



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:34 AM UTC

PDB ID : 8Z15 / pdb_00008z15
Title : Crystal structure of DiatB-NADP-6-DMAIAOx complex
Authors : Peng, M.; Wu, Q.L.
Deposited on : 2024-04-10
Resolution : 2.55 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

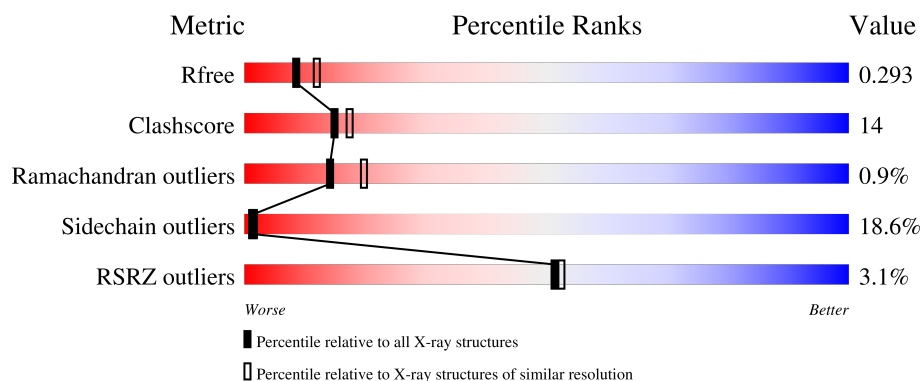
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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}	180053	1853 (2.58-2.54)
Clashscore	190562	1897 (2.58-2.54)
Ramachandran outliers	187476	1875 (2.58-2.54)
Sidechain outliers	187428	1875 (2.58-2.54)
RSRZ outliers	180081	1853 (2.58-2.54)

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	432	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 3403 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.

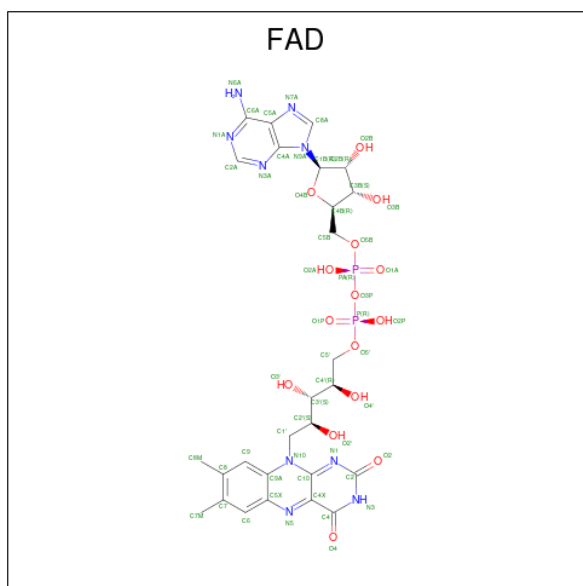
- Molecule 1 is a protein called Flavin-dependent monooxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	426	3255	2058	585	601	11	0	0	0

There is a discrepancy between the modelled and reference sequences:

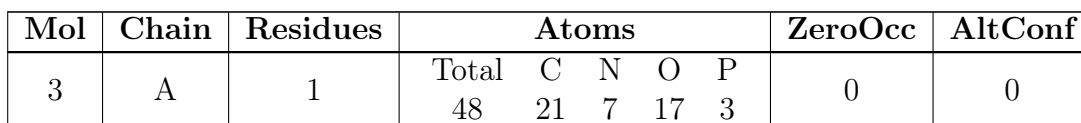
Chain	Residue	Modelled	Actual	Comment	Reference
A	333	MET	VAL	conflict	UNP A0A7T1BYC5

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



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

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



- # A1D7V

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			18	15	2	1		

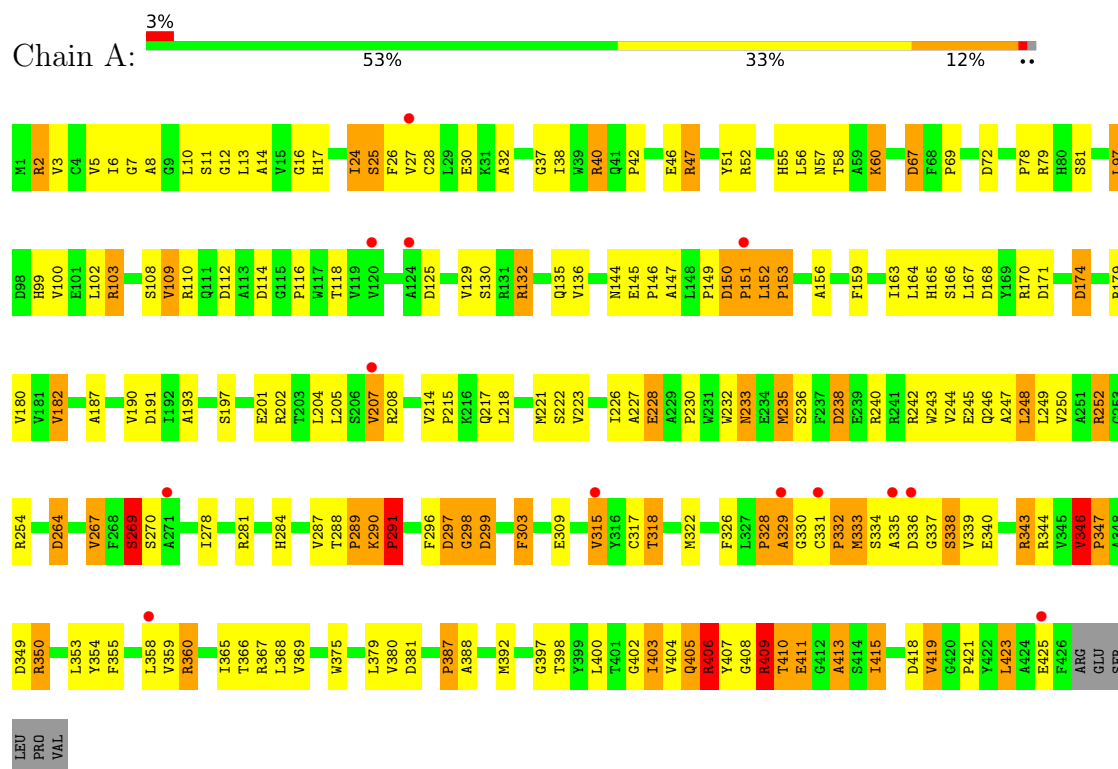
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	29	Total	O	0	0
			29	29		

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-dependent monooxygenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	66.62Å 66.62Å 374.18Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	52.37 – 2.55 52.37 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.9 (52.37-2.55) 97.9 (52.37-2.55)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.00 (at 2.55Å)	Xtriage
Refinement program	PHENIX (1.16_3549: ???)	Depositor
R, R_{free}	0.264 , 0.293 0.265 , 0.293	Depositor DCC
R_{free} test set	1719 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å ²)	49.4	Xtriage
Anisotropy	0.457	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 46.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.20$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	3403	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.07% of the height of the origin peak. No significant pseudotranslation is detected.*

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: NAP, A1D7V, FAD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.39	31/3337 (0.9%)	1.64	57/4547 (1.3%)

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	5

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	109	VAL	C-O	-8.07	1.15	1.23
1	A	13	LEU	C-O	-8.04	1.14	1.24
1	A	24	ILE	C-O	-7.61	1.15	1.24
1	A	112	ASP	CA-C	-7.45	1.42	1.53
1	A	16	GLY	C-O	-7.40	1.15	1.23
1	A	156	ALA	CA-C	7.33	1.62	1.52
1	A	25	SER	C-O	-7.25	1.15	1.23
1	A	214	VAL	CA-C	-6.56	1.46	1.52
1	A	5	VAL	C-O	-6.38	1.17	1.24
1	A	215	PRO	C-O	-6.31	1.16	1.23
1	A	58	THR	C-O	-6.21	1.16	1.23
1	A	136	VAL	CA-C	6.09	1.60	1.52
1	A	6	ILE	C-O	-6.05	1.16	1.23
1	A	248	LEU	CB-CG	-6.01	1.41	1.53
1	A	3	VAL	C-O	-6.01	1.17	1.24
1	A	397	GLY	C-O	-5.97	1.16	1.24
1	A	12	GLY	C-O	-5.90	1.16	1.23
1	A	214	VAL	C-O	-5.90	1.17	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	174	ASP	C-O	-5.87	1.16	1.24
1	A	72	ASP	N-CA	-5.84	1.39	1.46
1	A	415	ILE	CA-C	-5.75	1.45	1.52
1	A	171	ASP	CA-C	-5.73	1.45	1.52
1	A	24	ILE	CA-C	-5.56	1.46	1.52
1	A	108	SER	C-O	-5.56	1.17	1.23
1	A	254	ARG	CA-C	-5.53	1.46	1.52
1	A	227	ALA	N-CA	-5.43	1.38	1.46
1	A	110	ARG	C-O	-5.28	1.17	1.24
1	A	289	PRO	C-O	-5.25	1.17	1.23
1	A	24	ILE	CA-CB	-5.13	1.48	1.54
1	A	7	GLY	C-O	-5.12	1.17	1.23
1	A	14	ALA	N-CA	-5.01	1.39	1.46

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	207	VAL	CB-CA-C	-10.35	96.39	111.19
1	A	2	ARG	N-CA-C	9.97	121.91	111.14
1	A	346	VAL	N-CA-C	8.23	116.99	107.77
1	A	333	MET	N-CA-C	7.97	121.18	110.35
1	A	359	VAL	N-CA-C	7.66	119.63	109.21
1	A	332	PRO	CB-CA-C	7.35	123.69	111.56
1	A	387	PRO	CA-C-N	-6.38	111.11	120.75
1	A	387	PRO	C-N-CA	-6.38	111.11	120.75
1	A	332	PRO	N-CA-CB	-6.32	96.61	103.25
1	A	269	SER	N-CA-C	-6.28	105.20	112.92
1	A	151	PRO	N-CA-C	-6.25	99.59	112.47
1	A	406	ARG	N-CA-C	-6.23	105.99	113.97
1	A	381	ASP	CA-CB-CG	6.23	118.83	112.60
1	A	214	VAL	CA-C-N	-6.13	114.30	120.31
1	A	214	VAL	C-N-CA	-6.13	114.30	120.31
1	A	238	ASP	CB-CA-C	6.10	119.31	109.07
1	A	110	ARG	N-CA-C	6.02	123.62	110.80
1	A	112	ASP	CA-C-N	-5.97	111.03	122.61
1	A	112	ASP	C-N-CA	-5.97	111.03	122.61
1	A	411	GLU	N-CA-C	5.93	119.71	110.17
1	A	150	ASP	N-CA-CB	5.92	116.01	110.39
1	A	159	PHE	CA-CB-CG	5.89	119.69	113.80
1	A	303	PHE	N-CA-CB	-5.79	102.37	111.05
1	A	17	HIS	N-CA-C	-5.77	106.22	113.72
1	A	246	GLN	CB-CG-CD	-5.72	102.88	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	388	ALA	CA-C-N	5.65	128.12	120.38
1	A	388	ALA	C-N-CA	5.65	128.12	120.38
1	A	233	ASN	N-CA-C	-5.64	103.19	110.19
1	A	238	ASP	N-CA-C	-5.60	106.80	113.97
1	A	411	GLU	N-CA-CB	-5.60	101.51	110.63
1	A	299	ASP	CA-CB-CG	5.57	118.17	112.60
1	A	69	PRO	N-CA-CB	-5.53	98.53	103.35
1	A	191	ASP	CA-CB-CG	5.53	118.13	112.60
1	A	67	ASP	CB-CA-C	-5.53	100.86	110.09
1	A	360	ARG	CB-CA-C	-5.51	103.17	110.34
1	A	407	TYR	N-CA-C	-5.48	107.14	113.88
1	A	355	PHE	CA-CB-CG	5.45	119.25	113.80
1	A	410	THR	N-CA-C	-5.42	100.47	107.73
1	A	291	PRO	N-CA-CB	-5.41	97.57	103.25
1	A	328	PRO	N-CA-C	-5.37	101.41	112.47
1	A	405	GLN	CB-CA-C	5.36	118.02	109.02
1	A	347	PRO	N-CA-CB	-5.35	98.55	103.31
1	A	343	ARG	N-CA-C	-5.35	105.39	112.24
1	A	147	ALA	N-CA-C	5.34	117.91	108.24
1	A	55	HIS	CA-CB-CG	5.34	119.14	113.80
1	A	57	ASN	N-CA-C	-5.34	105.60	113.61
1	A	405	GLN	N-CA-CB	-5.27	103.89	110.90
1	A	317	CYS	CB-CA-C	5.24	118.92	111.74
1	A	246	GLN	CA-C-N	5.18	128.59	120.82
1	A	246	GLN	C-N-CA	5.18	128.59	120.82
1	A	40	ARG	N-CA-CB	-5.17	102.58	110.33
1	A	413	ALA	N-CA-C	-5.16	106.94	113.18
1	A	180	VAL	N-CA-C	5.15	117.26	108.86
1	A	42	PRO	N-CA-C	-5.11	101.94	112.47
1	A	297	ASP	CA-CB-CG	5.03	117.63	112.60
1	A	284	HIS	CA-CB-CG	5.02	118.82	113.80
1	A	230	PRO	N-CA-C	-5.01	107.01	113.57

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	103	ARG	Sidechain
1	A	281	ARG	Sidechain
1	A	367	ARG	Sidechain
1	A	406	ARG	Sidechain
1	A	409	ARG	Sidechain

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	3255	0	3190	91	0
2	A	53	0	31	1	0
3	A	48	0	25	0	0
4	A	18	0	0	1	0
5	A	29	0	0	2	0
All	All	3403	0	3246	91	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 14.

All (91) 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:56:LEU:HD12	1:A:78:PRO:HD2	1.32	1.12
1:A:47:ARG:HD2	1:A:168:ASP:HA	1.51	0.92
1:A:387:PRO:HG2	1:A:392:MET:HG3	1.50	0.91
1:A:368:LEU:HD11	1:A:419:VAL:HG12	1.61	0.83
1:A:358:LEU:O	1:A:415:ILE:HB	1.82	0.80
1:A:360:ARG:HB2	1:A:415:ILE:CD1	2.15	0.76
1:A:368:LEU:HA	1:A:423:LEU:HD11	1.70	0.71
1:A:331:CYS:O	1:A:333:MET:N	2.29	0.66
1:A:360:ARG:HB2	1:A:415:ILE:HD11	1.78	0.65
1:A:331:CYS:O	1:A:332:PRO:C	2.40	0.65
1:A:2:ARG:HB2	1:A:25:SER:HB3	1.78	0.65
1:A:226:ILE:HD11	4:A:503:A1D7V:CAQ	2.27	0.65
1:A:30:GLU:HG3	1:A:32:ALA:H	1.61	0.64
1:A:331:CYS:HB3	1:A:332:PRO:HD2	1.79	0.64
1:A:118:THR:HG22	1:A:132:ARG:HG3	1.79	0.64
1:A:326:PHE:O	1:A:328:PRO:HD3	1.97	0.63
1:A:291:PRO:HG2	1:A:303:PHE:HB3	1.80	0.62
1:A:418:ASP:HB3	1:A:421:PRO:HD2	1.80	0.62
1:A:360:ARG:HB2	1:A:415:ILE:HD12	1.81	0.62
1:A:387:PRO:HG2	1:A:392:MET:CG	2.27	0.61
1:A:244:VAL:HA	1:A:247:ALA:HB3	1.84	0.60
1:A:182:VAL:HG23	1:A:205:LEU:HA	1.84	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:334:SER:HB3	1:A:340:GLU:OE1	2.01	0.59
1:A:11:SER:HA	1:A:369:VAL:HG11	1.84	0.59
1:A:182:VAL:HG21	1:A:193:ALA:HB2	1.85	0.59
1:A:347:PRO:HG3	1:A:353:LEU:HB3	1.86	0.58
1:A:415:ILE:HD12	1:A:415:ILE:O	2.04	0.57
1:A:360:ARG:N	1:A:415:ILE:HD12	2.20	0.56
1:A:8:ALA:HB2	1:A:28:CYS:SG	2.47	0.55
1:A:26:PHE:C	1:A:26:PHE:CD1	2.84	0.55
1:A:244:VAL:HG11	1:A:267:VAL:HG21	1.88	0.54
1:A:331:CYS:C	1:A:333:MET:N	2.64	0.54
1:A:289:PRO:O	1:A:290:LYS:HD2	2.09	0.53
1:A:233:ASN:HA	1:A:240:ARG:HH21	1.73	0.53
1:A:37:GLY:HA2	2:A:501:FAD:O3B	2.09	0.52
1:A:347:PRO:HB2	1:A:350:ARG:HD2	1.91	0.52
1:A:297:ASP:O	1:A:298:GLY:C	2.54	0.51
1:A:2:ARG:HD3	1:A:24:ILE:HG23	1.92	0.51
1:A:365:ILE:HA	1:A:368:LEU:HD13	1.91	0.51
1:A:149:PRO:HD3	1:A:318:THR:HG21	1.93	0.50
1:A:40:ARG:HH22	1:A:46:GLU:CD	2.20	0.50
1:A:149:PRO:HG2	1:A:152:LEU:HD23	1.94	0.50
1:A:264:ASP:OD1	1:A:264:ASP:N	2.44	0.49
1:A:365:ILE:O	1:A:366:THR:C	2.54	0.49
1:A:40:ARG:NH2	1:A:46:GLU:OE2	2.46	0.49
1:A:114:ASP:C	1:A:116:PRO:HD3	2.38	0.49
1:A:343:ARG:NH2	1:A:425:GLU:O	2.47	0.48
1:A:245:GLU:O	1:A:249:LEU:HG	2.14	0.47
1:A:410:THR:HG22	1:A:411:GLU:H	1.79	0.47
1:A:109:VAL:O	1:A:328:PRO:HD2	2.15	0.47
1:A:346:VAL:HA	1:A:347:PRO:HD2	1.67	0.47
1:A:248:LEU:O	1:A:252:ARG:HG3	2.15	0.46
1:A:79:ARG:HE	1:A:81:SER:HB3	1.80	0.46
1:A:47:ARG:HA	1:A:47:ARG:HD3	1.52	0.46
1:A:150:ASP:HB3	1:A:151:PRO:HD3	1.97	0.46
1:A:170:ARG:HD3	1:A:174:ASP:OD2	2.16	0.45
1:A:329:ALA:O	1:A:330:GLY:C	2.59	0.45
1:A:242:ARG:O	1:A:243:TRP:C	2.59	0.45
1:A:343:ARG:HH21	1:A:425:GLU:HB2	1.82	0.44
1:A:135:GLN:OE1	1:A:354:TYR:HE2	2.01	0.44
1:A:218:LEU:HD23	1:A:247:ALA:HB1	1.99	0.44
1:A:375:TRP:O	1:A:379:LEU:HG	2.17	0.44
1:A:291:PRO:CG	1:A:303:PHE:HB3	2.48	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:TRP:O	1:A:235:MET:HB2	2.18	0.43
1:A:288:THR:HA	1:A:289:PRO:HD2	1.89	0.43
1:A:358:LEU:HD12	1:A:358:LEU:HA	1.90	0.43
1:A:226:ILE:C	1:A:228:GLU:N	2.74	0.43
1:A:267:VAL:C	1:A:269:SER:H	2.27	0.43
1:A:60:LYS:NZ	5:A:608:HOH:O	2.51	0.42
1:A:102:LEU:O	1:A:103:ARG:C	2.62	0.42
1:A:153:PRO:HB2	1:A:296:PHE:HE1	1.83	0.42
1:A:164:LEU:HG	1:A:315:VAL:HA	2.02	0.42
1:A:2:ARG:HB2	1:A:25:SER:CB	2.47	0.42
1:A:97:LEU:C	1:A:99:HIS:N	2.75	0.42
1:A:365:ILE:O	1:A:368:LEU:N	2.47	0.42
1:A:344:ARG:O	5:A:601:HOH:O	2.22	0.41
1:A:226:ILE:C	1:A:228:GLU:H	2.27	0.41
1:A:337:GLY:O	1:A:338:SER:C	2.63	0.41
1:A:400:LEU:C	1:A:402:GLY:N	2.77	0.41
1:A:100:VAL:HG12	1:A:102:LEU:HD22	2.02	0.41
1:A:408:GLY:O	1:A:409:ARG:C	2.63	0.41
1:A:146:PRO:HB2	1:A:165:HIS:CD2	2.55	0.41
1:A:187:ALA:HA	1:A:190:VAL:HG22	2.03	0.41
1:A:233:ASN:C	1:A:235:MET:N	2.78	0.41
1:A:247:ALA:O	1:A:250:VAL:HG12	2.19	0.41
1:A:368:LEU:HG	1:A:423:LEU:HD13	2.03	0.41
1:A:411:GLU:C	1:A:413:ALA:N	2.79	0.40
1:A:204:LEU:HD22	1:A:290:LYS:HD3	2.03	0.40
1:A:331:CYS:C	1:A:333:MET:H	2.28	0.40
1:A:52:ARG:HH22	1:A:79:ARG:HH22	1.70	0.40
1:A:403:ILE:HD13	1:A:403:ILE:HA	1.83	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	424/432 (98%)	382 (90%)	38 (9%)	4 (1%)	14 20

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	329	ALA
1	A	335	ALA
1	A	298	GLY
1	A	291	PRO

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	334/340 (98%)	272 (81%)	62 (19%)	1 1

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	LEU
1	A	27	VAL
1	A	38	ILE
1	A	47	ARG
1	A	51	TYR
1	A	60	LYS
1	A	67	ASP
1	A	97	LEU
1	A	125	ASP
1	A	129	VAL
1	A	130	SER
1	A	132	ARG
1	A	144	ASN
1	A	145	GLU
1	A	152	LEU
1	A	153	PRO
1	A	163	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	166	SER
1	A	167	LEU
1	A	179	ARG
1	A	182	VAL
1	A	197	SER
1	A	201	GLU
1	A	202	ARG
1	A	207	VAL
1	A	208	ARG
1	A	217	GLN
1	A	221	MET
1	A	222	SER
1	A	223	VAL
1	A	228	GLU
1	A	235	MET
1	A	236	SER
1	A	238	ASP
1	A	252	ARG
1	A	264	ASP
1	A	267	VAL
1	A	269	SER
1	A	270	SER
1	A	278	ILE
1	A	287	VAL
1	A	290	LYS
1	A	299	ASP
1	A	309	GLU
1	A	315	VAL
1	A	318	THR
1	A	322	MET
1	A	336	ASP
1	A	338	SER
1	A	339	VAL
1	A	346	VAL
1	A	349	ASP
1	A	350	ARG
1	A	380	VAL
1	A	398	THR
1	A	403	ILE
1	A	404	VAL
1	A	405	GLN
1	A	406	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	409	ARG
1	A	419	VAL
1	A	423	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	212	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

3 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	FAD	A	501	-	58,58,58	0.64	0	85,89,89	0.76	2 (2%)
3	NAP	A	502	-	50,52,52	0.64	1 (2%)	71,80,80	0.94	1 (1%)
4	A1D7V	A	503	-	18,19,19	4.86	12 (66%)	24,25,25	3.26	6 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	A	501	-	-	2/34/50/50	0/6/6/6
3	NAP	A	502	-	-	14/35/67/67	0/5/5/5
4	A1D7V	A	503	-	-	0/7/9/9	0/2/2/2

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	503	A1D7V	CAL-NAB	8.72	1.34	1.26
4	A	503	A1D7V	CAN-CAO	7.74	1.55	1.32
4	A	503	A1D7V	CAG-CAF	-7.47	1.32	1.41
4	A	503	A1D7V	CAM-CAD	-7.17	1.39	1.52
4	A	503	A1D7V	CAG-CAJ	-7.07	1.32	1.44
4	A	503	A1D7V	OAR-NAB	-6.19	1.27	1.40
4	A	503	A1D7V	CAH-CAG	-5.39	1.31	1.39
4	A	503	A1D7V	CAF-NAA	-3.87	1.31	1.37
4	A	503	A1D7V	CAI-NAA	-3.72	1.31	1.37
4	A	503	A1D7V	CAI-CAJ	-3.62	1.31	1.36
4	A	503	A1D7V	CAE-CAF	-3.51	1.34	1.39
3	A	502	NAP	C2N-N1N	2.79	1.38	1.35
4	A	503	A1D7V	CAM-CAN	2.52	1.56	1.50

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	503	A1D7V	OAR-NAB-CAL	11.04	122.05	111.70
4	A	503	A1D7V	CAM-CAN-CAO	-8.54	112.86	127.52
3	A	502	NAP	P2B-O2B-C2B	-5.73	108.14	123.43
4	A	503	A1D7V	CAJ-CAI-NAA	-3.44	106.53	110.31
4	A	503	A1D7V	CAM-CAD-CAE	3.42	126.81	120.51
4	A	503	A1D7V	CAD-CAM-CAN	3.02	121.11	114.04
4	A	503	A1D7V	CAG-CAJ-CAI	2.86	109.09	106.16
2	A	501	FAD	C4'-C3'-C2'	2.49	117.72	113.57
2	A	501	FAD	C2B-C1B-N9A	-2.12	108.03	113.30

There are no chirality outliers.

All (16) torsion outliers are listed below:

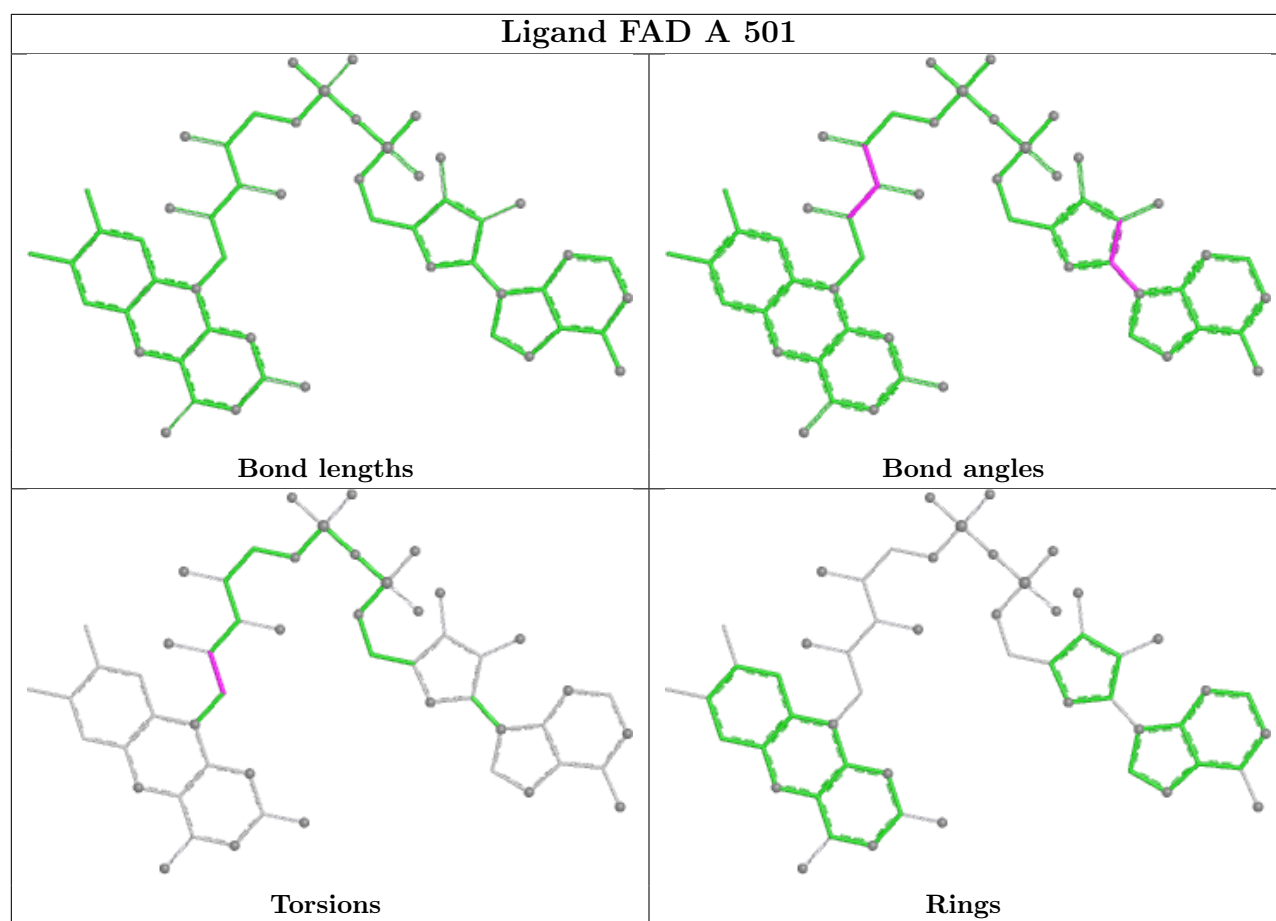
Mol	Chain	Res	Type	Atoms
2	A	501	FAD	N10-C1'-C2'-C3'
3	A	502	NAP	PA-O3-PN-O5D
3	A	502	NAP	C5D-O5D-PN-O3
3	A	502	NAP	C5D-O5D-PN-O2N
3	A	502	NAP	C2N-C3N-C7N-N7N
3	A	502	NAP	C2N-C3N-C7N-O7N
3	A	502	NAP	C4N-C3N-C7N-N7N
3	A	502	NAP	C4N-C3N-C7N-O7N
3	A	502	NAP	O4D-C4D-C5D-O5D
3	A	502	NAP	C3D-C4D-C5D-O5D
3	A	502	NAP	O4B-C4B-C5B-O5B
3	A	502	NAP	C3B-C4B-C5B-O5B
2	A	501	FAD	N10-C1'-C2'-O2'
3	A	502	NAP	C5B-O5B-PA-O1A
3	A	502	NAP	PA-O3-PN-O1N
3	A	502	NAP	PA-O3-PN-O2N

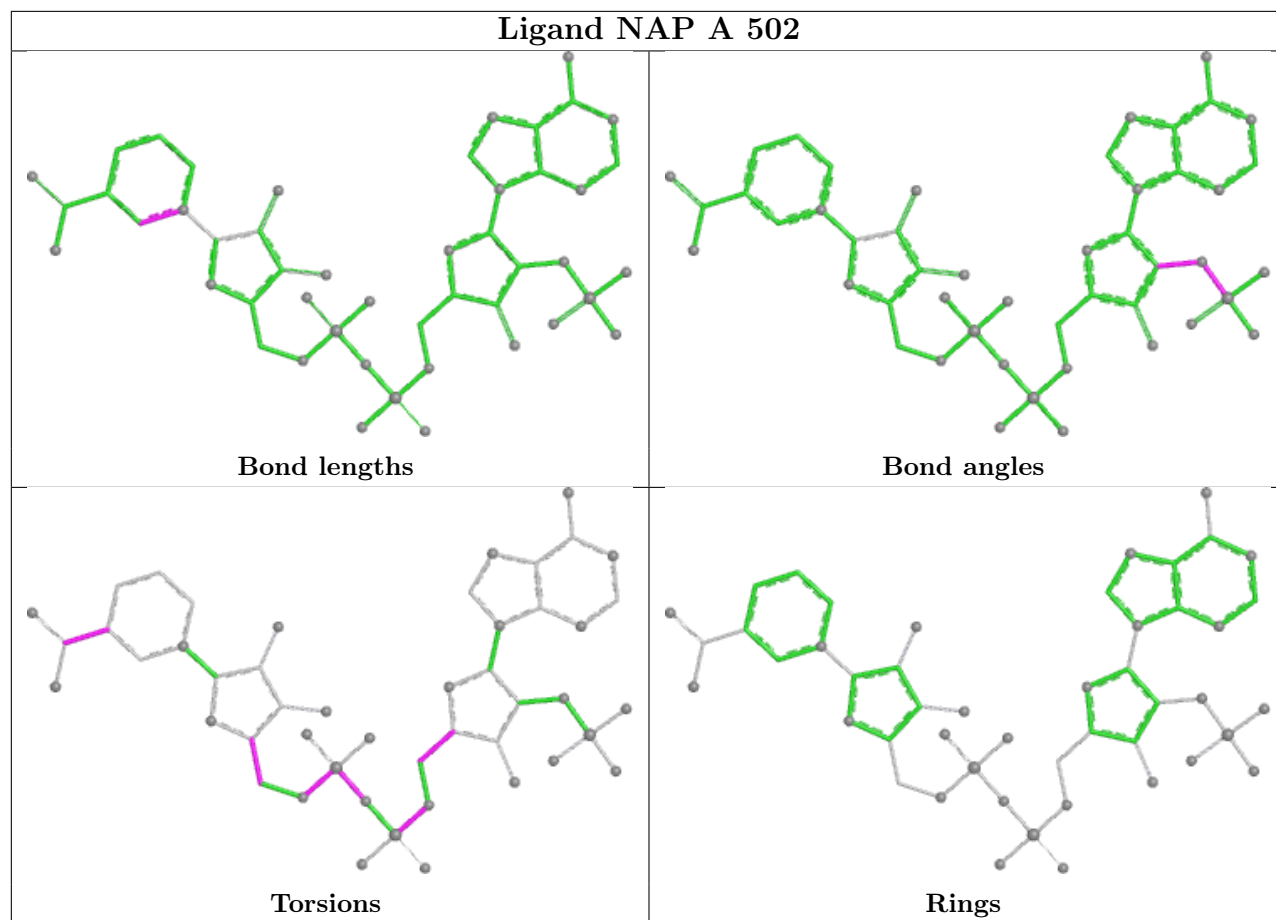
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	FAD	1	0
4	A	503	A1D7V	1	0

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

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	426/432 (98%)	0.51	13 (3%) 51 52	30, 49, 75, 95	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	335	ALA	3.7
1	A	358	LEU	3.6
1	A	151	PRO	3.5
1	A	331	CYS	3.5
1	A	27	VAL	3.5
1	A	207	VAL	2.5
1	A	124	ALA	2.4
1	A	271	ALA	2.2
1	A	329	ALA	2.2
1	A	425	GLU	2.2
1	A	315	VAL	2.2
1	A	336	ASP	2.2
1	A	120	VAL	2.1

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](#)

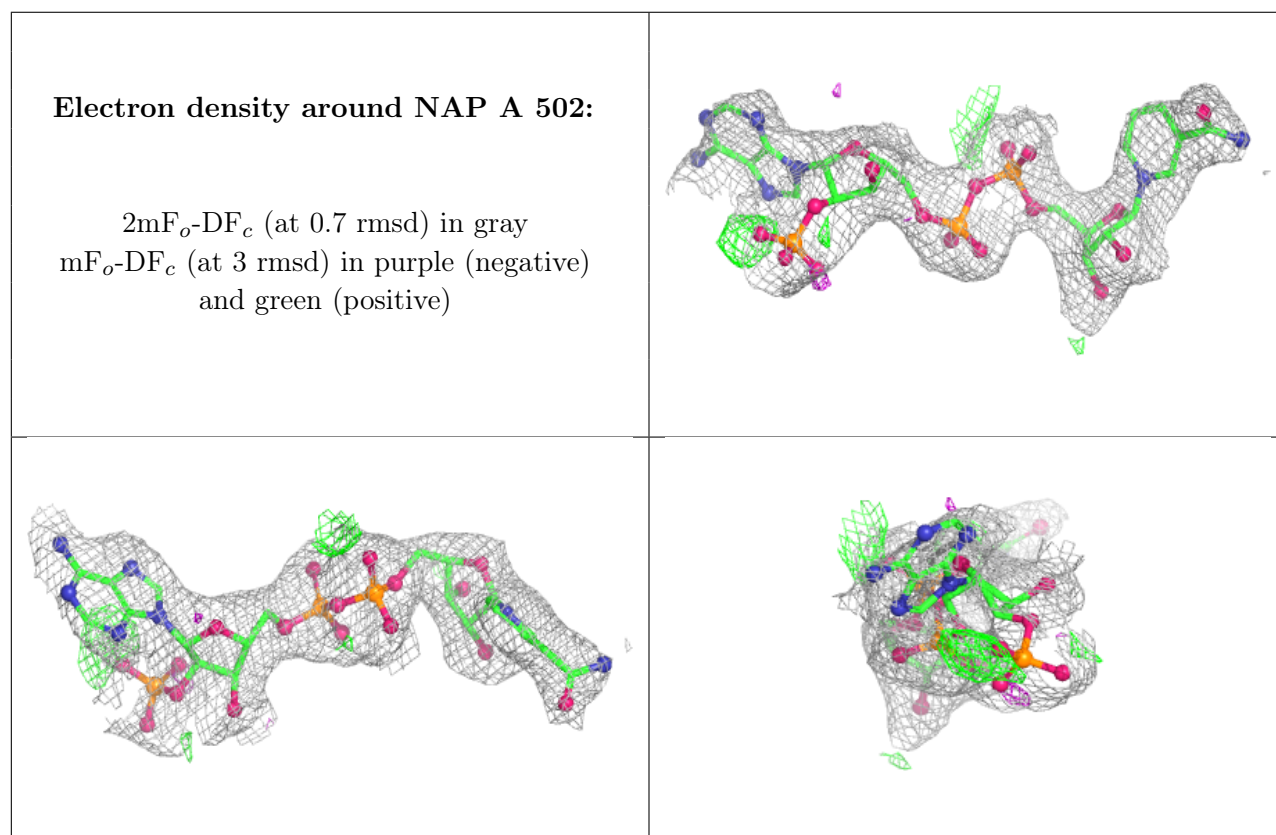
There are no oligosaccharides in this entry.

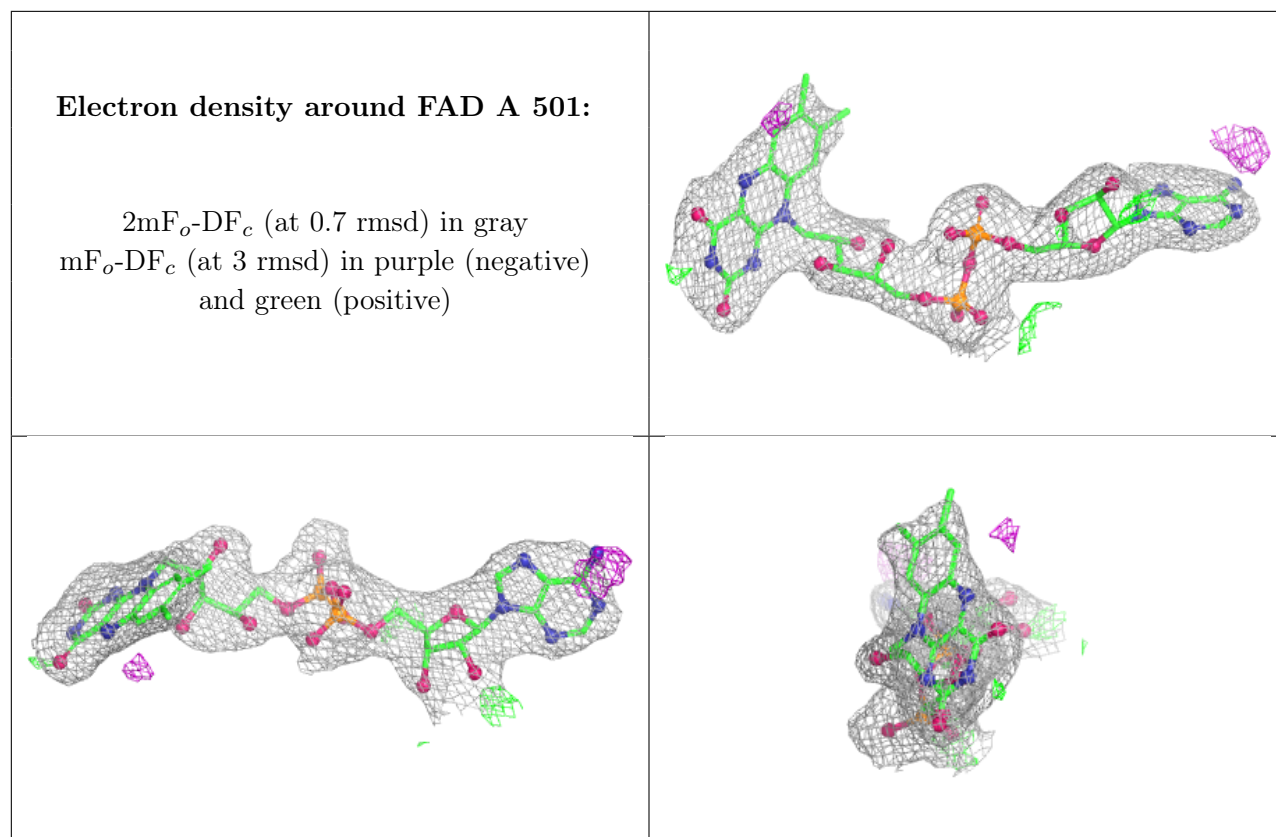
6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	A1D7V	A	503	18/18	0.58	0.22	42,64,67,67	0
3	NAP	A	502	48/48	0.89	0.11	42,54,79,81	0
2	FAD	A	501	53/53	0.94	0.09	39,47,55,56	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.