N-C3N	6.57	1.50	1.39
2	B	501	NAP	C4N-C3N	6.42	1.50	1.39
2	B	501	NAP	C2N-C3N	6.38	1.48	1.39
2	A	501	NAP	C2N-C3N	6.26	1.48	1.39
2	B	501	NAP	C5N-C4N	4.82	1.49	1.38
2	B	501	NAP	C6N-C5N	4.70	1.49	1.38
2	A	501	NAP	C6N-C5N	4.60	1.48	1.38
2	A	501	NAP	C5N-C4N	4.50	1.48	1.38
2	A	501	NAP	C3B-C2B	-4.46	1.43	1.52
2	B	501	NAP	C3B-C2B	-4.26	1.43	1.52
3	B	502	FAD	C4-C4X	4.17	1.48	1.41
3	A	502	FAD	C4-C4X	4.12	1.48	1.41
2	B	501	NAP	C6A-N6A	3.98	1.48	1.34
2	A	501	NAP	C6A-N6A	3.80	1.47	1.34
3	A	502	FAD	C9A-C5X	3.65	1.49	1.42
3	B	502	FAD	C9A-C5X	3.59	1.49	1.42
2	B	501	NAP	C6N-N1N	3.45	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	NAP	C6N-N1N	3.41	1.43	1.35
2	B	501	NAP	O2D-C2D	-3.33	1.35	1.43
3	B	502	FAD	C8-C7	3.20	1.48	1.40
3	A	502	FAD	C8-C7	3.18	1.48	1.40
2	A	501	NAP	O2D-C2D	-3.08	1.35	1.43
2	A	501	NAP	C2D-C3D	-3.02	1.45	1.53
2	B	501	NAP	C2D-C3D	-2.69	1.46	1.53
2	A	501	NAP	C2A-N3A	2.68	1.36	1.32
2	A	501	NAP	O3D-C3D	-2.60	1.36	1.43
2	B	501	NAP	O3D-C3D	-2.39	1.37	1.43
3	A	502	FAD	C5A-C4A	2.36	1.47	1.40
2	B	501	NAP	C2A-N3A	2.34	1.35	1.32
3	B	502	FAD	C5A-C4A	2.34	1.47	1.40
2	A	501	NAP	O4B-C4B	-2.19	1.40	1.45
2	B	501	NAP	P2B-O2B	2.13	1.63	1.59
3	A	502	FAD	C9A-N10	2.10	1.41	1.38
3	B	502	FAD	C9A-N10	2.09	1.41	1.38
2	B	501	NAP	C2D-C1D	-2.04	1.50	1.53

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	FAD	C4-N3-C2	8.54	122.35	115.14
3	B	502	FAD	C4-N3-C2	8.45	122.27	115.14
3	A	502	FAD	C1'-N10-C9A	5.94	122.97	118.29
3	B	502	FAD	C1'-N10-C9A	5.40	122.54	118.29
2	B	501	NAP	C5N-C4N-C3N	-5.29	114.08	120.34
2	A	501	NAP	C5N-C4N-C3N	-5.03	114.39	120.34
3	A	502	FAD	C4-C4X-C10	-5.01	116.63	119.95
3	B	502	FAD	C4-C4X-C10	-4.97	116.66	119.95
2	B	501	NAP	N3A-C2A-N1A	-4.42	121.76	128.68
2	A	501	NAP	N3A-C2A-N1A	-4.15	122.19	128.68
2	A	501	NAP	C2N-C3N-C4N	3.98	122.77	118.26
2	A	501	NAP	C2N-N1N-C1D	3.98	128.00	119.14
2	B	501	NAP	C2N-N1N-C1D	3.78	127.55	119.14
3	A	502	FAD	C4X-C4-N3	-3.77	118.28	123.43
3	B	502	FAD	C4X-C4-N3	-3.75	118.30	123.43
3	B	502	FAD	C4X-N5-C5X	3.62	120.39	116.77
3	A	502	FAD	C4X-N5-C5X	3.61	120.38	116.77
3	A	502	FAD	N3A-C2A-N1A	-3.30	123.53	128.68
2	B	501	NAP	C2N-C3N-C4N	3.29	121.99	118.26
3	A	502	FAD	C9A-N10-C10	-3.24	117.67	121.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	502	FAD	N3A-C2A-N1A	-3.20	123.67	128.68
3	B	502	FAD	C9A-N10-C10	-3.17	117.76	121.91
3	B	502	FAD	C4-C4X-N5	3.02	122.05	118.60
3	A	502	FAD	C4-C4X-N5	3.01	122.04	118.60
2	A	501	NAP	O5D-C5D-C4D	2.83	118.74	108.99
3	A	502	FAD	P-O3P-PA	-2.81	123.18	132.83
3	B	502	FAD	C4A-C5A-N7A	-2.77	106.51	109.40
3	A	502	FAD	C4A-C5A-N7A	-2.68	106.60	109.40
3	B	502	FAD	P-O3P-PA	-2.68	123.64	132.83
3	A	502	FAD	C5X-C9A-N10	2.64	119.63	117.72
2	A	501	NAP	C1B-N9A-C4A	-2.57	122.13	126.64
3	B	502	FAD	C5X-C9A-N10	2.45	119.49	117.72
2	B	501	NAP	C1B-N9A-C4A	-2.36	122.50	126.64
2	B	501	NAP	O5D-C5D-C4D	2.36	117.11	108.99

There are no chirality outliers.

All (12) torsion outliers are listed below:

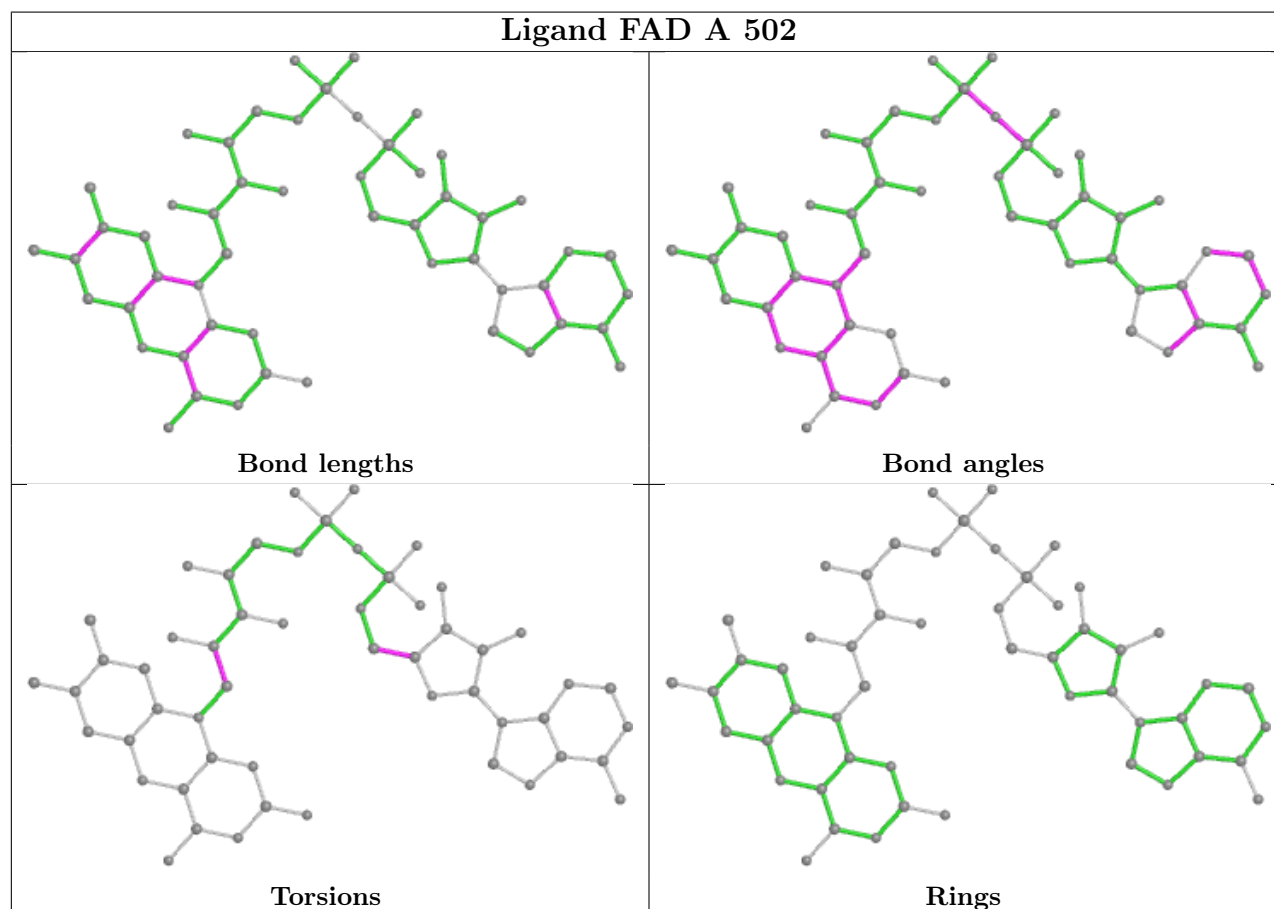
Mol	Chain	Res	Type	Atoms
3	A	502	FAD	N10-C1'-C2'-O2'
3	A	502	FAD	N10-C1'-C2'-C3'
3	B	502	FAD	N10-C1'-C2'-O2'
3	B	502	FAD	N10-C1'-C2'-C3'
3	A	502	FAD	O4B-C4B-C5B-O5B
2	A	501	NAP	C1B-C2B-O2B-P2B
3	B	502	FAD	O4B-C4B-C5B-O5B
2	A	501	NAP	C2B-O2B-P2B-O3X
2	B	501	NAP	C2B-O2B-P2B-O3X
2	A	501	NAP	O4B-C4B-C5B-O5B
2	B	501	NAP	O4B-C4B-C5B-O5B
2	A	501	NAP	C3B-C2B-O2B-P2B

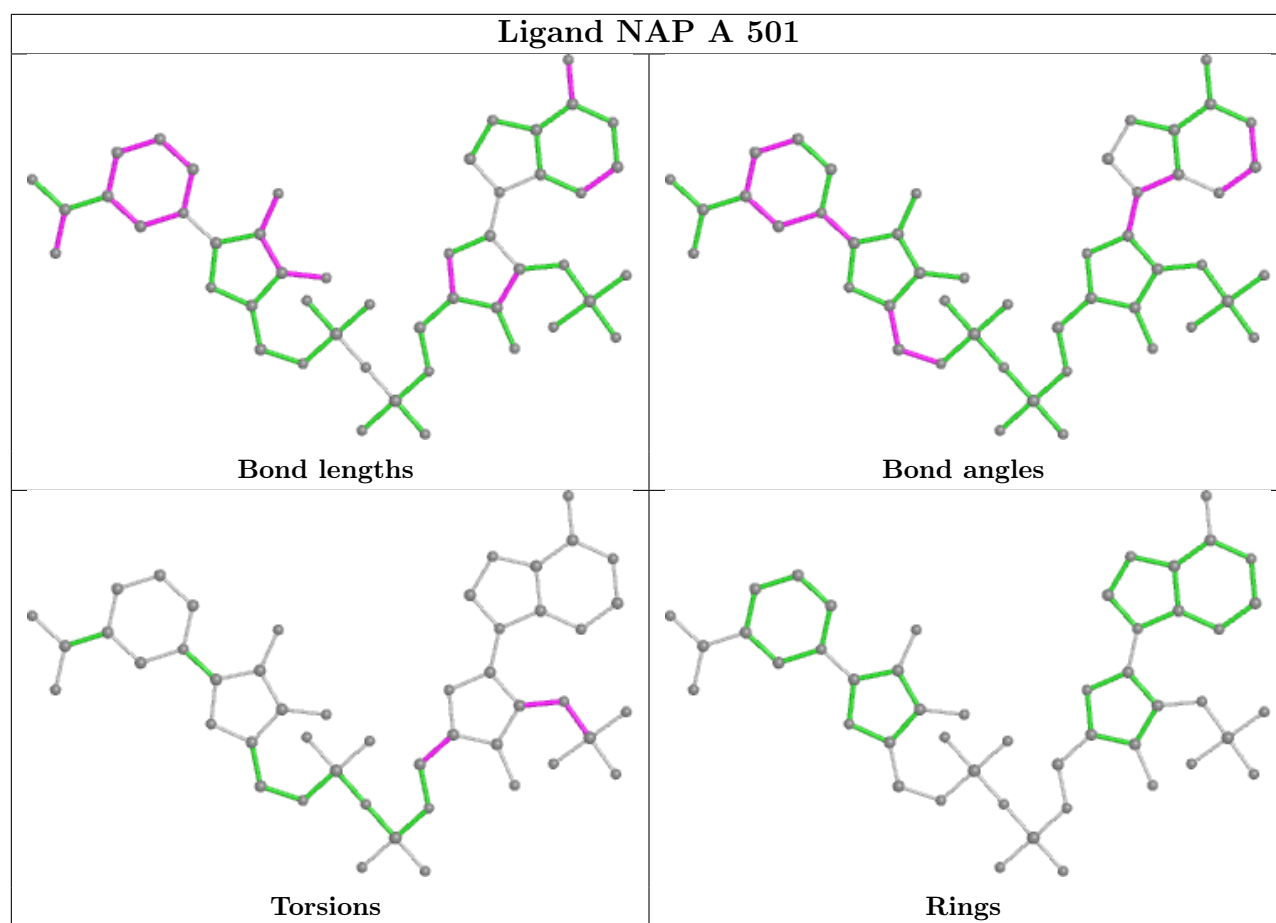
There are no ring outliers.

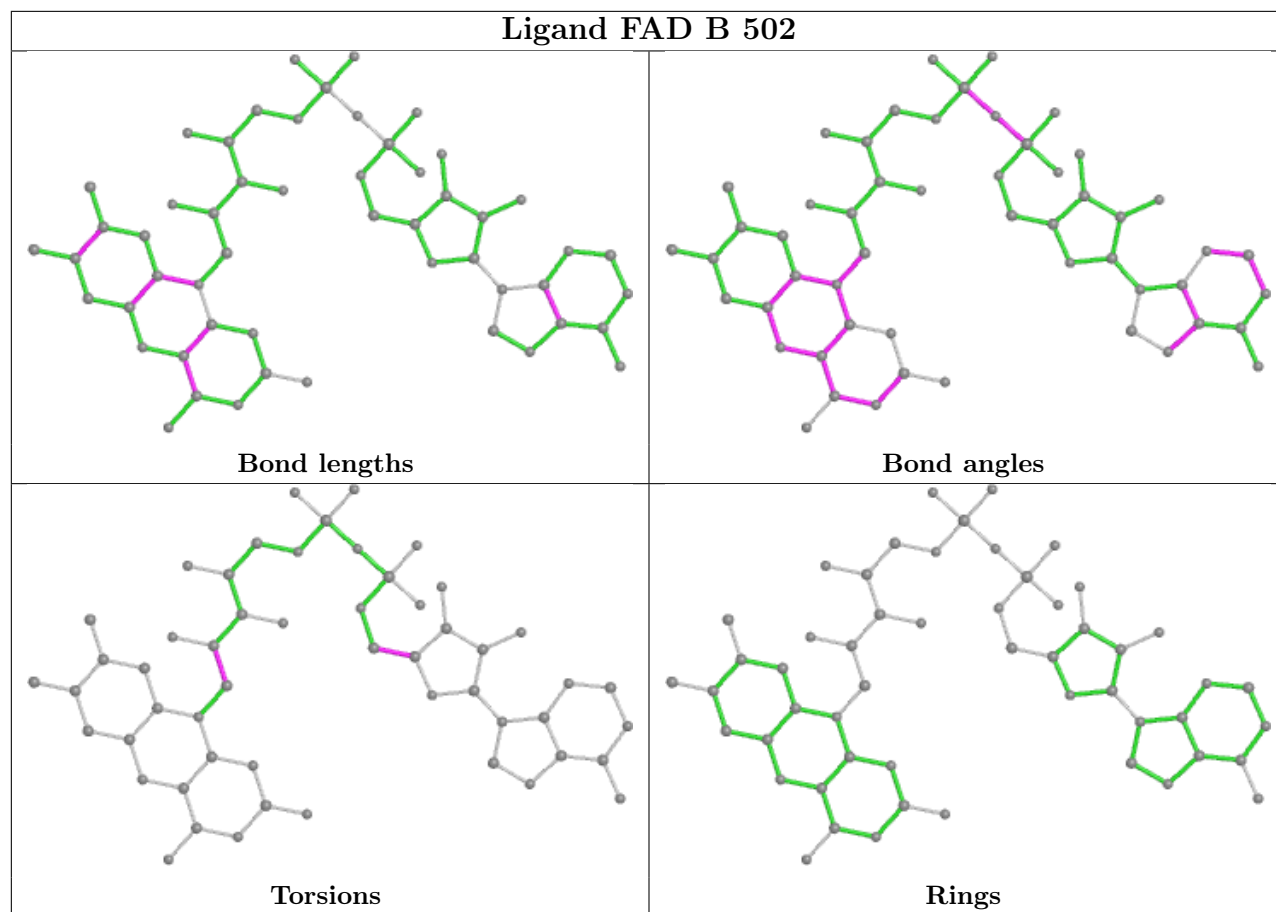
4 monomers are involved in 8 short contacts:

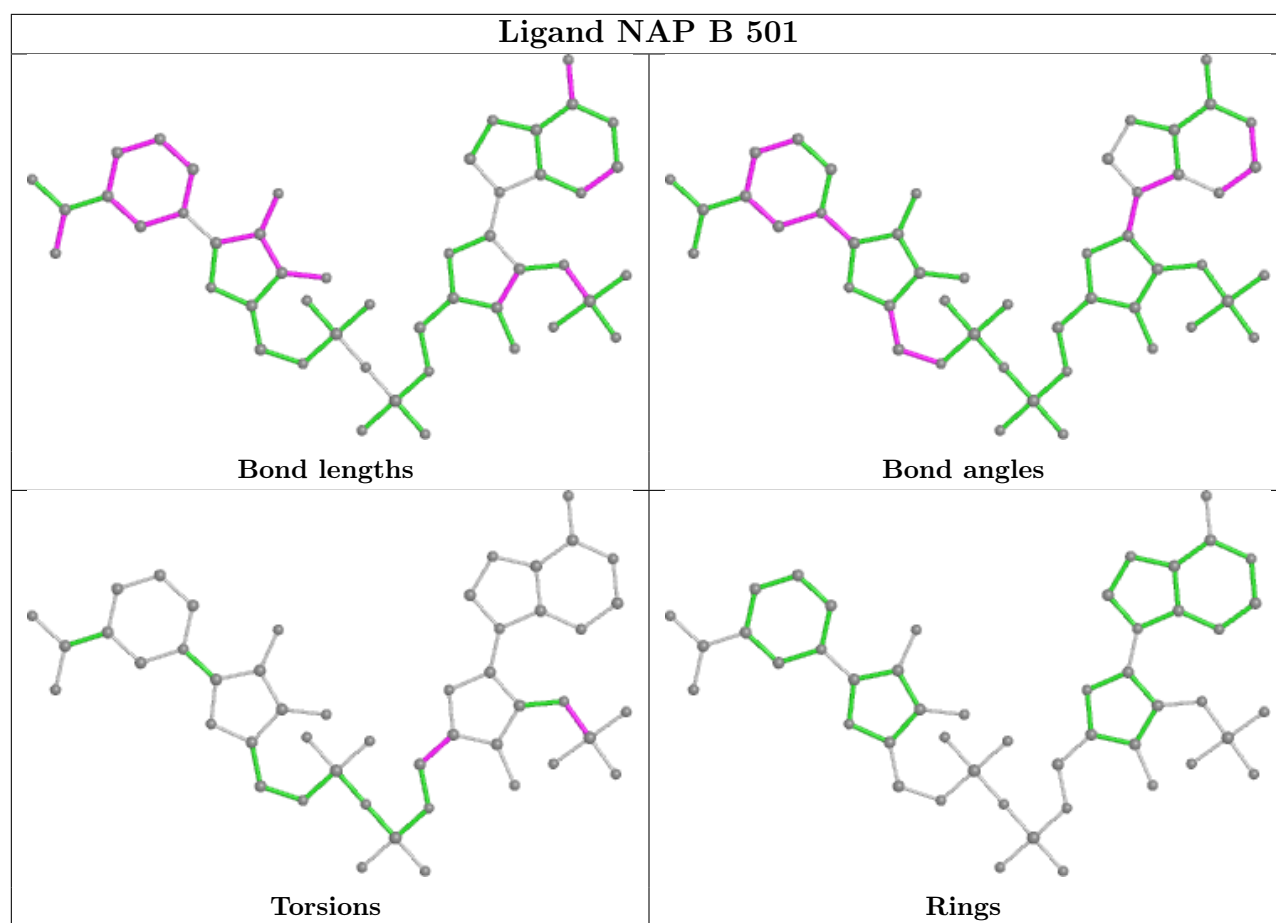
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	FAD	1	0
2	A	501	NAP	2	0
3	B	502	FAD	3	0
2	B	501	NAP	3	0

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









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, 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	444/464 (95%)	0.43	25 (5%) 24 19	19, 28, 41, 74	0
1	B	440/464 (94%)	0.48	23 (5%) 27 22	20, 29, 44, 78	0
All	All	884/928 (95%)	0.46	48 (5%) 25 20	19, 28, 43, 78	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	439	THR	4.9
1	A	442	ASN	4.6
1	B	441	LEU	4.4
1	A	438	LYS	3.7
1	B	399	HIS	3.6
1	A	337	ILE	3.5
1	A	444	ARG	3.4
1	B	440	PHE	3.4
1	B	434	ASP	3.2
1	A	167	ILE	3.2
1	B	426	HIS	3.1
1	B	430	GLU	3.0
1	A	342	ASP	2.9
1	A	233	LYS	2.7
1	B	335	ASP	2.7
1	B	433	MET	2.7
1	A	261	ASP	2.7
1	B	111	SER	2.7
1	A	237	GLY	2.7
1	A	132	ASN	2.7
1	B	424	VAL	2.6
1	B	112	LYS	2.6
1	A	256	ASP	2.6
1	A	131	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	399	HIS	2.5
1	B	261	ASP	2.5
1	A	151	THR	2.4
1	B	68	TYR	2.4
1	A	231	GLY	2.4
1	B	237	GLY	2.4
1	B	343	ASP	2.3
1	A	340	PRO	2.3
1	A	443	LYS	2.3
1	A	149	SER	2.3
1	A	287[A]	HIS	2.3
1	A	335	ASP	2.2
1	A	347	LYS	2.2
1	B	256	ASP	2.1
1	B	347	LYS	2.1
1	A	1	MET	2.1
1	A	318	THR	2.1
1	B	57	TYR	2.1
1	B	427	THR	2.1
1	B	131	ARG	2.1
1	B	436	SER	2.1
1	A	343	ASP	2.0
1	A	127	ASN	2.0
1	B	167	ILE	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](#)

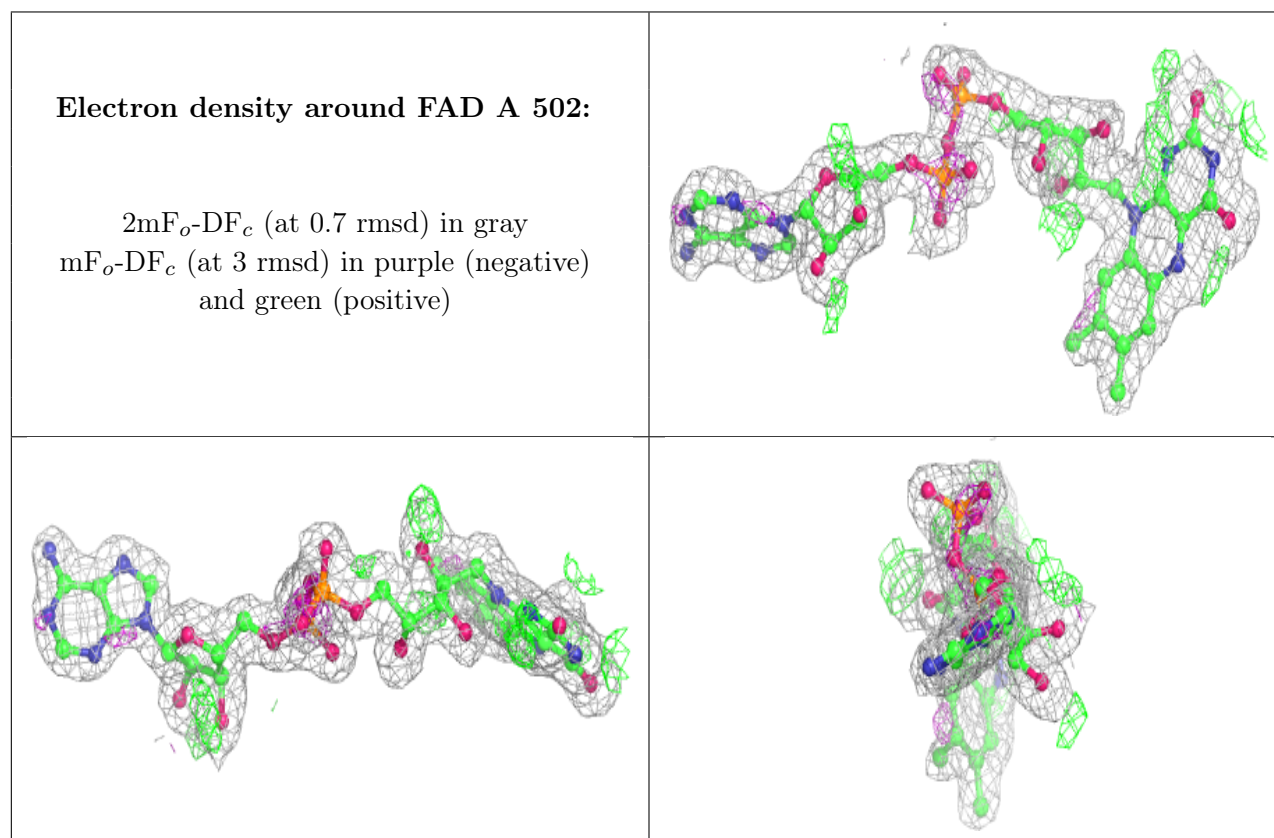
There are no monosaccharides in this entry.

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.

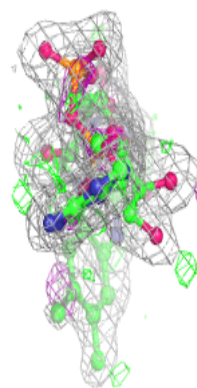
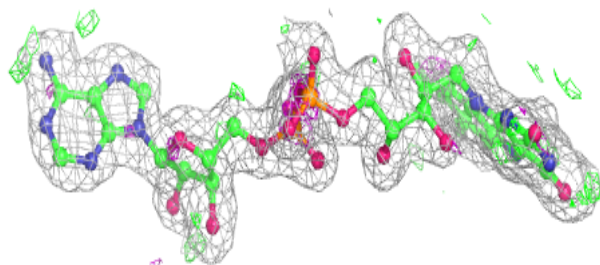
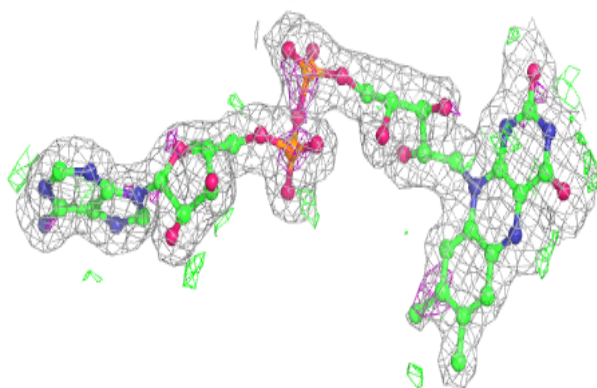
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	FAD	A	502	53/53	0.91	0.15	18,23,26,27	0
3	FAD	B	502	53/53	0.92	0.15	17,23,26,28	0
2	NAP	B	501	48/48	0.94	0.10	19,24,31,36	0
2	NAP	A	501	48/48	0.95	0.11	19,24,29,35	0

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.

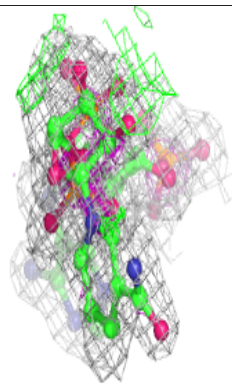
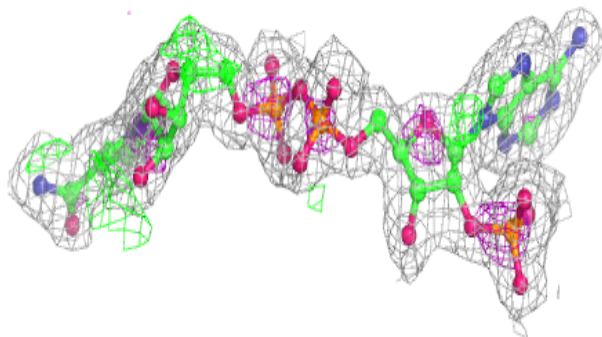
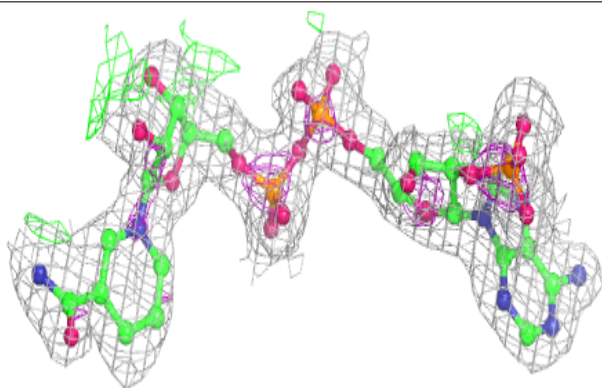


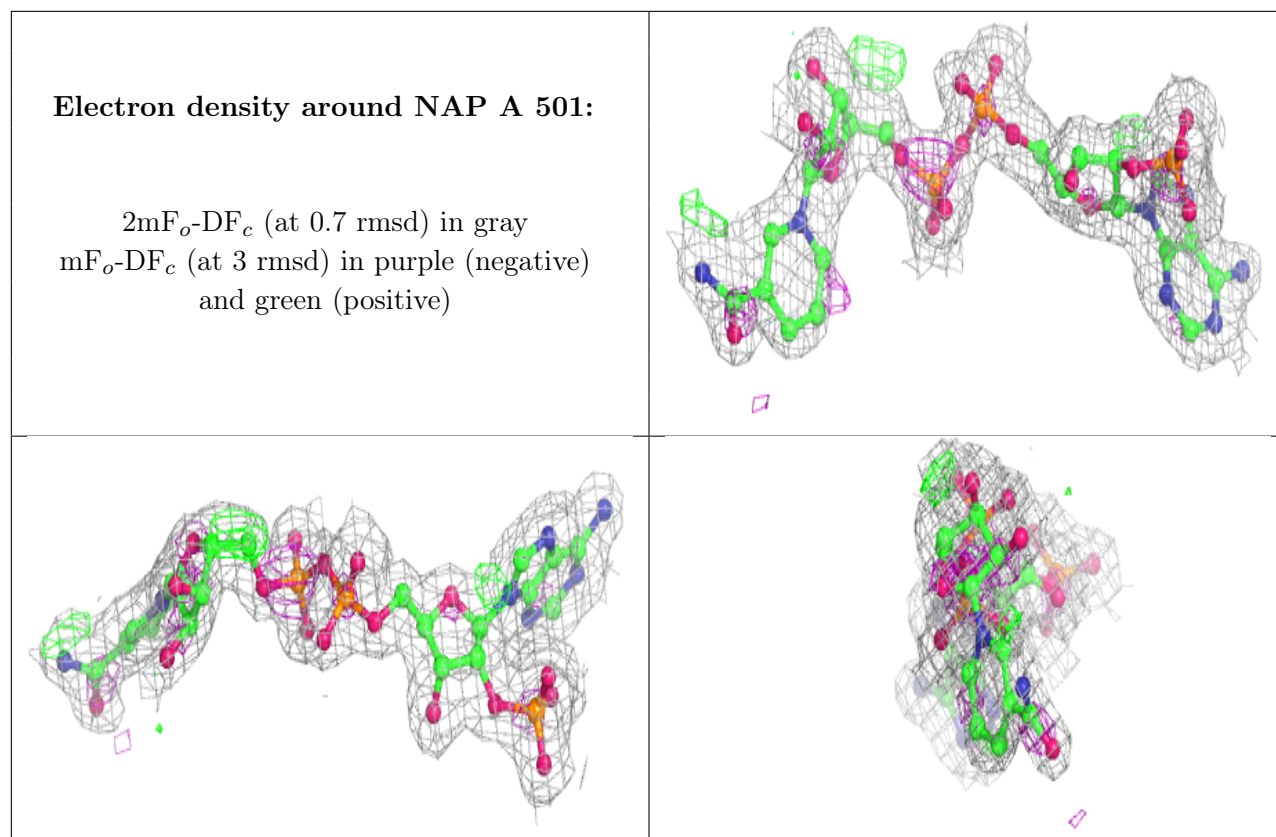
Electron density around FAD B 502:

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

**Electron density around NAP B 501:**

$2mF_o-DF_c$ (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.