



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:31 PM UTC

PDB ID : 7JVL / pdb_00007jvl
Title : Structure of the M101A variant of the SidA ornithine hydroxylase complexed with NADP and the FAD in the "out" conformation
Authors : Tanner, J.J.; Campbell, A.C.
Deposited on : 2020-08-21
Resolution : 2.10 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

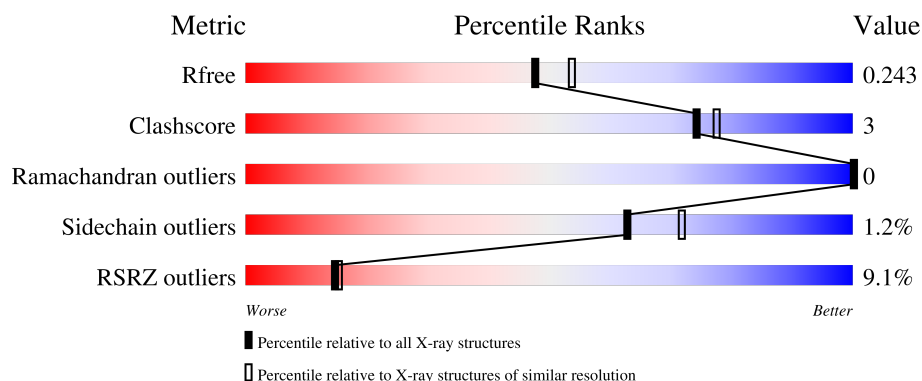
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	501	7% 79% 8% 12%
1	B	501	4% 82% 6% 12%
1	C	501	11% 80% 8% 12%
1	D	501	10% 79% 8% 12%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 14774 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.

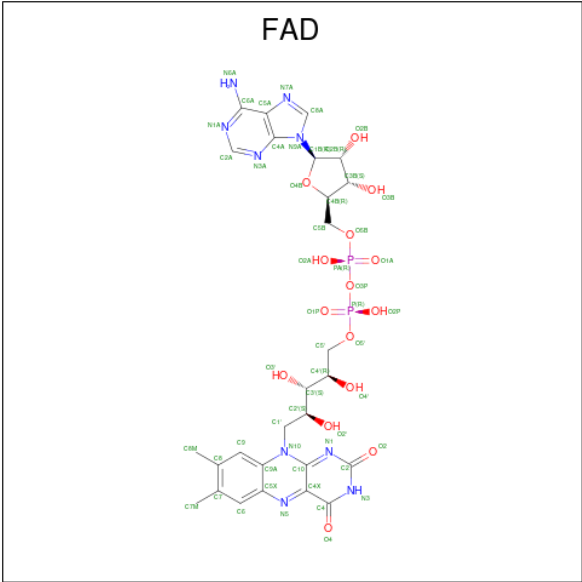
- Molecule 1 is a protein called L-ornithine N(5)-monooxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	439	Total	C	N	O	S	0	0	0
			3452	2177	625	635	15			
1	B	442	Total	C	N	O	S	0	0	0
			3464	2183	628	638	15			
1	C	441	Total	C	N	O	S	0	0	0
			3431	2165	622	629	15			
1	D	440	Total	C	N	O	S	0	0	0
			3418	2156	617	630	15			

There are 4 discrepancies between the modelled and reference sequences:

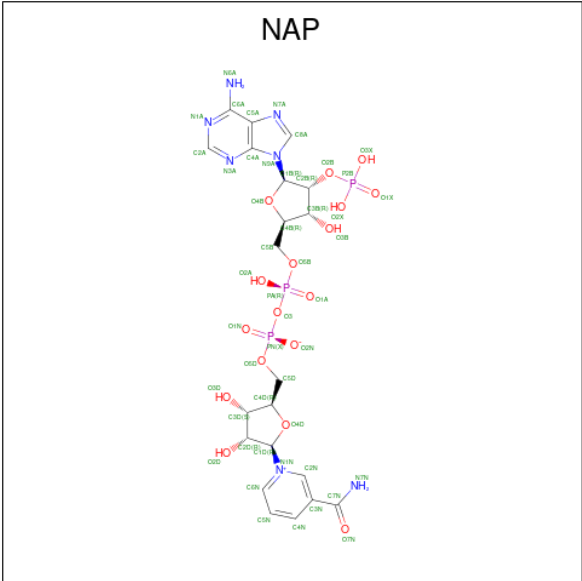
Chain	Residue	Modelled	Actual	Comment	Reference
A	101	ALA	MET	engineered mutation	UNP E9QYP0
B	101	ALA	MET	engineered mutation	UNP E9QYP0
C	101	ALA	MET	engineered mutation	UNP E9QYP0
D	101	ALA	MET	engineered mutation	UNP E9QYP0

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$) (labeled as "Ligand of Interest" by depositor).



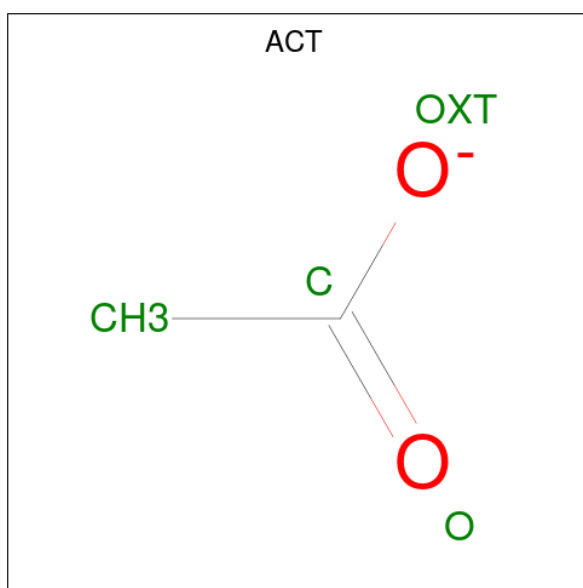
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃) (labeled as "Ligand of Interest" by depositor).



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 ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total 1	Ca 1	0	0
5	D	1	Total 1	Ca 1	0	0

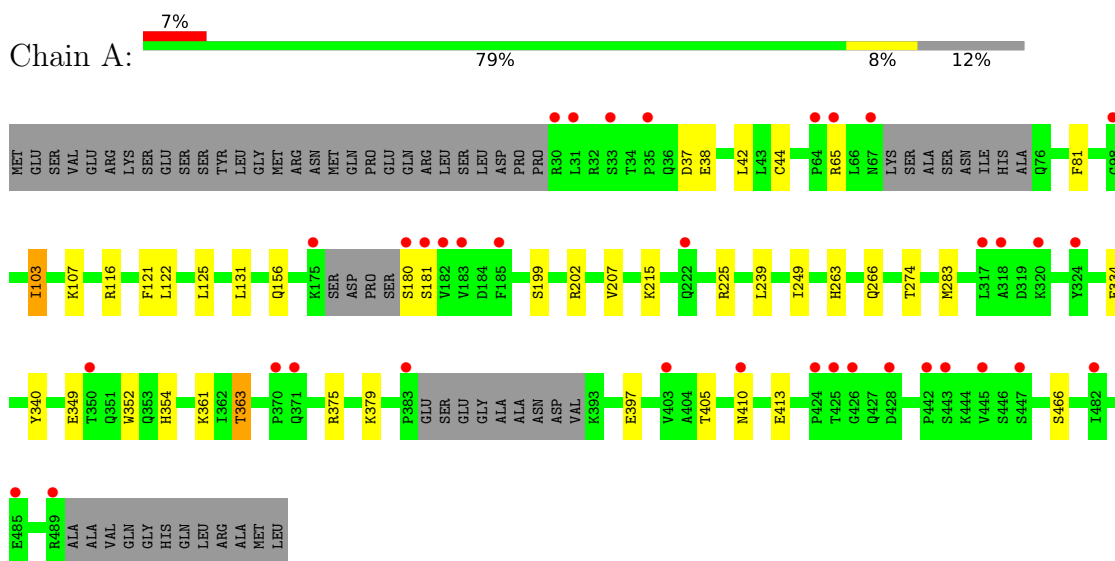
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	149	Total 149	O 149	0	0
6	B	168	Total 168	O 168	0	0
6	C	128	Total 128	O 128	0	0
6	D	126	Total 126	O 126	0	0

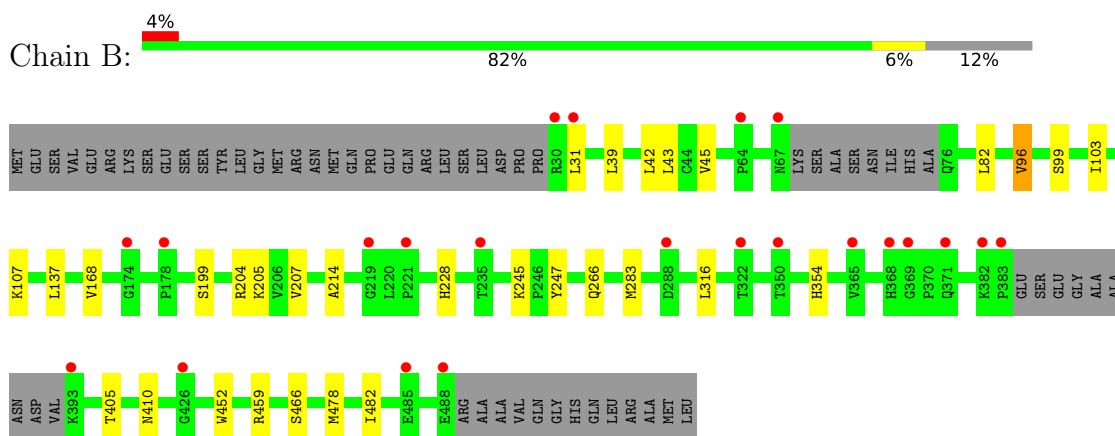
3 Residue-property plots [i](#)

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.

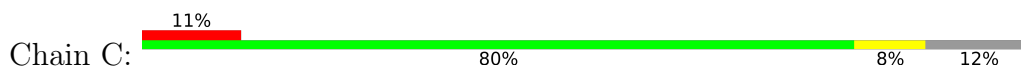
- Molecule 1: L-ornithine N(5)-monooxygenase

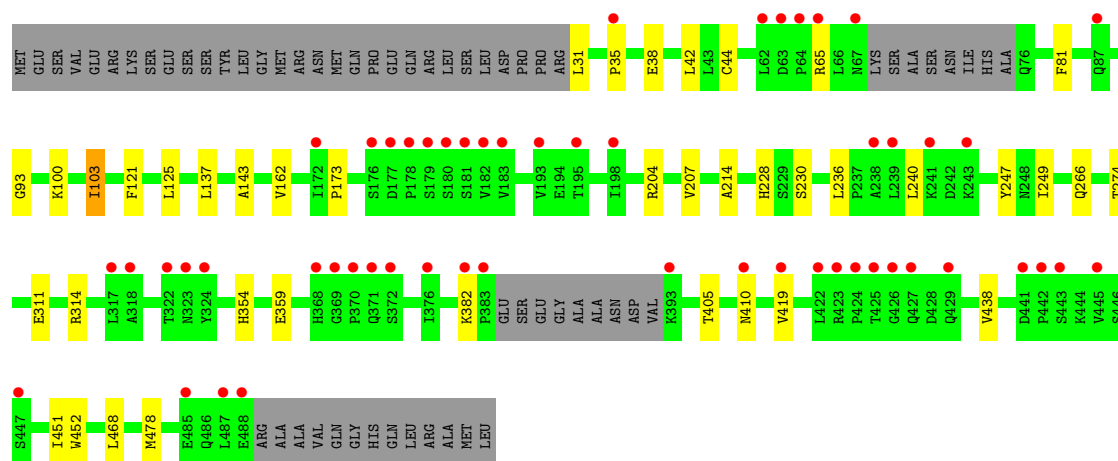


- Molecule 1: L-ornithine N(5)-monooxygenase

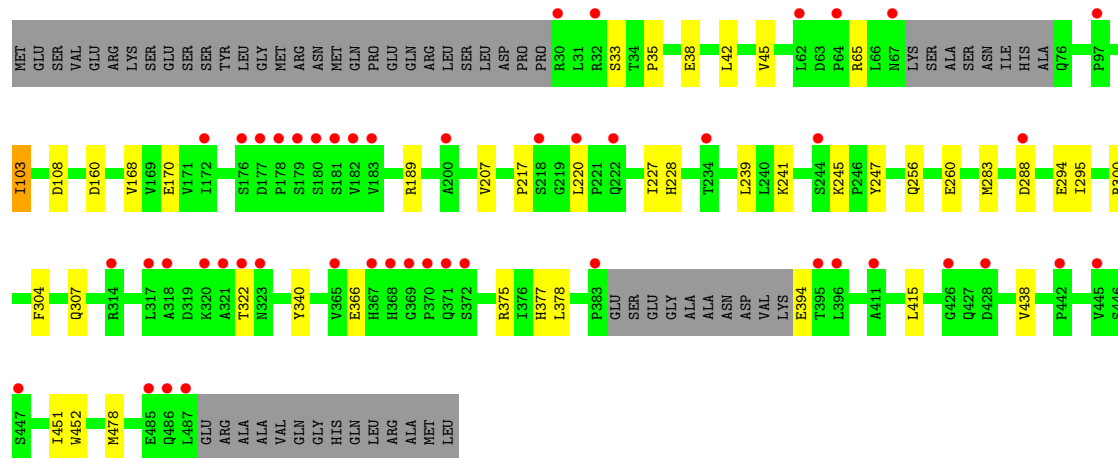
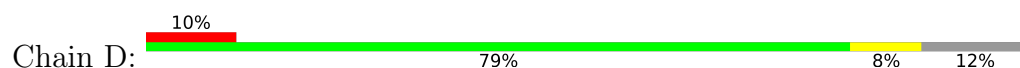


- Molecule 1: L-ornithine N(5)-monooxygenase





• Molecule 1: L-ornithine N(5)-monooxygenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	80.23Å 153.81Å 89.87Å 90.00° 109.28° 90.00°	Depositor
Resolution (Å)	62.89 – 2.10 62.89 – 2.10	Depositor EDS
% Data completeness (in resolution range)	94.4 (62.89-2.10) 95.3 (62.89-2.10)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.81 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.18	Depositor
R, R_{free}	0.204 , 0.241 0.206 , 0.243	Depositor DCC
R_{free} test set	2232 reflections (1.87%)	wwPDB-VP
Wilson B-factor (Å ²)	18.9	Xtriage
Anisotropy	0.167	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 35.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	14774	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.64% 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: ACT, FAD, CA, 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	0.34	0/3526	0.55	0/4774
1	B	0.35	0/3540	0.56	0/4795
1	C	0.32	0/3507	0.53	0/4756
1	D	0.32	0/3494	0.50	0/4742
All	All	0.34	0/14067	0.53	0/19067

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3452	0	3386	22	0
1	B	3464	0	3403	19	0
1	C	3431	0	3340	24	0
1	D	3418	0	3316	23	0
2	A	53	0	31	1	0
2	B	53	0	31	1	0
2	C	53	0	31	1	0
2	D	53	0	31	0	0
3	A	48	0	24	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	48	0	24	1	0
3	C	48	0	23	1	0
3	D	48	0	24	0	0
4	A	8	0	6	0	0
4	B	8	0	6	0	0
4	C	8	0	6	1	0
4	D	8	0	6	1	0
5	B	1	0	0	0	0
5	D	1	0	0	0	0
6	A	149	0	0	0	0
6	B	168	0	0	1	0
6	C	128	0	0	0	0
6	D	126	0	0	0	0
All	All	14774	0	13688	86	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 3.

All (86) 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:170:GLU:OE2	1:D:189:ARG:NH1	2.14	0.80
1:A:361:LYS:HE3	1:A:379:LYS:HE3	1.74	0.68
1:A:410:ASN:O	1:A:413:GLU:HG2	1.94	0.68
1:C:311:GLU:OE1	1:C:314:ARG:NH2	2.24	0.67
1:B:96:VAL:HG13	1:B:99:SER:HB3	1.78	0.66
1:D:304:PHE:HA	1:D:307:GLN:HE21	1.62	0.65
1:D:217:PRO:HD2	1:D:220:LEU:HD12	1.83	0.59
1:D:378:LEU:HB2	1:D:394:GLU:HG3	1.83	0.59
1:C:103:ILE:HD12	4:C:603:ACT:H2	1.86	0.56
1:A:42:LEU:HD11	1:A:207:VAL:HG23	1.90	0.54
1:A:215:LYS:HE2	1:A:405:THR:O	2.08	0.54
1:C:103:ILE:HD13	1:C:468:LEU:HB2	1.91	0.53
1:D:207:VAL:HG22	1:D:452:TRP:HB2	1.90	0.53
1:D:452:TRP:HB3	1:D:478:MET:HE1	1.92	0.52
1:C:65:ARG:HD3	1:D:65:ARG:O	2.10	0.52
1:A:363:THR:HG22	1:A:379:LYS:HG2	1.92	0.52
1:D:42:LEU:HD11	1:D:207:VAL:HG23	1.91	0.51
1:A:466:SER:OG	2:A:601:FAD:O2	2.20	0.51
1:A:65:ARG:NH2	1:A:116:ARG:O	2.28	0.51
1:D:295:ILE:HD11	1:D:322:THR:HG21	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:366:GLU:OE1	1:D:375:ARG:NH2	2.43	0.51
1:D:245:LYS:HE3	1:D:247:TYR:CE1	2.46	0.50
1:B:466:SER:OG	2:B:601:FAD:O2	2.16	0.50
1:C:359:GLU:OE1	1:C:382:LYS:HE3	2.12	0.50
1:C:93:GLY:HA3	1:C:230:SER:O	2.12	0.50
1:A:410:ASN:HB2	1:A:413:GLU:OE1	2.13	0.49
1:B:45:VAL:HG22	1:B:168:VAL:HG21	1.94	0.49
1:A:375:ARG:NH1	1:A:397:GLU:OE1	2.45	0.48
1:A:121:PHE:CE2	1:A:125:LEU:HD11	2.48	0.48
1:C:81:PHE:HB2	1:C:162:VAL:HG22	1.96	0.48
1:D:45:VAL:HG22	1:D:168:VAL:HG21	1.95	0.48
1:A:266:GLN:HG2	1:A:354:HIS:CE1	2.48	0.48
1:C:249:ILE:O	1:C:274:THR:HA	2.14	0.48
1:B:214:ALA:HB1	1:B:228:HIS:CG	2.48	0.47
1:C:42:LEU:HD11	1:C:207:VAL:HG23	1.95	0.47
1:D:256:GLN:O	1:D:260:GLU:HG3	2.14	0.47
1:C:35:PRO:HB2	1:C:38:GLU:HG3	1.95	0.47
1:C:266:GLN:HG2	1:C:354:HIS:CE1	2.48	0.47
1:B:266:GLN:HG2	1:B:354:HIS:CE1	2.50	0.47
1:B:42:LEU:HD11	1:B:207:VAL:HG23	1.96	0.47
1:A:180:SER:OG	1:A:181:SER:N	2.47	0.47
1:D:366:GLU:OE2	1:D:377:HIS:NE2	2.42	0.47
1:A:122:LEU:HD22	1:A:131:LEU:HD11	1.97	0.47
1:D:33:SER:HB3	1:D:160:ASP:O	2.15	0.47
1:A:249:ILE:O	1:A:274:THR:HA	2.16	0.46
1:D:294:GLU:O	1:D:300:ARG:HG3	2.16	0.46
1:A:225:ARG:HG2	1:A:239:LEU:HD11	1.97	0.45
1:B:245:LYS:HD3	1:B:247:TYR:CE1	2.51	0.45
1:A:263:HIS:CE1	1:A:334:GLU:HG2	2.52	0.45
1:C:31:LEU:HD23	1:C:31:LEU:HA	1.82	0.45
1:C:173:PRO:HG3	1:C:419:VAL:HG12	1.99	0.44
1:B:405:THR:HA	3:B:602:NAP:O4B	2.17	0.44
1:A:103:ILE:HG12	1:A:107:LYS:HB2	1.98	0.44
1:D:35:PRO:HB2	1:D:38:GLU:HG3	2.00	0.44
1:D:227:ILE:HG22	1:D:228:HIS:O	2.17	0.44
1:D:283:MET:HE3	1:D:283:MET:HB2	1.92	0.44
1:A:44:CYS:HB2	1:A:81:PHE:CD2	2.52	0.44
1:B:43:LEU:HD21	1:B:82:LEU:HD13	2.00	0.43
1:B:137:LEU:HD11	1:D:340:TYR:CD2	2.53	0.43
1:D:438:VAL:HG22	1:D:451:ILE:O	2.19	0.43
1:D:108:ASP:OD1	1:D:108:ASP:C	2.61	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:31:LEU:HD23	1:B:31:LEU:HA	1.92	0.42
1:C:266:GLN:HG2	1:C:354:HIS:CD2	2.55	0.42
1:B:316:LEU:HD11	1:B:459:ARG:HA	2.02	0.42
1:B:214:ALA:HB1	1:B:228:HIS:CD2	2.55	0.42
1:C:44:CYS:HB2	1:C:81:PHE:CD2	2.54	0.42
1:B:205:LYS:HD3	1:B:482:ILE:HG23	2.02	0.41
1:C:214:ALA:HB1	1:C:228:HIS:CG	2.55	0.41
1:C:405:THR:HA	3:C:602:NAP:O4B	2.20	0.41
1:B:266:GLN:HG2	1:B:354:HIS:CG	2.55	0.41
1:D:103:ILE:HG23	4:D:603:ACT:H2	2.01	0.41
1:A:340:TYR:CD2	1:C:137:LEU:HD11	2.55	0.41
1:A:349:GLU:HA	1:A:352:TRP:CE2	2.56	0.41
1:C:121:PHE:CE2	1:C:125:LEU:HD11	2.56	0.41
1:B:107:LYS:NZ	6:B:718:HOH:O	2.50	0.41
1:C:236:LEU:HA	1:C:236:LEU:HD12	1.84	0.41
1:B:452:TRP:HB3	1:B:478:MET:HE1	2.03	0.41
1:C:438:VAL:HG22	1:C:451:ILE:O	2.21	0.41
1:A:283:MET:HE3	1:A:283:MET:HB2	1.98	0.41
1:B:283:MET:HE3	1:B:283:MET:HB2	1.91	0.40
2:C:601:FAD:HM73	2:C:601:FAD:HM81	1.86	0.40
1:C:100:LYS:HD3	1:C:143:ALA:HA	2.04	0.40
1:C:452:TRP:HB3	1:C:478:MET:HE1	2.02	0.40
1:A:37:ASP:O	1:A:202:ARG:NH2	2.42	0.40
1:B:39:LEU:HD21	1:B:204:ARG:NE	2.36	0.40
1:C:240:LEU:HB3	1:C:247:TYR:CE2	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	431/501 (86%)	421 (98%)	10 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	436/501 (87%)	425 (98%)	11 (2%)	0	100	100
1	C	435/501 (87%)	423 (97%)	12 (3%)	0	100	100
1	D	434/501 (87%)	422 (97%)	12 (3%)	0	100	100
All	All	1736/2004 (87%)	1691 (97%)	45 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	370/441 (84%)	365 (99%)	5 (1%)	59	67
1	B	373/441 (85%)	369 (99%)	4 (1%)	65	74
1	C	363/441 (82%)	360 (99%)	3 (1%)	73	81
1	D	362/441 (82%)	357 (99%)	5 (1%)	59	67
All	All	1468/1764 (83%)	1451 (99%)	17 (1%)	63	72

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	GLU
1	A	103	ILE
1	A	156	GLN
1	A	199	SER
1	A	363	THR
1	B	96	VAL
1	B	103	ILE
1	B	199	SER
1	B	410	ASN
1	C	103	ILE
1	C	204	ARG
1	C	410	ASN
1	D	103	ILE

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Mol	Chain	Res	Type
1	D	239	LEU
1	D	241	LYS
1	D	288	ASP
1	D	415	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	420	GLN
1	B	36	GLN
1	B	337	ASN
1	C	126	HIS
1	C	480	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 2 are monoatomic - leaving 16 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
2	FAD	C	601	-	58,58,58	2.47	17 (29%)	85,89,89	1.81	18 (21%)
4	ACT	C	604	-	3,3,3	1.34	0	3,3,3	1.36	0
4	ACT	A	604	-	3,3,3	1.49	1 (33%)	3,3,3	1.25	0
4	ACT	C	603	-	3,3,3	1.12	0	3,3,3	1.61	1 (33%)
4	ACT	D	604	-	3,3,3	1.13	0	3,3,3	1.40	0
4	ACT	B	604	-	3,3,3	1.69	1 (33%)	3,3,3	1.30	0
4	ACT	A	603	-	3,3,3	1.62	1 (33%)	3,3,3	1.26	0
2	FAD	A	601	-	58,58,58	2.38	13 (22%)	85,89,89	1.76	17 (20%)
3	NAP	B	602	-	50,52,52	3.59	18 (36%)	71,80,80	1.82	15 (21%)
4	ACT	B	603	-	3,3,3	1.36	0	3,3,3	1.33	0
4	ACT	D	603	-	3,3,3	1.10	0	3,3,3	1.54	0
3	NAP	A	602	-	50,52,52	3.62	16 (32%)	71,80,80	1.74	10 (14%)
2	FAD	B	601	-	58,58,58	2.35	15 (25%)	85,89,89	1.77	20 (23%)
3	NAP	D	602	-	50,52,52	3.66	17 (34%)	71,80,80	1.82	14 (19%)
3	NAP	C	602	-	50,52,52	3.66	16 (32%)	71,80,80	1.74	15 (21%)
2	FAD	D	601	-	58,58,58	2.50	18 (31%)	85,89,89	1.83	20 (23%)

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	C	601	-	-	0/34/50/50	0/6/6/6
2	FAD	A	601	-	-	0/34/50/50	0/6/6/6
3	NAP	B	602	-	-	1/35/67/67	0/5/5/5
3	NAP	A	602	-	-	6/35/67/67	0/5/5/5
2	FAD	B	601	-	-	0/34/50/50	0/6/6/6
3	NAP	D	602	-	-	5/35/67/67	0/5/5/5
3	NAP	C	602	-	-	4/35/67/67	0/5/5/5
2	FAD	D	601	-	-	1/34/50/50	0/6/6/6

All (133) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	602	NAP	O4D-C1D	16.11	1.62	1.40
3	C	602	NAP	O4D-C1D	16.02	1.61	1.40
3	D	602	NAP	O4D-C1D	15.63	1.61	1.40
3	B	602	NAP	O4D-C1D	14.66	1.60	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	601	FAD	PA-O3P	-10.59	1.48	1.59
2	C	601	FAD	PA-O3P	-9.85	1.48	1.59
2	A	601	FAD	PA-O3P	-9.78	1.48	1.59
3	B	602	NAP	C2B-C1B	-9.14	1.30	1.53
3	A	602	NAP	C2B-C1B	-9.14	1.30	1.53
3	C	602	NAP	C2B-C1B	-8.98	1.31	1.53
3	D	602	NAP	C2B-C1B	-8.76	1.31	1.53
3	C	602	NAP	O4B-C1B	8.64	1.62	1.42
3	D	602	NAP	O4B-C1B	8.31	1.61	1.42
3	B	602	NAP	O4B-C1B	8.31	1.61	1.42
3	A	602	NAP	O4B-C1B	7.54	1.59	1.42
2	B	601	FAD	O4-C4	7.39	1.37	1.23
3	C	602	NAP	C7N-N7N	7.36	1.46	1.33
2	B	601	FAD	PA-O3P	-7.23	1.51	1.59
2	A	601	FAD	O4-C4	7.05	1.36	1.23
3	A	602	NAP	C7N-N7N	7.04	1.45	1.33
2	C	601	FAD	O4-C4	7.04	1.36	1.23
2	D	601	FAD	O4-C4	7.04	1.36	1.23
3	D	602	NAP	C7N-N7N	6.92	1.45	1.33
3	B	602	NAP	C7N-N7N	6.71	1.45	1.33
3	B	602	NAP	O4B-C4B	-6.34	1.30	1.45
3	A	602	NAP	O4B-C4B	-6.22	1.31	1.45
2	D	601	FAD	O2-C2	6.15	1.36	1.24
2	A	601	FAD	O2-C2	6.14	1.36	1.24
2	B	601	FAD	P-O3P	6.08	1.66	1.59
2	C	601	FAD	O2-C2	5.95	1.36	1.24
2	B	601	FAD	O2-C2	5.92	1.36	1.24
3	C	602	NAP	O4B-C4B	-5.90	1.31	1.45
3	B	602	NAP	O4D-C4D	-5.84	1.32	1.45
3	D	602	NAP	O4B-C4B	-5.84	1.32	1.45
3	C	602	NAP	O4D-C4D	-5.74	1.32	1.45
3	A	602	NAP	O4D-C4D	-5.74	1.32	1.45
3	D	602	NAP	O4D-C4D	-5.71	1.32	1.45
3	D	602	NAP	PN-O3	5.27	1.65	1.59
3	B	602	NAP	PN-O3	5.13	1.65	1.59
3	D	602	NAP	PA-O3	5.03	1.64	1.59
2	C	601	FAD	P-O3P	5.00	1.64	1.59
3	B	602	NAP	PA-O3	4.99	1.64	1.59
3	B	602	NAP	C6A-N6A	4.50	1.45	1.34
3	D	602	NAP	C6A-N6A	4.44	1.45	1.34
3	A	602	NAP	PA-O3	4.42	1.64	1.59
2	A	601	FAD	C6A-N6A	4.39	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	FAD	C4X-N5	4.38	1.40	1.30
2	D	601	FAD	C6A-N6A	4.34	1.45	1.34
3	C	602	NAP	C6A-N6A	4.31	1.45	1.34
2	B	601	FAD	C4X-N5	4.25	1.39	1.30
2	D	601	FAD	C4X-N5	4.24	1.39	1.30
3	A	602	NAP	C6A-N6A	4.10	1.44	1.34
2	C	601	FAD	C6A-N6A	4.01	1.44	1.34
3	A	602	NAP	PN-O3	3.89	1.63	1.59
2	B	601	FAD	C6A-N6A	3.87	1.44	1.34
2	D	601	FAD	C2-N1	3.85	1.45	1.36
2	C	601	FAD	C4X-N5	3.85	1.39	1.30
3	C	602	NAP	PA-O3	3.69	1.63	1.59
2	A	601	FAD	C2-N1	3.61	1.44	1.36
2	B	601	FAD	C2-N1	3.59	1.44	1.36
2	C	601	FAD	C2-N1	3.57	1.44	1.36
3	D	602	NAP	P2B-O2B	3.47	1.65	1.59
2	A	601	FAD	P-O3P	3.46	1.63	1.59
3	C	602	NAP	PN-O3	3.29	1.63	1.59
3	C	602	NAP	P2B-O2B	3.14	1.65	1.59
3	C	602	NAP	O2D-C2D	3.08	1.50	1.43
2	D	601	FAD	C10-N1	3.07	1.39	1.33
2	C	601	FAD	C10-N1	2.94	1.39	1.33
3	A	602	NAP	O3D-C3D	-2.93	1.35	1.43
3	D	602	NAP	O7N-C7N	-2.91	1.18	1.24
2	D	601	FAD	P-O3P	2.88	1.62	1.59
2	C	601	FAD	O4'-C4'	-2.86	1.37	1.43
3	D	602	NAP	C5A-C4A	-2.85	1.34	1.39
3	A	602	NAP	O2D-C2D	2.85	1.50	1.43
2	B	601	FAD	O4'-C4'	-2.84	1.37	1.43
2	A	601	FAD	C10-N1	2.80	1.38	1.33
3	D	602	NAP	C5A-N7A	-2.79	1.34	1.39
3	C	602	NAP	O3B-C3B	-2.78	1.36	1.43
3	C	602	NAP	C5A-C4A	-2.77	1.34	1.39
3	B	602	NAP	C5A-C4A	-2.77	1.34	1.39
3	B	602	NAP	O3D-C3D	-2.74	1.36	1.43
3	C	602	NAP	O3D-C3D	-2.72	1.36	1.43
3	D	602	NAP	O3D-C3D	-2.66	1.36	1.43
3	A	602	NAP	C5A-N7A	-2.63	1.34	1.39
2	D	601	FAD	O2'-C2'	-2.62	1.37	1.43
3	D	602	NAP	O2D-C2D	2.60	1.49	1.43
3	A	602	NAP	O7N-C7N	-2.57	1.19	1.24
3	A	602	NAP	P2B-O2B	2.56	1.64	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	602	NAP	C5A-N7A	-2.56	1.34	1.39
3	B	602	NAP	O2D-C2D	2.54	1.49	1.43
3	B	602	NAP	P2B-O2B	2.53	1.64	1.59
4	B	604	ACT	CH3-C	2.53	1.59	1.49
2	B	601	FAD	PA-O5B	-2.53	1.49	1.59
2	C	601	FAD	O2'-C2'	-2.49	1.38	1.43
2	C	601	FAD	PA-O5B	-2.49	1.49	1.59
2	D	601	FAD	O4'-C4'	-2.48	1.38	1.43
3	A	602	NAP	O3B-C3B	-2.47	1.36	1.43
3	B	602	NAP	C5A-N7A	-2.46	1.34	1.39
2	B	601	FAD	C10-N1	2.44	1.38	1.33
2	D	601	FAD	O4B-C4B	-2.42	1.39	1.45
2	C	601	FAD	C10-N10	2.41	1.42	1.37
2	A	601	FAD	O4'-C4'	-2.39	1.38	1.43
3	B	602	NAP	O3B-C3B	-2.35	1.37	1.43
2	C	601	FAD	O4B-C4B	-2.33	1.39	1.45
3	D	602	NAP	O3B-C3B	-2.32	1.37	1.43
2	C	601	FAD	C4A-N9A	2.31	1.42	1.37
3	A	602	NAP	C5A-C4A	-2.30	1.35	1.39
2	D	601	FAD	C1'-C2'	2.29	1.55	1.52
2	D	601	FAD	C4A-N9A	2.28	1.42	1.37
2	D	601	FAD	O2B-C2B	-2.28	1.37	1.43
2	B	601	FAD	PA-O2A	-2.27	1.44	1.55
2	D	601	FAD	PA-O5B	-2.26	1.50	1.59
2	D	601	FAD	PA-O2A	-2.25	1.44	1.55
2	C	601	FAD	PA-O2A	-2.23	1.45	1.55
4	A	604	ACT	CH3-C	2.21	1.57	1.49
2	D	601	FAD	P-O1P	2.20	1.58	1.50
3	B	602	NAP	C8A-N9A	-2.18	1.33	1.37
2	B	601	FAD	O2B-C2B	-2.18	1.37	1.43
4	A	603	ACT	CH3-C	2.16	1.57	1.49
2	A	601	FAD	O3B-C3B	-2.13	1.37	1.43
3	C	602	NAP	O7N-C7N	-2.12	1.20	1.24
3	B	602	NAP	C4N-C3N	-2.11	1.36	1.39
2	A	601	FAD	O4B-C4B	-2.10	1.40	1.45
2	D	601	FAD	C10-N10	2.10	1.41	1.37
2	B	601	FAD	O4B-C4B	-2.09	1.40	1.45
2	B	601	FAD	O3'-C3'	-2.09	1.37	1.43
3	B	602	NAP	O7N-C7N	-2.08	1.20	1.24
2	A	601	FAD	PA-O5B	-2.07	1.51	1.59
3	D	602	NAP	C8A-N9A	-2.07	1.34	1.37
2	B	601	FAD	C5A-C4A	2.07	1.42	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	FAD	P-O1P	2.06	1.57	1.50
2	C	601	FAD	P-O1P	2.05	1.57	1.50
2	C	601	FAD	C5A-C4A	2.04	1.42	1.39

All (130) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	601	FAD	N3A-C2A-N1A	-6.04	119.44	128.58
3	B	602	NAP	N3A-C2A-N1A	-6.04	119.44	128.58
2	D	601	FAD	N3A-C2A-N1A	-5.94	119.59	128.58
2	B	601	FAD	N3A-C2A-N1A	-5.91	119.63	128.58
3	C	602	NAP	N3A-C2A-N1A	-5.89	119.66	128.58
3	D	602	NAP	N3A-C2A-N1A	-5.77	119.85	128.58
2	A	601	FAD	N3A-C2A-N1A	-5.68	119.98	128.58
3	A	602	NAP	N3A-C2A-N1A	-5.67	120.00	128.58
3	D	602	NAP	C5A-C4A-N3A	-5.45	119.22	126.72
3	A	602	NAP	N6A-C6A-N1A	-5.34	106.49	118.38
2	A	601	FAD	C5A-C4A-N3A	-5.32	119.39	126.72
3	B	602	NAP	C5A-C4A-N3A	-5.14	119.64	126.72
2	C	601	FAD	C5A-C4A-N3A	-5.14	119.65	126.72
3	A	602	NAP	C5A-C4A-N3A	-5.01	119.82	126.72
2	D	601	FAD	C5A-C4A-N3A	-4.99	119.84	126.72
3	D	602	NAP	N6A-C6A-N1A	-4.94	107.37	118.38
2	D	601	FAD	O2A-PA-O3P	-4.89	94.07	107.27
3	C	602	NAP	N6A-C6A-N1A	-4.71	107.88	118.38
3	B	602	NAP	N6A-C6A-N1A	-4.59	108.16	118.38
2	B	601	FAD	C5A-C4A-N3A	-4.46	120.57	126.72
2	B	601	FAD	C4-C4X-N5	4.40	124.28	118.21
2	A	601	FAD	C5A-N7A-C8A	4.30	110.20	103.45
2	C	601	FAD	C5A-N7A-C8A	4.25	110.13	103.45
3	B	602	NAP	N9A-C8A-N7A	-4.24	107.92	113.94
2	B	601	FAD	N3A-C4A-N9A	4.22	134.35	127.17
3	C	602	NAP	C5A-C4A-N3A	-4.15	121.00	126.72
2	D	601	FAD	C5A-N7A-C8A	4.10	109.90	103.45
2	D	601	FAD	N3A-C4A-N9A	4.05	134.06	127.17
2	C	601	FAD	N3A-C4A-N9A	4.02	134.01	127.17
3	C	602	NAP	N9A-C8A-N7A	-3.99	108.27	113.94
2	A	601	FAD	N3A-C4A-N9A	3.99	133.95	127.17
3	A	602	NAP	C5A-C6A-N6A	3.94	133.05	123.29
3	D	602	NAP	N9A-C8A-N7A	-3.93	108.36	113.94
2	C	601	FAD	C2A-N3A-C4A	3.88	121.31	111.83
3	A	602	NAP	N9A-C8A-N7A	-3.88	108.44	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	602	NAP	N3A-C4A-N9A	3.87	133.75	127.17
3	C	602	NAP	C5A-C6A-N6A	3.83	132.78	123.29
2	A	601	FAD	C2A-N3A-C4A	3.81	121.13	111.83
2	D	601	FAD	C2A-N3A-C4A	3.78	121.06	111.83
2	A	601	FAD	C4-C4X-N5	3.78	123.42	118.21
3	D	602	NAP	N3A-C4A-N9A	3.75	133.54	127.17
2	B	601	FAD	C5A-N7A-C8A	3.72	109.29	103.45
3	D	602	NAP	C5A-C6A-N6A	3.70	132.46	123.29
3	B	602	NAP	C5A-C6A-N6A	3.56	132.09	123.29
2	A	601	FAD	C4A-C5A-N7A	-3.55	106.52	110.58
2	C	601	FAD	C4A-C5A-N7A	-3.53	106.54	110.58
3	C	602	NAP	C6N-N1N-C2N	-3.50	118.90	121.88
3	B	602	NAP	C2A-N3A-C4A	3.48	120.33	111.83
3	D	602	NAP	C2A-N3A-C4A	3.44	120.23	111.83
3	A	602	NAP	C6N-N1N-C2N	-3.42	118.97	121.88
2	B	601	FAD	C4X-C10-N10	3.35	121.28	116.48
2	B	601	FAD	C2A-N3A-C4A	3.35	120.02	111.83
3	A	602	NAP	N3A-C4A-N9A	3.34	132.85	127.17
2	C	601	FAD	N9A-C8A-N7A	-3.29	109.27	113.94
3	A	602	NAP	C2A-N3A-C4A	3.29	119.86	111.83
2	C	601	FAD	C4-N3-C2	-3.27	119.83	125.64
2	A	601	FAD	N9A-C8A-N7A	-3.27	109.30	113.94
2	D	601	FAD	C4A-C5A-N7A	-3.22	106.90	110.58
2	D	601	FAD	N9A-C8A-N7A	-3.21	109.38	113.94
3	D	602	NAP	C2B-C1B-N9A	-3.19	108.49	113.75
2	A	601	FAD	C4-N3-C2	-3.12	120.11	125.64
2	B	601	FAD	N9A-C8A-N7A	-3.06	109.59	113.94
3	C	602	NAP	C2A-N3A-C4A	3.04	119.26	111.83
2	B	601	FAD	C10-C4X-N5	-3.03	118.62	124.81
2	B	601	FAD	C4-N3-C2	-2.95	120.40	125.64
2	D	601	FAD	C4X-C4-N3	2.91	120.67	113.25
3	B	602	NAP	C4A-N9A-C8A	2.90	108.78	105.74
3	C	602	NAP	N3A-C4A-N9A	2.90	132.09	127.17
3	B	602	NAP	C6N-N1N-C2N	-2.86	119.45	121.88
2	C	601	FAD	C4X-C10-N1	-2.84	117.64	124.59
2	C	601	FAD	C4X-C4-N3	2.83	120.47	113.25
3	D	602	NAP	C5A-N7A-C8A	2.83	107.89	103.45
3	B	602	NAP	C5A-N7A-C8A	2.81	107.87	103.45
3	D	602	NAP	C6N-N1N-C2N	-2.79	119.50	121.88
2	D	601	FAD	C4'-C3'-C2'	2.79	118.22	113.57
2	A	601	FAD	C4X-C4-N3	2.77	120.29	113.25
2	D	601	FAD	C4-N3-C2	-2.75	120.76	125.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602	NAP	C5A-N7A-C8A	2.70	107.69	103.45
3	C	602	NAP	C2N-C3N-C4N	2.67	121.37	118.26
2	C	601	FAD	O2A-PA-O3P	-2.64	100.14	107.27
2	C	601	FAD	C4-C4X-N5	2.61	121.81	118.21
3	D	602	NAP	C6A-C5A-C4A	2.60	120.73	117.18
2	D	601	FAD	O3P-PA-O1A	2.58	118.47	110.70
3	C	602	NAP	C4A-N9A-C8A	2.58	108.44	105.74
2	B	601	FAD	O2A-PA-O3P	-2.56	100.36	107.27
3	B	602	NAP	C4D-O4D-C1D	-2.53	107.61	109.92
2	D	601	FAD	C5X-C9A-N10	2.50	120.23	117.97
2	D	601	FAD	C4-C4X-N5	2.50	121.66	118.21
2	B	601	FAD	C4X-C4-N3	2.49	119.59	113.25
2	C	601	FAD	O2P-P-O3P	-2.49	100.55	107.27
3	D	602	NAP	C4D-O4D-C1D	-2.46	107.67	109.92
2	C	601	FAD	C10-C4X-N5	-2.46	119.78	124.81
3	C	602	NAP	C4D-O4D-C1D	-2.45	107.68	109.92
3	C	602	NAP	C2B-C1B-N9A	-2.45	109.72	113.75
2	A	601	FAD	C10-C4X-N5	-2.44	119.82	124.81
3	B	602	NAP	C6A-C5A-C4A	2.44	120.51	117.18
2	B	601	FAD	O5'-P-O1P	2.43	118.57	108.94
2	A	601	FAD	C4X-C10-N10	2.43	119.96	116.48
2	B	601	FAD	O2P-P-O5'	-2.41	96.65	107.57
3	C	602	NAP	C5A-N7A-C8A	2.39	107.21	103.45
2	D	601	FAD	C4X-C10-N1	-2.36	118.81	124.59
2	D	601	FAD	O3P-P-O1P	2.35	117.76	110.70
2	B	601	FAD	C4X-C10-N1	-2.30	118.94	124.59
2	D	601	FAD	C1'-C2'-C3'	2.30	115.89	109.66
2	A	601	FAD	O4-C4-C4X	-2.29	120.48	126.53
2	B	601	FAD	C1'-C2'-C3'	2.28	115.84	109.66
3	B	602	NAP	C2N-C3N-C4N	2.28	120.91	118.26
3	D	602	NAP	C2N-C3N-C4N	2.26	120.89	118.26
2	B	601	FAD	O4-C4-N3	-2.26	115.87	120.11
2	A	601	FAD	O3P-P-O1P	2.24	117.44	110.70
3	A	602	NAP	C3N-C7N-N7N	2.22	120.47	117.74
2	B	601	FAD	C2A-N1A-C6A	2.22	122.37	118.73
2	A	601	FAD	C2B-C3B-C4B	2.21	106.89	102.61
2	B	601	FAD	C5'-C4'-C3'	2.18	116.33	112.22
2	C	601	FAD	O3P-P-O1P	2.17	117.23	110.70
3	C	602	NAP	C5N-C4N-C3N	-2.15	118.25	120.36
3	D	602	NAP	C4A-N9A-C8A	2.12	107.96	105.74
4	C	603	ACT	O-C-CH3	-2.12	113.86	122.53
2	D	601	FAD	C2A-N1A-C6A	2.11	122.19	118.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	FAD	C4A-C5A-N7A	-2.10	108.18	110.58
2	A	601	FAD	C4X-C10-N1	-2.09	119.46	124.59
2	D	601	FAD	O3'-C3'-C4'	-2.07	104.22	108.93
2	D	601	FAD	O2P-P-O5'	-2.07	98.18	107.57
2	A	601	FAD	C5X-C9A-N10	2.06	119.83	117.97
3	B	602	NAP	P2B-O2B-C2B	-2.05	117.95	123.43
3	B	602	NAP	C2B-C1B-N9A	-2.03	110.42	113.75
3	C	602	NAP	C6A-C5A-C4A	2.02	119.94	117.18
2	C	601	FAD	C5X-C9A-N10	2.02	119.79	117.97
2	C	601	FAD	C1'-C2'-C3'	2.01	115.12	109.66
2	C	601	FAD	O2P-P-O5'	-2.01	98.48	107.57

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	602	NAP	C5D-O5D-PN-O3
3	D	602	NAP	C3B-C2B-O2B-P2B
3	A	602	NAP	PA-O3-PN-O5D
3	C	602	NAP	PA-O3-PN-O5D
3	D	602	NAP	PA-O3-PN-O5D
3	A	602	NAP	C1B-C2B-O2B-P2B
3	A	602	NAP	C3B-C2B-O2B-P2B
3	A	602	NAP	C2B-O2B-P2B-O3X
3	D	602	NAP	C1B-C2B-O2B-P2B
3	C	602	NAP	O4B-C4B-C5B-O5B
2	D	601	FAD	O4B-C4B-C5B-O5B
3	A	602	NAP	O4B-C4B-C5B-O5B
3	C	602	NAP	C2B-O2B-P2B-O3X
3	D	602	NAP	C2B-O2B-P2B-O3X
3	A	602	NAP	PN-O3-PA-O2A
3	C	602	NAP	PN-O3-PA-O2A
3	D	602	NAP	PN-O3-PA-O2A

There are no ring outliers.

7 monomers are involved in 7 short contacts:

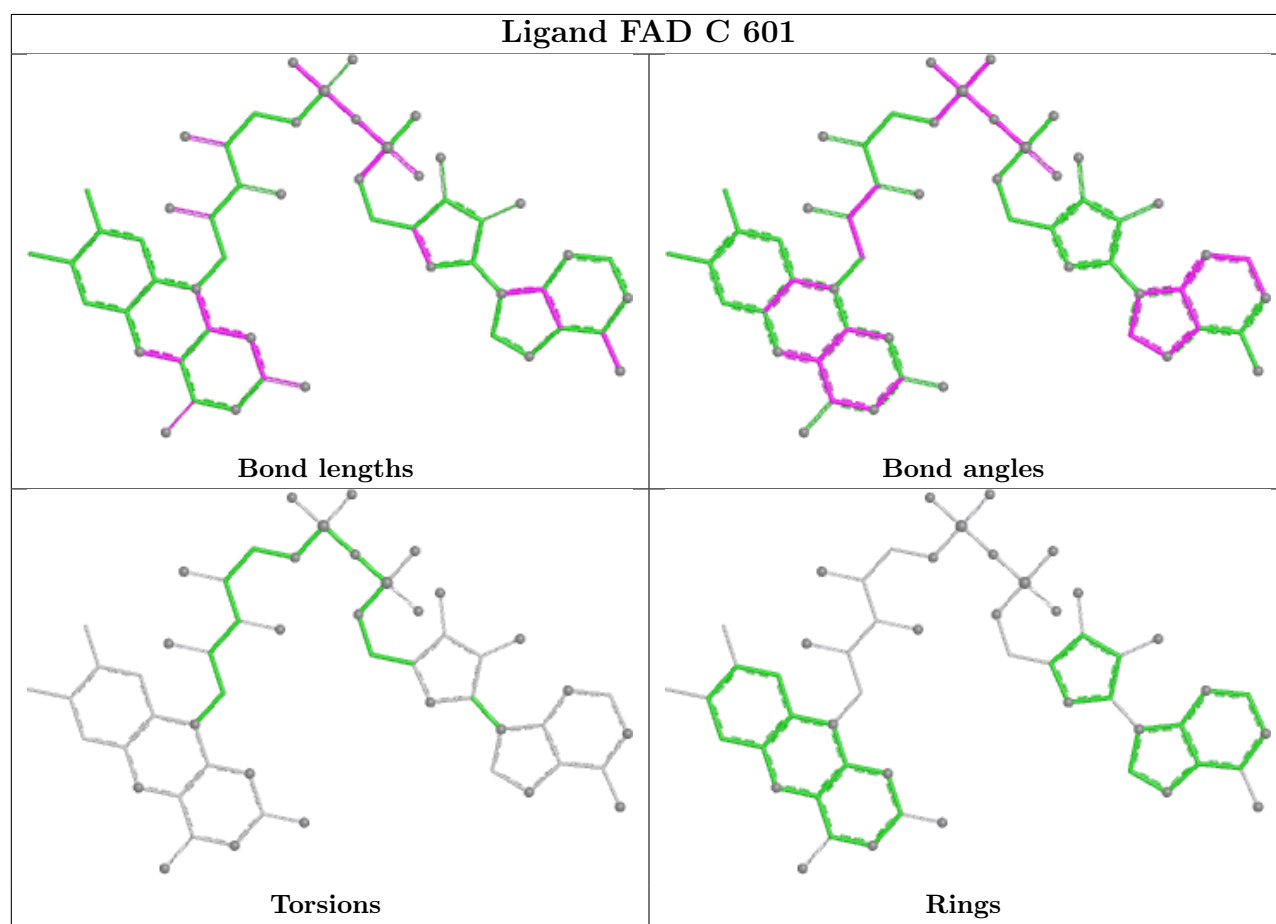
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	601	FAD	1	0
4	C	603	ACT	1	0
2	A	601	FAD	1	0

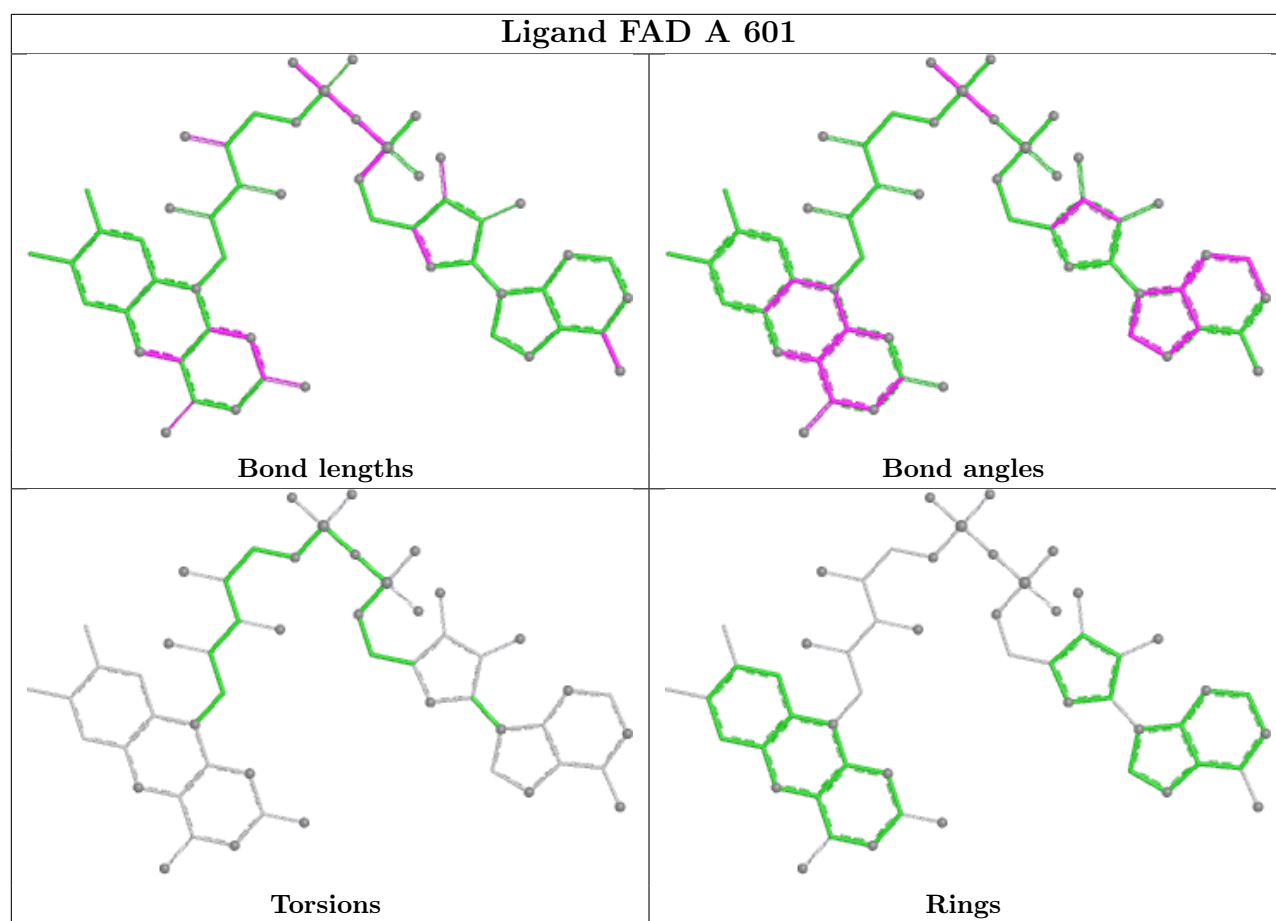
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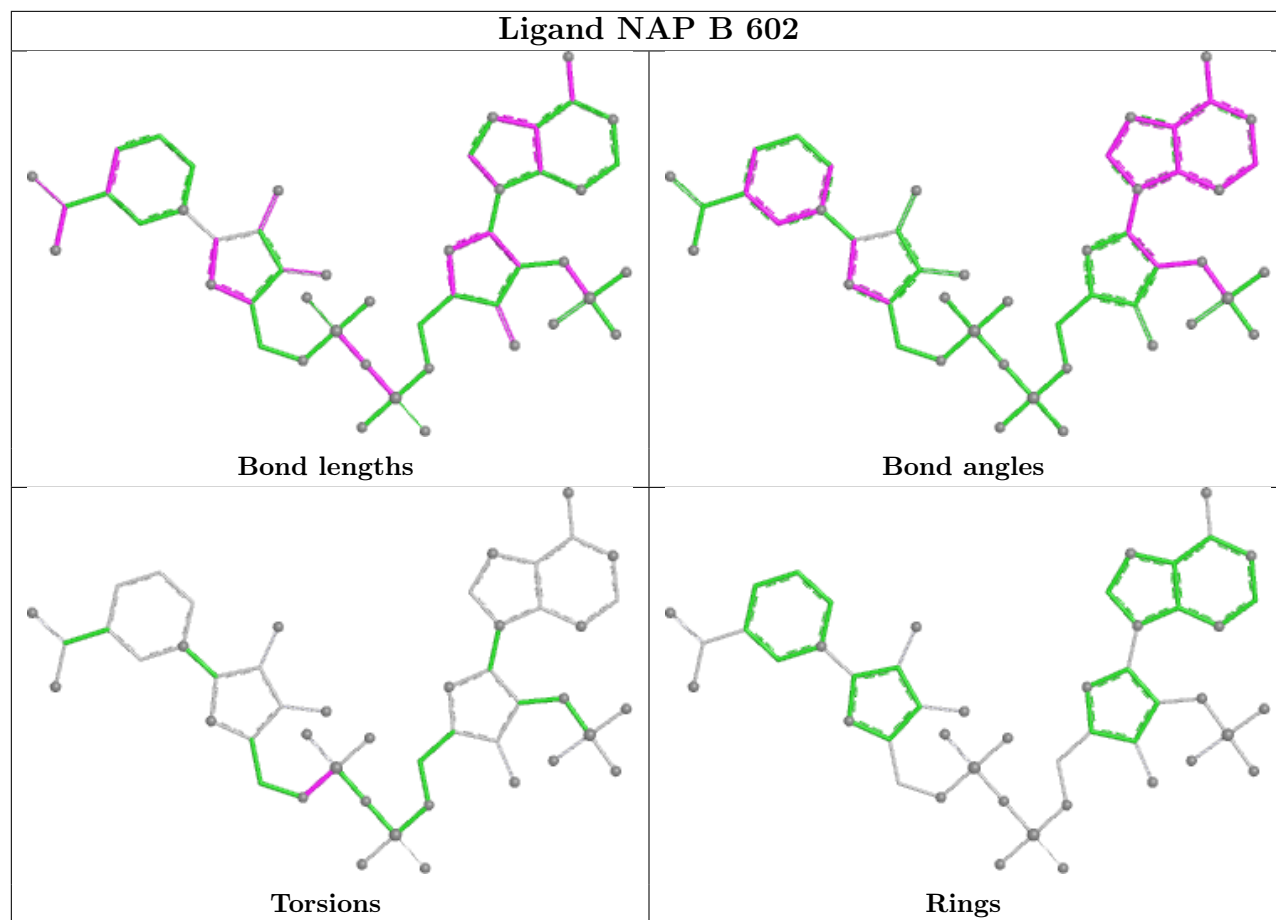
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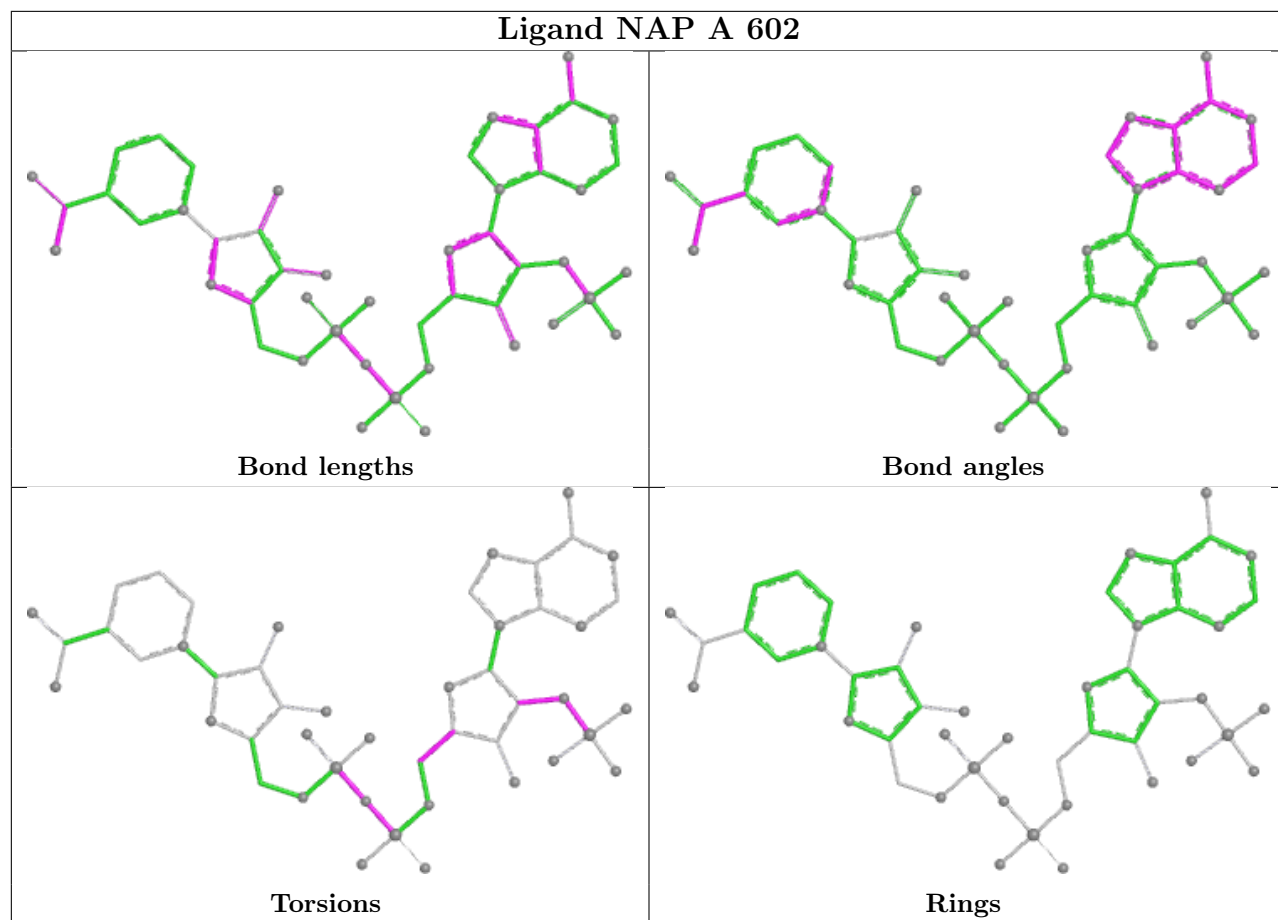
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	602	NAP	1	0
4	D	603	ACT	1	0
2	B	601	FAD	1	0
3	C	602	NAP	1	0

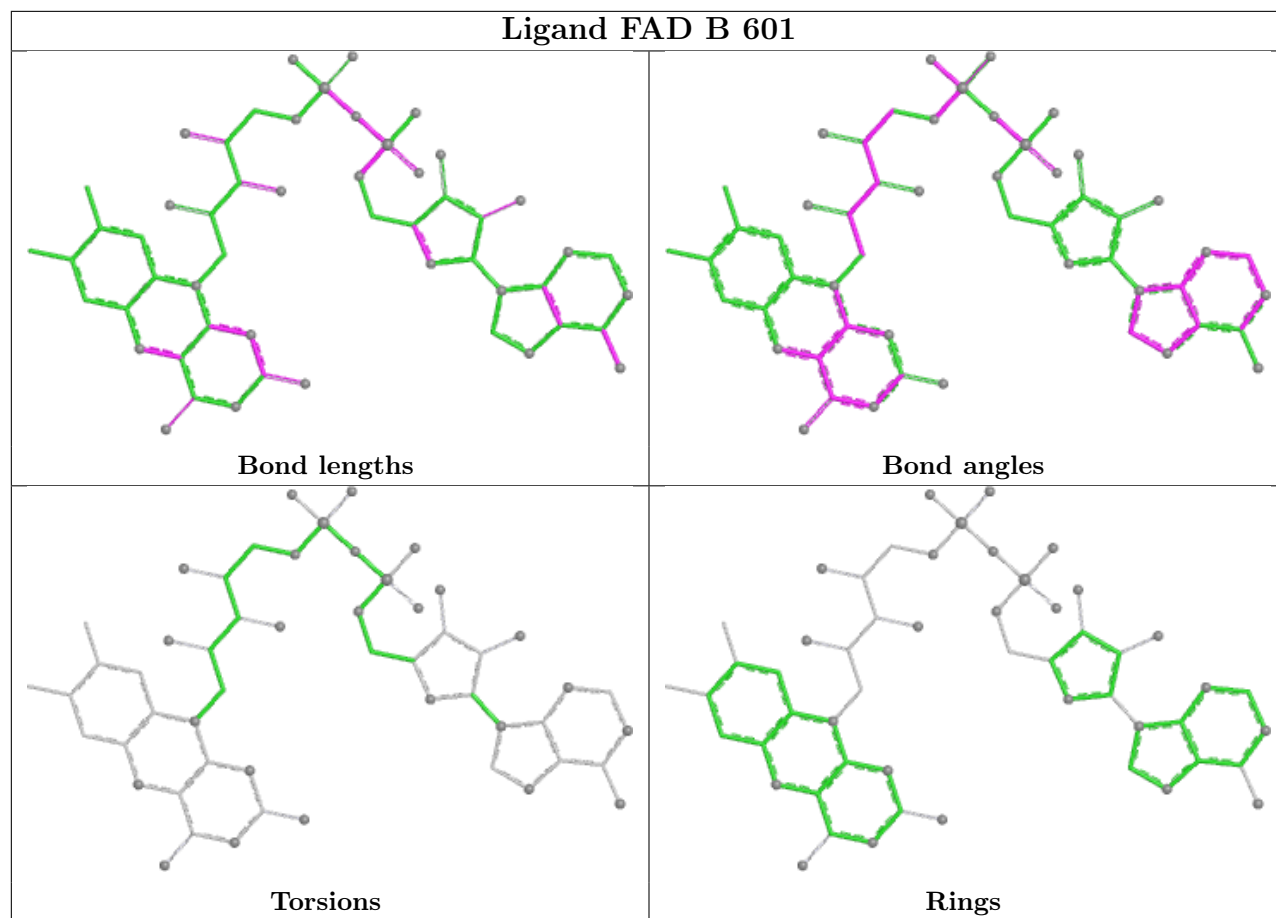
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

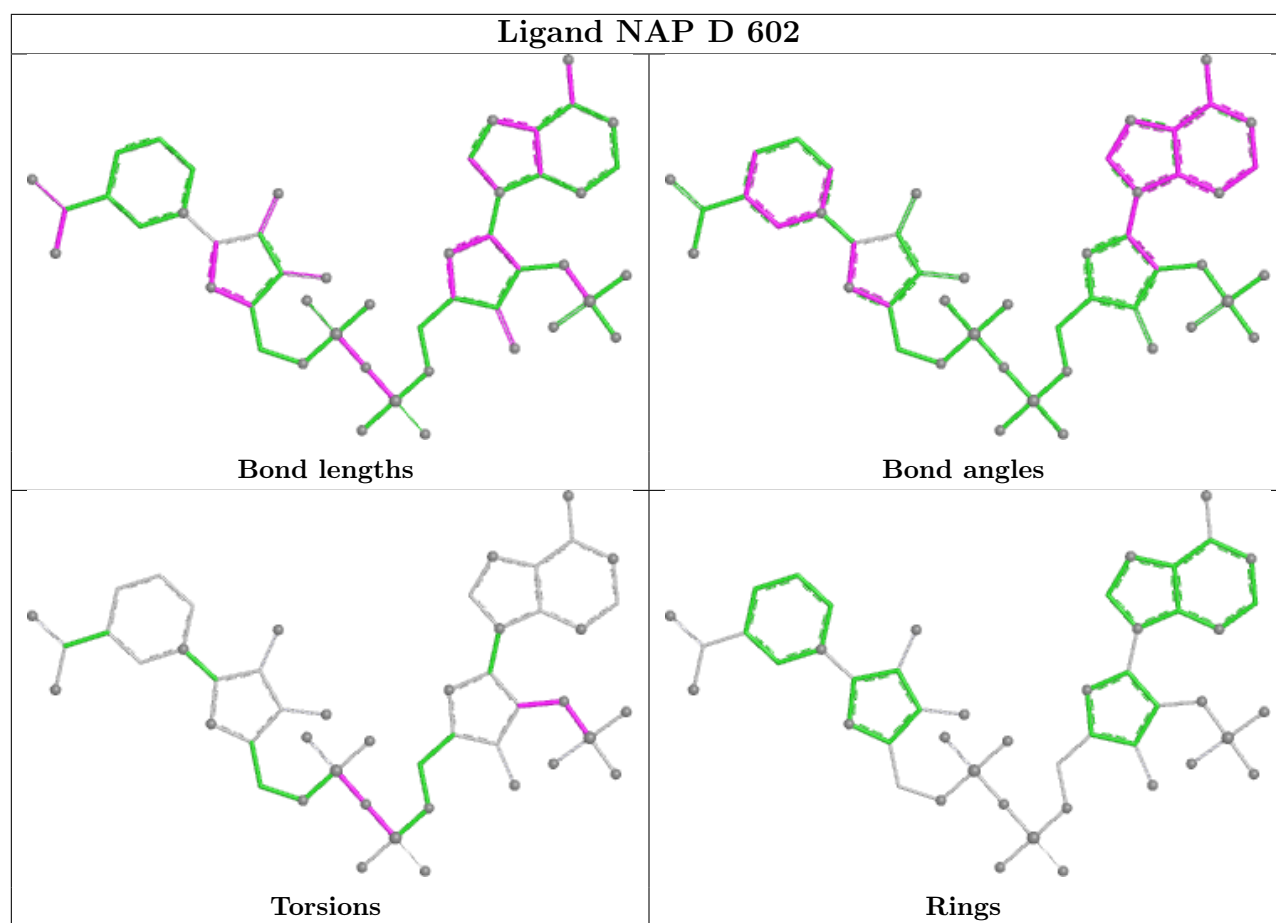


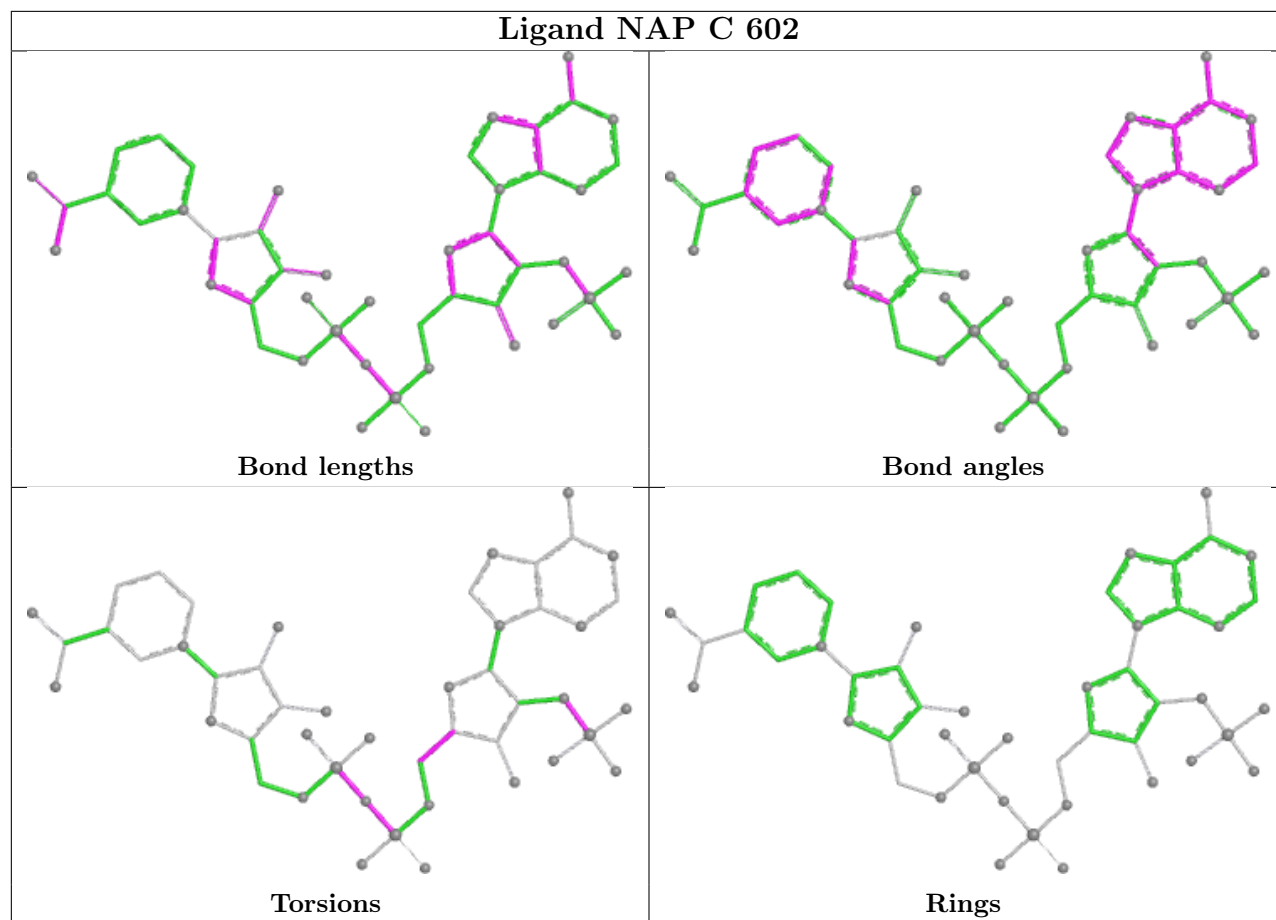


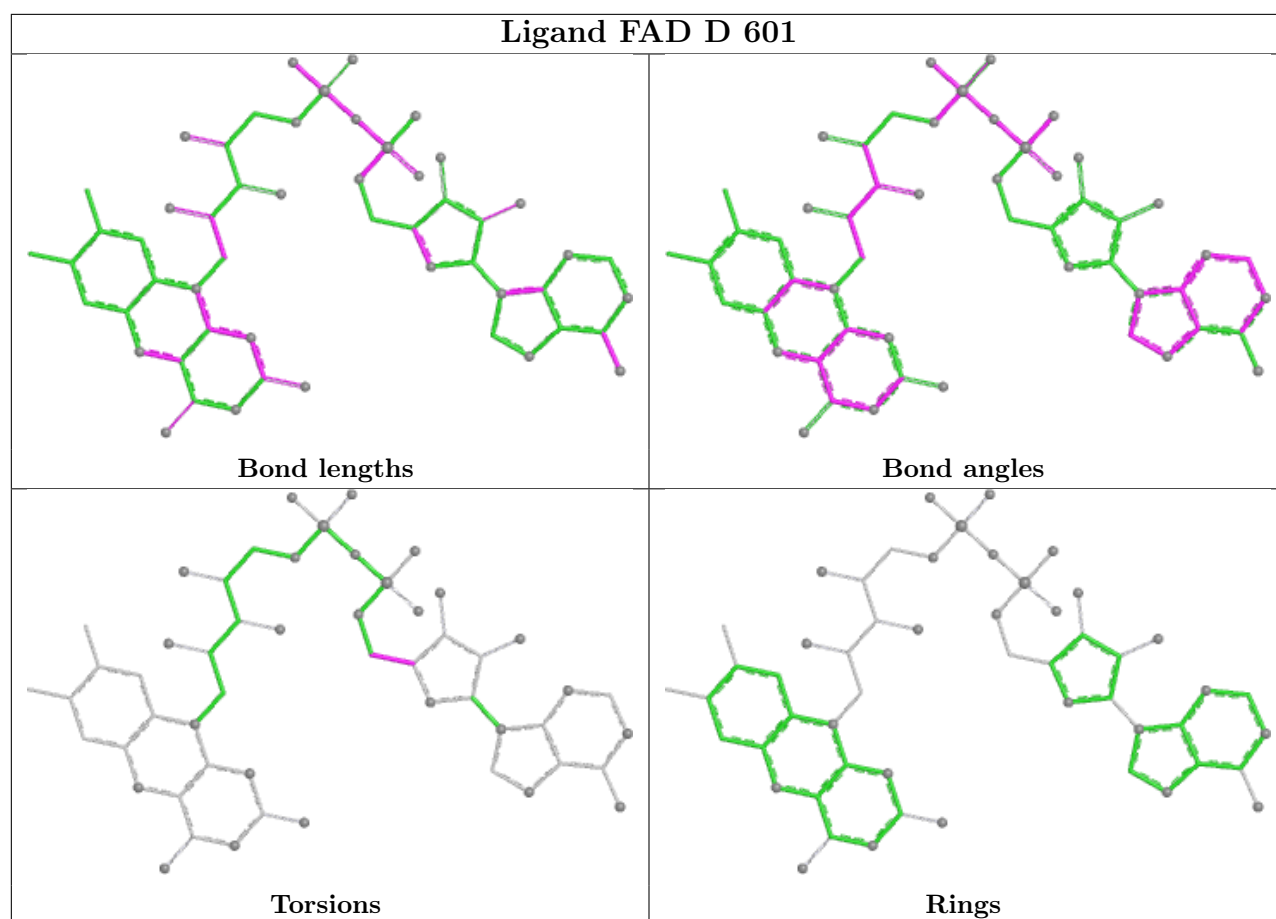












5.7 Other polymers [i](#)

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 ⓘ

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	439/501 (87%)	0.77	36 (8%) 17 18	15, 27, 45, 58	0
1	B	442/501 (88%)	0.63	22 (4%) 34 36	16, 24, 40, 55	0
1	C	441/501 (88%)	0.95	54 (12%) 8 8	17, 29, 50, 71	0
1	D	440/501 (87%)	0.90	48 (10%) 10 11	17, 28, 48, 80	0
All	All	1762/2004 (87%)	0.81	160 (9%) 15 15	15, 27, 46, 80	0

All (160) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	370	PRO	6.2
1	C	425	THR	5.6
1	C	369	GLY	4.7
1	A	489	ARG	4.7
1	A	425	THR	4.4
1	C	182	VAL	4.4
1	A	67	ASN	4.2
1	A	383	PRO	4.0
1	D	426	GLY	3.9
1	D	179	SER	3.9
1	D	368	HIS	3.8
1	A	371	GLN	3.8
1	D	487	LEU	3.8
1	C	393	LYS	3.8
1	D	371	GLN	3.6
1	B	67	ASN	3.6
1	C	371	GLN	3.6
1	C	177	ASP	3.6
1	B	383	PRO	3.5
1	C	427	GLN	3.5
1	C	487	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	180	SER	3.5
1	D	181	SER	3.4
1	D	369	GLY	3.4
1	A	182	VAL	3.4
1	D	30	ARG	3.3
1	A	181	SER	3.3
1	C	67	ASN	3.3
1	C	370	PRO	3.3
1	A	180	SER	3.3
1	D	383	PRO	3.3
1	C	368	HIS	3.2
1	D	67	ASN	3.2
1	C	447	SER	3.2
1	C	323	ASN	3.2
1	C	179	SER	3.1
1	C	383	PRO	3.1
1	C	65	ARG	3.1
1	B	488	GLU	3.1
1	C	181	SER	3.1
1	C	488	GLU	3.1
1	C	178	PRO	3.0
1	B	368	HIS	3.0
1	D	64	PRO	2.9
1	D	288	ASP	2.9
1	C	426	GLY	2.9
1	D	178	PRO	2.8
1	A	222	GLN	2.8
1	A	320	LYS	2.8
1	D	372	SER	2.8
1	B	64	PRO	2.8
1	C	64	PRO	2.7
1	D	365	VAL	2.7
1	B	485	GLU	2.6
1	C	183	VAL	2.6
1	C	318	ALA	2.6
1	D	234	THR	2.6
1	D	322	THR	2.6
1	C	35	PRO	2.6
1	A	65	ARG	2.6
1	A	447	SER	2.6
1	B	365	VAL	2.6
1	C	324	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	445	VAL	2.6
1	D	222	GLN	2.6
1	D	323	ASN	2.5
1	A	442	PRO	2.5
1	A	350	THR	2.5
1	D	395	THR	2.5
1	C	238	ALA	2.5
1	D	182	VAL	2.5
1	C	63	ASP	2.5
1	B	371	GLN	2.5
1	B	235	THR	2.5
1	D	180	SER	2.5
1	B	221	PRO	2.4
1	A	30	ARG	2.4
1	B	30	ARG	2.4
1	D	177	ASP	2.4
1	C	372	SER	2.4
1	A	443	SER	2.4
1	D	32	ARG	2.4
1	C	376	ILE	2.4
1	C	424	PRO	2.4
1	C	423	ARG	2.3
1	D	183	VAL	2.3
1	C	485	GLU	2.3
1	D	442	PRO	2.3
1	D	318	ALA	2.3
1	D	220	LEU	2.3
1	D	396	LEU	2.3
1	D	367	HIS	2.3
1	A	183	VAL	2.3
1	C	195	THR	2.3
1	B	288	ASP	2.3
1	A	426	GLY	2.3
1	A	485	GLU	2.2
1	C	442	PRO	2.2
1	D	445	VAL	2.2
1	B	31	LEU	2.2
1	D	176	SER	2.2
1	A	424	PRO	2.2
1	B	393	LYS	2.2
1	C	317	LEU	2.2
1	B	382	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	410	ASN	2.2
1	A	185	PHE	2.2
1	A	428	ASP	2.2
1	C	193	VAL	2.2
1	C	422	LEU	2.2
1	C	176	SER	2.2
1	D	218	SER	2.2
1	D	314	ARG	2.2
1	A	324	TYR	2.2
1	C	172	ILE	2.1
1	A	445	VAL	2.1
1	D	200	ALA	2.1
1	A	31	LEU	2.1
1	A	317	LEU	2.1
1	D	62	LEU	2.1
1	C	443	SER	2.1
1	C	243	LYS	2.1
1	D	485	GLU	2.1
1	A	35	PRO	2.1
1	C	429	GLN	2.1
1	B	174	GLY	2.1
1	C	419	VAL	2.1
1	A	318	ALA	2.1
1	D	447	SER	2.1
1	A	410	ASN	2.1
1	D	428	ASP	2.1
1	A	64	PRO	2.1
1	A	370	PRO	2.1
1	C	87	GLN	2.1
1	B	426	GLY	2.1
1	D	172	ILE	2.1
1	C	241	LYS	2.1
1	D	320	LYS	2.1
1	D	411	ALA	2.1
1	A	33	SER	2.1
1	D	486	GLN	2.1
1	B	322	THR	2.1
1	D	97	PRO	2.1
1	C	198	ILE	2.1
1	C	382	LYS	2.1
1	A	403	VAL	2.1
1	C	62	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	317	LEU	2.0
1	C	441	ASP	2.0
1	B	178	PRO	2.0
1	B	350	THR	2.0
1	C	322	THR	2.0
1	A	175	LYS	2.0
1	A	482	ILE	2.0
1	D	244	SER	2.0
1	D	321	ALA	2.0
1	C	239	LEU	2.0
1	A	98	GLY	2.0
1	B	219	GLY	2.0
1	B	369	GLY	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 oligosaccharides 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
4	ACT	C	604	4/4	0.81	0.17	23,27,28,32	0
5	CA	D	605	1/1	0.82	0.13	57,57,57,57	0
4	ACT	D	604	4/4	0.87	0.13	24,24,27,29	0
4	ACT	A	603	4/4	0.87	0.14	24,26,26,32	0
4	ACT	B	604	4/4	0.88	0.11	20,21,22,25	0
4	ACT	B	603	4/4	0.89	0.12	20,22,23,24	0
4	ACT	C	603	4/4	0.90	0.11	21,22,24,24	0
4	ACT	D	603	4/4	0.92	0.09	21,22,22,26	0
5	CA	B	605	1/1	0.93	0.07	46,46,46,46	0
2	FAD	C	601	53/53	0.93	0.09	19,23,29,41	0

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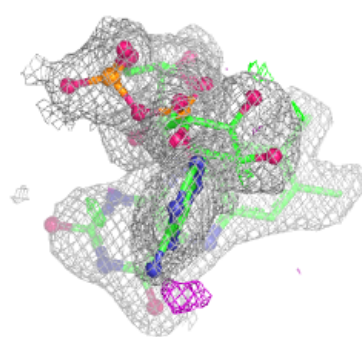
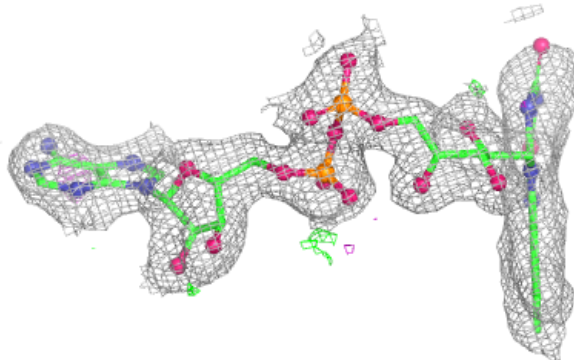
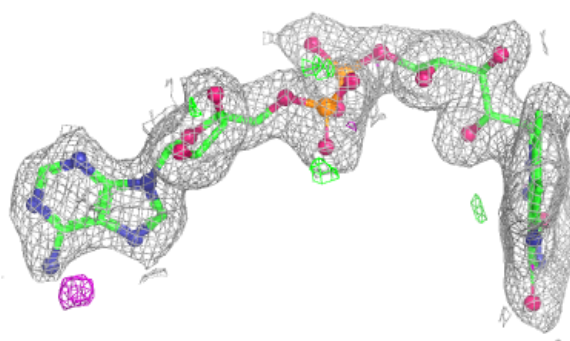
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FAD	D	601	53/53	0.94	0.10	18,24,31,35	0
3	NAP	A	602	48/48	0.94	0.08	18,23,30,33	0
3	NAP	B	602	48/48	0.94	0.08	17,23,31,34	0
3	NAP	C	602	48/48	0.94	0.09	17,25,32,39	0
3	NAP	D	602	48/48	0.94	0.09	20,26,34,40	0
2	FAD	B	601	53/53	0.94	0.09	13,18,25,31	0
2	FAD	A	601	53/53	0.94	0.08	17,23,30,35	0
4	ACT	A	604	4/4	0.96	0.06	18,21,21,22	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.

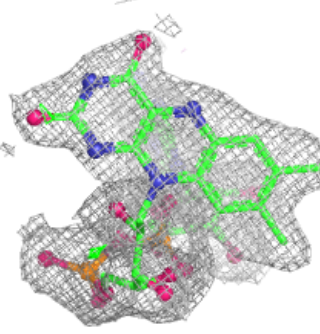
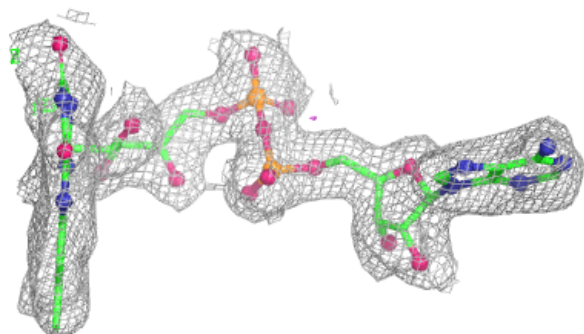
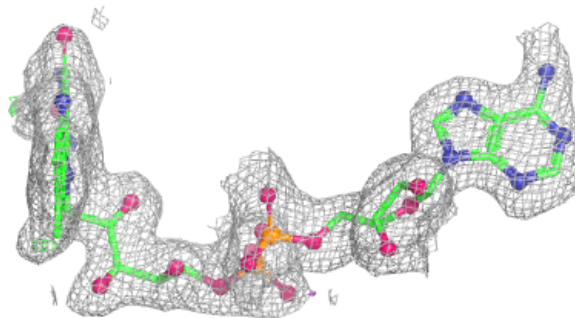
Electron density around FAD C 601:

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

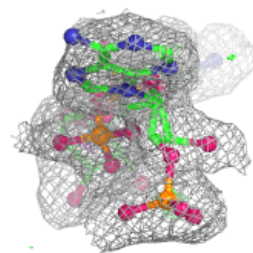
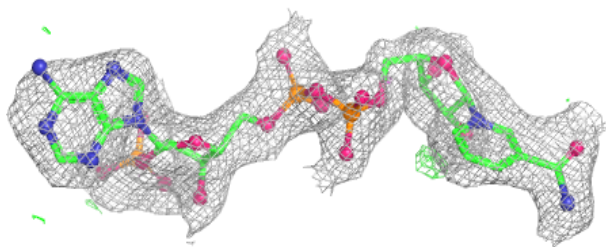
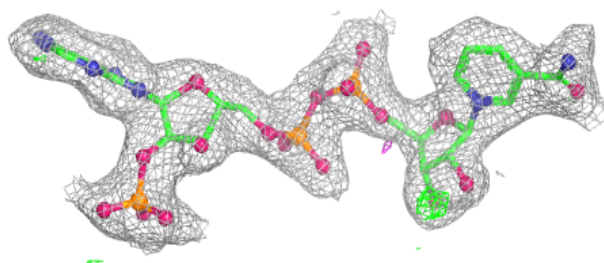


Electron density around FAD D 601:

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

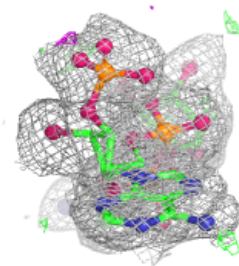
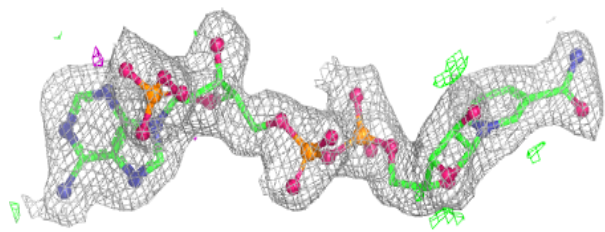
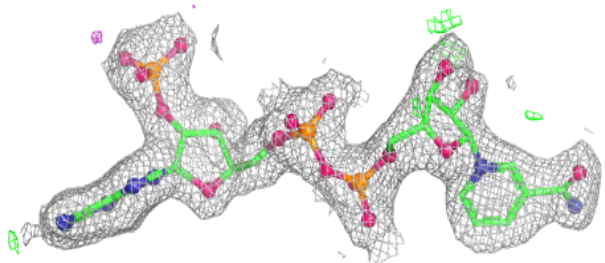
**Electron density around NAP A 602:**

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

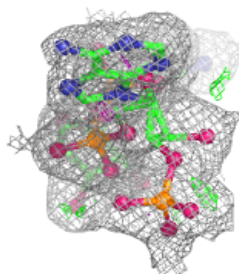
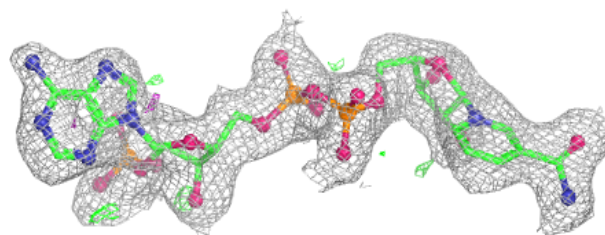
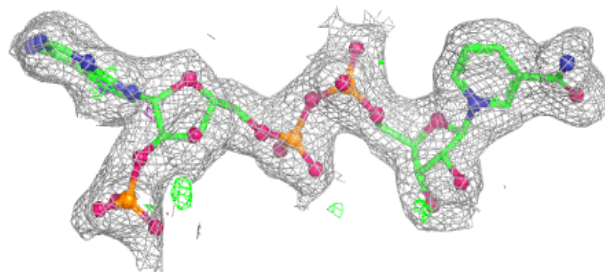


Electron density around NAP B 602:

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

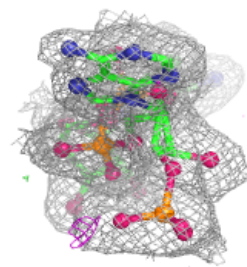
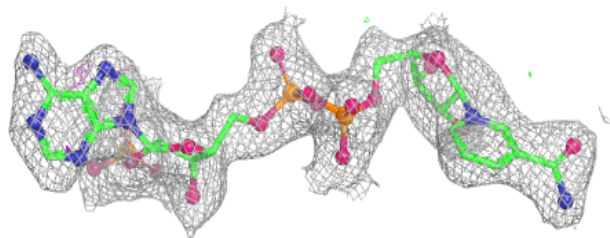
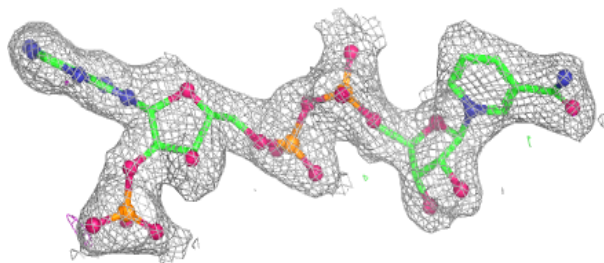
**Electron density around NAP C 602:**

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

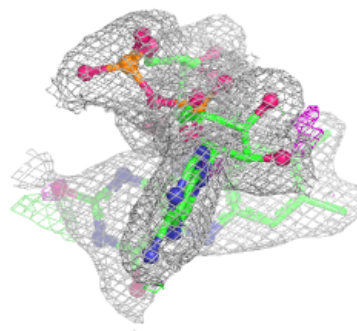
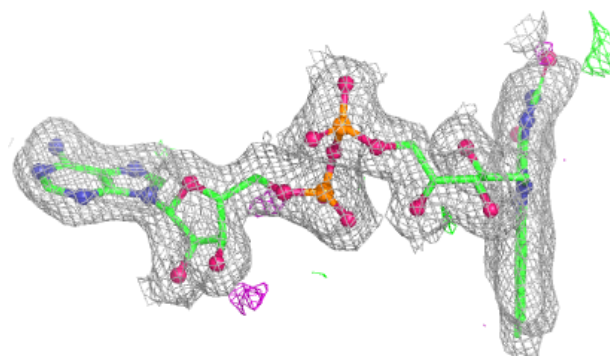
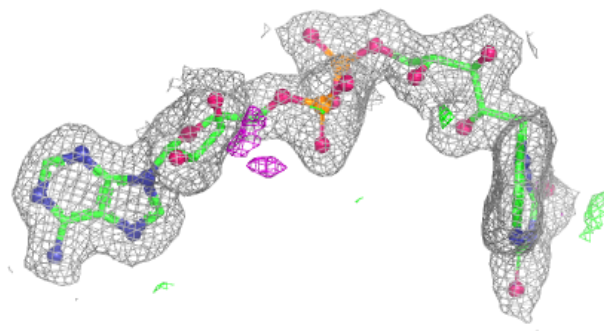


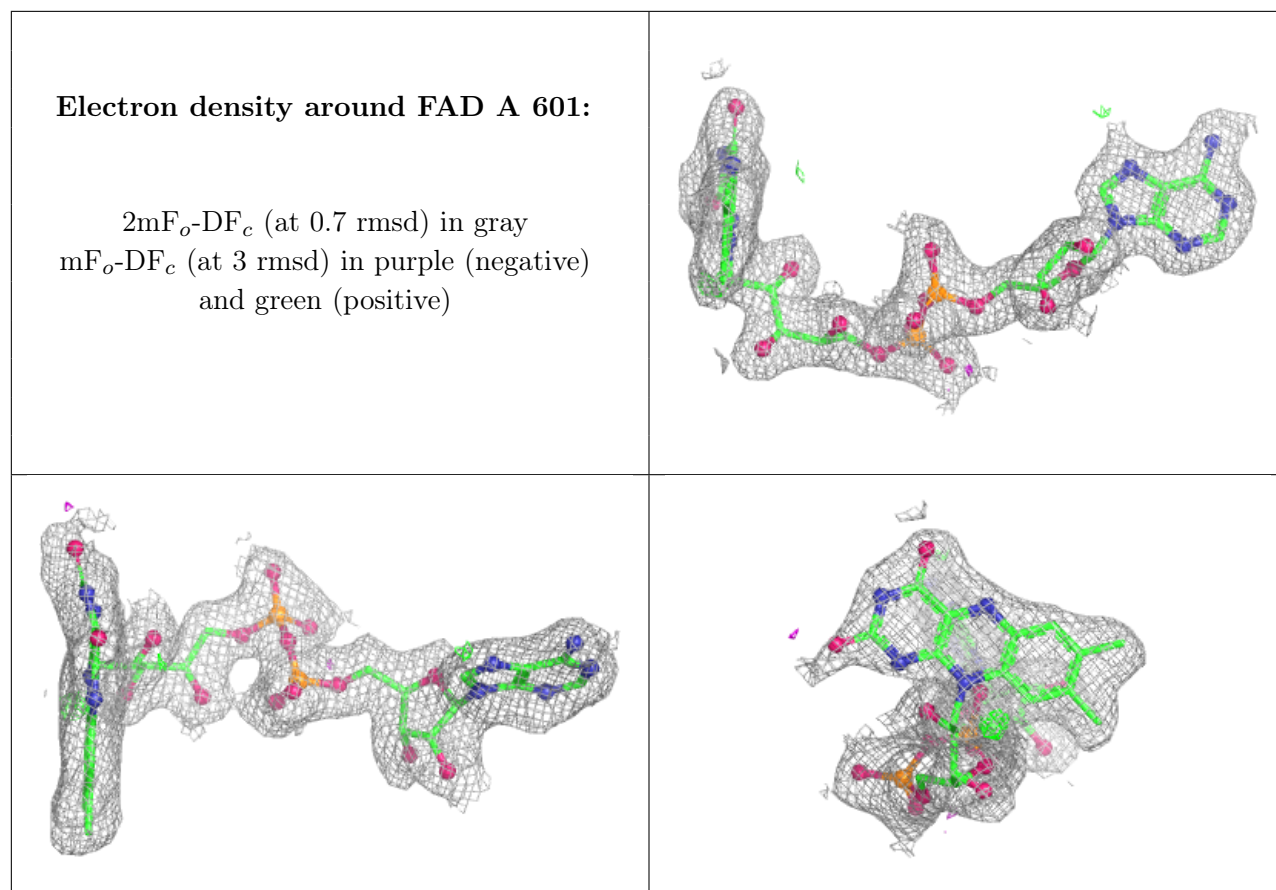
Electron density around NAP D 602:

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

**Electron density around FAD B 601:**

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





6.5 Other polymers ⓘ

There are no such residues in this entry.