



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 8, 2024 – 07:55 am GMT

PDB ID : 5NMX
Title : Crystal Structure of the pyrrolizidine alkaloid N-oxygenase from *Zonocerus variegatus* in complex with FAD and NADP+
Authors : Scheidig, A.; Kubitzka, C.; Faust, A.; Ober, D.
Deposited on : 2017-04-07
Resolution : 1.60 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 : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

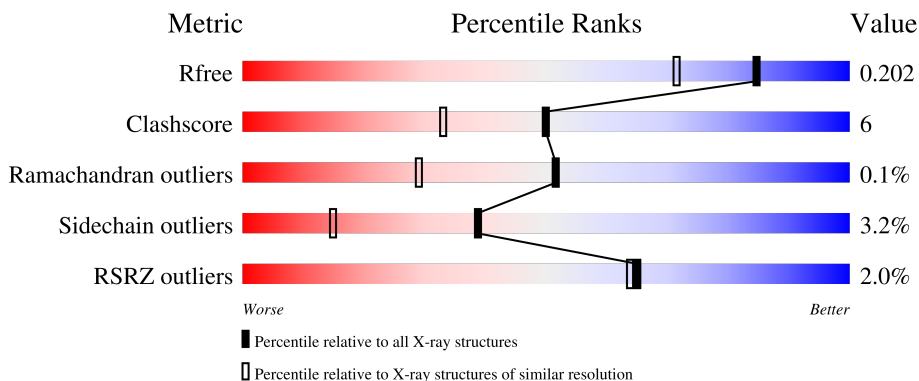
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

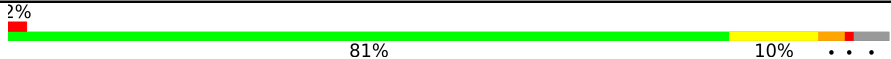



The reported resolution of this entry is 1.60 Å.

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	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	425	 2% 81% 10% . . .
1	B	425	 2% 85% 9% . .
1	C	425	 2% 82% 13% . .
1	D	425	 2% 83% 12% . .

2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 15289 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	406	3323	2138	552	608	25	0	1	0
1	B	407	3323	2139	550	609	25	0	0	0
1	C	406	3323	2138	552	608	25	0	1	0
1	D	409	3341	2148	556	612	25	0	1	0

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	414	TYR	-	expression tag	UNP L0N8S9
A	415	ALA	-	expression tag	UNP L0N8S9
A	416	ALA	-	expression tag	UNP L0N8S9
A	417	ALA	-	expression tag	UNP L0N8S9
A	418	LEU	-	expression tag	UNP L0N8S9
A	419	GLU	-	expression tag	UNP L0N8S9
A	420	HIS	-	expression tag	UNP L0N8S9
A	421	HIS	-	expression tag	UNP L0N8S9
A	422	HIS	-	expression tag	UNP L0N8S9
A	423	HIS	-	expression tag	UNP L0N8S9
A	424	HIS	-	expression tag	UNP L0N8S9
A	425	HIS	-	expression tag	UNP L0N8S9
B	414	TYR	-	expression tag	UNP L0N8S9
B	415	ALA	-	expression tag	UNP L0N8S9
B	416	ALA	-	expression tag	UNP L0N8S9
B	417	ALA	-	expression tag	UNP L0N8S9
B	418	LEU	-	expression tag	UNP L0N8S9
B	419	GLU	-	expression tag	UNP L0N8S9
B	420	HIS	-	expression tag	UNP L0N8S9
B	421	HIS	-	expression tag	UNP L0N8S9
B	422	HIS	-	expression tag	UNP L0N8S9

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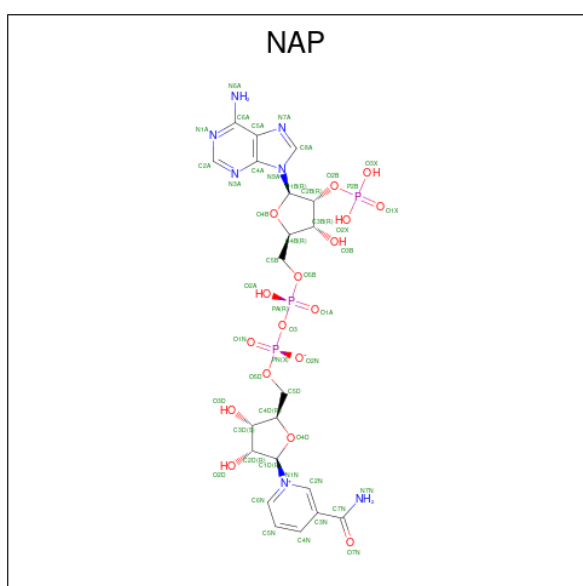
Chain	Residue	Modelled	Actual	Comment	Reference
B	423	HIS	-	expression tag	UNP L0N8S9
B	424	HIS	-	expression tag	UNP L0N8S9
B	425	HIS	-	expression tag	UNP L0N8S9
C	414	TYR	-	expression tag	UNP L0N8S9
C	415	ALA	-	expression tag	UNP L0N8S9
C	416	ALA	-	expression tag	UNP L0N8S9
C	417	ALA	-	expression tag	UNP L0N8S9
C	418	LEU	-	expression tag	UNP L0N8S9
C	419	GLU	-	expression tag	UNP L0N8S9
C	420	HIS	-	expression tag	UNP L0N8S9
C	421	HIS	-	expression tag	UNP L0N8S9
C	422	HIS	-	expression tag	UNP L0N8S9
C	423	HIS	-	expression tag	UNP L0N8S9
C	424	HIS	-	expression tag	UNP L0N8S9
C	425	HIS	-	expression tag	UNP L0N8S9
D	414	TYR	-	expression tag	UNP L0N8S9
D	415	ALA	-	expression tag	UNP L0N8S9
D	416	ALA	-	expression tag	UNP L0N8S9
D	417	ALA	-	expression tag	UNP L0N8S9
D	418	LEU	-	expression tag	UNP L0N8S9
D	419	GLU	-	expression tag	UNP L0N8S9
D	420	HIS	-	expression tag	UNP L0N8S9
D	421	HIS	-	expression tag	UNP L0N8S9
D	422	HIS	-	expression tag	UNP L0N8S9
D	423	HIS	-	expression tag	UNP L0N8S9
D	424	HIS	-	expression tag	UNP L0N8S9
D	425	HIS	-	expression tag	UNP L0N8S9

- 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		
			Total	C	N	O			P	
2	A	1	Total	53	27	9	15	2	0	0
2	B	1	Total	53	27	9	15	2	0	0
2	C	1	Total	53	27	9	15	2	0	0
2	D	1	Total	53	27	9	15	2	0	0

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).



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		
3	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Mg	0	0
			1	1		
4	C	1	Total	Mg	0	0
			1	1		
4	D	1	Total	Mg	0	0
			1	1		

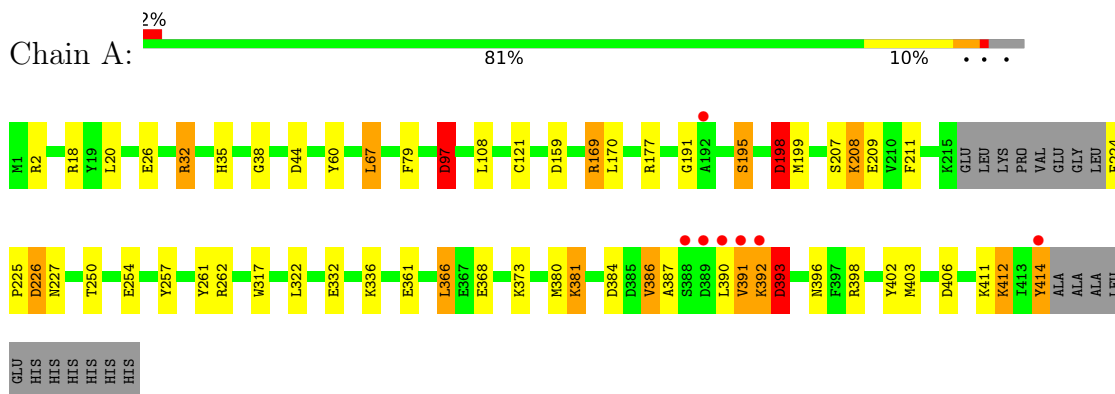
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	402	Total	O	0	0
			402	402		
5	B	448	Total	O	0	0
			448	448		
5	C	371	Total	O	0	0
			371	371		
5	D	351	Total	O	0	0
			351	351		

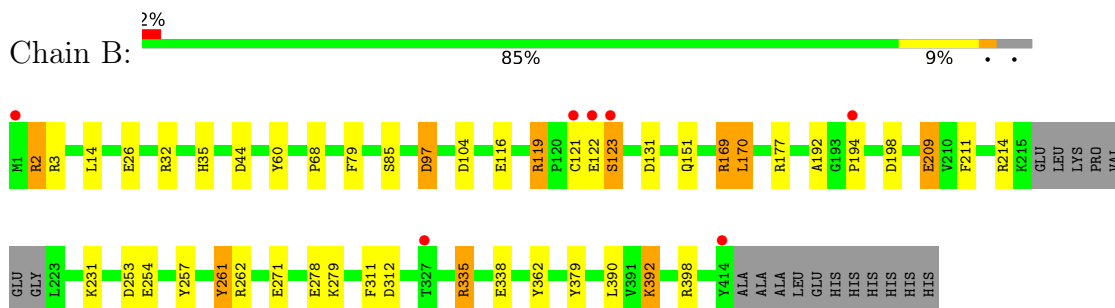
3 Residue-property plots

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.

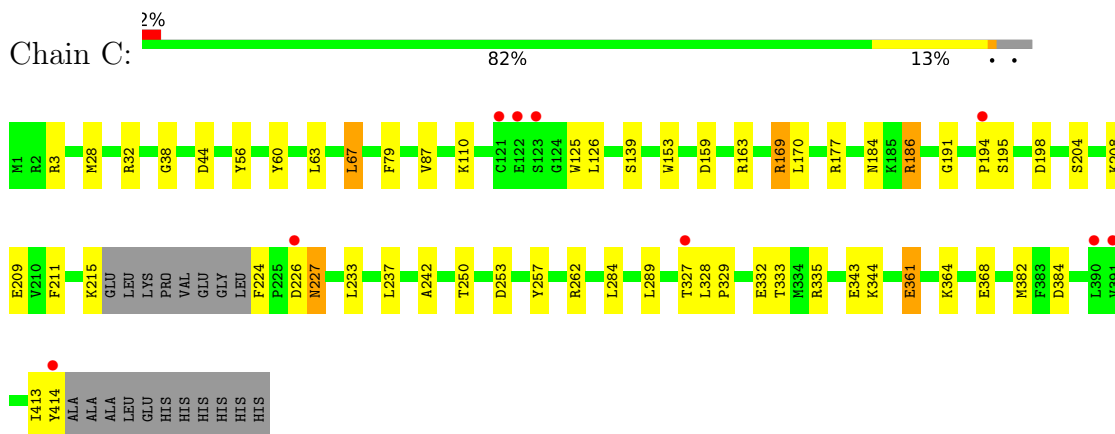
- Molecule 1: Flavin-containing monooxygenase



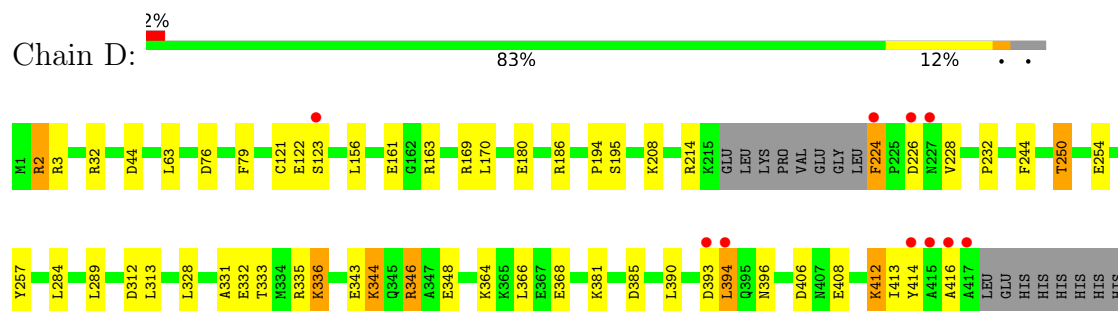
- Molecule 1: Flavin-containing monooxygenase



- Molecule 1: Flavin-containing monooxygenase



● Molecule 1: Flavin-containing monooxygenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	74.08Å 76.08Å 81.67Å 71.81° 81.64° 82.04°	Depositor
Resolution (Å)	77.13 – 1.60 77.13 – 1.60	Depositor EDS
% Data completeness (in resolution range)	96.1 (77.13-1.60) 96.1 (77.13-1.60)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.38 (at 1.59Å)	Xtrriage
Refinement program	REFMAC 5.7.0032, REFMAC 5.7.0032	Depositor
R, R_{free}	0.174 , 0.202 0.173 , 0.202	Depositor DCC
R_{free} test set	10741 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	17.2	Xtrriage
Anisotropy	0.071	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 37.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	15289	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.32% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	1.24	8/3422 (0.2%)	1.25	23/4639 (0.5%)
1	B	1.19	5/3419 (0.1%)	1.19	18/4636 (0.4%)
1	C	1.18	3/3422 (0.1%)	1.20	15/4639 (0.3%)
1	D	1.13	0/3437	1.15	8/4660 (0.2%)
All	All	1.19	16/13700 (0.1%)	1.20	64/18574 (0.3%)

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	1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	60	TYR	CE1-CZ	7.58	1.48	1.38
1	A	332	GLU	CD-OE1	6.54	1.32	1.25
1	B	362	TYR	CE2-CZ	6.31	1.46	1.38
1	A	332	GLU	CD-OE2	6.30	1.32	1.25
1	C	56	TYR	CE1-CZ	5.82	1.46	1.38
1	C	153	TRP	CE3-CZ3	5.50	1.47	1.38
1	B	209	GLU	CD-OE2	5.42	1.31	1.25
1	A	225	PRO	N-CD	5.39	1.55	1.47
1	A	317	TRP	N-CA	5.33	1.57	1.46
1	B	271	GLU	CG-CD	5.29	1.59	1.51
1	B	379	TYR	CZ-OH	5.27	1.46	1.37
1	A	257	TYR	CG-CD1	-5.26	1.32	1.39
1	A	195	SER	CA-CB	5.17	1.60	1.52
1	B	338	GLU	CD-OE1	5.14	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	125	TRP	CB-CG	-5.14	1.41	1.50
1	A	361	GLU	CG-CD	5.04	1.59	1.51

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	18	ARG	NE-CZ-NH1	9.72	125.16	120.30
1	A	18	ARG	NE-CZ-NH2	-9.03	115.78	120.30
1	B	44	ASP	CB-CG-OD1	8.85	126.26	118.30
1	A	97	ASP	CB-CG-OD2	-8.82	110.37	118.30
1	A	366	LEU	CB-CG-CD1	8.15	124.86	111.00
1	B	253	ASP	CB-CG-OD2	7.75	125.28	118.30
1	A	393	ASP	N-CA-CB	-7.65	96.82	110.60
1	C	186[A]	ARG	NE-CZ-NH1	-7.62	116.49	120.30
1	C	186[B]	ARG	NE-CZ-NH1	-7.62	116.49	120.30
1	A	393	ASP	N-CA-C	7.38	130.91	111.00
1	D	366	LEU	CB-CG-CD2	7.19	123.22	111.00
1	D	76	ASP	CB-CG-OD1	7.16	124.74	118.30
1	A	67	LEU	CA-CB-CG	7.13	131.69	115.30
1	B	116	GLU	OE1-CD-OE2	-6.96	114.95	123.30
1	C	335	ARG	NE-CZ-NH2	-6.73	116.93	120.30
1	B	262	ARG	NE-CZ-NH2	-6.67	116.97	120.30
1	C	382	MET	CG-SD-CE	6.62	110.80	100.20
1	C	67	LEU	CA-CB-CG	6.56	130.40	115.30
1	C	44	ASP	CB-CG-OD1	6.54	124.19	118.30
1	A	406	ASP	CB-CG-OD1	6.49	124.14	118.30
1	D	44	ASP	CB-CG-OD1	6.46	124.11	118.30
1	B	312	ASP	CB-CG-OD2	-6.34	112.59	118.30
1	C	253	ASP	CB-CG-OD2	6.23	123.90	118.30
1	D	406	ASP	CB-CG-OD1	6.18	123.86	118.30
1	C	177	ARG	NE-CZ-NH2	-6.09	117.26	120.30
1	D	156	LEU	CB-CG-CD2	-5.93	100.92	111.00
1	A	44	ASP	CB-CG-OD2	-5.90	112.99	118.30
1	B	169	ARG	NE-CZ-NH2	-5.85	117.37	120.30
1	B	311	PHE	CB-CG-CD2	-5.83	116.72	120.80
1	B	177	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	A	169	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	A	177	ARG	NE-CZ-NH2	-5.68	117.46	120.30
1	B	131	ASP	CB-CG-OD1	5.67	123.40	118.30
1	B	312	ASP	CB-CG-OD1	5.67	123.40	118.30
1	B	261	TYR	CG-CD1-CE1	-5.63	116.80	121.30
1	A	44	ASP	CB-CG-OD1	5.62	123.36	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	261	TYR	CD1-CE1-CZ	-5.59	114.77	119.80
1	D	312	ASP	CB-CG-OD1	5.53	123.28	118.30
1	C	253	ASP	CB-CG-OD1	-5.53	113.33	118.30
1	A	261	TYR	CZ-CE2-CD2	5.53	124.77	119.80
1	A	198	ASP	CB-CA-C	5.51	121.42	110.40
1	D	406	ASP	CB-CG-OD2	-5.44	113.41	118.30
1	C	169	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	A	97	ASP	CB-CG-OD1	5.39	123.16	118.30
1	B	97	ASP	CB-CG-OD2	-5.38	113.46	118.30
1	B	231	LYS	CD-CE-NZ	-5.36	99.38	111.70
1	B	335	ARG	NE-CZ-NH1	-5.36	117.62	120.30
1	B	14	LEU	CB-CG-CD2	5.35	120.10	111.00
1	C	186[A]	ARG	NE-CZ-NH2	5.30	122.95	120.30
1	C	186[B]	ARG	NE-CZ-NH2	5.30	122.95	120.30
1	B	104	ASP	CB-CG-OD2	-5.29	113.53	118.30
1	B	177	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	C	87	VAL	CG1-CB-CG2	-5.27	102.47	110.90
1	D	44	ASP	CB-CG-OD2	-5.24	113.59	118.30
1	A	108	LEU	CB-CG-CD1	-5.23	102.11	111.00
1	A	224	PHE	C-N-CD	5.22	139.37	128.40
1	A	67	LEU	CB-CG-CD2	-5.20	102.15	111.00
1	A	412	LYS	CB-CA-C	-5.20	100.00	110.40
1	C	262	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	B	398	ARG	NE-CZ-NH2	-5.15	117.72	120.30
1	A	20	LEU	CB-CG-CD1	-5.12	102.30	111.00
1	A	322	LEU	CB-CG-CD1	-5.12	102.30	111.00
1	A	384	ASP	CB-CG-OD1	5.03	122.82	118.30
1	C	384	ASP	CB-CG-OD1	5.02	122.82	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	32	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	3323	0	3212	53	0
1	B	3323	0	3210	27	0
1	C	3323	0	3212	40	0
1	D	3341	0	3226	40	0
2	A	53	0	31	1	0
2	B	53	0	31	1	0
2	C	53	0	31	2	0
2	D	53	0	31	1	0
3	A	48	0	25	2	0
3	B	48	0	25	4	0
3	C	48	0	25	6	0
3	D	48	0	25	2	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	402	0	0	13	0
5	B	448	0	0	6	0
5	C	371	0	0	5	0
5	D	351	0	0	6	0
All	All	15289	0	13084	155	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 (155) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:343:GLU:HA	1:D:346:ARG:NH1	1.85	0.92
1:B:170:LEU:HD21	1:B:257:TYR:HE2	1.36	0.90
1:A:403:MET:HE2	1:A:411:LYS:HE3	1.51	0.90
1:D:343:GLU:HA	1:D:346:ARG:HH12	1.38	0.87
1:B:170:LEU:HD21	1:B:257:TYR:CE2	2.11	0.85
1:B:214:ARG:HG3	5:B:850:HOH:O	1.75	0.84
1:D:393:ASP:OD2	1:D:396:ASN:HB2	1.76	0.83
1:D:3[A]:ARG:NH1	5:D:601:HOH:O	2.06	0.83
1:A:403:MET:CE	1:A:411:LYS:HE3	2.09	0.82
1:D:412:LYS:O	1:D:413:ILE:HG23	1.79	0.81
3:C:502:NAP:O2D	5:C:601:HOH:O	1.78	0.81
1:A:402:TYR:HE1	1:A:412:LYS:HG2	1.46	0.81
1:A:198:ASP:HB3	5:A:606:HOH:O	1.81	0.79
1:B:335:ARG:HD3	5:B:601:HOH:O	1.81	0.79
1:A:402:TYR:CE1	1:A:412:LYS:HD3	2.18	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:390:LEU:HA	5:A:641:HOH:O	1.83	0.78
1:C:169:ARG:NH2	5:C:603:HOH:O	2.16	0.78
1:D:180:GLU:HG2	5:D:878:HOH:O	1.82	0.78
1:A:402:TYR:CE1	1:A:412:LYS:HG2	2.20	0.77
1:A:402:TYR:HE1	1:A:412:LYS:CG	1.99	0.76
1:A:402:TYR:HE1	1:A:412:LYS:CD	1.99	0.75
1:A:380:MET:CE	1:D:332:GLU:HG3	2.18	0.74
1:A:402:TYR:HE1	1:A:412:LYS:HD3	1.52	0.74
1:D:224:PHE:CD1	1:D:224:PHE:N	2.56	0.72
1:B:35:HIS:CE1	1:B:97:ASP:OD2	2.43	0.71
1:C:343:GLU:OE2	5:C:602:HOH:O	2.09	0.70
1:B:3:ARG:HD2	1:B:26:GLU:OE2	1.92	0.69
1:D:333:THR:HG23	1:D:336:LYS:HE3	1.76	0.67
1:D:331:ALA:O	1:D:335:ARG:HG3	1.94	0.67
1:C:204:SER:O	1:C:227:ASN:OD1	2.13	0.66
1:A:169:ARG:NH1	1:A:254:GLU:OE1	2.29	0.66
1:C:170:LEU:HD22	1:C:257:TYR:HE2	1.61	0.66
1:A:387:ALA:HA	1:A:390:LEU:HD12	1.76	0.66
1:B:35:HIS:HE1	1:B:97:ASP:OD2	1.79	0.66
1:D:169:ARG:HD3	1:D:254:GLU:OE1	1.95	0.66
1:C:204:SER:HB2	1:C:227:ASN:HB3	1.78	0.66
1:A:392:LYS:HB3	1:A:393:ASP:HB2	1.77	0.65
1:C:170:LEU:HD11	5:C:763:HOH:O	1.96	0.65
1:D:170:LEU:HD11	1:D:257:TYR:HE2	1.61	0.65
1:C:186[A]:ARG:HG3	1:C:208:LYS:HE3	1.79	0.65
1:A:373:LYS:HE3	5:A:613:HOH:O	1.97	0.64
1:A:226:ASP:OD2	1:C:414:TYR:CB	2.46	0.63
1:B:198:ASP:HB3	5:B:614:HOH:O	1.98	0.63
1:B:60:TYR:OH	3:B:502:NAP:H4N	1.99	0.62
1:D:170:LEU:HD11	1:D:257:TYR:CE2	2.35	0.61
1:A:262[B]:ARG:NH2	5:A:603:HOH:O	2.33	0.61
1:A:35:HIS:HE1	1:A:97:ASP:OD2	1.83	0.61
1:C:170:LEU:HD22	1:C:257:TYR:CE2	2.36	0.60
1:A:391:VAL:HG12	1:A:391:VAL:O	2.02	0.59
1:D:385:ASP:OD2	1:D:412:LYS:HE2	2.03	0.59
1:A:35:HIS:CE1	1:A:97:ASP:OD2	2.56	0.59
1:C:28:MET:CE	1:C:110:LYS:NZ	2.65	0.59
1:C:28:MET:CE	1:C:110:LYS:HZ3	2.16	0.58
1:B:119:ARG:HD2	5:B:790:HOH:O	2.03	0.58
1:A:208:LYS:NZ	1:A:208:LYS:HB3	2.18	0.58
1:A:226:ASP:OD2	1:C:414:TYR:HB3	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:LEU:HD11	5:A:664:HOH:O	2.03	0.57
1:B:194:PRO:HG2	3:B:502:NAP:H2D	1.86	0.57
1:C:126:LEU:HD11	1:C:139:SER:OG	2.05	0.57
1:C:344:LYS:NZ	5:C:607:HOH:O	2.36	0.57
1:C:209:GLU:HG3	1:C:211:PHE:CZ	2.39	0.57
1:A:226:ASP:OD2	1:C:414:TYR:HB2	2.04	0.57
1:D:121:CYS:O	1:D:122:GLU:HG2	2.05	0.57
1:D:194:PRO:HD2	3:D:502:NAP:O1N	2.06	0.55
1:C:224:PHE:N	1:C:224:PHE:CD1	2.74	0.55
1:B:169:ARG:HD3	1:B:254:GLU:OE1	2.07	0.55
1:D:186:ARG:HG2	1:D:208:LYS:HE2	1.89	0.55
1:A:390:LEU:C	1:A:392:LYS:H	2.10	0.55
1:C:63:LEU:HD11	2:C:501:FAD:H6	1.88	0.55
1:A:198:ASP:CB	5:A:606:HOH:O	2.48	0.54
1:D:333:THR:O	1:D:336:LYS:HG3	2.06	0.54
1:D:346:ARG:NH2	5:D:603:HOH:O	2.40	0.54
1:D:2:ARG:HG3	1:D:3[A]:ARG:HG3	1.88	0.54
1:A:380:MET:HE3	1:D:332:GLU:HG3	1.89	0.54
1:C:361:GLU:CD	1:C:361:GLU:H	2.11	0.53
1:C:194:PRO:HG2	3:C:502:NAP:H2D	1.90	0.53
1:D:381:LYS:NZ	1:D:408:GLU:O	2.34	0.53
1:C:186[B]:ARG:HG3	1:C:208:LYS:HE3	1.89	0.52
1:D:344:LYS:O	1:D:348:GLU:HB2	2.10	0.52
1:B:2:ARG:HB2	1:B:2:ARG:NH1	2.24	0.52
1:A:398:ARG:NH2	3:A:502:NAP:H72N	2.07	0.52
1:B:192:ALA:HB2	1:B:214:ARG:HG2	1.91	0.52
1:B:192:ALA:CB	1:B:214:ARG:HG2	2.40	0.52
1:D:63:LEU:HD11	2:D:501:FAD:H6	1.91	0.51
1:A:209:GLU:HG3	1:A:211:PHE:CE2	2.46	0.51
1:A:393:ASP:CG	1:A:396:ASN:HB2	2.31	0.51
1:D:414:TYR:CE2	1:D:416:ALA:HA	2.45	0.51
1:A:402:TYR:CE1	1:A:412:LYS:CG	2.85	0.50
1:A:198:ASP:CG	5:A:606:HOH:O	2.49	0.50
1:D:250:THR:HG22	5:D:800:HOH:O	2.11	0.50
1:A:211:PHE:CZ	1:A:250:THR:HG21	2.47	0.49
1:A:386:VAL:O	1:A:390:LEU:HG	2.12	0.49
1:C:209:GLU:HG3	1:C:211:PHE:CE1	2.47	0.49
1:A:393:ASP:O	1:A:396:ASN:N	2.41	0.49
1:D:343:GLU:CA	1:D:346:ARG:HH12	2.17	0.49
1:D:412:LYS:O	1:D:413:ILE:CG2	2.57	0.49
1:A:336:LYS:HE2	5:A:955:HOH:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:329:PRO:HB2	1:C:333:THR:HB	1.94	0.48
1:B:278:GLU:HG3	5:B:809:HOH:O	2.13	0.48
1:A:380:MET:HE1	1:D:332:GLU:HG3	1.94	0.48
1:D:170:LEU:HD21	1:D:257:TYR:CE2	2.48	0.48
1:D:224:PHE:HB2	1:D:228:VAL:HB	1.95	0.48
1:C:191:GLY:HA2	3:C:502:NAP:N3A	2.29	0.47
1:A:381:LYS:HE3	1:A:381:LYS:HB2	1.67	0.47
1:D:343:GLU:HG2	5:D:703:HOH:O	2.15	0.47
1:A:67:LEU:HD12	1:A:386:VAL:HG21	1.97	0.47
1:D:390:LEU:O	1:D:394:LEU:HD22	2.15	0.47
1:B:121:CYS:O	1:B:123:SER:N	2.48	0.47
1:A:393:ASP:OD2	1:A:396:ASN:HB2	2.15	0.46
1:C:184:ASN:O	1:C:208:LYS:HE2	2.16	0.46
1:A:169:ARG:NH2	5:A:609:HOH:O	2.46	0.46
1:C:215:LYS:HB3	1:C:233:LEU:HD13	1.96	0.46
1:A:414:TYR:HB2	1:C:226:ASP:OD1	2.15	0.46
1:B:392:LYS:HZ3	1:B:392:LYS:HG2	1.57	0.46
1:B:122:GLU:CD	1:B:122:GLU:H	2.19	0.46
1:C:28:MET:HE1	1:C:110:LYS:NZ	2.30	0.46
2:B:501:FAD:C6	3:B:502:NAP:C2N	2.93	0.46
1:B:261:TYR:O	1:B:279:LYS:HE2	2.16	0.45
1:A:195:SER:O	1:A:199:MET:HB2	2.16	0.45
1:D:161:GLU:HG3	5:D:680:HOH:O	2.17	0.45
1:B:194:PRO:HB3	1:B:390:LEU:HD21	1.98	0.45
1:C:195:SER:HA	3:C:502:NAP:H5N	1.98	0.45
1:A:368:GLU:HG3	5:A:939:HOH:O	2.17	0.45
1:C:413:ILE:HG22	1:C:414:TYR:N	2.32	0.45
1:D:284:LEU:HA	1:D:289:LEU:O	2.16	0.45
1:C:237:LEU:HD23	1:C:242:ALA:HA	2.00	0.44
1:A:2:ARG:HD2	1:A:26:GLU:OE1	2.18	0.44
1:A:373:LYS:CE	5:A:613:HOH:O	2.61	0.44
1:C:284:LEU:HA	1:C:289:LEU:O	2.17	0.44
1:A:67:LEU:CD2	5:A:842:HOH:O	2.65	0.44
1:C:28:MET:HE2	1:C:110:LYS:NZ	2.32	0.44
1:A:191:GLY:HA2	3:A:502:NAP:N3A	2.34	0.43
1:C:60:TYR:OH	3:C:502:NAP:H4N	2.18	0.43
1:B:121:CYS:O	1:B:122:GLU:C	2.56	0.43
1:B:209:GLU:HG3	1:B:211:PHE:CE2	2.53	0.43
1:A:38:GLY:HA2	2:A:501:FAD:O3B	2.18	0.43
1:A:390:LEU:C	1:A:392:LYS:N	2.72	0.43
1:B:2:ARG:HB2	1:B:2:ARG:HH11	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:361:GLU:CD	1:C:361:GLU:N	2.73	0.42
1:B:198:ASP:OD2	3:B:502:NAP:O7N	2.38	0.42
1:C:3:ARG:HE	1:C:3:ARG:HB2	1.62	0.42
1:C:364:LYS:O	1:C:368:GLU:HG2	2.20	0.42
1:A:207:SER:O	1:A:227:ASN:ND2	2.53	0.41
1:B:2:ARG:NH2	5:B:622:HOH:O	2.53	0.41
1:C:163:ARG:HG3	1:C:163:ARG:HH11	1.85	0.41
1:D:122:GLU:HB2	1:D:123:SER:H	1.61	0.41
1:D:364:LYS:O	1:D:368:GLU:HG2	2.21	0.41
1:D:244:PHE:HE2	1:D:250:THR:HG23	1.86	0.41
1:A:386:VAL:CG2	5:A:674:HOH:O	2.67	0.41
1:C:38:GLY:HA2	2:C:501:FAD:O3B	2.21	0.41
1:C:194:PRO:HB2	3:C:502:NAP:H2D	2.02	0.41
1:B:68:PRO:HB3	1:B:85:SER:HB3	2.03	0.40
1:A:227:ASN:OD1	1:A:227:ASN:N	2.50	0.40
1:D:313:LEU:HD23	1:D:313:LEU:HA	1.97	0.40
1:D:195:SER:HA	3:D:502:NAP:H5N	2.03	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	403/425 (95%)	385 (96%)	17 (4%)	1 (0%)	47	26
1	B	403/425 (95%)	385 (96%)	18 (4%)	0	100	100
1	C	403/425 (95%)	387 (96%)	16 (4%)	0	100	100
1	D	406/425 (96%)	382 (94%)	23 (6%)	1 (0%)	47	26
All	All	1615/1700 (95%)	1539 (95%)	74 (5%)	2 (0%)	51	29

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	232	PRO
1	A	391	VAL

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	364/378 (96%)	350 (96%)	14 (4%)	33	10
1	B	364/378 (96%)	356 (98%)	8 (2%)	52	27
1	C	364/378 (96%)	353 (97%)	11 (3%)	41	16
1	D	364/378 (96%)	350 (96%)	14 (4%)	33	10
All	All	1456/1512 (96%)	1409 (97%)	47 (3%)	39	15

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	ARG
1	A	79	PHE
1	A	97	ASP
1	A	121	CYS
1	A	159	ASP
1	A	198	ASP
1	A	208	LYS
1	A	226	ASP
1	A	366	LEU
1	A	381	LYS
1	A	386	VAL
1	A	392	LYS
1	A	393	ASP
1	A	414	TYR
1	B	2	ARG
1	B	32	ARG
1	B	79	PHE
1	B	119	ARG
1	B	123	SER
1	B	151	GLN

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Mol	Chain	Res	Type
1	B	170	LEU
1	B	392	LYS
1	C	32	ARG
1	C	67	LEU
1	C	79	PHE
1	C	159	ASP
1	C	198	ASP
1	C	227	ASN
1	C	250	THR
1	C	327	THR
1	C	328	LEU
1	C	332	GLU
1	C	361	GLU
1	D	2	ARG
1	D	32	ARG
1	D	79	PHE
1	D	163	ARG
1	D	214	ARG
1	D	224	PHE
1	D	226	ASP
1	D	250	THR
1	D	328	LEU
1	D	336	LYS
1	D	344	LYS
1	D	346	ARG
1	D	394	LEU
1	D	412	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	35	HIS
1	B	117	ASN
1	B	151	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](#)

Of 11 ligands modelled in this entry, 3 are monoatomic - leaving 8 for Mogul analysis.

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	B	502	-	45,52,52	1.30	3 (6%)	56,80,80	1.95	14 (25%)
3	NAP	D	502	-	45,52,52	1.21	7 (15%)	56,80,80	1.49	10 (17%)
3	NAP	C	502	-	45,52,52	1.25	6 (13%)	56,80,80	1.78	12 (21%)
3	NAP	A	502	-	45,52,52	1.40	5 (11%)	56,80,80	1.75	13 (23%)
2	FAD	B	501	-	53,58,58	1.59	15 (28%)	68,89,89	1.90	17 (25%)
2	FAD	A	501	-	53,58,58	1.49	8 (15%)	68,89,89	1.66	12 (17%)
2	FAD	D	501	-	53,58,58	1.76	13 (24%)	68,89,89	1.52	14 (20%)
2	FAD	C	501	-	53,58,58	1.58	11 (20%)	68,89,89	1.78	13 (19%)

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	B	502	-	-	1/31/67/67	0/5/5/5
3	NAP	D	502	-	-	1/31/67/67	0/5/5/5
3	NAP	C	502	-	-	2/31/67/67	0/5/5/5
3	NAP	A	502	-	-	3/31/67/67	0/5/5/5
2	FAD	B	501	-	-	1/30/50/50	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	A	501	-	-	2/30/50/50	0/6/6/6
2	FAD	D	501	-	-	1/30/50/50	0/6/6/6
2	FAD	C	501	-	-	1/30/50/50	0/6/6/6

All (68) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	FAD	C2'-C3'	-4.75	1.44	1.53
2	C	501	FAD	C9A-C5X	4.42	1.48	1.41
3	A	502	NAP	C2A-N3A	4.27	1.39	1.32
2	D	501	FAD	C9A-C5X	4.07	1.48	1.41
3	B	502	NAP	C2A-N3A	3.98	1.38	1.32
2	C	501	FAD	C2-N3	-3.93	1.29	1.39
3	A	502	NAP	P2B-O2B	3.87	1.66	1.59
3	B	502	NAP	P2B-O2B	3.86	1.66	1.59
2	D	501	FAD	C8-C7	3.80	1.50	1.40
2	C	501	FAD	C4-N3	-3.59	1.32	1.38
2	B	501	FAD	C9A-C5X	3.56	1.47	1.41
3	B	502	NAP	O4D-C1D	3.49	1.45	1.41
2	A	501	FAD	C9A-C5X	3.47	1.47	1.41
2	C	501	FAD	C2B-C1B	-3.45	1.48	1.53
3	A	502	NAP	O4B-C1B	3.41	1.45	1.41
2	A	501	FAD	C4X-N5	3.28	1.37	1.30
2	A	501	FAD	C2-N3	-3.26	1.31	1.39
3	C	502	NAP	C2A-N3A	3.21	1.37	1.32
2	B	501	FAD	C4-N3	-3.20	1.32	1.38
2	C	501	FAD	C6-C7	3.17	1.44	1.39
2	A	501	FAD	C2'-C3'	-3.15	1.47	1.53
2	D	501	FAD	C5X-N5	-3.11	1.33	1.39
2	A	501	FAD	C4A-N3A	3.11	1.39	1.35
2	B	501	FAD	C2'-C3'	-3.11	1.47	1.53
2	D	501	FAD	C4-N3	-2.95	1.33	1.38
2	B	501	FAD	C10-N10	2.93	1.43	1.37
2	D	501	FAD	C9A-N10	-2.89	1.36	1.41
3	C	502	NAP	C7N-N7N	2.88	1.38	1.33
2	D	501	FAD	C5A-C4A	2.87	1.48	1.40
3	C	502	NAP	O4D-C1D	2.86	1.45	1.41
2	D	501	FAD	C4X-N5	2.80	1.36	1.30
3	A	502	NAP	C5A-C4A	2.79	1.48	1.40
2	A	501	FAD	O3B-C3B	2.76	1.49	1.43
2	D	501	FAD	C2A-N3A	2.75	1.36	1.32
2	B	501	FAD	C2-N3	-2.73	1.32	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	FAD	C8-C7	2.72	1.47	1.40
3	D	502	NAP	C5A-C4A	2.68	1.48	1.40
2	C	501	FAD	C8-C7	2.61	1.47	1.40
3	D	502	NAP	C2A-N3A	2.58	1.36	1.32
2	C	501	FAD	C2A-N3A	2.53	1.36	1.32
2	B	501	FAD	C5'-C4'	-2.53	1.48	1.51
2	D	501	FAD	C9-C8	-2.50	1.35	1.39
2	B	501	FAD	C4X-N5	2.37	1.35	1.30
3	D	502	NAP	O3D-C3D	2.36	1.48	1.43
3	C	502	NAP	P2B-O2B	2.34	1.63	1.59
3	C	502	NAP	C5A-C4A	2.33	1.47	1.40
2	C	501	FAD	C2'-C3'	-2.32	1.49	1.53
2	B	501	FAD	C6-C7	2.31	1.43	1.39
2	C	501	FAD	C5A-C4A	2.28	1.47	1.40
2	B	501	FAD	O4B-C1B	2.28	1.44	1.41
3	C	502	NAP	C8A-N7A	2.24	1.38	1.34
3	D	502	NAP	C7N-N7N	2.22	1.37	1.33
3	A	502	NAP	C2N-N1N	2.19	1.37	1.35
2	D	501	FAD	C9-C9A	-2.17	1.36	1.39
2	D	501	FAD	C6-C7	2.16	1.42	1.39
2	B	501	FAD	C2A-N3A	2.16	1.35	1.32
3	D	502	NAP	O4D-C1D	2.15	1.44	1.41
2	B	501	FAD	C8M-C8	2.12	1.55	1.51
2	C	501	FAD	O2-C2	-2.10	1.20	1.24
3	D	502	NAP	O4B-C1B	2.09	1.44	1.41
2	A	501	FAD	O2'-C2'	2.08	1.47	1.43
2	D	501	FAD	C1'-C2'	-2.08	1.49	1.52
2	B	501	FAD	C4A-N3A	2.07	1.38	1.35
2	B	501	FAD	P-O2P	-2.06	1.45	1.55
2	A	501	FAD	C2A-N1A	2.05	1.37	1.33
3	D	502	NAP	C2A-N1A	2.04	1.37	1.33
2	B	501	FAD	C10-N1	-2.03	1.29	1.33
2	C	501	FAD	C8M-C8	2.03	1.55	1.51

All (105) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	502	NAP	O7N-C7N-C3N	-6.41	111.97	119.63
2	A	501	FAD	N3A-C2A-N1A	-5.71	119.75	128.68
2	C	501	FAD	C5'-C4'-C3'	-5.64	101.31	112.20
3	B	502	NAP	O7N-C7N-C3N	-5.35	113.23	119.63
2	B	501	FAD	O4-C4-C4X	-5.19	112.82	126.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	502	NAP	C1B-N9A-C4A	-5.18	117.54	126.64
2	C	501	FAD	O4-C4-C4X	-5.01	113.30	126.60
2	D	501	FAD	C5'-C4'-C3'	-4.97	102.61	112.20
2	A	501	FAD	C5'-C4'-C3'	-4.79	102.95	112.20
3	B	502	NAP	C3N-C7N-N7N	4.70	123.39	117.75
2	C	501	FAD	C9A-C5X-N5	-4.48	117.56	122.43
2	B	501	FAD	O4B-C1B-C2B	-4.45	100.43	106.93
2	B	501	FAD	C5'-C4'-C3'	-4.34	103.81	112.20
3	A	502	NAP	N3A-C2A-N1A	-4.32	121.92	128.68
2	B	501	FAD	C4-C4X-N5	4.20	124.21	118.23
3	B	502	NAP	C4A-C5A-N7A	-4.20	105.02	109.40
3	B	502	NAP	N3A-C2A-N1A	-4.19	122.13	128.68
2	B	501	FAD	C9A-C5X-N5	-4.10	117.97	122.43
3	B	502	NAP	C1B-N9A-C4A	-4.10	119.44	126.64
3	D	502	NAP	O4B-C1B-C2B	-3.99	99.66	106.59
2	B	501	FAD	N3A-C2A-N1A	-3.95	122.51	128.68
3	D	502	NAP	N3A-C2A-N1A	-3.90	122.58	128.68
2	A	501	FAD	O4B-C4B-C3B	3.82	112.68	105.11
2	C	501	FAD	C4X-C4-N3	3.69	122.56	113.19
3	A	502	NAP	PN-O3-PA	-3.68	120.22	132.83
3	A	502	NAP	N6A-C6A-N1A	3.63	126.11	118.57
3	C	502	NAP	N3A-C2A-N1A	-3.59	123.06	128.68
3	A	502	NAP	C1B-N9A-C4A	-3.49	120.50	126.64
2	C	501	FAD	C4-C4X-N5	3.44	123.13	118.23
3	D	502	NAP	C4A-C5A-N7A	-3.38	105.87	109.40
3	D	502	NAP	C1B-N9A-C4A	-3.37	120.72	126.64
3	A	502	NAP	C2A-N1A-C6A	3.32	124.44	118.75
3	C	502	NAP	C3N-C7N-N7N	3.32	121.73	117.75
2	A	501	FAD	O4-C4-C4X	-3.31	117.83	126.60
3	B	502	NAP	C2D-C3D-C4D	3.30	109.05	102.64
3	D	502	NAP	PN-O3-PA	-3.30	121.52	132.83
2	D	501	FAD	C1B-N9A-C4A	-3.29	120.86	126.64
2	D	501	FAD	N3A-C2A-N1A	-3.26	123.58	128.68
3	B	502	NAP	O4B-C4B-C5B	-3.20	98.83	109.37
2	C	501	FAD	C10-N1-C2	3.16	123.22	116.90
2	B	501	FAD	C4X-C4-N3	3.13	121.13	113.19
3	A	502	NAP	C3N-C7N-N7N	-3.12	114.01	117.75
2	C	501	FAD	O2'-C2'-C1'	3.11	117.32	109.80
3	B	502	NAP	O3D-C3D-C2D	-3.10	101.81	111.82
2	A	501	FAD	C4-C4X-N5	3.04	122.56	118.23
2	B	501	FAD	O4-C4-N3	3.00	125.87	120.12
2	A	501	FAD	C2A-N1A-C6A	2.99	123.87	118.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	FAD	O4-C4-C4X	-2.93	118.83	126.60
2	B	501	FAD	C2A-N1A-C6A	2.92	123.75	118.75
2	B	501	FAD	C5X-C9A-N10	2.91	120.96	117.95
3	A	502	NAP	O7N-C7N-N7N	2.88	126.67	122.58
2	D	501	FAD	O4'-C4'-C5'	-2.88	103.44	109.92
2	D	501	FAD	O4B-C1B-C2B	-2.87	102.73	106.93
2	C	501	FAD	C4-C4X-C10	-2.85	112.01	116.79
2	A	501	FAD	C4X-C10-N10	2.80	120.57	116.48
3	A	502	NAP	O2A-PA-O1A	2.75	125.85	112.24
3	D	502	NAP	O2D-C2D-C3D	2.74	120.69	111.82
2	C	501	FAD	O4B-C1B-C2B	-2.74	102.92	106.93
2	D	501	FAD	C9-C9A-N10	-2.73	118.15	121.84
2	D	501	FAD	C5X-C9A-N10	2.71	120.76	117.95
2	B	501	FAD	C10-N1-C2	2.68	122.26	116.90
2	C	501	FAD	N3A-C2A-N1A	-2.63	124.57	128.68
3	A	502	NAP	O3X-P2B-O2X	2.61	117.61	107.64
3	B	502	NAP	O4B-C1B-C2B	-2.61	102.07	106.59
2	C	501	FAD	C3B-C2B-C1B	2.59	104.87	100.98
2	B	501	FAD	C4-C4X-C10	-2.58	112.46	116.79
2	A	501	FAD	C3B-C2B-C1B	2.57	104.84	100.98
3	B	502	NAP	C5N-C4N-C3N	-2.55	117.32	120.34
2	B	501	FAD	C9A-C9-C8	2.54	124.41	119.30
2	A	501	FAD	O2-C2-N1	-2.47	117.74	121.83
3	A	502	NAP	O3B-C3B-C4B	-2.44	104.00	111.05
3	C	502	NAP	O3B-C3B-C4B	-2.42	104.05	111.05
3	C	502	NAP	O7N-C7N-N7N	2.40	125.99	122.58
3	B	502	NAP	O2X-P2B-O1X	2.38	119.98	110.68
2	D	501	FAD	O2-C2-N1	-2.36	117.91	121.83
3	A	502	NAP	C5A-C6A-N6A	-2.34	116.79	120.35
3	D	502	NAP	O5B-C5B-C4B	-2.34	100.94	108.99
3	C	502	NAP	PN-O3-PA	-2.33	124.82	132.83
3	D	502	NAP	O3X-P2B-O2X	2.33	116.53	107.64
2	D	501	FAD	C2A-N1A-C6A	2.32	122.73	118.75
2	B	501	FAD	C5X-N5-C4X	2.31	121.92	118.07
2	A	501	FAD	C2B-C3B-C4B	-2.29	98.20	102.64
3	C	502	NAP	O3X-P2B-O2X	2.27	116.30	107.64
3	D	502	NAP	O3X-P2B-O2B	-2.24	95.94	105.99
2	A	501	FAD	O4-C4-N3	2.23	124.39	120.12
2	C	501	FAD	C8M-C8-C7	-2.21	116.20	120.74
2	D	501	FAD	O4-C4-N3	2.20	124.34	120.12
3	D	502	NAP	O2N-PN-O1N	2.20	123.12	112.24
3	B	502	NAP	C6N-N1N-C2N	-2.18	119.98	121.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	NAP	O4B-C4B-C5B	-2.18	102.20	109.37
3	C	502	NAP	O3B-C3B-C2B	-2.18	104.98	111.17
2	D	501	FAD	C4-C4X-N5	2.15	121.30	118.23
3	C	502	NAP	O2A-PA-O1A	2.14	122.84	112.24
2	B	501	FAD	C6-C5X-N5	2.14	122.25	118.51
2	B	501	FAD	C3B-C2B-C1B	2.14	104.20	100.98
2	C	501	FAD	C8M-C8-C9	2.12	123.41	119.49
2	B	501	FAD	O3'-C3'-C4'	-2.08	103.78	108.81
3	C	502	NAP	C2D-C3D-C4D	2.08	106.68	102.64
2	A	501	FAD	O3'-C3'-C2'	-2.07	103.80	108.81
3	A	502	NAP	O4B-C4B-C3B	2.07	109.20	105.11
3	C	502	NAP	C4A-C5A-N7A	-2.06	107.25	109.40
3	B	502	NAP	C3B-C2B-C1B	-2.06	99.01	102.89
2	D	501	FAD	C1'-N10-C9A	2.05	123.94	120.51
2	D	501	FAD	N6A-C6A-N1A	2.02	122.77	118.57
3	B	502	NAP	O4D-C1D-C2D	2.00	109.85	106.93

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502	NAP	C4N-C3N-C7N-O7N
3	A	502	NAP	C2N-C3N-C7N-O7N
3	C	502	NAP	C4N-C3N-C7N-N7N
2	A	501	FAD	O3'-C3'-C4'-C5'
2	A	501	FAD	O4B-C4B-C5B-O5B
2	B	501	FAD	O4B-C4B-C5B-O5B
2	C	501	FAD	O4B-C4B-C5B-O5B
2	D	501	FAD	O4B-C4B-C5B-O5B
3	A	502	NAP	O4B-C4B-C5B-O5B
3	B	502	NAP	O4B-C4B-C5B-O5B
3	C	502	NAP	O4B-C4B-C5B-O5B
3	D	502	NAP	O4B-C4B-C5B-O5B

There are no ring outliers.

8 monomers are involved in 18 short contacts:

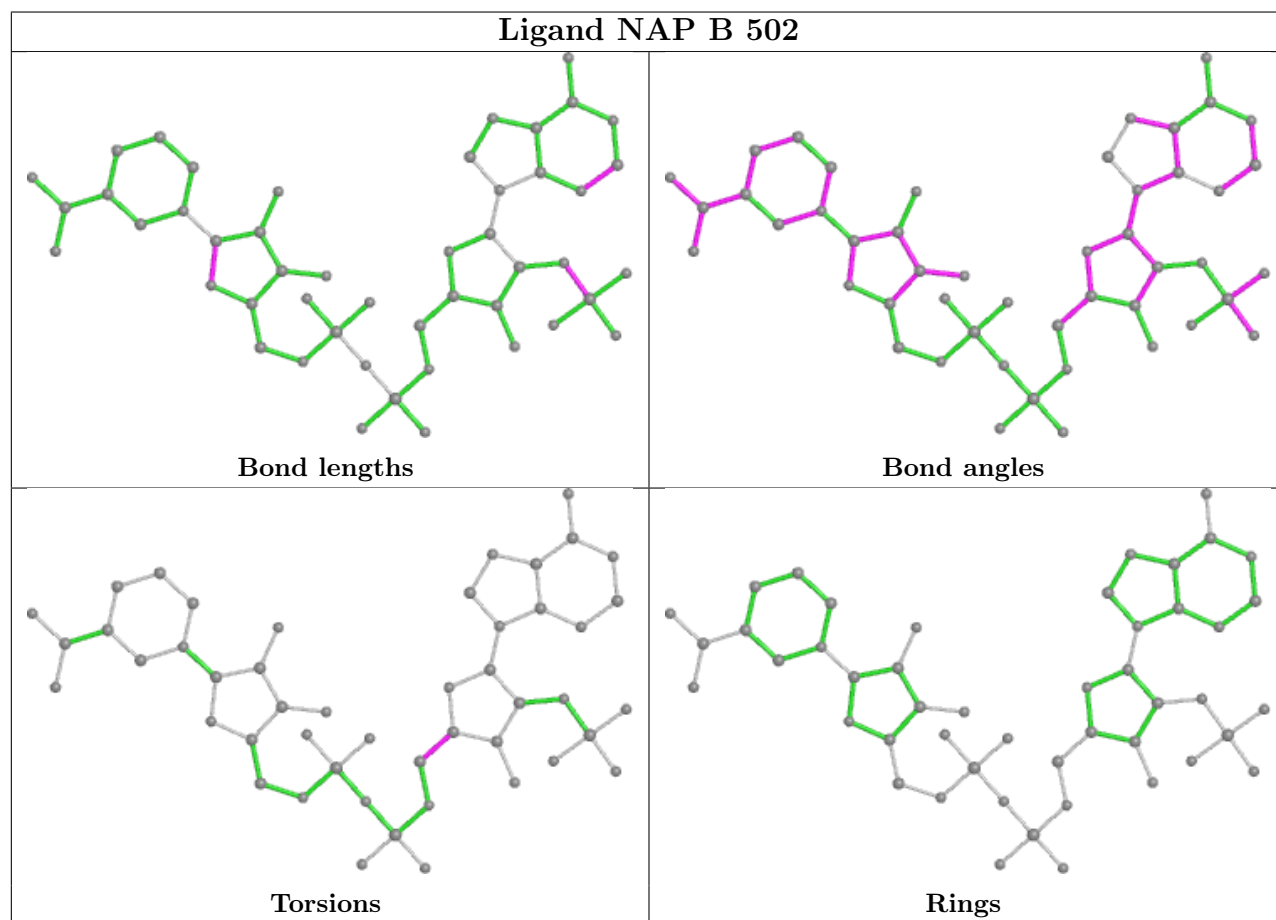
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	502	NAP	4	0
3	D	502	NAP	2	0
3	C	502	NAP	6	0

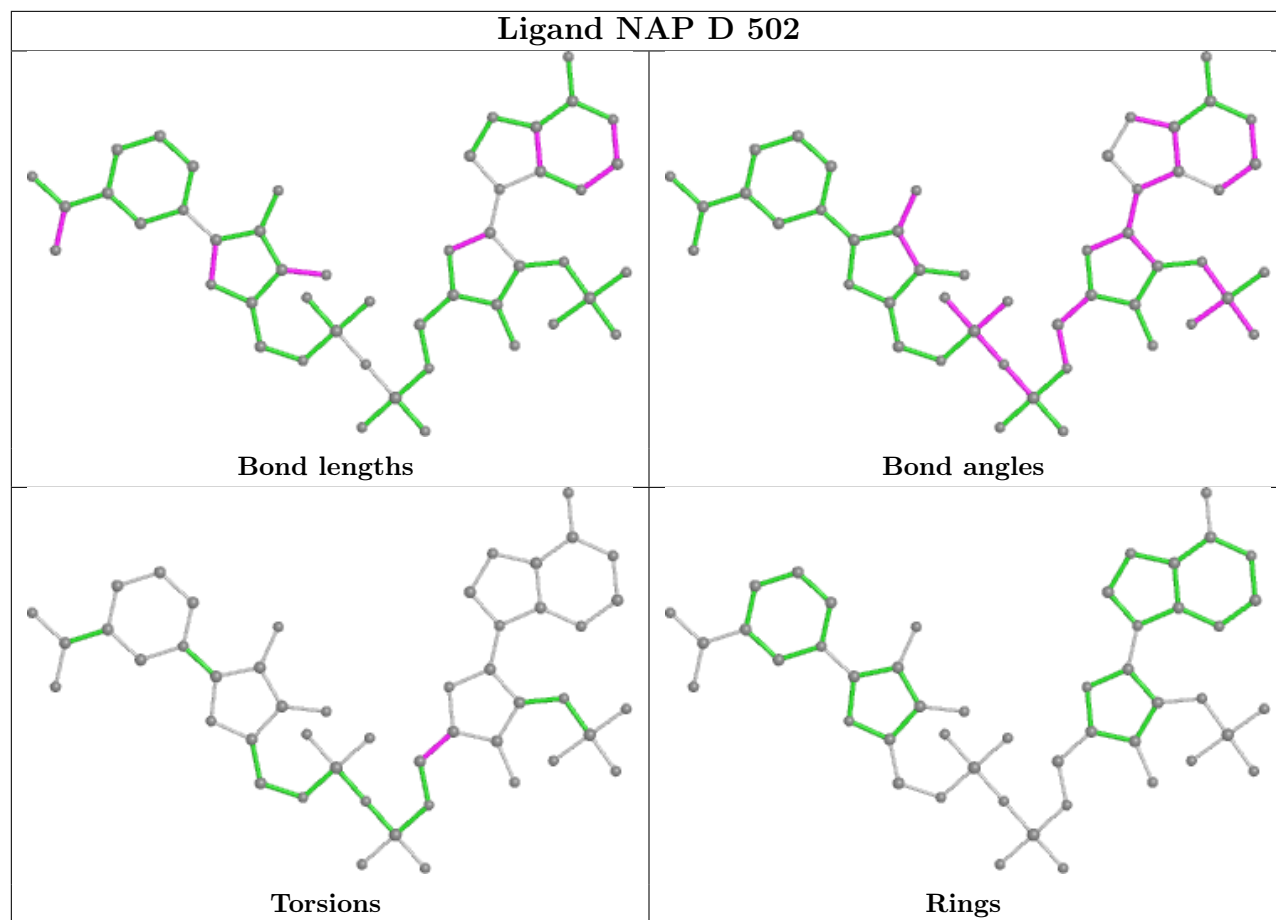
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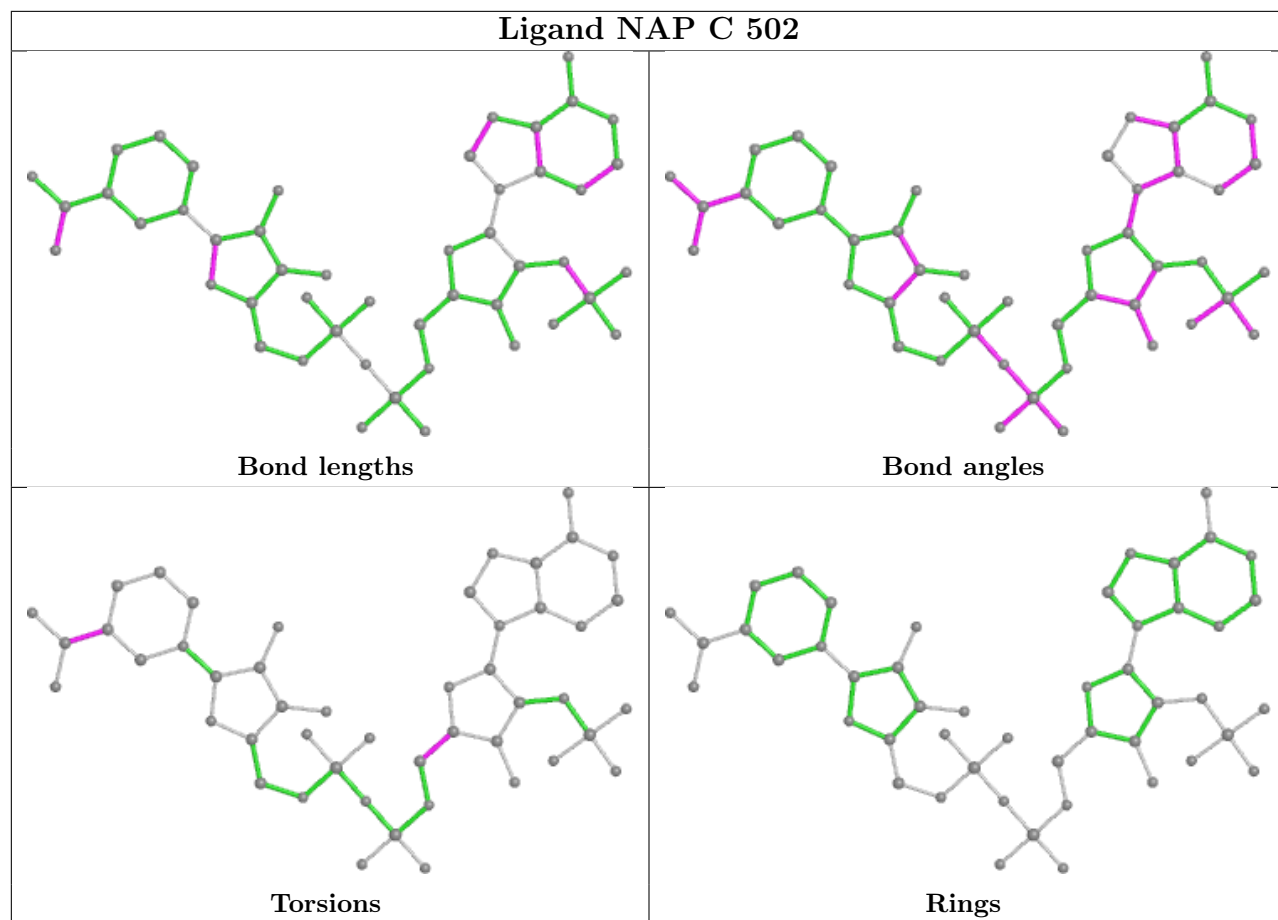
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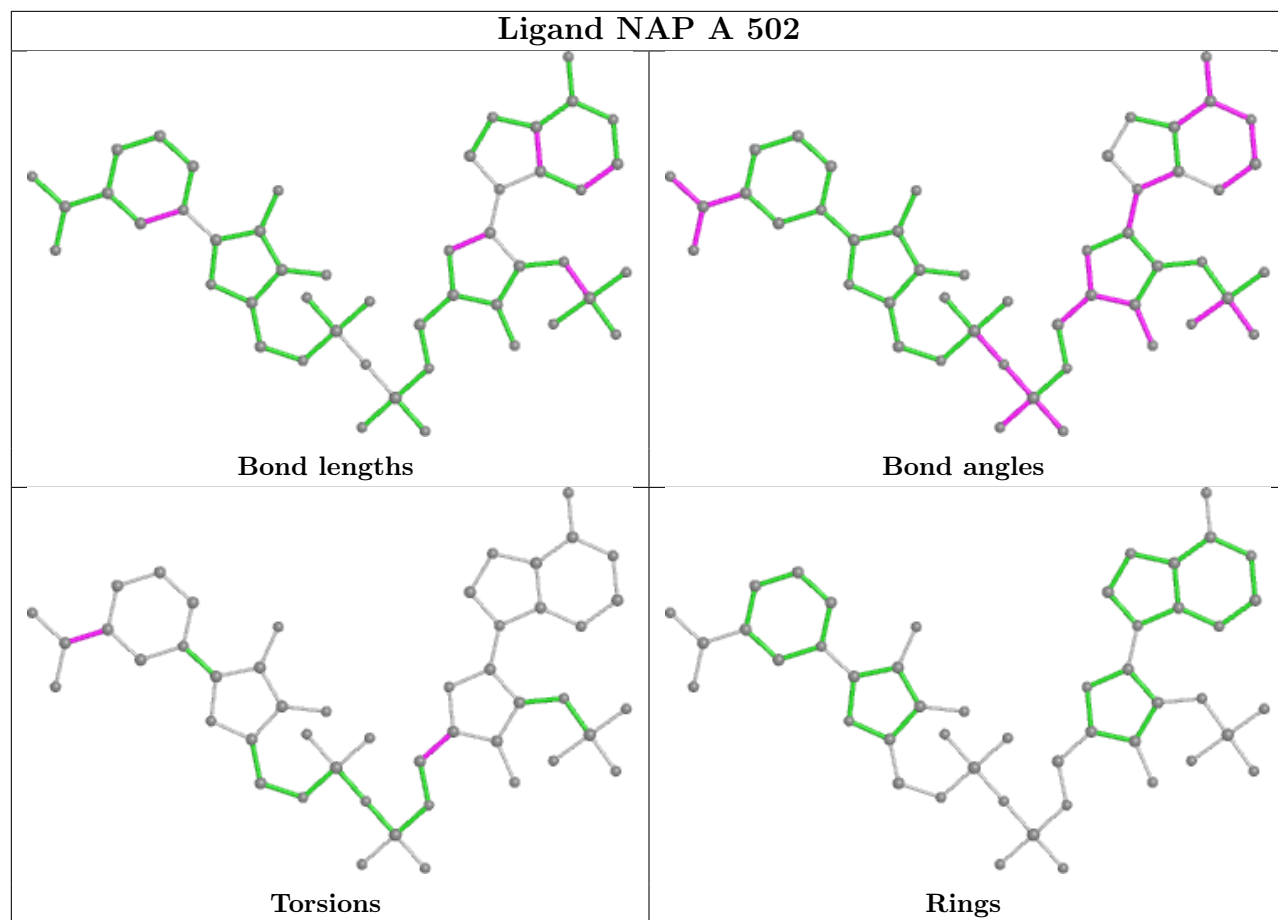
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	NAP	2	0
2	B	501	FAD	1	0
2	A	501	FAD	1	0
2	D	501	FAD	1	0
2	C	501	FAD	2	0

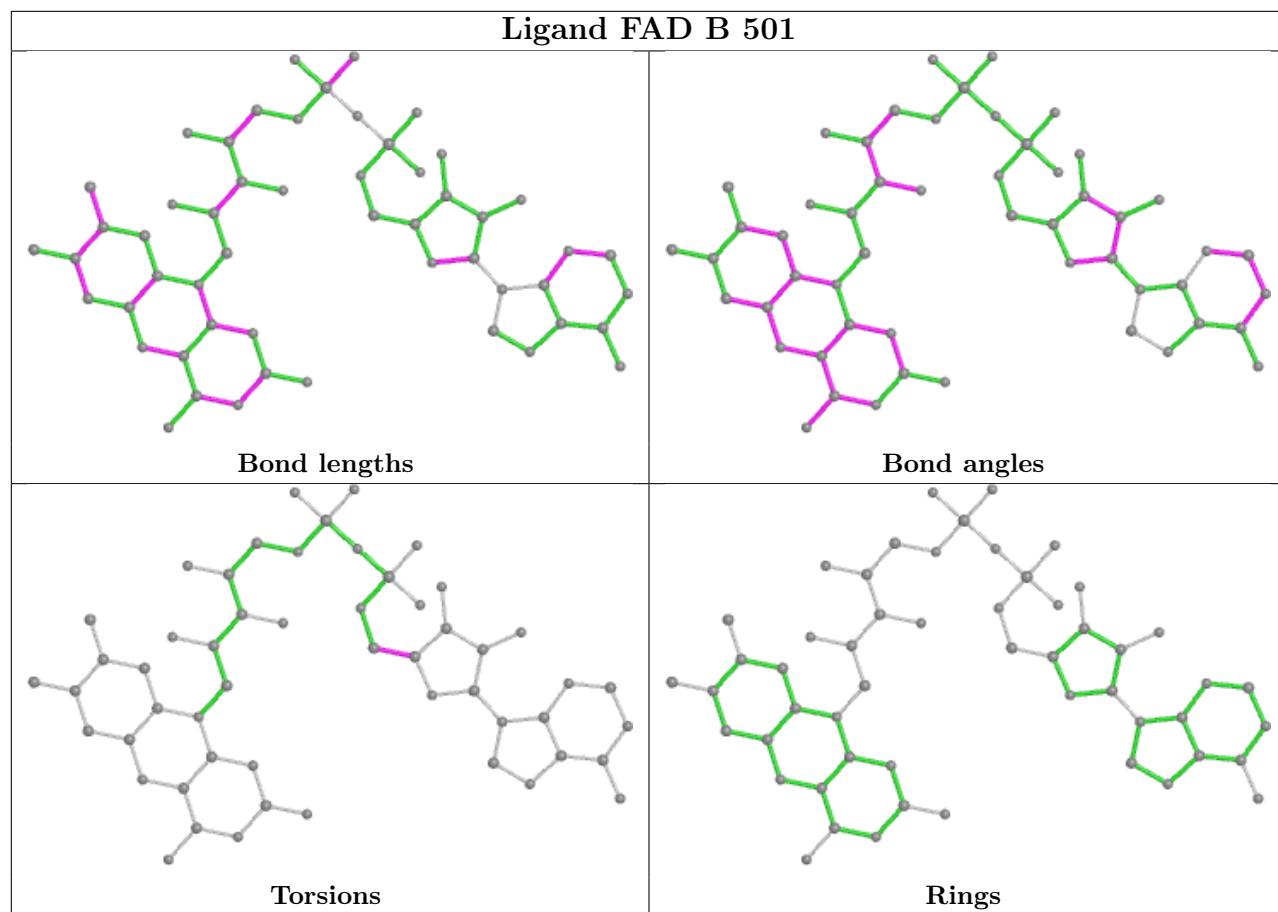
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

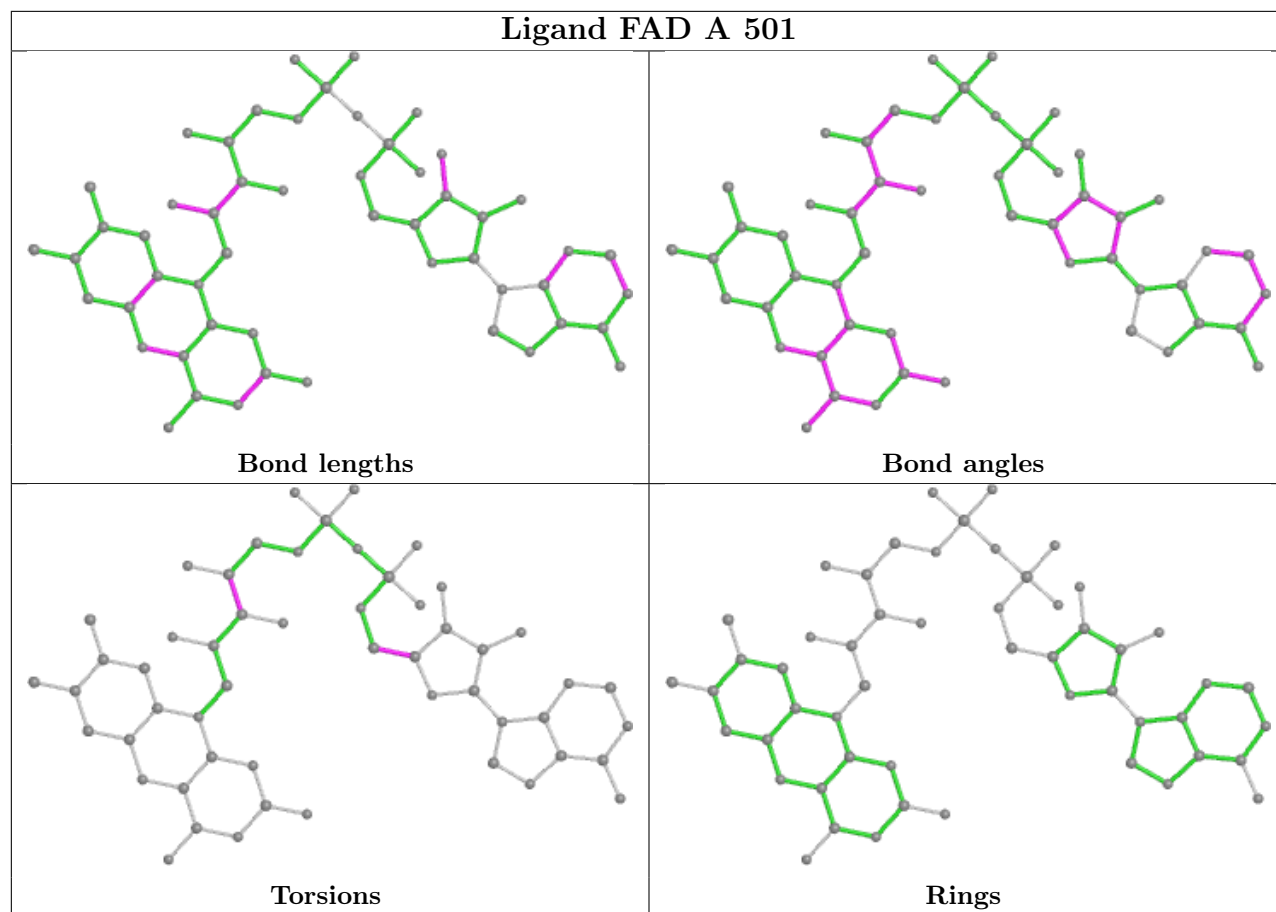


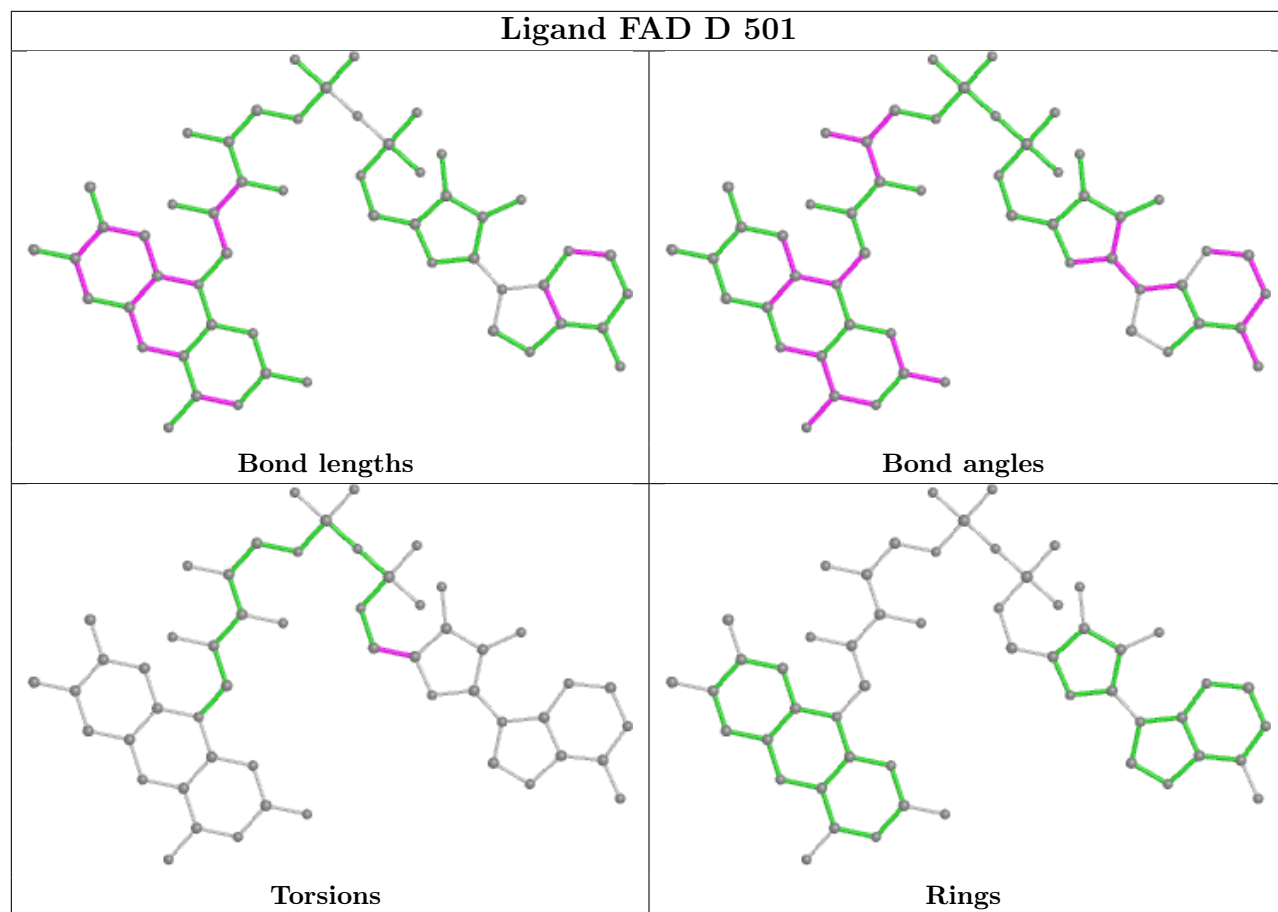


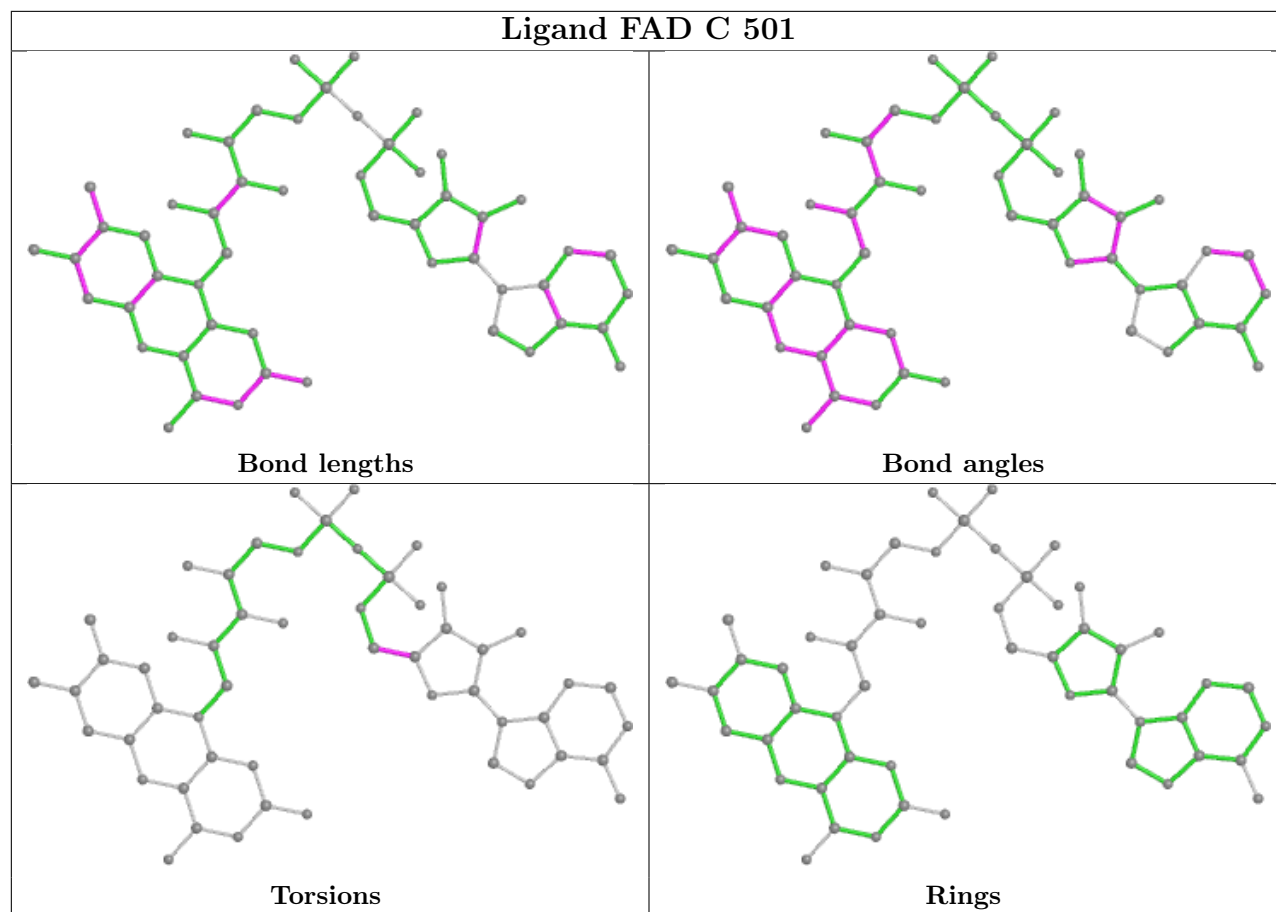












5.7 Other polymers [i](#)

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	406/425 (95%)	-0.31	7 (1%) 70 69	8, 17, 41, 80	2 (0%)
1	B	407/425 (95%)	-0.39	7 (1%) 70 69	9, 17, 34, 86	1 (0%)
1	C	406/425 (95%)	-0.29	9 (2%) 62 60	10, 19, 43, 76	1 (0%)
1	D	409/425 (96%)	-0.28	10 (2%) 59 56	9, 18, 43, 67	1 (0%)
All	All	1628/1700 (95%)	-0.32	33 (2%) 65 64	8, 18, 41, 86	5 (0%)

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	414	TYR	8.5
1	C	414	TYR	5.5
1	A	391	VAL	5.2
1	B	327	THR	4.8
1	D	226	ASP	4.4
1	B	122	GLU	4.3
1	A	389	ASP	4.1
1	D	417	ALA	4.1
1	B	123	SER	4.1
1	D	416	ALA	4.0
1	C	122	GLU	3.7
1	A	392	LYS	3.6
1	C	123	SER	3.5
1	D	394	LEU	3.3
1	A	390	LEU	3.2
1	C	121	CYS	3.1
1	B	1	MET	3.0
1	A	192	ALA	3.0
1	C	194	PRO	3.0
1	D	414	TYR	3.0
1	A	388	SER	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	123	SER	2.9
1	B	414	TYR	2.8
1	B	194	PRO	2.5
1	C	226	ASP	2.4
1	D	415	ALA	2.3
1	D	224	PHE	2.3
1	D	227	ASN	2.3
1	C	391	VAL	2.2
1	C	390	LEU	2.2
1	D	393	ASP	2.2
1	C	327	THR	2.1
1	B	121	CYS	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](#)

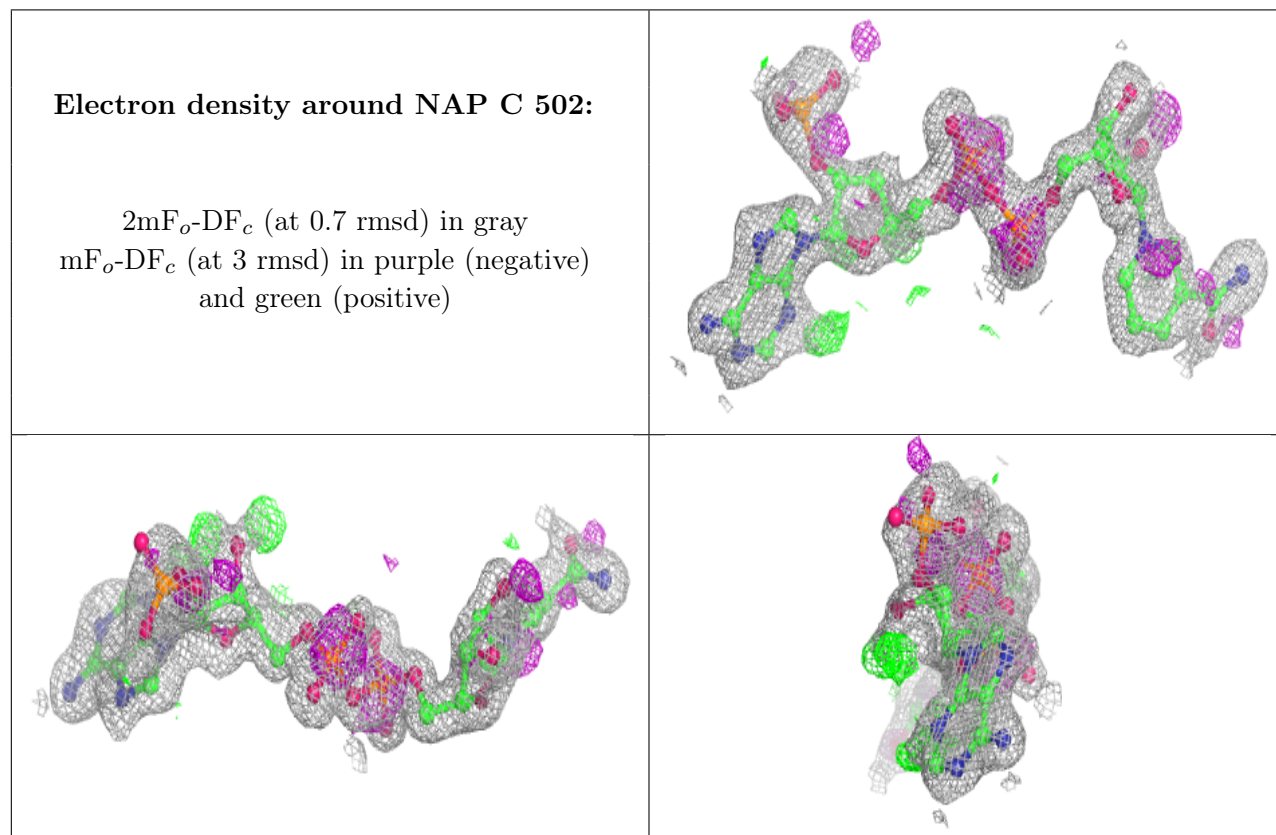
There are no monosaccharides in this entry.

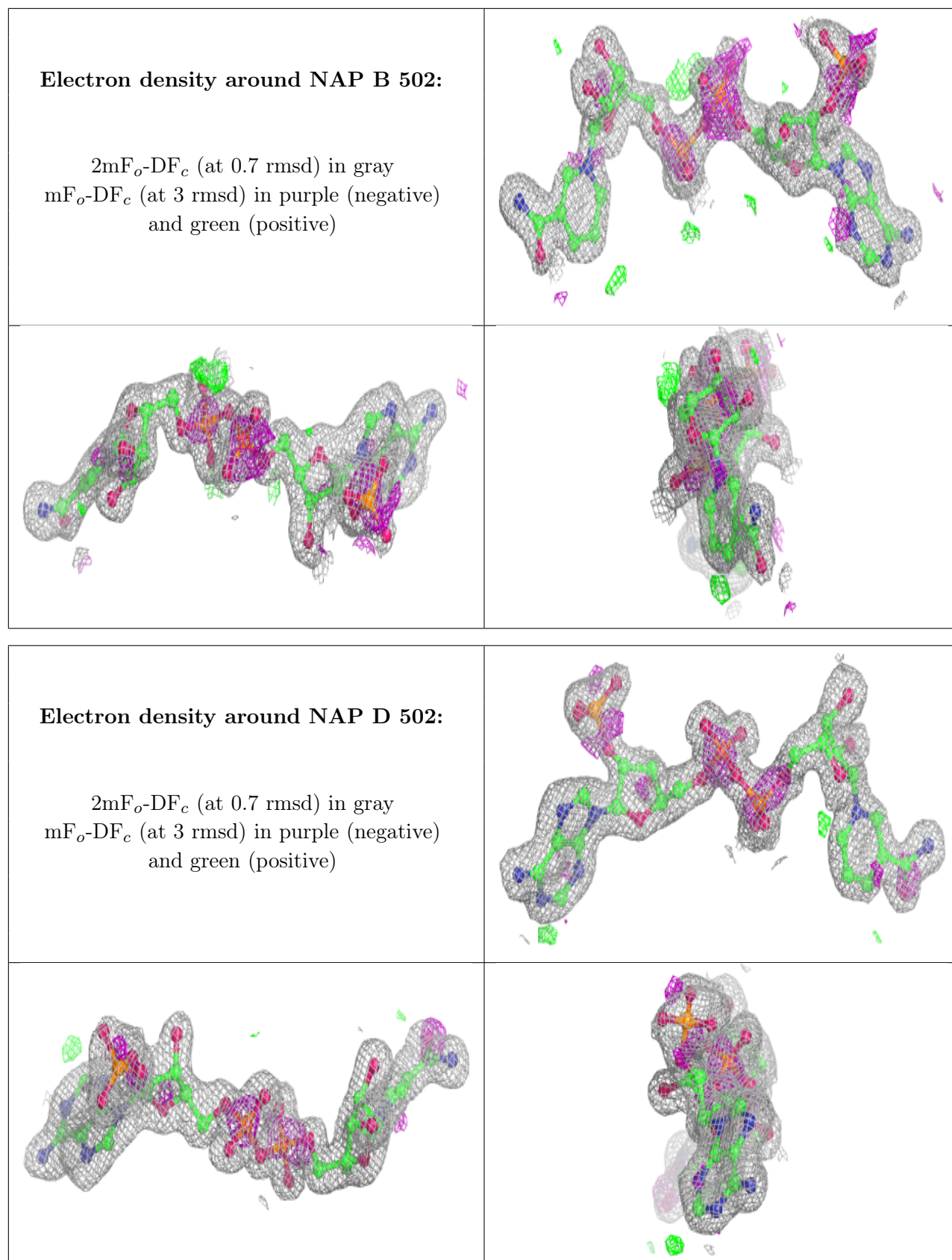
6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAP	C	502	48/48	0.89	0.18	19,31,48,56	0
3	NAP	B	502	48/48	0.93	0.17	17,28,40,48	0
3	NAP	D	502	48/48	0.93	0.15	19,25,44,50	0
3	NAP	A	502	48/48	0.94	0.17	17,25,40,50	0
2	FAD	C	501	53/53	0.98	0.07	9,12,19,21	0
2	FAD	D	501	53/53	0.98	0.07	8,11,20,24	0
4	MG	B	503	1/1	0.98	0.14	27,27,27,27	0
2	FAD	B	501	53/53	0.99	0.06	7,10,17,20	0
2	FAD	A	501	53/53	0.99	0.06	7,10,17,18	0
4	MG	C	503	1/1	0.99	0.07	23,23,23,23	0
4	MG	D	503	1/1	0.99	0.03	19,19,19,19	0

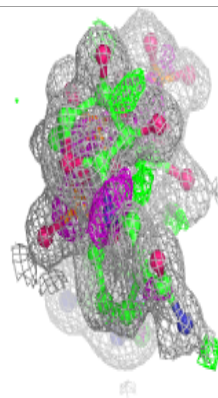
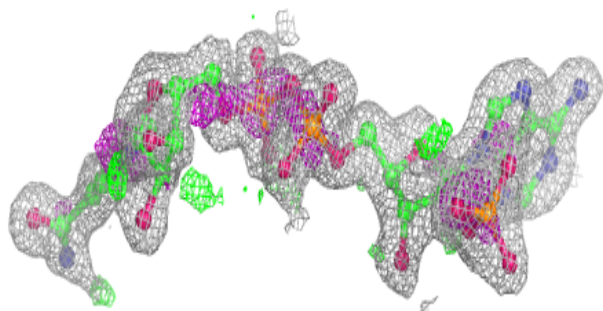
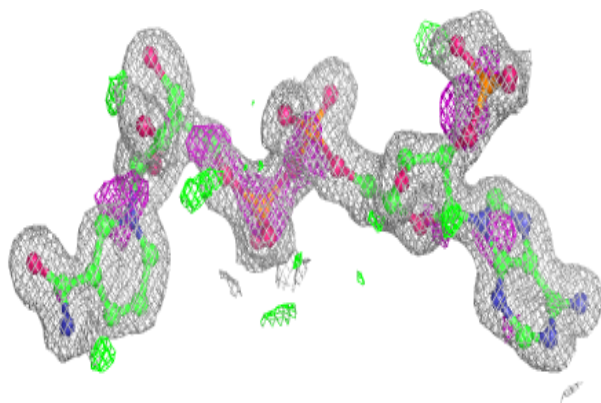
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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



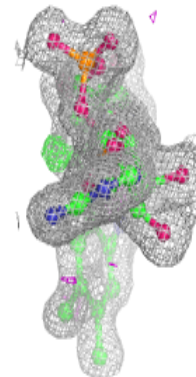
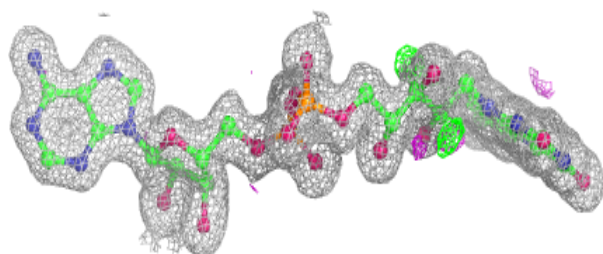
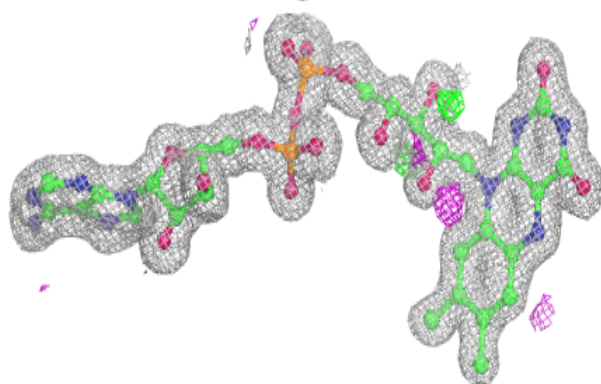


Electron density around NAP A 502:

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

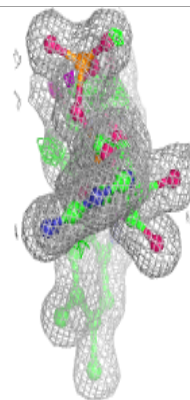
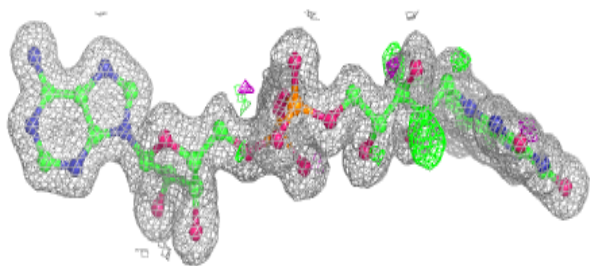
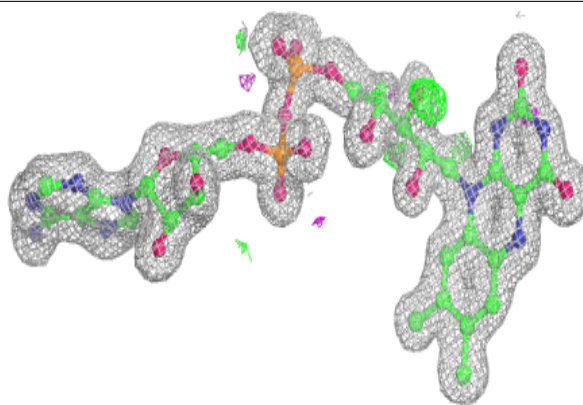
**Electron density around FAD C 501:**

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

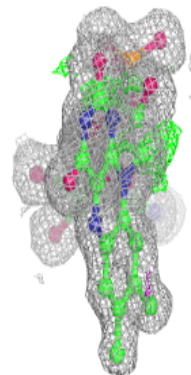
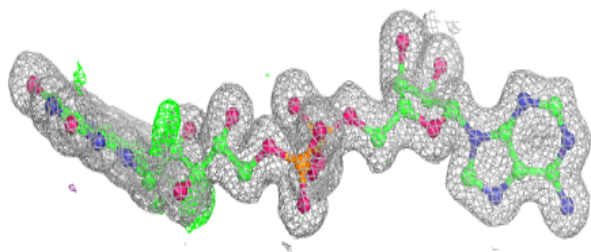
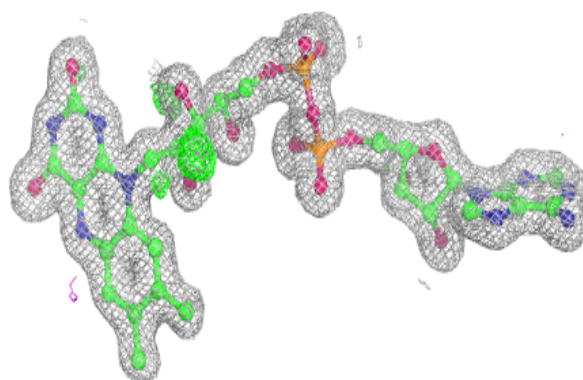


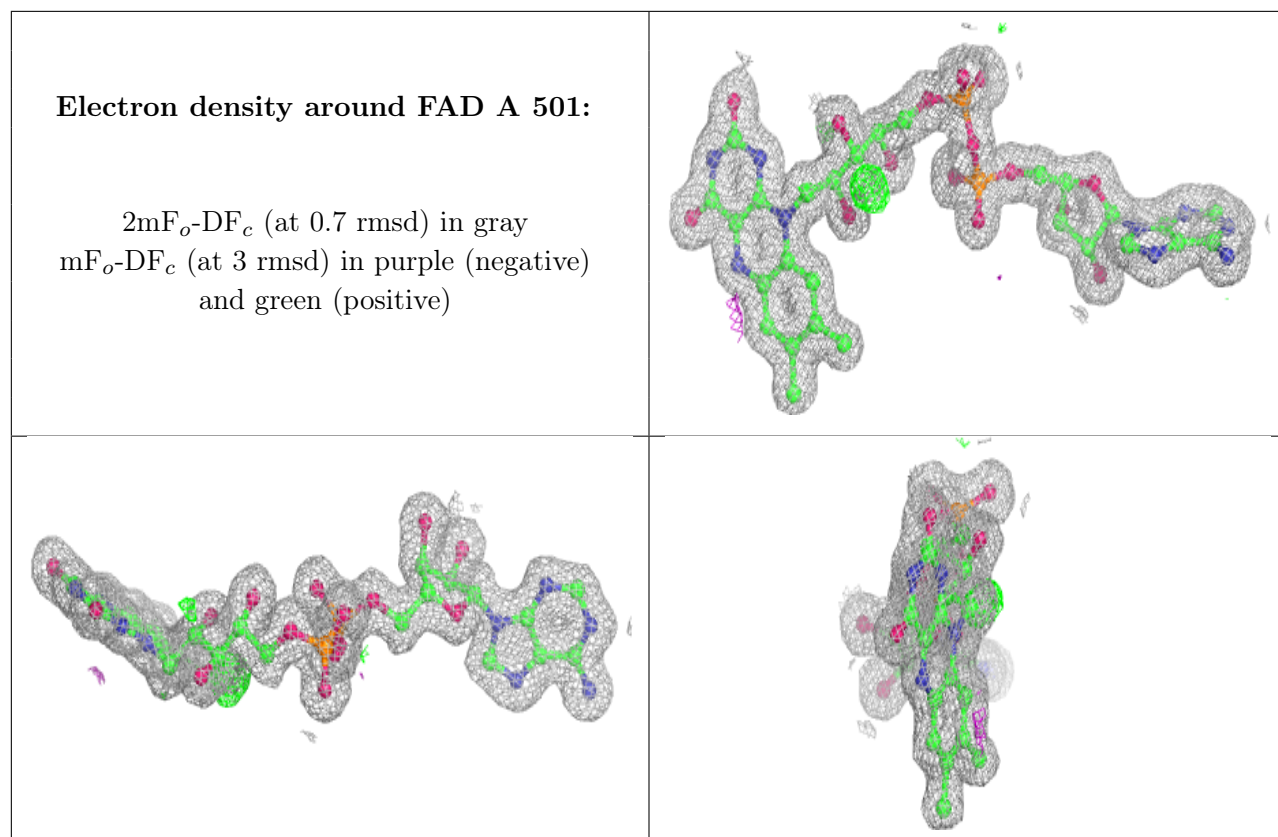
Electron density around FAD D 501:

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

**Electron density around FAD B 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.