



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 11:36 PM UTC

PDB ID : 5EAI / pdb_00005eai
Title : Crystal Structure of NAD(P)H dehydrogenase, quinone 1 complexed with a
chemotherapeutic naphthoquinone E6a
Authors : Pidugu, L.S.; Mbimba, J.E.; Ahmad, M.; Pozharski, E.; Sausville, E.A.;
Emadi, A.; Toth, E.A.
Deposited on : 2015-10-16
Resolution : 2.90 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

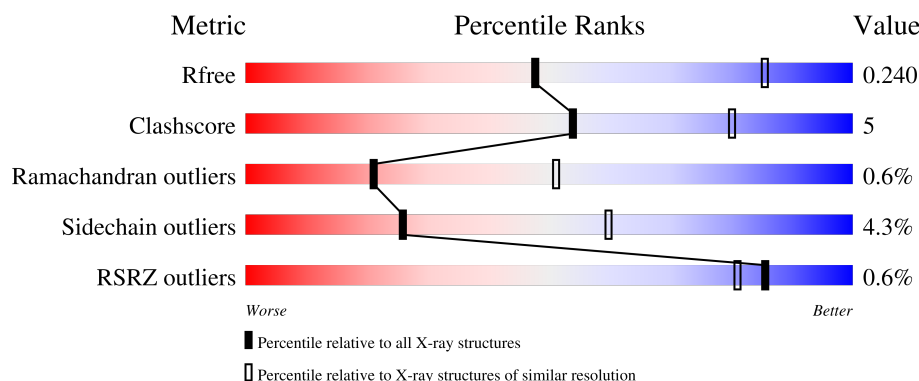
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	277	
1	B	277	
1	C	277	
1	D	277	

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Mol	Chain	Length	Quality of chain
1	E	277	% 79% 16% ..
1	F	277	% 83% 13% ..
1	G	277	% 77% 18% ..
1	H	277	84% 12% ..
1	I	277	78% 18% ...
1	J	277	% 83% 13% ..
1	K	277	81% 14% ..
1	L	277	% 84% 12% ..
1	M	277	82% 15% ...
1	N	277	80% 15% ..

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 31021 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 NAD(P)H dehydrogenase [quinone] 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	270	Total	C	N	O	S	46	0	0
			2134	1386	356	385	7			
1	B	270	Total	C	N	O	S	78	0	0
			2122	1379	353	383	7			
1	C	272	Total	C	N	O	S	61	0	0
			2161	1405	362	387	7			
1	D	271	Total	C	N	O	S	45	0	0
			2164	1407	363	387	7			
1	E	271	Total	C	N	O	S	55	0	0
			2155	1402	361	385	7			
1	F	271	Total	C	N	O	S	63	0	0
			2152	1400	359	386	7			
1	G	272	Total	C	N	O	S	78	0	0
			2139	1389	362	381	7			
1	H	271	Total	C	N	O	S	77	0	0
			2158	1403	362	386	7			
1	I	272	Total	C	N	O	S	31	0	0
			2163	1406	363	387	7			
1	J	271	Total	C	N	O	S	62	0	0
			2148	1396	361	384	7			
1	K	271	Total	C	N	O	S	69	0	0
			2154	1401	361	385	7			
1	L	273	Total	C	N	O	S	69	0	0
			2164	1406	364	387	7			
1	M	273	Total	C	N	O	S	80	0	0
			2151	1398	360	386	7			
1	N	271	Total	C	N	O	S	53	0	0
			2134	1391	351	385	7			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP P15559

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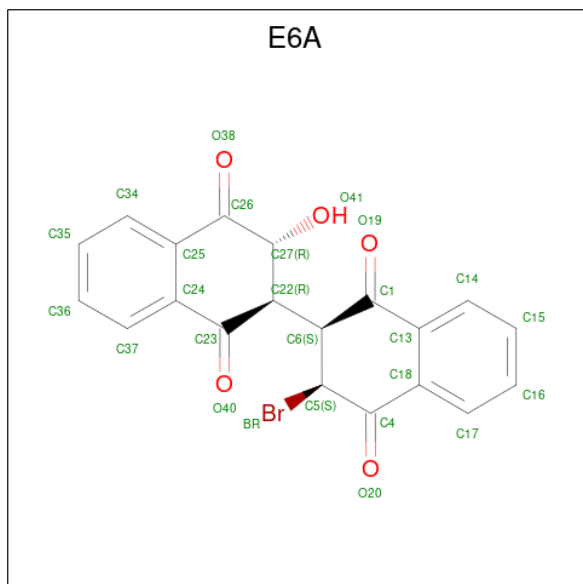
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	PRO	-	expression tag	UNP P15559
A	-1	HIS	-	expression tag	UNP P15559
B	-3	GLY	-	expression tag	UNP P15559
B	-2	PRO	-	expression tag	UNP P15559
B	-1	HIS	-	expression tag	UNP P15559
C	-3	GLY	-	expression tag	UNP P15559
C	-2	PRO	-	expression tag	UNP P15559
C	-1	HIS	-	expression tag	UNP P15559
D	-3	GLY	-	expression tag	UNP P15559
D	-2	PRO	-	expression tag	UNP P15559
D	-1	HIS	-	expression tag	UNP P15559
E	-3	GLY	-	expression tag	UNP P15559
E	-2	PRO	-	expression tag	UNP P15559
E	-1	HIS	-	expression tag	UNP P15559
F	-3	GLY	-	expression tag	UNP P15559
F	-2	PRO	-	expression tag	UNP P15559
F	-1	HIS	-	expression tag	UNP P15559
G	-3	GLY	-	expression tag	UNP P15559
G	-2	PRO	-	expression tag	UNP P15559
G	-1	HIS	-	expression tag	UNP P15559
H	-3	GLY	-	expression tag	UNP P15559
H	-2	PRO	-	expression tag	UNP P15559
H	-1	HIS	-	expression tag	UNP P15559
I	-3	GLY	-	expression tag	UNP P15559
I	-2	PRO	-	expression tag	UNP P15559
I	-1	HIS	-	expression tag	UNP P15559
J	-3	GLY	-	expression tag	UNP P15559
J	-2	PRO	-	expression tag	UNP P15559
J	-1	HIS	-	expression tag	UNP P15559
K	-3	GLY	-	expression tag	UNP P15559
K	-2	PRO	-	expression tag	UNP P15559
K	-1	HIS	-	expression tag	UNP P15559
L	-3	GLY	-	expression tag	UNP P15559
L	-2	PRO	-	expression tag	UNP P15559
L	-1	HIS	-	expression tag	UNP P15559
M	-3	GLY	-	expression tag	UNP P15559
M	-2	PRO	-	expression tag	UNP P15559
M	-1	HIS	-	expression tag	UNP P15559
N	-3	GLY	-	expression tag	UNP P15559
N	-2	PRO	-	expression tag	UNP P15559
N	-1	HIS	-	expression tag	UNP P15559

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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		
2	E	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	F	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	G	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	H	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	I	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	J	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	K	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	L	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	M	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	N	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is (2 {R},3 {R})-2-[(2 {S},3 {S})-3-bromanyl-1,4-bis(oxidanylidene)-2,3-dihydronaphthalen-2-yl]-3-oxidanyl-2,3-dihydronaphthalene-1,4-dione (CCD ID: E6A) (formula: C₂₀H₁₃BrO₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	Br	C	O	0	0
			26	1	20	5		
3	E	1	Total	Br	C	O	0	0
			26	1	20	5		
3	H	1	Total	Br	C	O	0	0
			26	1	20	5		
3	K	1	Total	Br	C	O	0	0
			26	1	20	5		
3	M	1	Total	Br	C	O	0	0
			26	1	20	5		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	4	Total	O	0	0
			4	4		
4	B	4	Total	O	0	0
			4	4		
4	C	1	Total	O	0	0
			1	1		
4	D	4	Total	O	0	0
			4	4		
4	E	6	Total	O	0	0
			6	6		

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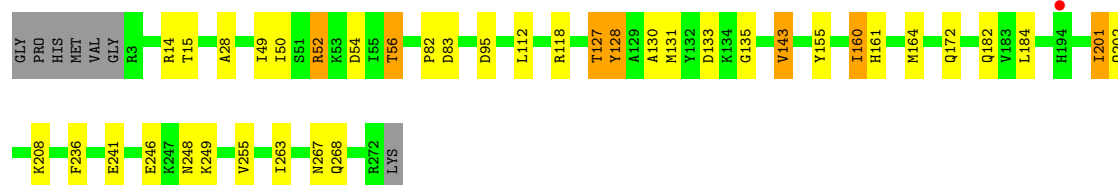
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	F	2	Total 2	O 2	0	0
4	G	1	Total 1	O 1	0	0
4	H	3	Total 3	O 3	0	0
4	I	8	Total 8	O 8	0	0
4	J	4	Total 4	O 4	0	0
4	K	3	Total 3	O 3	0	0
4	L	4	Total 4	O 4	0	0
4	M	3	Total 3	O 3	0	0
4	N	3	Total 3	O 3	0	0

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.

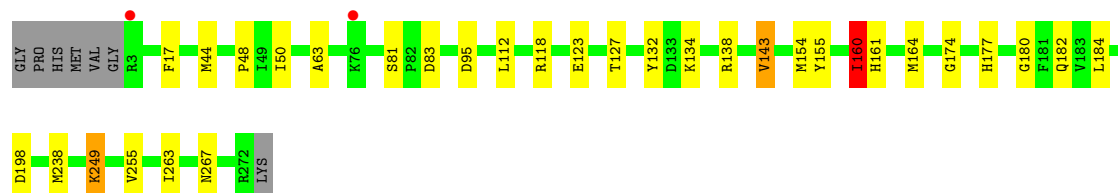
- Molecule 1: NAD(P)H dehydrogenase [quinone] 1

Chain A:  83% 12% . .



- Molecule 1: NAD(P)H dehydrogenase [quinone] 1

Chain B:  86% 10% . .



- Molecule 1: NAD(P)H dehydrogenase [quinone] 1

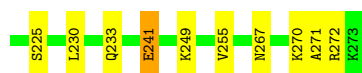
Chain C:  83% 13% . .



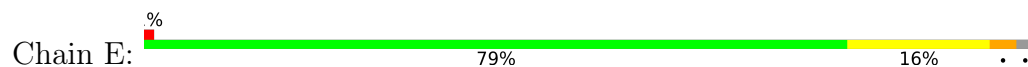
- Molecule 1: NAD(P)H dehydrogenase [quinone] 1

Chain D:  83% 12% . .

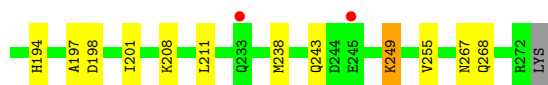
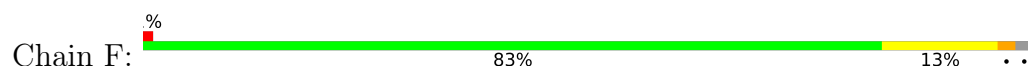




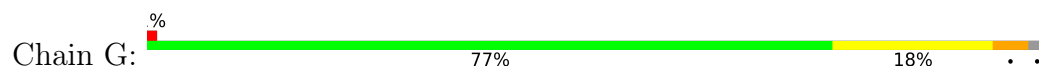
- Molecule 1: NAD(P)H dehydrogenase [quinone] 1



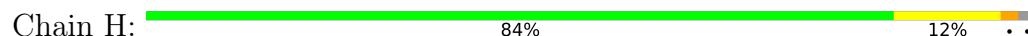
- Molecule 1: NAD(P)H dehydrogenase [quinone] 1



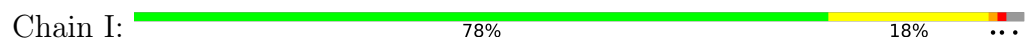
- Molecule 1: NAD(P)H dehydrogenase [quinone] 1

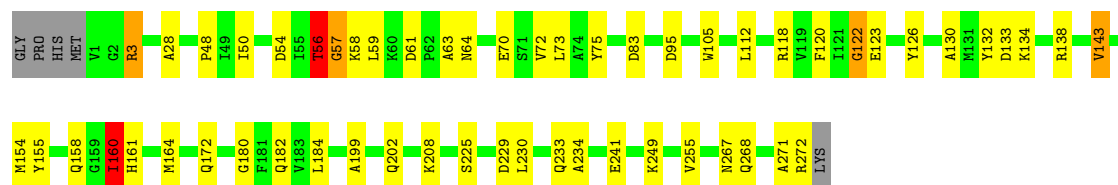


- Molecule 1: NAD(P)H dehydrogenase [quinone] 1

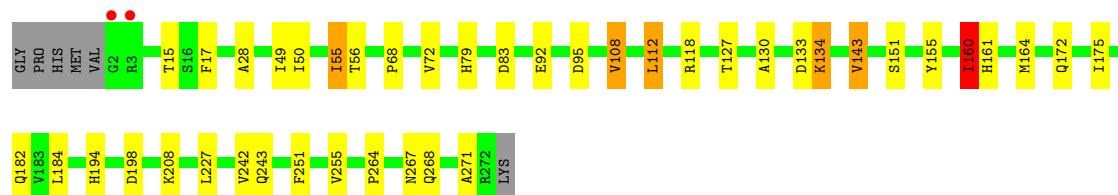
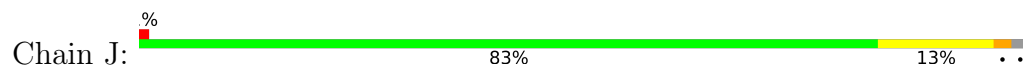


- Molecule 1: NAD(P)H dehydrogenase [quinone] 1

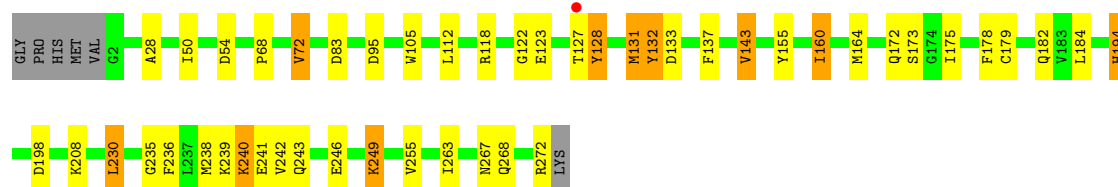
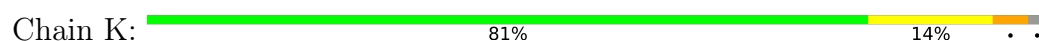




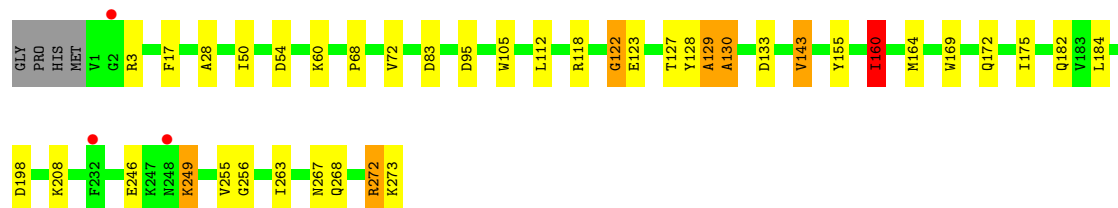
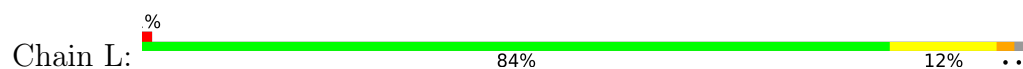
- Molecule 1: NAD(P)H dehydrogenase [quinone] 1



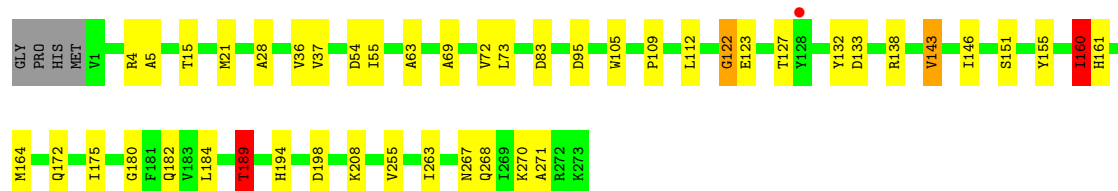
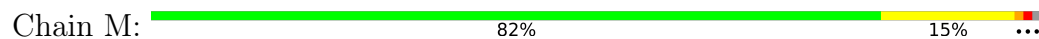
- Molecule 1: NAD(P)H dehydrogenase [quinone] 1



- Molecule 1: NAD(P)H dehydrogenase [quinone] 1



- Molecule 1: NAD(P)H dehydrogenase [quinone] 1



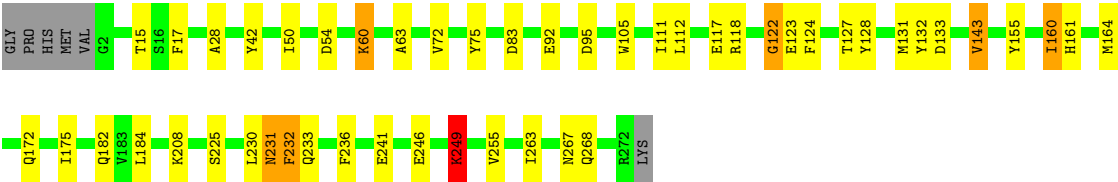
- Molecule 1: NAD(P)H dehydrogenase [quinone] 1

Chain N:

80%

15%

••



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	95.60Å 210.77Å 228.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	95.67 – 2.90 95.67 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.9 (95.67-2.90) 99.9 (95.67-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.24 (at 2.91Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.183 , 0.220 0.205 , 0.240	Depositor DCC
R_{free} test set	4972 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	60.8	Xtriage
Anisotropy	0.625	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 76.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	31021	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.04% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FAD, E6A

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	0.88	0/2190	1.34	7/2961 (0.2%)
1	B	0.84	0/2179	1.35	9/2951 (0.3%)
1	C	0.91	1/2219 (0.0%)	1.36	9/3000 (0.3%)
1	D	0.87	0/2222	1.39	15/3000 (0.5%)
1	E	0.89	0/2213	1.33	10/2990 (0.3%)
1	F	0.90	0/2210	1.37	15/2987 (0.5%)
1	G	0.88	0/2195	1.41	16/2967 (0.5%)
1	H	0.89	0/2216	1.35	13/2994 (0.4%)
1	I	0.87	0/2221	1.36	11/3001 (0.4%)
1	J	0.86	1/2205 (0.0%)	1.34	6/2979 (0.2%)
1	K	0.88	0/2212	1.34	11/2989 (0.4%)
1	L	0.91	1/2221 (0.0%)	1.40	9/2999 (0.3%)
1	M	0.87	0/2209	1.40	13/2989 (0.4%)
1	N	0.90	0/2192	1.37	13/2966 (0.4%)
All	All	0.88	3/30904 (0.0%)	1.37	157/41773 (0.4%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	3	ARG	CA-C	6.37	1.61	1.52
1	J	271	ALA	CA-C	6.02	1.60	1.53
1	C	271	ALA	C-N	5.03	1.40	1.33

All (157) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	129	ALA	CA-C-N	12.23	143.72	121.70
1	L	129	ALA	C-N-CA	12.23	143.72	121.70
1	F	92	GLU	CB-CG-CD	9.71	129.12	112.60
1	M	123	GLU	CA-C-N	8.54	131.92	120.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	123	GLU	C-N-CA	8.54	131.92	120.65
1	K	240	LYS	CA-C-N	7.77	131.58	120.79
1	K	240	LYS	C-N-CA	7.77	131.58	120.79
1	G	234	ALA	N-CA-C	-7.22	105.00	113.88
1	D	55	ILE	CA-C-N	6.96	130.17	120.29
1	D	55	ILE	C-N-CA	6.96	130.17	120.29
1	F	160	ILE	N-CA-CB	6.78	119.77	110.54
1	E	83	ASP	CA-CB-CG	6.66	119.26	112.60
1	L	160	ILE	N-CA-CB	6.65	119.58	110.54
1	F	129	ALA	N-CA-C	-6.65	96.64	110.80
1	M	270	LYS	CA-C-N	6.62	129.81	120.28
1	M	270	LYS	C-N-CA	6.62	129.81	120.28
1	G	133	ASP	CA-CB-CG	6.61	119.21	112.60
1	I	271	ALA	N-CA-C	6.60	122.42	113.97
1	M	271	ALA	N-CA-C	6.57	119.27	111.71
1	E	160	ILE	N-CA-CB	6.47	119.34	110.54
1	J	160	ILE	N-CA-CB	6.46	119.32	110.54
1	F	249	LYS	CA-C-N	6.43	128.89	120.28
1	F	249	LYS	C-N-CA	6.43	128.89	120.28
1	D	270	LYS	CA-C-N	6.41	133.79	121.54
1	D	270	LYS	C-N-CA	6.41	133.79	121.54
1	I	160	ILE	N-CA-CB	6.39	119.23	110.54
1	G	232	PHE	CA-C-N	6.34	133.66	121.54
1	G	232	PHE	C-N-CA	6.34	133.66	121.54
1	G	233	GLN	N-CA-C	-6.34	97.29	110.80
1	C	55	ILE	CA-C-N	6.26	129.18	120.29
1	C	55	ILE	C-N-CA	6.26	129.18	120.29
1	N	75	TYR	CA-C-N	6.22	128.90	120.38
1	N	75	TYR	C-N-CA	6.22	128.90	120.38
1	B	249	LYS	CA-C-N	6.15	128.53	120.28
1	B	249	LYS	C-N-CA	6.15	128.53	120.28
1	M	55	ILE	CA-C-N	6.12	128.98	120.29
1	M	55	ILE	C-N-CA	6.12	128.98	120.29
1	D	45	ASN	CA-CB-CG	6.11	118.71	112.60
1	H	69	ALA	CA-C-N	6.11	128.75	120.44
1	H	69	ALA	C-N-CA	6.11	128.75	120.44
1	G	270	LYS	CA-C-N	6.10	130.88	121.19
1	G	270	LYS	C-N-CA	6.10	130.88	121.19
1	G	126	TYR	CA-C-N	6.08	133.14	121.54
1	G	126	TYR	C-N-CA	6.08	133.14	121.54
1	D	83	ASP	CA-CB-CG	6.07	118.67	112.60
1	K	241	GLU	CA-C-N	5.99	128.11	120.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	241	GLU	C-N-CA	5.99	128.11	120.56
1	K	160	ILE	N-CA-CB	5.98	118.67	110.54
1	M	160	ILE	N-CA-CB	5.97	118.66	110.54
1	C	160	ILE	N-CA-CB	5.96	118.65	110.54
1	E	95	ASP	N-CA-C	-5.91	104.82	112.68
1	J	83	ASP	CA-CB-CG	5.91	118.51	112.60
1	L	83	ASP	CA-CB-CG	5.88	118.48	112.60
1	C	188	LEU	CA-C-N	-5.87	114.78	123.11
1	C	188	LEU	C-N-CA	-5.87	114.78	123.11
1	D	160	ILE	N-CA-CB	5.87	117.80	110.47
1	B	160	ILE	N-CA-CB	5.86	118.51	110.54
1	F	45	ASN	CA-CB-CG	5.85	118.45	112.60
1	D	198	ASP	CA-CB-CG	5.81	118.41	112.60
1	G	129	ALA	CA-C-N	5.81	132.64	121.54
1	G	129	ALA	C-N-CA	5.81	132.64	121.54
1	N	83	ASP	CA-CB-CG	5.79	118.39	112.60
1	G	83	ASP	CA-CB-CG	5.78	118.38	112.60
1	G	95	ASP	N-CA-C	-5.78	105.90	113.12
1	F	83	ASP	CA-CB-CG	5.75	118.35	112.60
1	I	83	ASP	CA-CB-CG	5.73	118.33	112.60
1	L	123	GLU	CA-C-N	5.72	127.88	120.44
1	L	123	GLU	C-N-CA	5.72	127.88	120.44
1	M	83	ASP	CA-CB-CG	5.68	118.28	112.60
1	H	83	ASP	CA-CB-CG	5.68	118.28	112.60
1	G	160	ILE	N-CA-CB	5.65	118.23	110.54
1	H	160	ILE	N-CA-CB	5.65	118.23	110.54
1	N	160	ILE	N-CA-CB	5.65	118.23	110.54
1	N	123	GLU	CA-C-N	5.64	128.10	120.44
1	N	123	GLU	C-N-CA	5.64	128.10	120.44
1	N	232	PHE	N-CA-C	-5.63	105.15	111.28
1	I	95	ASP	N-CA-C	-5.62	106.10	113.12
1	A	127	THR	CA-C-N	5.53	132.11	121.54
1	A	127	THR	C-N-CA	5.53	132.11	121.54
1	K	95	ASP	N-CA-C	-5.51	106.23	113.12
1	H	95	ASP	N-CA-C	-5.51	106.24	113.12
1	H	249	LYS	CA-C-N	5.50	127.97	120.54
1	H	249	LYS	C-N-CA	5.50	127.97	120.54
1	F	182	GLN	N-CA-C	-5.50	100.22	108.96
1	M	54	ASP	CA-CB-CG	5.49	118.09	112.60
1	L	182	GLN	N-CA-C	-5.49	100.23	108.96
1	A	54	ASP	CA-CB-CG	5.46	118.06	112.60
1	M	182	GLN	N-CA-C	-5.46	100.28	108.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	95	ASP	N-CA-C	-5.45	106.30	113.12
1	B	134	LYS	CA-C-N	5.45	130.42	121.87
1	B	134	LYS	C-N-CA	5.45	130.42	121.87
1	A	95	ASP	N-CA-C	-5.43	106.33	113.12
1	K	83	ASP	CA-CB-CG	5.43	118.03	112.60
1	N	54	ASP	CA-CB-CG	5.42	118.03	112.60
1	J	95	ASP	N-CA-C	-5.41	106.36	113.12
1	B	182	GLN	N-CA-C	-5.40	100.37	108.96
1	N	95	ASP	N-CA-C	-5.40	106.37	113.12
1	D	272	ARG	CA-C-N	5.40	131.42	121.70
1	D	272	ARG	C-N-CA	5.40	131.42	121.70
1	B	83	ASP	CA-CB-CG	5.40	118.00	112.60
1	C	83	ASP	CA-CB-CG	5.40	118.00	112.60
1	C	189	THR	CB-CA-C	5.38	119.56	110.79
1	D	182	GLN	N-CA-C	-5.36	100.43	108.96
1	D	123	GLU	CA-C-N	5.32	127.87	120.63
1	D	123	GLU	C-N-CA	5.32	127.87	120.63
1	I	120	PHE	CA-CB-CG	5.32	119.12	113.80
1	A	182	GLN	N-CA-C	-5.32	100.50	108.96
1	A	160	ILE	N-CA-CB	5.32	117.77	110.54
1	I	249	LYS	CA-C-N	5.29	127.37	120.28
1	I	249	LYS	C-N-CA	5.29	127.37	120.28
1	H	182	GLN	N-CA-C	-5.27	100.58	108.96
1	H	244	ASP	CA-C-N	5.26	127.33	120.28
1	H	244	ASP	C-N-CA	5.26	127.33	120.28
1	H	54	ASP	CA-CB-CG	5.26	117.86	112.60
1	A	83	ASP	CA-CB-CG	5.25	117.85	112.60
1	B	95	ASP	N-CA-C	-5.24	106.57	113.12
1	H	55	ILE	CA-C-N	5.24	128.27	120.31
1	H	55	ILE	C-N-CA	5.24	128.27	120.31
1	F	149	GLY	CA-C-N	5.22	125.64	120.31
1	F	149	GLY	C-N-CA	5.22	125.64	120.31
1	K	182	GLN	N-CA-C	-5.22	100.66	108.96
1	N	182	GLN	N-CA-C	-5.22	100.67	108.96
1	L	54	ASP	CA-CB-CG	5.19	117.79	112.60
1	B	174	GLY	N-CA-C	5.18	119.16	112.83
1	M	189	THR	CB-CA-C	5.18	120.21	111.41
1	D	95	ASP	N-CA-C	-5.17	106.66	113.12
1	M	95	ASP	N-CA-C	-5.17	106.66	113.12
1	E	249	LYS	CA-C-N	5.16	127.20	120.28
1	E	249	LYS	C-N-CA	5.16	127.20	120.28
1	C	101	PHE	N-CA-C	5.16	114.77	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	182	GLN	N-CA-C	-5.15	100.77	108.96
1	K	173	SER	CA-C-N	5.15	125.69	119.98
1	K	173	SER	C-N-CA	5.15	125.69	119.98
1	D	163	ASP	N-CA-C	5.14	118.01	110.30
1	I	75	TYR	CA-C-N	5.13	127.11	120.44
1	I	75	TYR	C-N-CA	5.13	127.11	120.44
1	E	173	SER	CA-C-N	5.12	125.66	119.98
1	E	173	SER	C-N-CA	5.12	125.66	119.98
1	N	133	ASP	CA-CB-CG	5.12	117.72	112.60
1	E	54	ASP	CA-CB-CG	5.10	117.70	112.60
1	N	249	LYS	CA-C-N	5.10	127.12	120.28
1	N	249	LYS	C-N-CA	5.10	127.12	120.28
1	E	101	PHE	N-CA-C	5.09	114.68	108.11
1	F	197	ALA	CA-C-N	5.09	127.10	120.28
1	F	197	ALA	C-N-CA	5.09	127.10	120.28
1	I	182	GLN	N-CA-C	-5.09	100.87	108.96
1	J	182	GLN	N-CA-C	-5.07	100.89	108.96
1	G	54	ASP	CA-CB-CG	5.07	117.67	112.60
1	G	182	GLN	N-CA-C	-5.07	100.91	108.96
1	K	54	ASP	CA-CB-CG	5.06	117.66	112.60
1	I	54	ASP	CA-CB-CG	5.05	117.65	112.60
1	F	95	ASP	N-CA-C	-5.05	106.81	113.12
1	F	128	TYR	CA-C-N	5.05	131.18	121.54
1	F	128	TYR	C-N-CA	5.05	131.18	121.54
1	J	55	ILE	CA-C-N	5.04	127.30	120.44
1	J	55	ILE	C-N-CA	5.04	127.30	120.44
1	E	189	THR	CB-CA-C	5.03	119.95	111.41

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2134	0	2119	23	0
1	B	2122	0	2085	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2161	0	2155	21	0
1	D	2164	0	2164	24	0
1	E	2155	0	2150	28	0
1	F	2152	0	2143	25	0
1	G	2139	0	2133	31	0
1	H	2158	0	2154	17	0
1	I	2163	0	2159	32	0
1	J	2148	0	2143	26	0
1	K	2154	0	2148	24	0
1	L	2164	0	2166	20	0
1	M	2151	0	2125	23	0
1	N	2134	0	2108	28	0
2	A	53	0	31	1	0
2	B	53	0	31	1	0
2	C	53	0	31	0	0
2	D	53	0	31	1	0
2	E	53	0	31	0	0
2	F	53	0	31	1	0
2	G	53	0	31	0	0
2	H	53	0	31	1	0
2	I	53	0	31	0	0
2	J	53	0	31	1	0
2	K	53	0	31	0	0
2	L	53	0	31	1	0
2	M	53	0	31	0	0
2	N	53	0	31	1	0
3	B	26	0	12	2	0
3	E	26	0	12	2	0
3	H	26	0	12	3	0
3	K	26	0	12	2	0
3	M	26	0	12	2	0
4	A	4	0	0	0	0
4	B	4	0	0	0	0
4	C	1	0	0	0	0
4	D	4	0	0	0	0
4	E	6	0	0	0	0
4	F	2	0	0	0	0
4	G	1	0	0	0	0
4	H	3	0	0	0	0
4	I	8	0	0	0	0
4	J	4	0	0	0	0
4	K	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	L	4	0	0	0	0
4	M	3	0	0	0	0
4	N	3	0	0	0	0
All	All	31021	0	30446	291	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 5.

All (291) 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:L:72:VAL:HG22	1:L:122:GLY:HA3	1.36	1.08
3:E:602:E6A:H5	3:E:602:E6A:BR	2.15	1.01
1:G:72:VAL:HG22	1:G:122:GLY:HA3	1.43	0.97
3:B:302:E6A:H5	3:B:302:E6A:BR	2.21	0.95
1:C:154:MET:HE1	1:D:128:TYR:HE2	1.34	0.93
1:J:108:VAL:HG13	1:J:112:LEU:HB3	1.49	0.91
1:E:60:LYS:HD3	1:K:240:LYS:HB2	1.56	0.87
1:I:72:VAL:HG22	1:I:122:GLY:HA3	1.56	0.86
3:K:602:E6A:H5	3:K:602:E6A:BR	2.33	0.84
1:K:68:PRO:O	1:K:72:VAL:HG23	1.77	0.84
1:D:72:VAL:HG22	1:D:122:GLY:HA3	1.62	0.82
1:G:272:ARG:HH11	1:G:272:ARG:HB3	1.46	0.80
1:J:130:ALA:HB1	1:J:134:LYS:O	1.81	0.79
1:L:127:THR:HB	1:L:130:ALA:HB3	1.67	0.77
1:K:236:PHE:HB3	1:L:160:ILE:HD11	1.68	0.76
1:M:72:VAL:HG22	1:M:122:GLY:HA3	1.68	0.76
1:C:154:MET:HE1	1:D:128:TYR:CE2	2.20	0.76
1:E:48:PRO:HG3	1:F:49:ILE:HD11	1.71	0.73
1:G:130:ALA:O	1:G:135:GLY:HA2	1.87	0.73
1:J:108:VAL:CG1	1:J:112:LEU:HB3	2.18	0.73
1:H:72:VAL:HG22	1:H:122:GLY:HA3	1.68	0.73
1:G:272:ARG:HB3	1:G:272:ARG:NH1	2.04	0.72
3:E:602:E6A:BR	3:E:602:E6A:C27	2.93	0.70
3:B:302:E6A:BR	3:B:302:E6A:C27	2.94	0.69
1:A:49:ILE:HD11	1:B:48:PRO:HG3	1.75	0.69
1:M:69:ALA:O	1:M:73:LEU:HD13	1.93	0.68
1:G:188:LEU:HD11	1:G:269:ILE:HG12	1.75	0.67
1:A:128:TYR:CD1	1:A:128:TYR:N	2.62	0.67
1:F:29:LEU:CD1	1:F:211:LEU:HB3	2.24	0.67
1:E:127:THR:HG23	1:E:130:ALA:H	1.60	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:72:VAL:HG22	1:N:122:GLY:HA3	1.76	0.66
1:J:127:THR:HG23	1:J:130:ALA:H	1.61	0.66
3:H:302:E6A:BR	3:H:302:E6A:H5	2.51	0.66
3:M:602:E6A:H5	3:M:602:E6A:BR	2.51	0.66
1:M:161:HIS:HD2	1:N:132:TYR:OH	1.79	0.65
1:F:29:LEU:HD11	1:F:211:LEU:HB3	1.79	0.65
1:N:72:VAL:CG2	1:N:122:GLY:HA3	2.29	0.61
1:N:42:TYR:CE1	1:N:111:ILE:HG21	2.36	0.60
1:A:161:HIS:HD2	1:B:132:TYR:OH	1.84	0.60
1:E:71:SER:HB2	1:E:121:ILE:HD12	1.84	0.60
1:A:56:THR:HG23	1:F:83:ASP:HB3	1.83	0.60
1:A:127:THR:HB	1:A:130:ALA:HB3	1.84	0.59
3:K:602:E6A:BR	3:K:602:E6A:C27	3.04	0.59
1:E:231:ASN:OD1	1:E:233:GLN:HB2	2.03	0.59
1:B:138:ARG:HA	1:B:180:GLY:O	2.03	0.58
1:E:131:MET:CE	1:F:160:ILE:HG13	2.34	0.58
1:H:72:VAL:HG13	1:H:123:GLU:H	1.69	0.58
1:D:127:THR:HG23	1:D:130:ALA:HB3	1.86	0.58
1:K:239:LYS:HB2	1:K:242:VAL:HG23	1.84	0.58
1:D:83:ASP:HB3	1:I:56:THR:HG23	1.87	0.57
1:L:155:TYR:HB3	1:L:164:MET:HB2	1.87	0.57
1:D:130:ALA:HB1	1:D:134:LYS:O	2.05	0.57
1:C:132:TYR:OH	1:D:161:HIS:HD2	1.88	0.57
1:H:17:PHE:HB2	2:H:301:FAD:H51A	1.88	0.56
1:M:155:TYR:HB3	1:M:164:MET:HB2	1.88	0.56
1:I:3:ARG:HE	1:I:3:ARG:HA	1.71	0.56
1:L:28:ALA:HB2	1:L:208:LYS:HG2	1.88	0.56
1:H:128:TYR:HA	1:H:131:MET:HG3	1.88	0.55
1:C:28:ALA:HB2	1:C:208:LYS:HG2	1.89	0.55
1:F:28:ALA:HB2	1:F:208:LYS:HG2	1.89	0.55
1:A:236:PHE:HB3	1:B:160:ILE:HG13	1.88	0.55
1:B:155:TYR:HB3	1:B:164:MET:HB2	1.88	0.55
1:N:155:TYR:HB3	1:N:164:MET:HB2	1.89	0.55
1:H:155:TYR:HB3	1:H:164:MET:HB2	1.88	0.54
1:C:155:TYR:HB3	1:C:164:MET:HB2	1.90	0.54
1:E:155:TYR:HB3	1:E:164:MET:HB2	1.88	0.54
1:K:155:TYR:HB3	1:K:164:MET:HB2	1.89	0.54
1:I:154:MET:HB3	1:I:161:HIS:CD2	2.42	0.54
1:K:131:MET:HE3	1:K:230:LEU:HD23	1.90	0.54
1:F:17:PHE:HB2	2:F:301:FAD:H51A	1.90	0.54
1:H:68:PRO:O	1:H:72:VAL:HG23	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:155:TYR:HB3	1:J:164:MET:HB2	1.89	0.53
1:A:201:ILE:HD12	2:A:601:FAD:H2A	1.90	0.53
1:G:28:ALA:HB2	1:G:208:LYS:HG2	1.91	0.53
1:A:82:PRO:HB3	1:F:56:THR:HG22	1.90	0.53
1:A:155:TYR:HB3	1:A:164:MET:HB2	1.89	0.53
1:G:151:SER:HB2	1:J:194:HIS:HB3	1.90	0.53
1:G:155:TYR:HB3	1:G:164:MET:HB2	1.91	0.53
1:E:131:MET:HE3	1:F:160:ILE:HG13	1.90	0.53
1:J:28:ALA:HB2	1:J:208:LYS:HG2	1.91	0.53
1:H:28:ALA:HB2	1:H:208:LYS:HG2	1.90	0.53
1:M:255:VAL:HG23	1:M:267:ASN:HD22	1.73	0.53
1:E:28:ALA:HB2	1:E:208:LYS:HG2	1.90	0.53
1:F:155:TYR:HB3	1:F:164:MET:HB2	1.90	0.53
1:H:255:VAL:HG23	1:H:267:ASN:HD22	1.74	0.52
1:I:138:ARG:HA	1:I:180:GLY:O	2.09	0.52
1:G:194:HIS:HB3	1:J:151:SER:HB2	1.91	0.52
1:D:155:TYR:HB3	1:D:164:MET:HB2	1.91	0.52
1:N:28:ALA:HB2	1:N:208:LYS:HG2	1.91	0.52
1:B:17:PHE:HB2	2:B:301:FAD:H51A	1.91	0.52
1:N:17:PHE:HB2	2:N:301:FAD:H51A	1.91	0.52
1:C:255:VAL:HG23	1:C:267:ASN:HD22	1.75	0.52
1:B:154:MET:HE2	1:B:161:HIS:NE2	2.25	0.52
1:E:138:ARG:HA	1:E:180:GLY:O	2.09	0.52
1:L:17:PHE:HB2	2:L:301:FAD:H51A	1.91	0.52
1:N:143:VAL:HG13	1:N:184:LEU:HB2	1.92	0.52
1:G:164:MET:HG3	1:G:269:ILE:HD11	1.91	0.52
1:I:28:ALA:HB2	1:I:208:LYS:HG2	1.91	0.51
1:G:146:ILE:O	1:G:189:THR:HG23	2.10	0.51
1:H:143:VAL:HG13	1:H:184:LEU:HB2	1.91	0.51
1:N:246:GLU:HA	1:N:249:LYS:HG3	1.93	0.51
1:E:132:TYR:OH	1:F:161:HIS:HD2	1.94	0.51
1:E:143:VAL:HG13	1:E:184:LEU:HB2	1.93	0.51
1:L:129:ALA:HB3	1:L:130:ALA:CB	2.41	0.51
1:I:50:ILE:CG2	1:I:118:ARG:HG2	2.40	0.50
1:B:143:VAL:HG13	1:B:184:LEU:HB2	1.94	0.50
1:G:143:VAL:HG13	1:G:184:LEU:HB2	1.92	0.50
1:M:263:ILE:HD11	1:N:263:ILE:HD11	1.93	0.50
1:J:255:VAL:HG23	1:J:267:ASN:HD22	1.76	0.50
1:K:143:VAL:HG13	1:K:184:LEU:HB2	1.94	0.50
1:K:246:GLU:HA	1:K:249:LYS:HG3	1.93	0.50
1:L:143:VAL:HG13	1:L:184:LEU:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:172:GLN:HB2	1:J:268:GLN:NE2	2.27	0.50
1:A:143:VAL:HG13	1:A:184:LEU:HB2	1.93	0.50
1:I:56:THR:HG22	1:I:57:GLY:N	2.26	0.50
1:C:143:VAL:HG13	1:C:184:LEU:HB2	1.93	0.50
1:I:50:ILE:HG22	1:I:118:ARG:HG2	1.94	0.50
1:N:255:VAL:HG23	1:N:267:ASN:HD22	1.77	0.50
1:G:255:VAL:HG23	1:G:267:ASN:HD22	1.76	0.49
1:I:143:VAL:HG13	1:I:184:LEU:HB2	1.94	0.49
1:I:230:LEU:HD21	1:J:160:ILE:HG21	1.94	0.49
1:I:255:VAL:HG23	1:I:267:ASN:HD22	1.76	0.49
1:H:121:ILE:O	1:H:122:GLY:O	2.30	0.49
1:C:236:PHE:HB3	1:D:160:ILE:HG13	1.93	0.49
1:M:28:ALA:HB2	1:M:208:LYS:HG2	1.94	0.49
1:I:155:TYR:HB3	1:I:164:MET:HB2	1.93	0.49
1:C:160:ILE:HD13	1:D:131:MET:HE1	1.94	0.49
1:F:143:VAL:HG13	1:F:184:LEU:HB2	1.94	0.49
1:I:229:ASP:HB2	1:I:234:ALA:HB1	1.94	0.49
1:M:143:VAL:HG13	1:M:184:LEU:HB2	1.94	0.49
1:C:194:HIS:HB3	1:M:151:SER:HB2	1.94	0.49
1:C:151:SER:HB2	1:M:194:HIS:HB3	1.95	0.48
1:J:143:VAL:HG13	1:J:184:LEU:HB2	1.95	0.48
1:K:28:ALA:HB2	1:K:208:LYS:HG2	1.94	0.48
1:N:92:GLU:HG3	1:N:124:PHE:HE1	1.79	0.48
1:A:130:ALA:O	1:A:135:GLY:HA2	2.12	0.48
1:E:255:VAL:HG23	1:E:267:ASN:HD22	1.77	0.48
1:L:172:GLN:HB2	1:L:268:GLN:NE2	2.28	0.48
1:L:255:VAL:HG23	1:L:267:ASN:HD22	1.78	0.48
1:D:82:PRO:HG2	1:I:56:THR:HG21	1.94	0.48
1:C:161:HIS:HD2	1:D:132:TYR:OH	1.96	0.48
1:E:50:ILE:CG2	1:E:118:ARG:HG2	2.44	0.48
1:E:21:MET:HE2	1:E:189:THR:HG21	1.95	0.48
1:F:29:LEU:HD11	1:F:211:LEU:HD22	1.95	0.48
1:F:172:GLN:HB2	1:F:268:GLN:NE2	2.28	0.48
1:G:272:ARG:HH11	1:G:272:ARG:CB	2.22	0.48
1:M:160:ILE:HG13	1:N:236:PHE:HB3	1.95	0.48
1:D:17:PHE:HB2	2:D:301:FAD:H51A	1.94	0.48
3:H:302:E6A:BR	3:H:302:E6A:C27	3.17	0.48
1:I:132:TYR:OH	1:J:161:HIS:HD2	1.97	0.48
1:A:255:VAL:HG23	1:A:267:ASN:HD22	1.78	0.48
1:E:172:GLN:HB2	1:E:268:GLN:NE2	2.28	0.48
1:E:246:GLU:HA	1:E:249:LYS:HG3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:225:SER:HB2	1:I:230:LEU:HD11	1.96	0.47
1:N:225:SER:HB2	1:N:230:LEU:HD11	1.95	0.47
1:A:236:PHE:HB3	1:B:160:ILE:CG1	2.43	0.47
1:D:131:MET:HE3	1:D:178:PHE:HE1	1.79	0.47
1:F:50:ILE:CG2	1:F:118:ARG:HG2	2.44	0.47
1:H:238:MET:HE2	1:H:243:GLN:HG2	1.96	0.47
1:B:50:ILE:CG2	1:B:118:ARG:HG2	2.44	0.47
1:F:255:VAL:HG23	1:F:267:ASN:HD22	1.79	0.47
1:K:236:PHE:HB3	1:L:160:ILE:CD1	2.40	0.47
1:C:50:ILE:CG2	1:C:118:ARG:HG2	2.44	0.47
1:F:25:ALA:O	1:F:29:LEU:HD22	2.15	0.47
1:C:172:GLN:HB2	1:C:268:GLN:NE2	2.29	0.47
1:G:105:TRP:HB3	1:H:175:ILE:HG12	1.97	0.47
1:J:17:PHE:HB2	2:J:301:FAD:H51A	1.94	0.47
1:K:50:ILE:CG2	1:K:118:ARG:HG2	2.45	0.47
1:K:255:VAL:HG23	1:K:267:ASN:HD22	1.78	0.47
1:A:50:ILE:CG2	1:A:118:ARG:HG2	2.44	0.47
1:A:28:ALA:HB2	1:A:208:LYS:HG2	1.96	0.47
1:L:272:ARG:O	1:L:273:LYS:HG3	2.15	0.47
1:D:225:SER:HB2	1:D:230:LEU:HD11	1.97	0.47
1:D:241:GLU:HG3	1:N:60:LYS:HG2	1.97	0.47
1:K:172:GLN:HB2	1:K:268:GLN:NE2	2.29	0.47
1:D:143:VAL:HG13	1:D:184:LEU:HB2	1.96	0.47
1:A:263:ILE:HD11	1:B:263:ILE:HD11	1.96	0.46
1:B:132:TYR:HA	1:B:177:HIS:O	2.16	0.46
1:N:231:ASN:HB2	1:N:233:GLN:HB2	1.96	0.46
1:K:105:TRP:HB3	1:L:175:ILE:HG12	1.98	0.46
1:G:229:ASP:OD2	1:G:239:LYS:HG2	2.16	0.46
1:I:3:ARG:HA	1:I:3:ARG:NE	2.30	0.46
1:F:194:HIS:NE2	1:K:235:GLY:HA2	2.30	0.46
1:G:175:ILE:HG12	1:H:105:TRP:HB3	1.98	0.46
1:N:172:GLN:HB2	1:N:268:GLN:NE2	2.30	0.46
1:A:172:GLN:HB2	1:A:268:GLN:NE2	2.31	0.46
1:B:255:VAL:HG23	1:B:267:ASN:HD22	1.81	0.46
1:C:138:ARG:HA	1:C:180:GLY:O	2.16	0.46
1:D:255:VAL:HG23	1:D:267:ASN:HD22	1.81	0.46
1:E:32:LYS:HD3	1:E:212:GLU:HG2	1.97	0.46
1:I:154:MET:HB3	1:I:161:HIS:HD2	1.79	0.46
1:I:132:TYR:O	1:I:180:GLY:HA2	2.16	0.45
1:I:172:GLN:HB2	1:I:268:GLN:NE2	2.31	0.45
1:E:3:ARG:HE	1:E:3:ARG:HA	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:68:PRO:O	1:E:72:VAL:HG23	2.15	0.45
1:F:138:ARG:HA	1:F:180:GLY:O	2.16	0.45
1:L:246:GLU:HA	1:L:249:LYS:HG3	1.99	0.45
1:G:21:MET:HE2	1:G:189:THR:HG21	1.97	0.45
1:I:130:ALA:HB1	1:I:134:LYS:O	2.16	0.45
1:J:50:ILE:CG2	1:J:118:ARG:HG2	2.47	0.45
1:I:105:TRP:HB3	1:J:175:ILE:HG12	1.98	0.45
1:A:246:GLU:HA	1:A:249:LYS:HG3	1.98	0.45
1:G:172:GLN:HB2	1:G:268:GLN:NE2	2.32	0.45
1:G:50:ILE:CG2	1:G:118:ARG:HG2	2.47	0.45
1:J:251:PHE:CD2	1:J:264:PRO:HA	2.52	0.45
1:G:68:PRO:O	1:G:72:VAL:HG23	2.17	0.45
1:E:236:PHE:HB3	1:F:160:ILE:HD11	1.98	0.45
1:E:238:MET:HE2	1:E:243:GLN:HG2	1.99	0.45
1:G:188:LEU:CD1	1:G:269:ILE:HG12	2.45	0.45
1:M:21:MET:HE2	1:M:189:THR:HG21	1.99	0.45
1:M:63:ALA:O	1:N:15:THR:HG21	2.17	0.45
1:M:172:GLN:HB2	1:M:268:GLN:NE2	2.32	0.45
1:L:68:PRO:O	1:L:72:VAL:HG23	2.18	0.44
1:M:132:TYR:OH	1:N:161:HIS:HD2	2.00	0.44
1:M:138:ARG:HA	1:M:180:GLY:O	2.16	0.44
1:D:127:THR:CG2	1:D:130:ALA:HB3	2.48	0.44
1:G:15:THR:HG21	1:H:63:ALA:O	2.17	0.44
1:G:138:ARG:HA	1:G:180:GLY:O	2.18	0.44
1:G:169:TRP:CZ2	1:G:256:GLY:HA3	2.52	0.44
1:H:172:GLN:HB2	1:H:268:GLN:NE2	2.32	0.44
1:M:175:ILE:HG12	1:N:105:TRP:HB3	1.98	0.44
1:G:106:PHE:CD1	1:G:106:PHE:N	2.85	0.44
3:M:602:E6A:BR	3:M:602:E6A:C27	3.20	0.44
1:K:238:MET:HE2	1:K:243:GLN:HG2	2.00	0.44
1:N:50:ILE:CG2	1:N:118:ARG:HG2	2.47	0.44
1:A:50:ILE:HG22	1:A:118:ARG:HG2	2.00	0.43
1:L:127:THR:HB	1:L:130:ALA:CB	2.43	0.43
1:D:72:VAL:CG2	1:D:122:GLY:HA3	2.42	0.43
1:I:56:THR:HG22	1:I:57:GLY:H	1.82	0.43
1:M:146:ILE:O	1:M:189:THR:HG23	2.17	0.43
1:G:109:PRO:HA	1:H:117:GLU:OE2	2.18	0.43
1:I:48:PRO:HG3	1:J:49:ILE:HD11	2.00	0.43
1:I:58:LYS:HE3	1:I:59:LEU:O	2.19	0.43
1:H:127:THR:O	1:H:128:TYR:HB2	2.18	0.43
1:D:68:PRO:O	1:D:72:VAL:HG23	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:50:ILE:HG22	1:E:118:ARG:HG2	2.00	0.43
1:B:123:GLU:HA	1:B:127:THR:HG22	2.00	0.43
1:J:251:PHE:HD2	1:J:264:PRO:HA	1.84	0.43
1:M:5:ALA:HB3	1:M:36:VAL:HG22	2.01	0.43
1:F:238:MET:HE2	1:F:243:GLN:HG2	2.01	0.42
1:I:199:ALA:HA	1:I:202:GLN:HE21	1.83	0.42
1:N:128:TYR:O	1:N:131:MET:HE2	2.19	0.42
1:D:50:ILE:CG2	1:D:118:ARG:HG2	2.49	0.42
1:K:194:HIS:CD2	1:K:194:HIS:N	2.88	0.42
1:I:122:GLY:O	1:I:126:TYR:O	2.37	0.42
1:M:161:HIS:CD2	1:N:132:TYR:OH	2.67	0.42
1:B:50:ILE:HG22	1:B:118:ARG:HG2	2.00	0.42
1:F:52:ARG:H	1:F:52:ARG:HG2	1.72	0.42
1:B:44:MET:HA	1:E:82:PRO:HG2	2.02	0.42
1:E:146:ILE:O	1:E:189:THR:HG23	2.19	0.42
1:K:50:ILE:HG22	1:K:118:ARG:HG2	2.01	0.42
1:D:122:GLY:HA2	1:D:126:TYR:CZ	2.54	0.42
1:J:55:ILE:HG23	1:J:79:HIS:CD2	2.54	0.42
1:C:238:MET:HE2	1:C:243:GLN:HG2	2.02	0.42
1:M:105:TRP:HB3	1:N:175:ILE:HG12	2.01	0.42
1:E:132:TYR:OH	1:F:161:HIS:CD2	2.73	0.41
1:G:50:ILE:HG22	1:G:118:ARG:HG2	2.02	0.41
1:K:128:TYR:HA	1:K:131:MET:HG2	2.02	0.41
1:K:263:ILE:HD11	1:L:263:ILE:HD11	2.01	0.41
1:K:132:TYR:CD1	1:K:178:PHE:HA	2.55	0.41
1:M:15:THR:HG21	1:N:63:ALA:O	2.20	0.41
1:M:109:PRO:HA	1:N:117:GLU:OE2	2.20	0.41
1:A:15:THR:HG21	1:B:63:ALA:O	2.20	0.41
1:G:149:GLY:HA3	3:H:302:E6A:BR	2.74	0.41
1:I:158:GLN:HG2	1:J:243:GLN:OE1	2.20	0.41
1:N:50:ILE:HG22	1:N:118:ARG:HG2	2.03	0.41
1:C:50:ILE:HG22	1:C:118:ARG:HG2	2.01	0.41
1:E:72:VAL:HG13	1:E:123:GLU:HB2	2.03	0.41
1:J:50:ILE:HG22	1:J:118:ARG:HG2	2.02	0.41
1:A:52:ARG:H	1:A:52:ARG:HG2	1.68	0.41
1:A:161:HIS:CD2	1:B:132:TYR:OH	2.69	0.41
1:C:160:ILE:HG21	1:D:230:LEU:HD21	2.02	0.41
1:E:125:ALA:C	1:E:136:PRO:HG2	2.46	0.41
1:F:50:ILE:HG22	1:F:118:ARG:HG2	2.02	0.41
1:L:50:ILE:CG2	1:L:118:ARG:HG2	2.49	0.41
1:C:200:ARG:HA	1:C:203:ILE:HD12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:68:PRO:O	1:J:72:VAL:HG23	2.20	0.41
1:G:225:SER:HB2	1:G:230:LEU:HD11	2.04	0.40
1:I:63:ALA:O	1:J:15:THR:HG21	2.21	0.40
1:J:227:LEU:HB3	1:J:242:VAL:HG11	2.02	0.40
1:K:175:ILE:HG12	1:L:105:TRP:HB3	2.04	0.40
1:G:200:ARG:HA	1:G:203:ILE:HD12	2.03	0.40
1:I:61:ASP:OD2	1:I:64:ASN:HB3	2.21	0.40
1:J:56:THR:HB	1:J:79:HIS:HB2	2.04	0.40
1:C:68:PRO:O	1:C:72:VAL:HG23	2.21	0.40
1:C:150:GLY:HA2	1:N:232:PHE:HE2	1.85	0.40
1:K:72:VAL:HG13	1:K:123:GLU:H	1.86	0.40
1:K:137:PHE:CD2	1:K:179:CYS:HB3	2.56	0.40
1:I:154:MET:HE2	1:I:160:ILE:HD11	2.04	0.40
1:A:56:THR:CG2	1:F:83:ASP:HB3	2.49	0.40
1:L:169:TRP:CZ2	1:L:256:GLY:HA3	2.56	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	268/277 (97%)	254 (95%)	14 (5%)	0	100	100
1	B	268/277 (97%)	256 (96%)	12 (4%)	0	100	100
1	C	270/277 (98%)	259 (96%)	10 (4%)	1 (0%)	30	59
1	D	269/277 (97%)	255 (95%)	12 (4%)	2 (1%)	18	48
1	E	269/277 (97%)	255 (95%)	12 (4%)	2 (1%)	18	48
1	F	269/277 (97%)	259 (96%)	10 (4%)	0	100	100
1	G	270/277 (98%)	249 (92%)	16 (6%)	5 (2%)	6	23
1	H	269/277 (97%)	253 (94%)	14 (5%)	2 (1%)	18	48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	270/277 (98%)	260 (96%)	7 (3%)	3 (1%)	11	36
1	J	269/277 (97%)	253 (94%)	16 (6%)	0	100	100
1	K	269/277 (97%)	256 (95%)	11 (4%)	2 (1%)	18	48
1	L	271/277 (98%)	255 (94%)	12 (4%)	4 (2%)	8	28
1	M	271/277 (98%)	260 (96%)	10 (4%)	1 (0%)	30	59
1	N	269/277 (97%)	251 (93%)	17 (6%)	1 (0%)	30	59
All	All	3771/3878 (97%)	3575 (95%)	173 (5%)	23 (1%)	21	51

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	271	ALA
1	E	131	MET
1	G	130	ALA
1	H	122	GLY
1	I	56	THR
1	L	272	ARG
1	D	122	GLY
1	G	122	GLY
1	G	233	GLN
1	H	128	TYR
1	I	57	GLY
1	I	122	GLY
1	K	122	GLY
1	L	122	GLY
1	L	128	TYR
1	L	130	ALA
1	G	127	THR
1	G	232	PHE
1	C	123	GLU
1	E	32	LYS
1	K	132	TYR
1	N	122	GLY
1	M	122	GLY

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	221/230 (96%)	208 (94%)	13 (6%)	18	48
1	B	218/230 (95%)	211 (97%)	7 (3%)	34	68
1	C	225/230 (98%)	216 (96%)	9 (4%)	28	62
1	D	226/230 (98%)	215 (95%)	11 (5%)	22	54
1	E	224/230 (97%)	214 (96%)	10 (4%)	24	58
1	F	224/230 (97%)	214 (96%)	10 (4%)	24	58
1	G	220/230 (96%)	208 (94%)	12 (6%)	19	50
1	H	225/230 (98%)	219 (97%)	6 (3%)	39	73
1	I	225/230 (98%)	213 (95%)	12 (5%)	20	52
1	J	223/230 (97%)	215 (96%)	8 (4%)	31	65
1	K	224/230 (97%)	211 (94%)	13 (6%)	18	49
1	L	225/230 (98%)	218 (97%)	7 (3%)	35	69
1	M	221/230 (96%)	212 (96%)	9 (4%)	27	61
1	N	220/230 (96%)	212 (96%)	8 (4%)	31	65
All	All	3121/3220 (97%)	2986 (96%)	135 (4%)	26	60

All (135) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	ARG
1	A	52	ARG
1	A	56	THR
1	A	112	LEU
1	A	128	TYR
1	A	131	MET
1	A	133	ASP
1	A	143	VAL
1	A	160	ILE
1	A	201	ILE
1	A	202	GLN
1	A	241	GLU
1	A	248	ASN
1	B	81	SER
1	B	112	LEU
1	B	143	VAL

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Mol	Chain	Res	Type
1	B	160	ILE
1	B	198	ASP
1	B	238	MET
1	B	249	LYS
1	C	112	LEU
1	C	123	GLU
1	C	128	TYR
1	C	143	VAL
1	C	160	ILE
1	C	189	THR
1	C	198	ASP
1	C	241	GLU
1	C	249	LYS
1	D	73	LEU
1	D	112	LEU
1	D	123	GLU
1	D	127	THR
1	D	131	MET
1	D	133	ASP
1	D	143	VAL
1	D	160	ILE
1	D	233	GLN
1	D	241	GLU
1	D	249	LYS
1	E	3	ARG
1	E	4	ARG
1	E	31	LYS
1	E	112	LEU
1	E	123	GLU
1	E	143	VAL
1	E	160	ILE
1	E	189	THR
1	E	201	ILE
1	E	244	ASP
1	F	29	LEU
1	F	92	GLU
1	F	112	LEU
1	F	127	THR
1	F	133	ASP
1	F	143	VAL
1	F	160	ILE
1	F	198	ASP

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Mol	Chain	Res	Type
1	F	201	ILE
1	F	249	LYS
1	G	3	ARG
1	G	38	GLU
1	G	56	THR
1	G	127	THR
1	G	139	SER
1	G	143	VAL
1	G	160	ILE
1	G	189	THR
1	G	241	GLU
1	G	249	LYS
1	G	269	ILE
1	G	272	ARG
1	H	73	LEU
1	H	112	LEU
1	H	131	MET
1	H	143	VAL
1	H	160	ILE
1	H	248	ASN
1	I	3	ARG
1	I	56	THR
1	I	70	GLU
1	I	73	LEU
1	I	112	LEU
1	I	123	GLU
1	I	133	ASP
1	I	143	VAL
1	I	160	ILE
1	I	233	GLN
1	I	241	GLU
1	I	272	ARG
1	J	92	GLU
1	J	108	VAL
1	J	112	LEU
1	J	133	ASP
1	J	134	LYS
1	J	143	VAL
1	J	160	ILE
1	J	198	ASP
1	K	72	VAL
1	K	112	LEU

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Mol	Chain	Res	Type
1	K	127	THR
1	K	128	TYR
1	K	131	MET
1	K	133	ASP
1	K	143	VAL
1	K	160	ILE
1	K	194	HIS
1	K	198	ASP
1	K	230	LEU
1	K	249	LYS
1	K	272	ARG
1	L	60	LYS
1	L	112	LEU
1	L	133	ASP
1	L	143	VAL
1	L	160	ILE
1	L	198	ASP
1	L	249	LYS
1	M	4	ARG
1	M	37	VAL
1	M	112	LEU
1	M	127	THR
1	M	133	ASP
1	M	143	VAL
1	M	160	ILE
1	M	189	THR
1	M	198	ASP
1	N	60	LYS
1	N	112	LEU
1	N	127	THR
1	N	143	VAL
1	N	160	ILE
1	N	231	ASN
1	N	241	GLU
1	N	249	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (70) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	161	HIS
1	A	172	GLN
1	A	231	ASN

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Mol	Chain	Res	Type
1	A	267	ASN
1	A	268	GLN
1	B	45	ASN
1	B	172	GLN
1	B	267	ASN
1	B	268	GLN
1	C	161	HIS
1	C	172	GLN
1	C	267	ASN
1	C	268	GLN
1	D	45	ASN
1	D	88	GLN
1	D	104	GLN
1	D	161	HIS
1	D	172	GLN
1	D	267	ASN
1	D	268	GLN
1	E	172	GLN
1	E	267	ASN
1	E	268	GLN
1	F	161	HIS
1	F	172	GLN
1	F	194	HIS
1	F	243	GLN
1	F	267	ASN
1	F	268	GLN
1	G	172	GLN
1	G	267	ASN
1	G	268	GLN
1	H	64	ASN
1	H	79	HIS
1	H	172	GLN
1	H	267	ASN
1	H	268	GLN
1	I	172	GLN
1	I	202	GLN
1	I	267	ASN
1	I	268	GLN
1	J	79	HIS
1	J	161	HIS
1	J	194	HIS
1	J	267	ASN

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Mol	Chain	Res	Type
1	J	268	GLN
1	K	45	ASN
1	K	79	HIS
1	K	172	GLN
1	K	194	HIS
1	K	267	ASN
1	K	268	GLN
1	L	45	ASN
1	L	64	ASN
1	L	172	GLN
1	L	231	ASN
1	L	267	ASN
1	L	268	GLN
1	M	64	ASN
1	M	161	HIS
1	M	172	GLN
1	M	194	HIS
1	M	267	ASN
1	M	268	GLN
1	N	66	GLN
1	N	161	HIS
1	N	177	HIS
1	N	231	ASN
1	N	267	ASN
1	N	268	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

19 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FAD	F	301	-	58,58,58	0.42	0	85,89,89	0.48	0
2	FAD	B	301	-	58,58,58	0.36	0	85,89,89	0.49	0
2	FAD	N	301	-	58,58,58	0.43	0	85,89,89	0.48	0
2	FAD	A	601	-	58,58,58	0.39	0	85,89,89	0.56	0
2	FAD	C	601	-	58,58,58	0.41	0	85,89,89	0.54	1 (1%)
3	E6A	M	602	-	26,29,29	1.81	5 (19%)	31,44,44	2.60	11 (35%)
2	FAD	K	601	-	58,58,58	0.40	0	85,89,89	0.56	1 (1%)
3	E6A	B	302	-	26,29,29	1.75	4 (15%)	31,44,44	2.46	10 (32%)
3	E6A	H	302	-	26,29,29	1.76	4 (15%)	31,44,44	2.40	11 (35%)
3	E6A	K	602	-	26,29,29	1.71	5 (19%)	31,44,44	2.39	9 (29%)
2	FAD	L	301	-	58,58,58	0.44	0	85,89,89	0.45	0
2	FAD	E	601	-	58,58,58	0.35	0	85,89,89	0.58	1 (1%)
2	FAD	D	301	-	58,58,58	0.46	0	85,89,89	0.51	1 (1%)
3	E6A	E	602	-	26,29,29	1.96	5 (19%)	31,44,44	2.22	11 (35%)
2	FAD	H	301	-	58,58,58	0.47	0	85,89,89	0.48	0
2	FAD	M	601	-	58,58,58	0.35	0	85,89,89	0.49	0
2	FAD	G	601	-	58,58,58	0.30	0	85,89,89	0.56	0
2	FAD	J	301	-	58,58,58	0.30	0	85,89,89	0.47	0
2	FAD	I	601	-	58,58,58	0.39	0	85,89,89	0.53	0

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	F	301	-	-	7/34/50/50	0/6/6/6
2	FAD	B	301	-	-	7/34/50/50	0/6/6/6
2	FAD	N	301	-	-	9/34/50/50	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	A	601	-	-	4/34/50/50	0/6/6/6
2	FAD	C	601	-	-	5/34/50/50	0/6/6/6
3	E6A	M	602	-	-	2/4/44/44	0/4/4/4
2	FAD	K	601	-	-	4/34/50/50	0/6/6/6
3	E6A	B	302	-	-	2/4/44/44	0/4/4/4
3	E6A	H	302	-	-	2/4/44/44	0/4/4/4
3	E6A	K	602	-	-	2/4/44/44	0/4/4/4
2	FAD	L	301	-	-	9/34/50/50	0/6/6/6
2	FAD	E	601	-	-	4/34/50/50	0/6/6/6
2	FAD	D	301	-	-	7/34/50/50	0/6/6/6
3	E6A	E	602	-	-	2/4/44/44	0/4/4/4
2	FAD	H	301	-	-	6/34/50/50	0/6/6/6
2	FAD	M	601	-	-	4/34/50/50	0/6/6/6
2	FAD	G	601	-	-	4/34/50/50	0/6/6/6
2	FAD	J	301	-	-	6/34/50/50	0/6/6/6
2	FAD	I	601	-	-	4/34/50/50	0/6/6/6

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	602	E6A	C25-C24	6.04	1.50	1.40
3	B	302	E6A	C25-C24	5.54	1.49	1.40
3	M	602	E6A	C25-C24	5.50	1.49	1.40
3	H	302	E6A	C25-C24	5.26	1.49	1.40
3	K	602	E6A	C25-C24	5.18	1.49	1.40
3	K	602	E6A	C13-C18	4.50	1.48	1.40
3	M	602	E6A	C13-C18	4.44	1.47	1.40
3	E	602	E6A	C13-C18	4.18	1.47	1.40
3	H	302	E6A	C13-C18	3.90	1.47	1.40
3	B	302	E6A	C13-C18	3.84	1.47	1.40
3	E	602	E6A	C25-C26	3.09	1.53	1.48
3	H	302	E6A	C24-C23	2.86	1.53	1.48
3	H	302	E6A	C6-C22	2.76	1.60	1.55
3	E	602	E6A	C6-C22	2.63	1.60	1.55
3	E	602	E6A	C24-C23	2.59	1.52	1.48
3	M	602	E6A	C24-C23	2.45	1.52	1.48
3	K	602	E6A	C25-C26	2.36	1.52	1.48
3	B	302	E6A	C24-C23	2.31	1.52	1.48
3	M	602	E6A	C25-C26	2.28	1.52	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	K	602	E6A	C24-C23	2.18	1.52	1.48
3	K	602	E6A	C13-C1	2.08	1.51	1.48
3	M	602	E6A	BR-C5	2.06	2.05	1.97
3	B	302	E6A	C13-C1	2.03	1.51	1.48

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	602	E6A	BR-C5-C6	6.94	119.11	109.41
3	M	602	E6A	C18-C13-C1	-6.68	114.12	120.75
3	K	602	E6A	BR-C5-C6	6.51	118.52	109.41
3	B	302	E6A	C13-C18-C4	-6.25	114.55	120.75
3	K	602	E6A	C18-C13-C1	-6.06	114.73	120.75
3	H	302	E6A	BR-C5-C6	5.99	117.78	109.41
3	M	602	E6A	C13-C18-C4	-5.81	114.99	120.75
3	B	302	E6A	C18-C13-C1	-5.73	115.06	120.75
3	E	602	E6A	C13-C18-C4	-5.52	115.27	120.75
3	B	302	E6A	BR-C5-C6	5.47	117.06	109.41
3	H	302	E6A	C13-C18-C4	-5.08	115.71	120.75
3	H	302	E6A	C18-C13-C1	-5.07	115.72	120.75
3	K	602	E6A	C13-C18-C4	-4.99	115.79	120.75
3	B	302	E6A	C14-C13-C1	4.72	126.48	119.89
3	E	602	E6A	C18-C13-C1	-4.71	116.08	120.75
3	M	602	E6A	C17-C18-C4	4.13	125.67	119.89
3	K	602	E6A	C14-C13-C1	4.06	125.56	119.89
3	E	602	E6A	BR-C5-C6	4.03	115.05	109.41
3	B	302	E6A	C17-C18-C4	3.98	125.45	119.89
3	M	602	E6A	C14-C13-C1	3.97	125.44	119.89
3	H	302	E6A	O40-C23-C24	-3.63	116.56	122.18
3	H	302	E6A	O20-C4-C18	-3.51	116.75	122.18
3	E	602	E6A	O40-C23-C24	-3.36	116.98	122.18
3	K	602	E6A	C17-C18-C4	3.28	124.47	119.89
3	H	302	E6A	C14-C13-C1	3.17	124.32	119.89
3	E	602	E6A	C14-C13-C1	3.16	124.31	119.89
3	B	302	E6A	O40-C23-C24	-3.08	117.42	122.18
3	H	302	E6A	C24-C25-C26	-2.99	117.78	120.75
3	K	602	E6A	O20-C4-C18	-2.87	117.74	122.18
3	M	602	E6A	C24-C25-C26	-2.85	117.92	120.75
3	E	602	E6A	O20-C4-C18	-2.82	117.82	122.18
3	E	602	E6A	O38-C26-C27	-2.80	116.98	119.88
3	K	602	E6A	C25-C24-C23	-2.64	118.13	120.75
3	E	602	E6A	C17-C18-C4	2.63	123.56	119.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	602	E6A	O40-C23-C24	-2.61	118.15	122.18
3	H	302	E6A	O38-C26-C25	-2.58	118.18	122.18
3	H	302	E6A	C17-C18-C4	2.57	123.47	119.89
3	M	602	E6A	C34-C25-C26	2.42	123.27	119.89
2	E	601	FAD	O5B-PA-O1A	2.36	118.30	108.94
3	B	302	E6A	C24-C25-C26	-2.36	118.41	120.75
3	E	602	E6A	O41-C27-C26	-2.33	106.01	111.43
3	B	302	E6A	O19-C1-C13	-2.33	118.58	122.18
3	M	602	E6A	C25-C24-C23	-2.30	118.47	120.75
3	E	602	E6A	O19-C1-C13	-2.30	118.63	122.18
3	M	602	E6A	O20-C4-C18	-2.29	118.64	122.18
3	M	602	E6A	O41-C27-C26	-2.26	106.17	111.43
3	H	302	E6A	O41-C27-C26	-2.20	106.31	111.43
3	H	302	E6A	C34-C25-C26	2.19	122.95	119.89
3	K	602	E6A	C24-C25-C26	-2.17	118.60	120.75
2	D	301	FAD	O5B-PA-O1A	2.15	117.47	108.94
2	C	601	FAD	O5B-PA-O1A	2.14	117.43	108.94
2	K	601	FAD	O5B-PA-O1A	2.14	117.42	108.94
3	M	602	E6A	O40-C23-C24	-2.13	118.89	122.18
3	E	602	E6A	C24-C25-C26	-2.05	118.71	120.75
3	B	302	E6A	C25-C24-C23	-2.03	118.73	120.75
3	B	302	E6A	O20-C4-C18	-2.03	119.04	122.18

There are no chirality outliers.

All (90) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	L	301	FAD	C5B-O5B-PA-O3P
3	B	302	E6A	C23-C22-C6-C1
3	B	302	E6A	C27-C22-C6-C5
3	E	602	E6A	C23-C22-C6-C1
3	E	602	E6A	C27-C22-C6-C5
3	H	302	E6A	C23-C22-C6-C1
3	H	302	E6A	C27-C22-C6-C5
3	K	602	E6A	C23-C22-C6-C1
3	K	602	E6A	C27-C22-C6-C5
3	M	602	E6A	C23-C22-C6-C1
3	M	602	E6A	C27-C22-C6-C5
2	L	301	FAD	O4B-C4B-C5B-O5B
2	N	301	FAD	O4B-C4B-C5B-O5B
2	F	301	FAD	O4B-C4B-C5B-O5B
2	H	301	FAD	O4B-C4B-C5B-O5B

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Mol	Chain	Res	Type	Atoms
2	F	301	FAD	C2B-C1B-N9A-C8A
2	B	301	FAD	O4B-C4B-C5B-O5B
2	J	301	FAD	O4B-C4B-C5B-O5B
2	B	301	FAD	C2B-C1B-N9A-C8A
2	D	301	FAD	C2B-C1B-N9A-C8A
2	H	301	FAD	C2B-C1B-N9A-C8A
2	J	301	FAD	C2B-C1B-N9A-C8A
2	L	301	FAD	C2B-C1B-N9A-C8A
2	N	301	FAD	C2B-C1B-N9A-C8A
2	F	301	FAD	PA-O3P-P-O1P
2	J	301	FAD	PA-O3P-P-O1P
2	L	301	FAD	PA-O3P-P-O1P
2	A	601	FAD	C2B-C1B-N9A-C8A
2	C	601	FAD	C2B-C1B-N9A-C8A
2	E	601	FAD	C2B-C1B-N9A-C8A
2	G	601	FAD	C2B-C1B-N9A-C8A
2	I	601	FAD	C2B-C1B-N9A-C8A
2	K	601	FAD	C2B-C1B-N9A-C8A
2	M	601	FAD	C2B-C1B-N9A-C8A
2	B	301	FAD	PA-O3P-P-O1P
2	H	301	FAD	PA-O3P-P-O1P
2	N	301	FAD	PA-O3P-P-O1P
2	N	301	FAD	C5B-O5B-PA-O3P
2	A	601	FAD	PA-O3P-P-O2P
2	C	601	FAD	PA-O3P-P-O2P
2	E	601	FAD	PA-O3P-P-O2P
2	G	601	FAD	PA-O3P-P-O2P
2	I	601	FAD	PA-O3P-P-O2P
2	K	601	FAD	PA-O3P-P-O2P
2	M	601	FAD	PA-O3P-P-O2P
2	B	301	FAD	C2B-C1B-N9A-C4A
2	J	301	FAD	C2B-C1B-N9A-C4A
2	L	301	FAD	C2B-C1B-N9A-C4A
2	D	301	FAD	C4'-C5'-O5'-P
2	D	301	FAD	C2B-C1B-N9A-C4A
2	F	301	FAD	C2B-C1B-N9A-C4A
2	H	301	FAD	C2B-C1B-N9A-C4A
2	N	301	FAD	C2B-C1B-N9A-C4A
2	C	601	FAD	O4B-C1B-N9A-C8A
2	E	601	FAD	O4B-C1B-N9A-C8A
2	D	301	FAD	O4B-C4B-C5B-O5B
2	A	601	FAD	PA-O3P-P-O1P

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Mol	Chain	Res	Type	Atoms
2	D	301	FAD	PA-O3P-P-O1P
2	A	601	FAD	O4B-C1B-N9A-C8A
2	G	601	FAD	O4B-C1B-N9A-C8A
2	M	601	FAD	O4B-C1B-N9A-C8A
2	L	301	FAD	C3B-C4B-C5B-O5B
2	N	301	FAD	C3B-C4B-C5B-O5B
2	K	601	FAD	O4B-C1B-N9A-C8A
2	L	301	FAD	C4'-C5'-O5'-P
2	I	601	FAD	O4B-C1B-N9A-C8A
2	B	301	FAD	PA-O3P-P-O2P
2	C	601	FAD	PA-O3P-P-O1P
2	D	301	FAD	PA-O3P-P-O2P
2	F	301	FAD	PA-O3P-P-O2P
2	H	301	FAD	PA-O3P-P-O2P
2	I	601	FAD	PA-O3P-P-O1P
2	L	301	FAD	PA-O3P-P-O2P
2	H	301	FAD	O4B-C1B-N9A-C8A
2	N	301	FAD	C4'-C5'-O5'-P
2	B	301	FAD	O4B-C1B-N9A-C8A
2	D	301	FAD	O4B-C1B-N9A-C8A
2	F	301	FAD	O4B-C1B-N9A-C8A
2	J	301	FAD	O4B-C1B-N9A-C8A
2	L	301	FAD	O4B-C1B-N9A-C8A
2	N	301	FAD	O4B-C1B-N9A-C8A
2	B	301	FAD	C4'-C5'-O5'-P
2	F	301	FAD	C4'-C5'-O5'-P
2	C	601	FAD	C4'-C5'-O5'-P
2	E	601	FAD	PA-O3P-P-O1P
2	G	601	FAD	PA-O3P-P-O1P
2	J	301	FAD	PA-O3P-P-O2P
2	K	601	FAD	PA-O3P-P-O1P
2	M	601	FAD	PA-O3P-P-O1P
2	N	301	FAD	PA-O3P-P-O2P

There are no ring outliers.

13 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	301	FAD	1	0
2	B	301	FAD	1	0
2	N	301	FAD	1	0
2	A	601	FAD	1	0

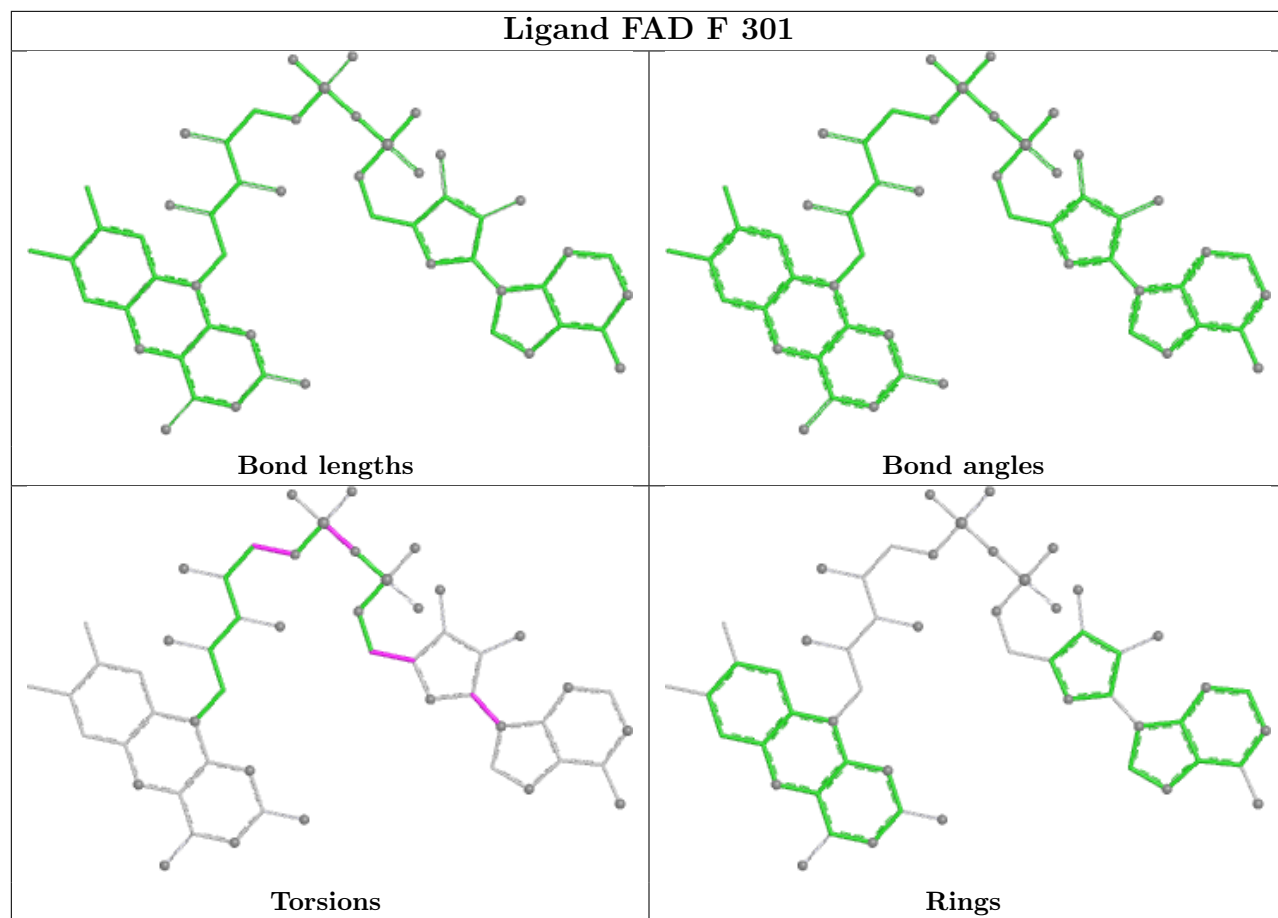
Continued on next page...

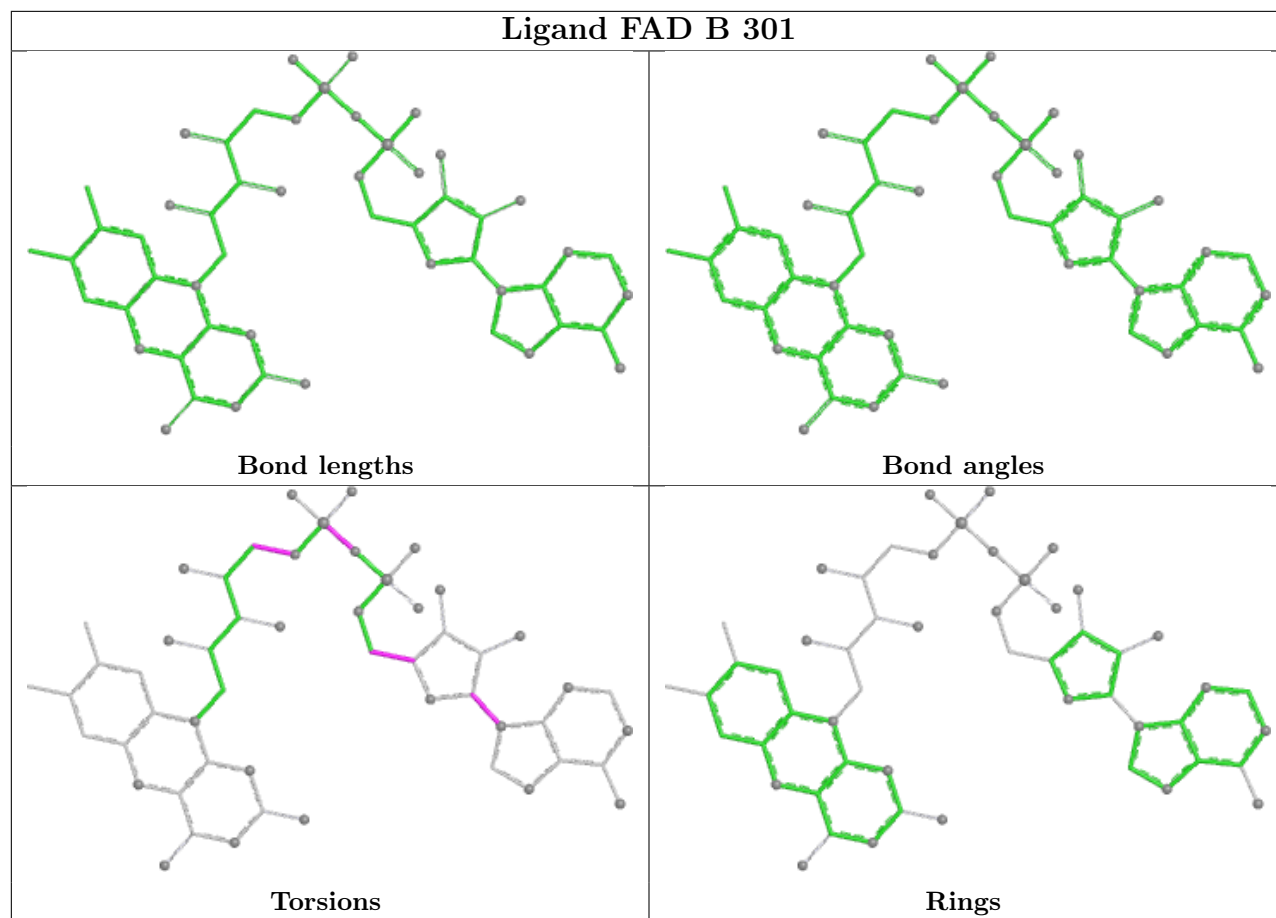
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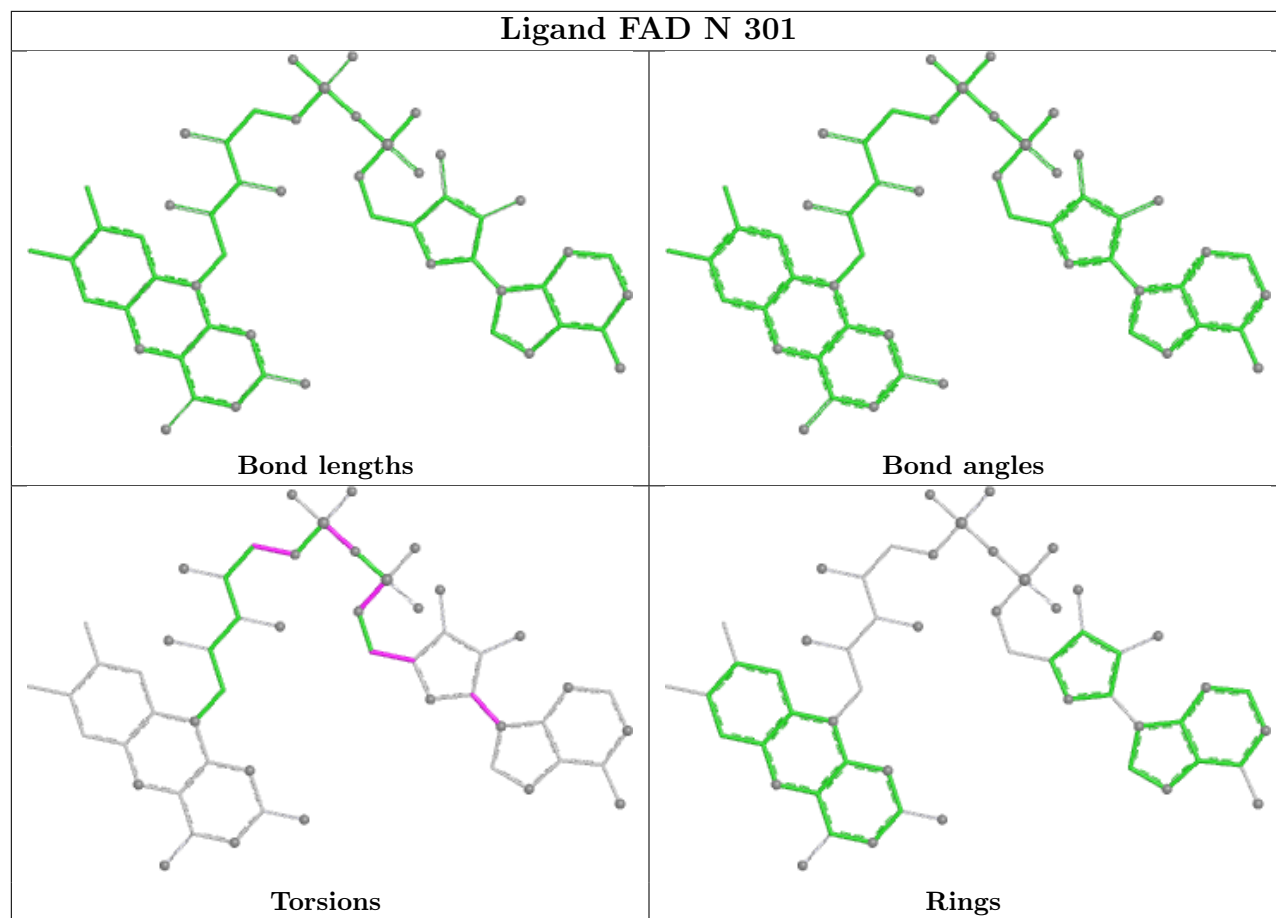
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	M	602	E6A	2	0
3	B	302	E6A	2	0
3	H	302	E6A	3	0
3	K	602	E6A	2	0
2	L	301	FAD	1	0
2	D	301	FAD	1	0
3	E	602	E6A	2	0
2	H	301	FAD	1	0
2	J	301	FAD	1	0

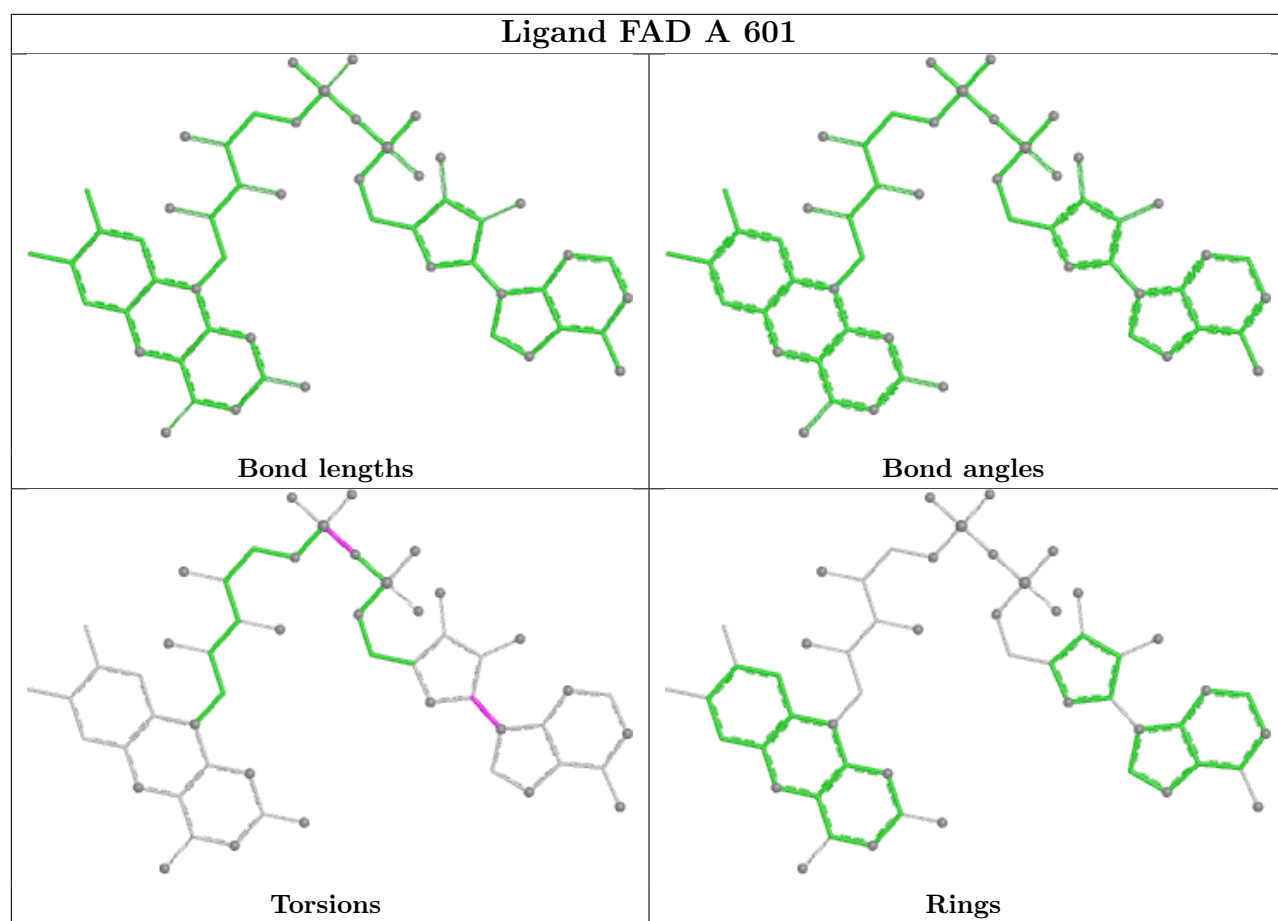
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand FAD F 301

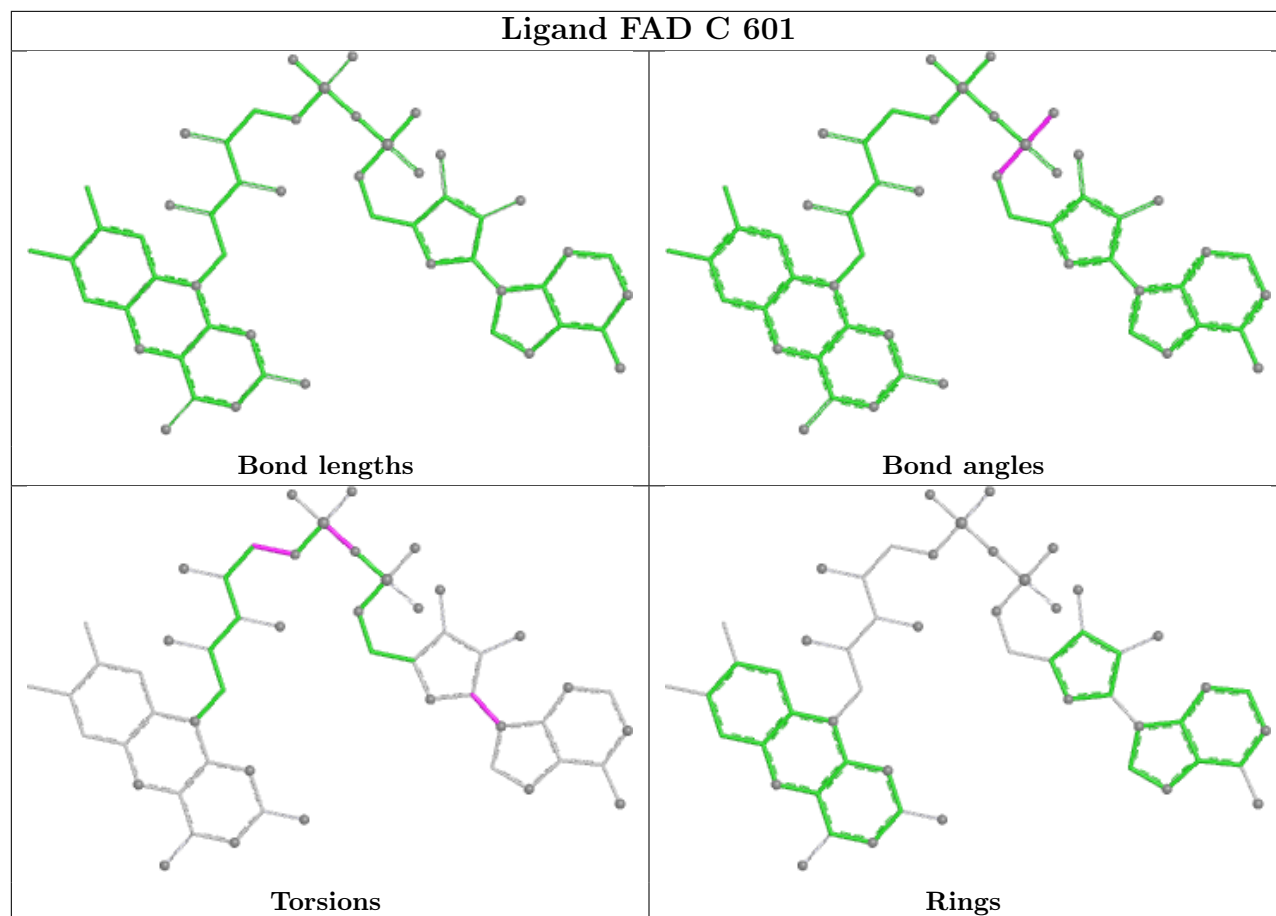




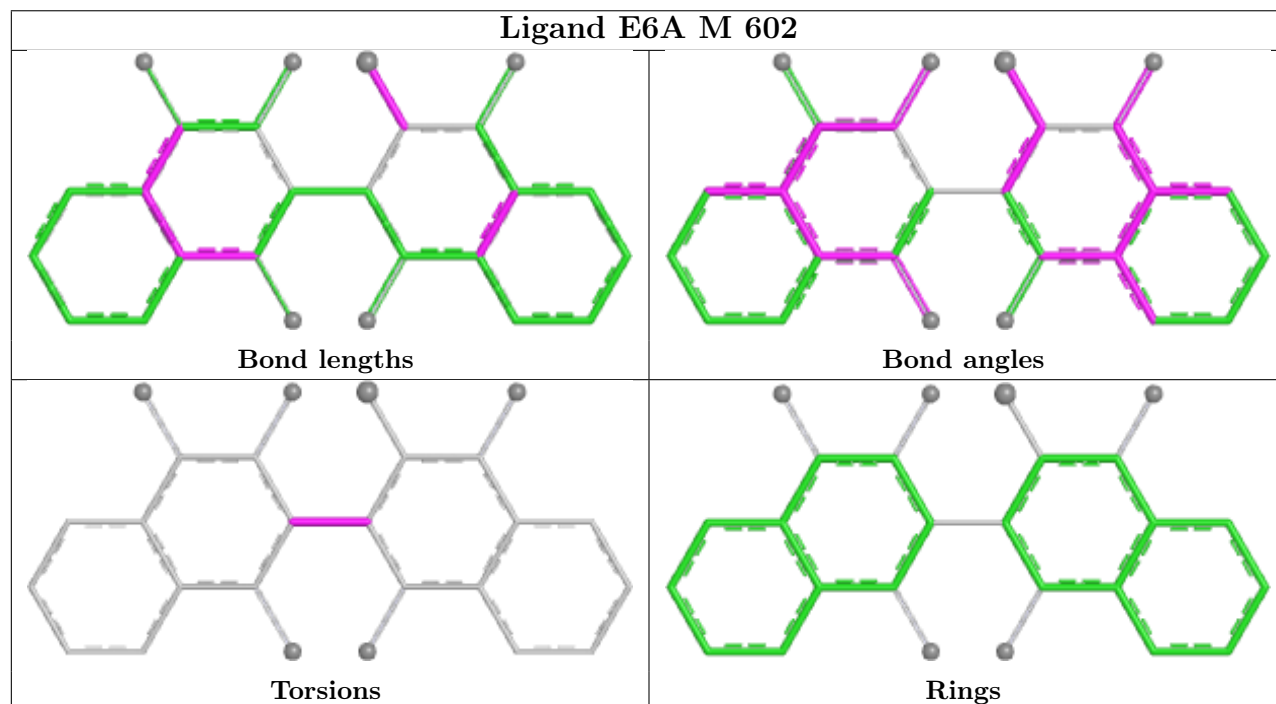




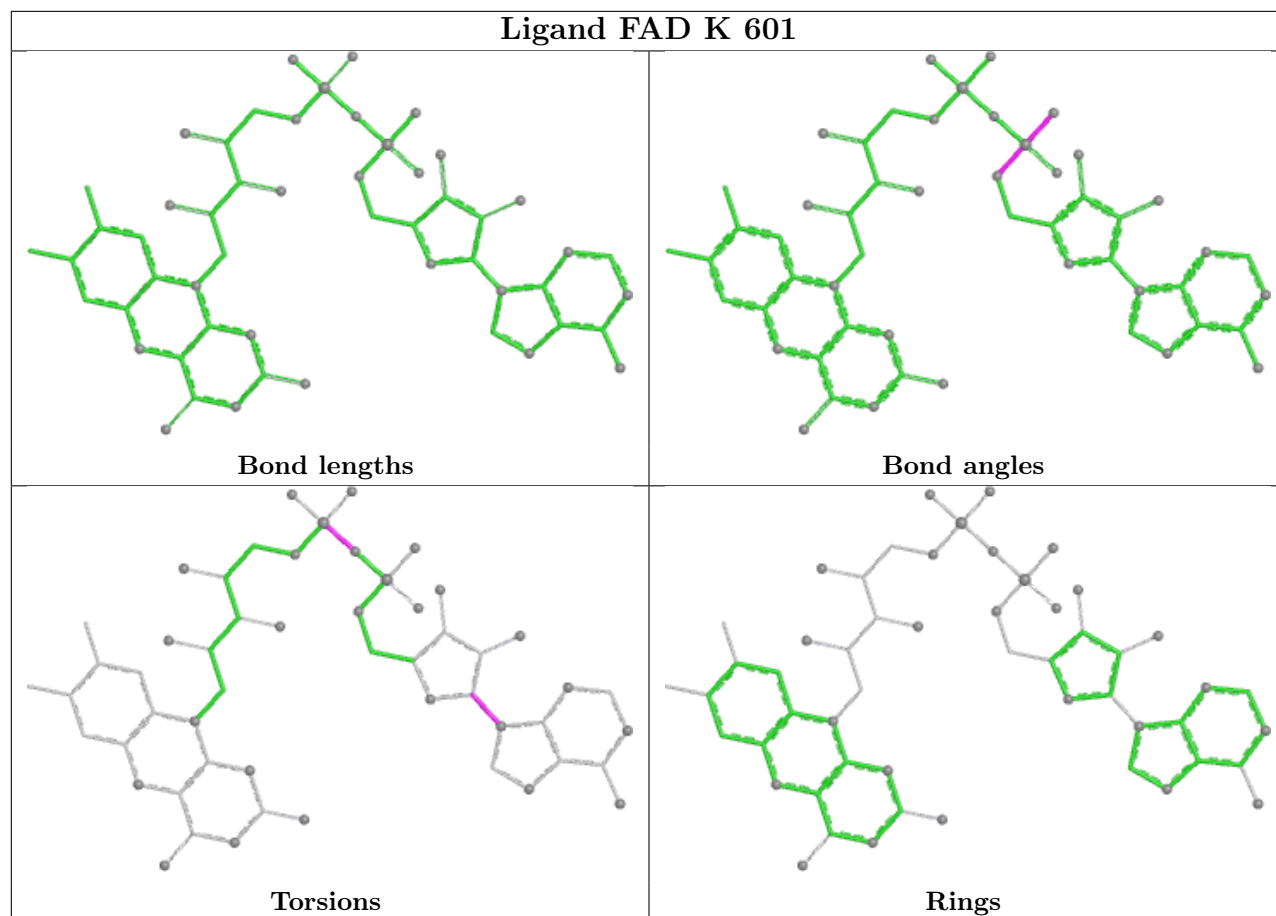
Ligand FAD C 601



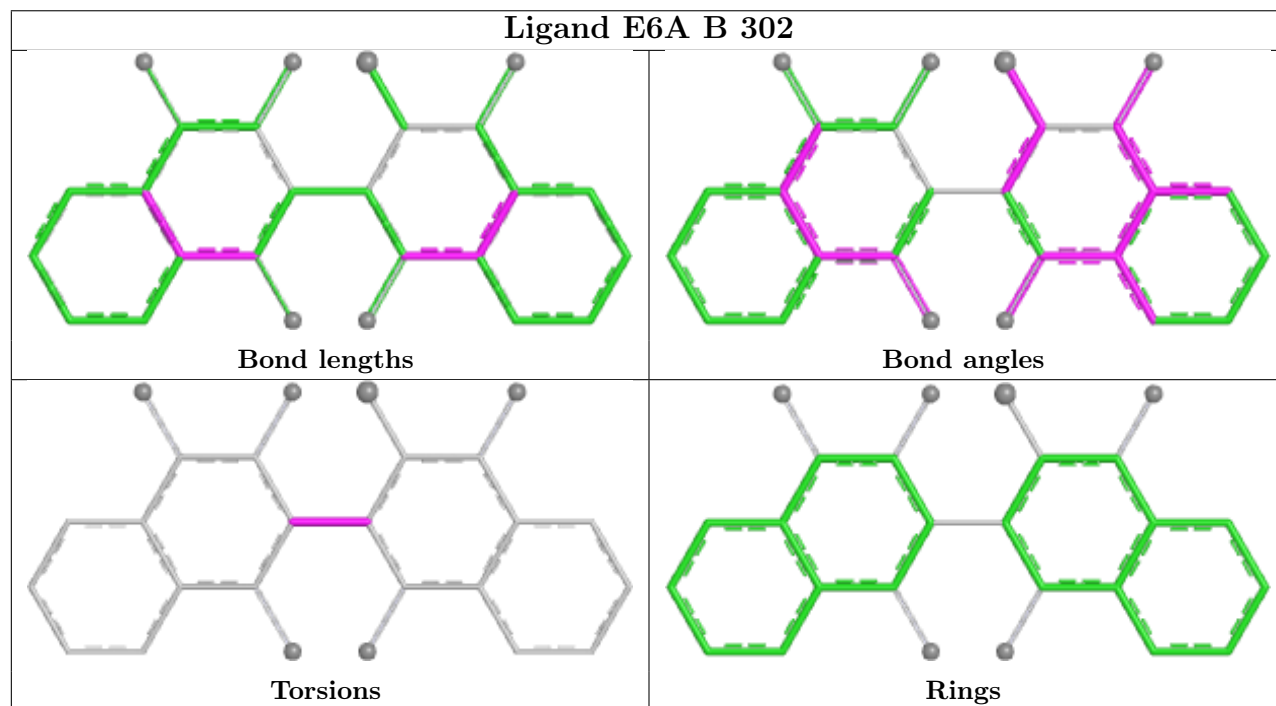
Ligand E6A M 602

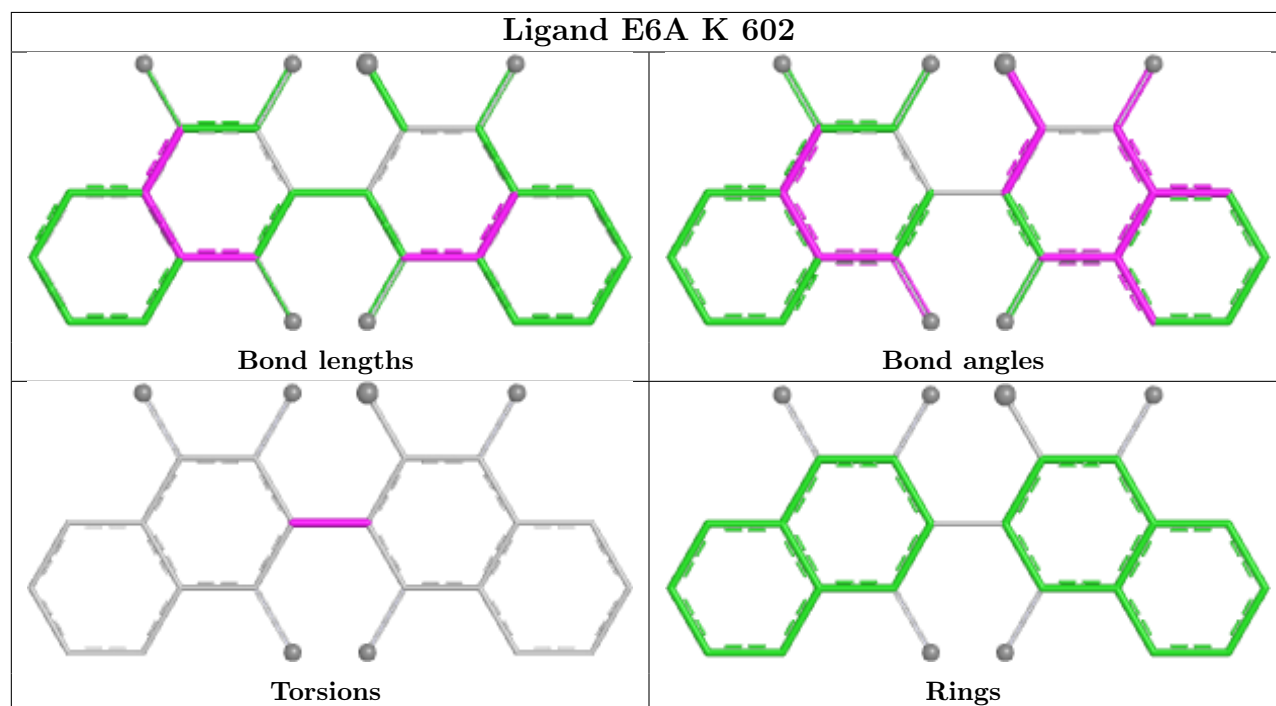
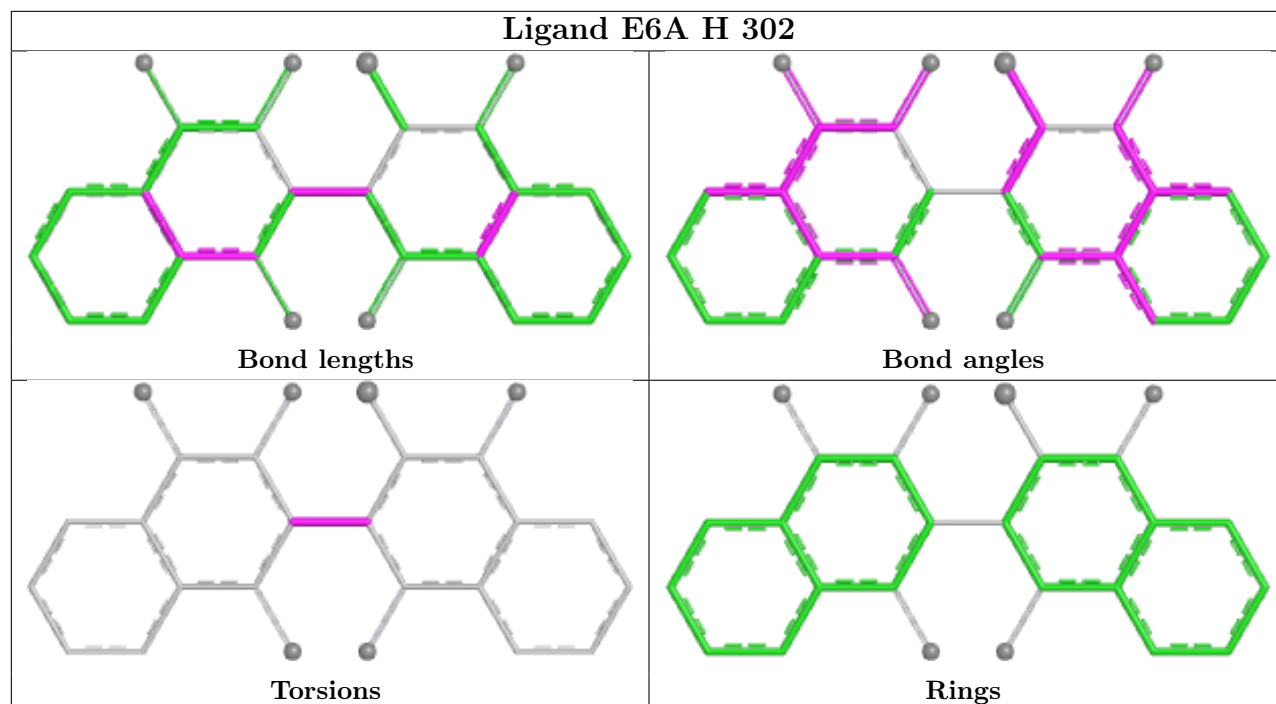


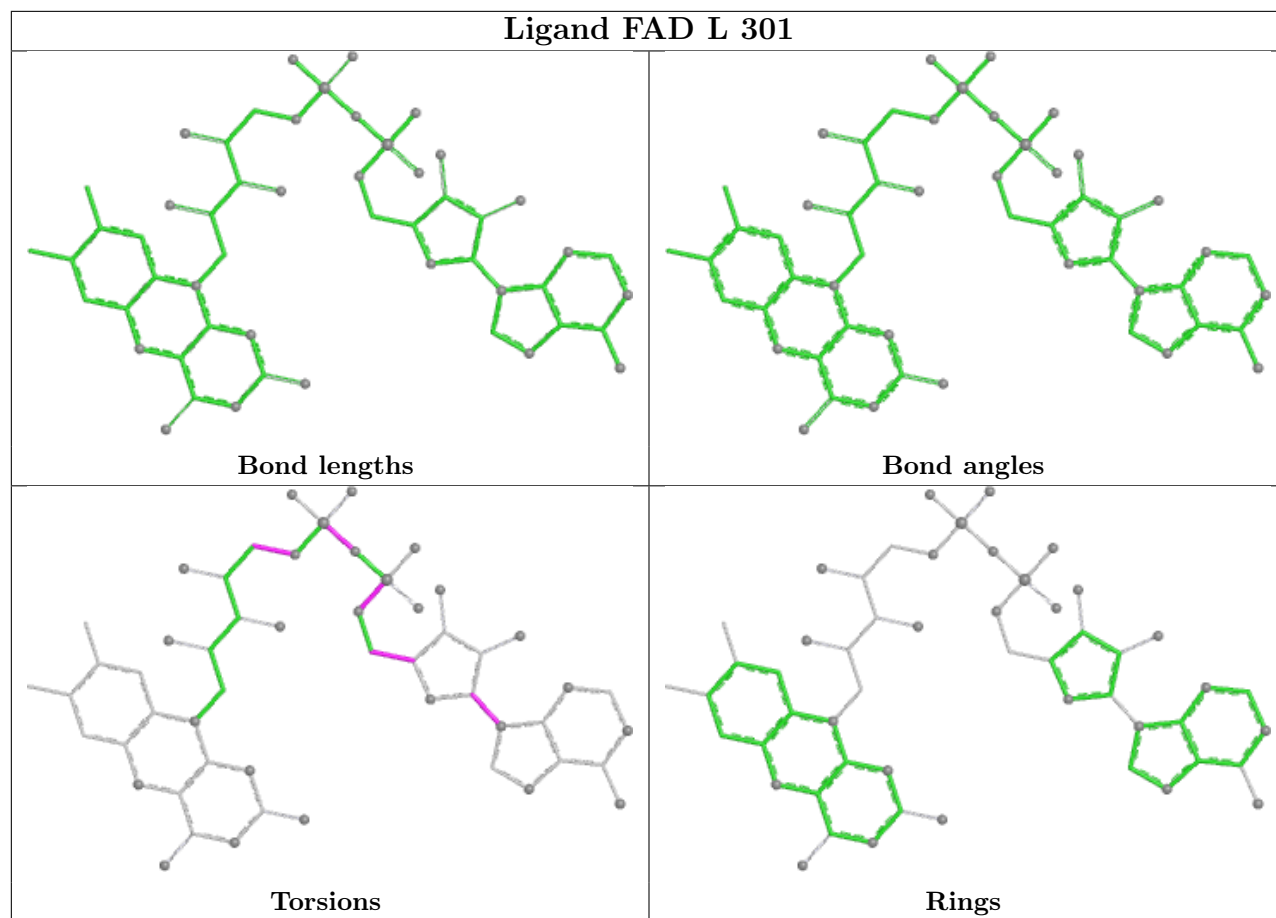
Ligand FAD K 601



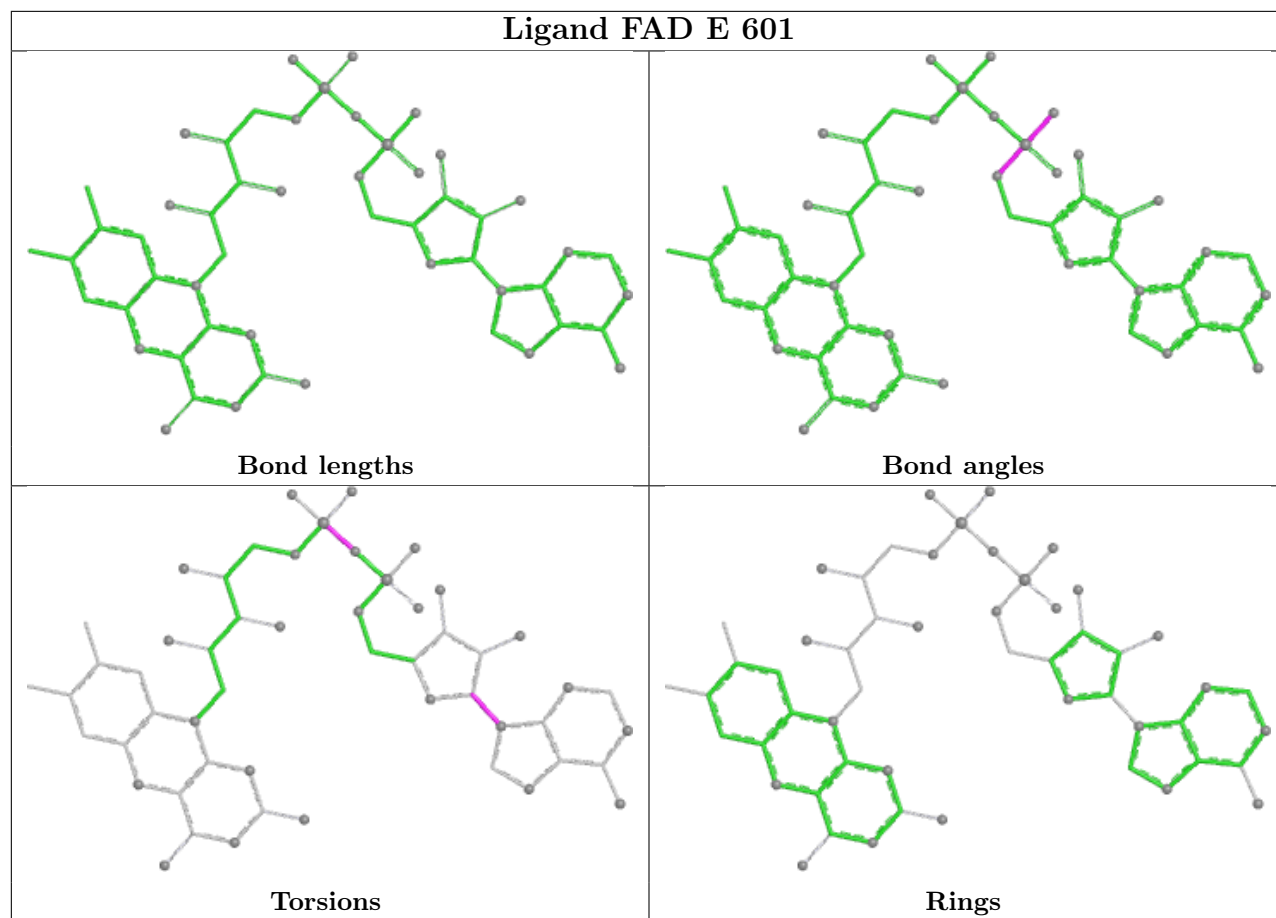
Ligand E6A B 302



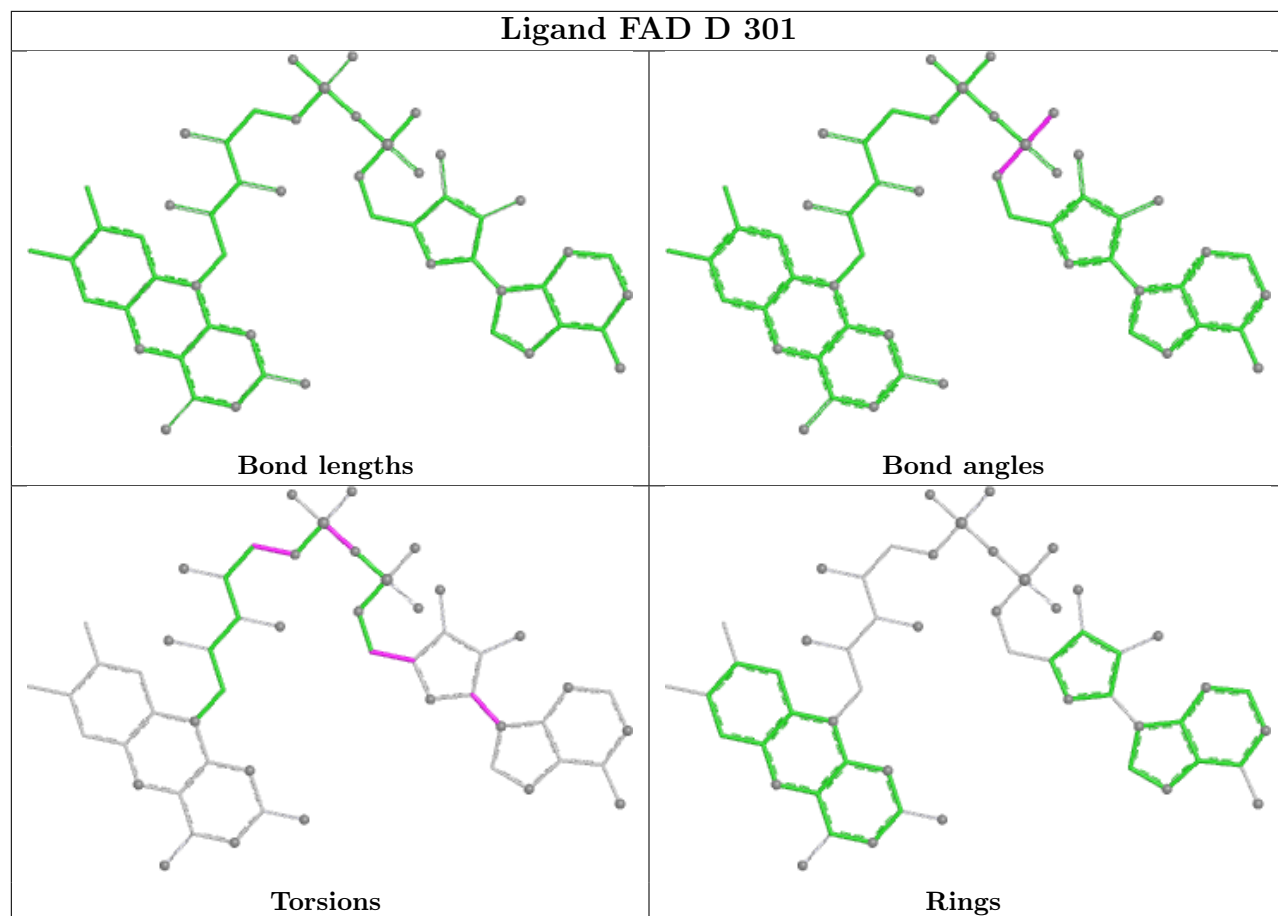




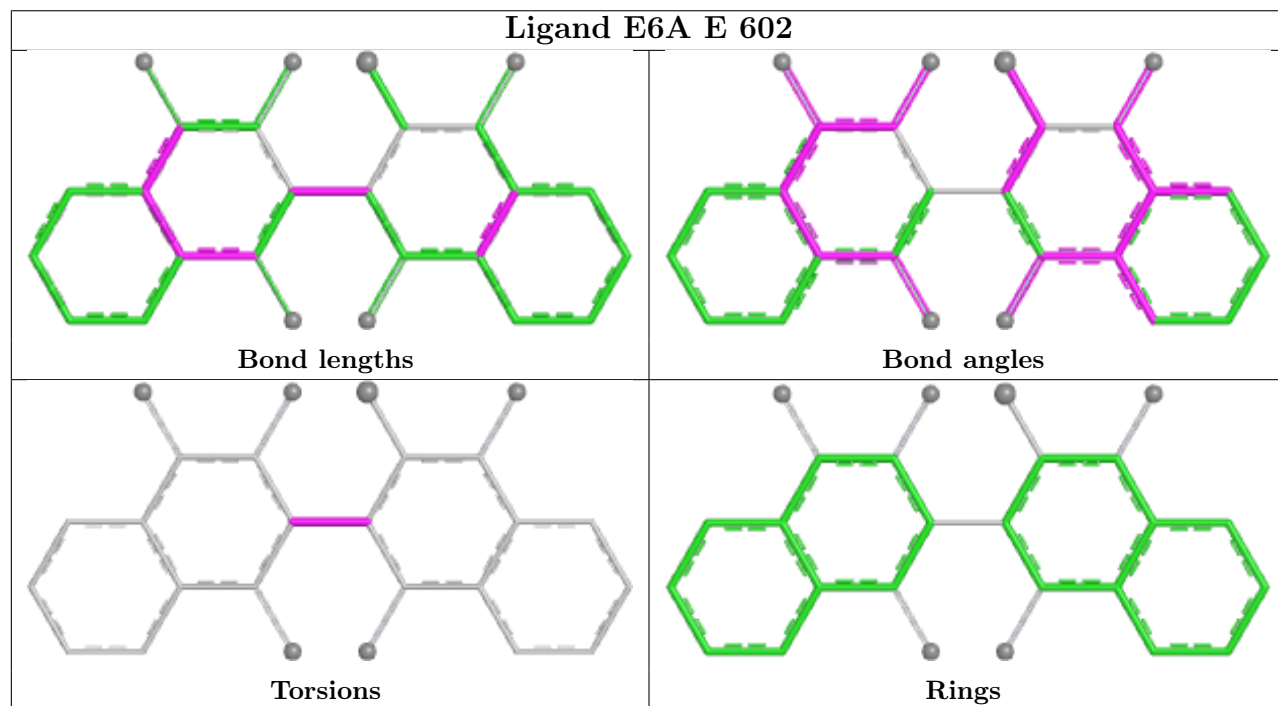
Ligand FAD E 601

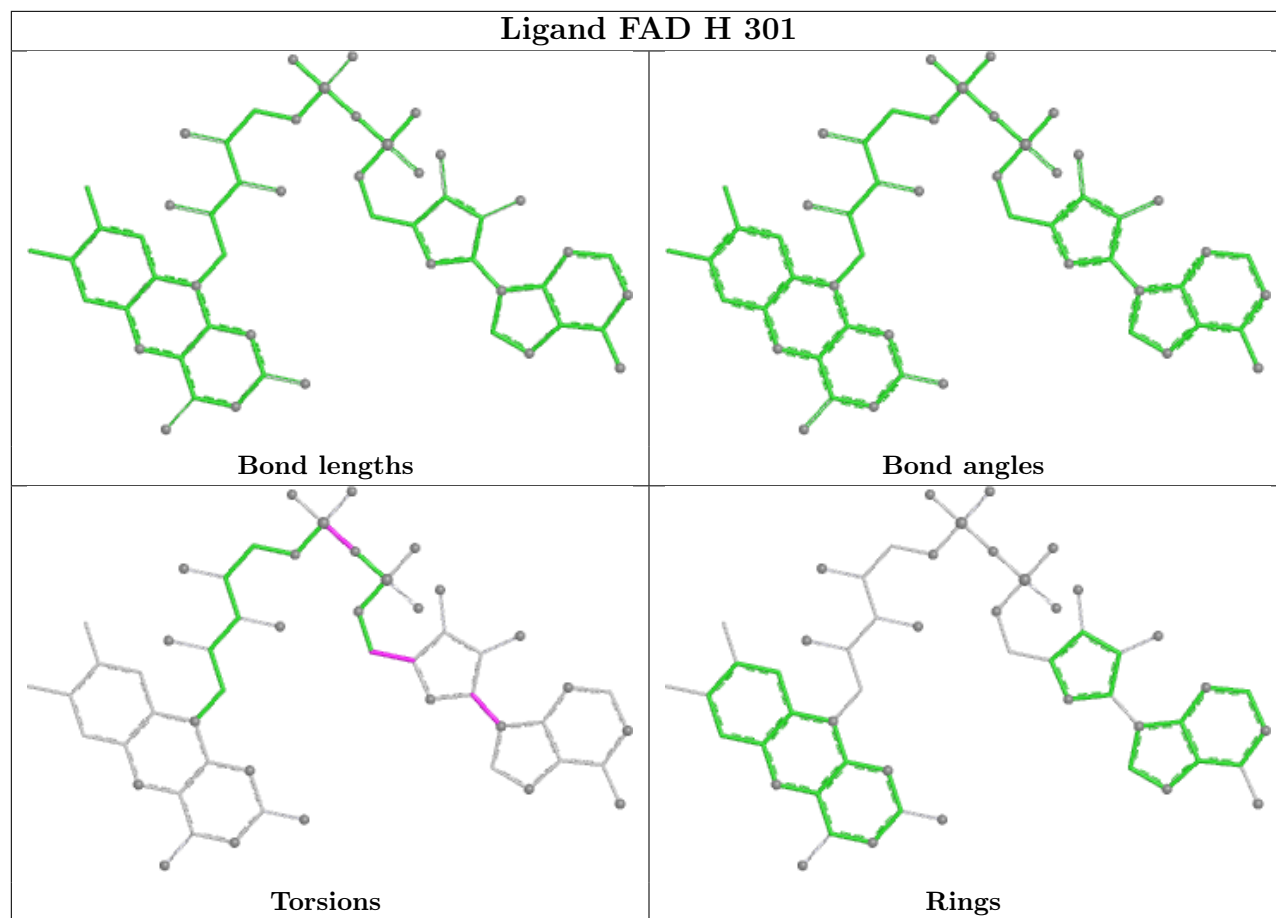


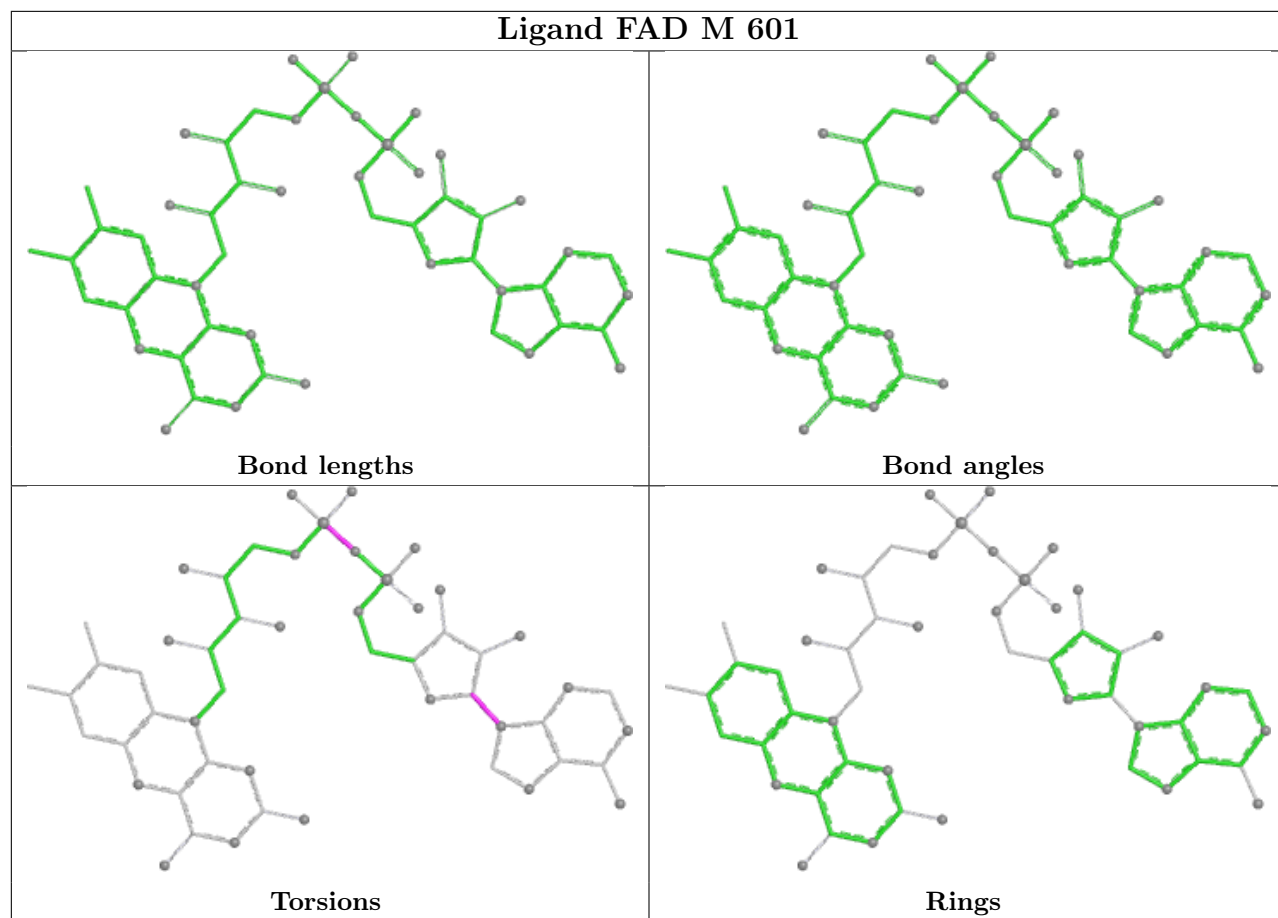
Ligand FAD D 301

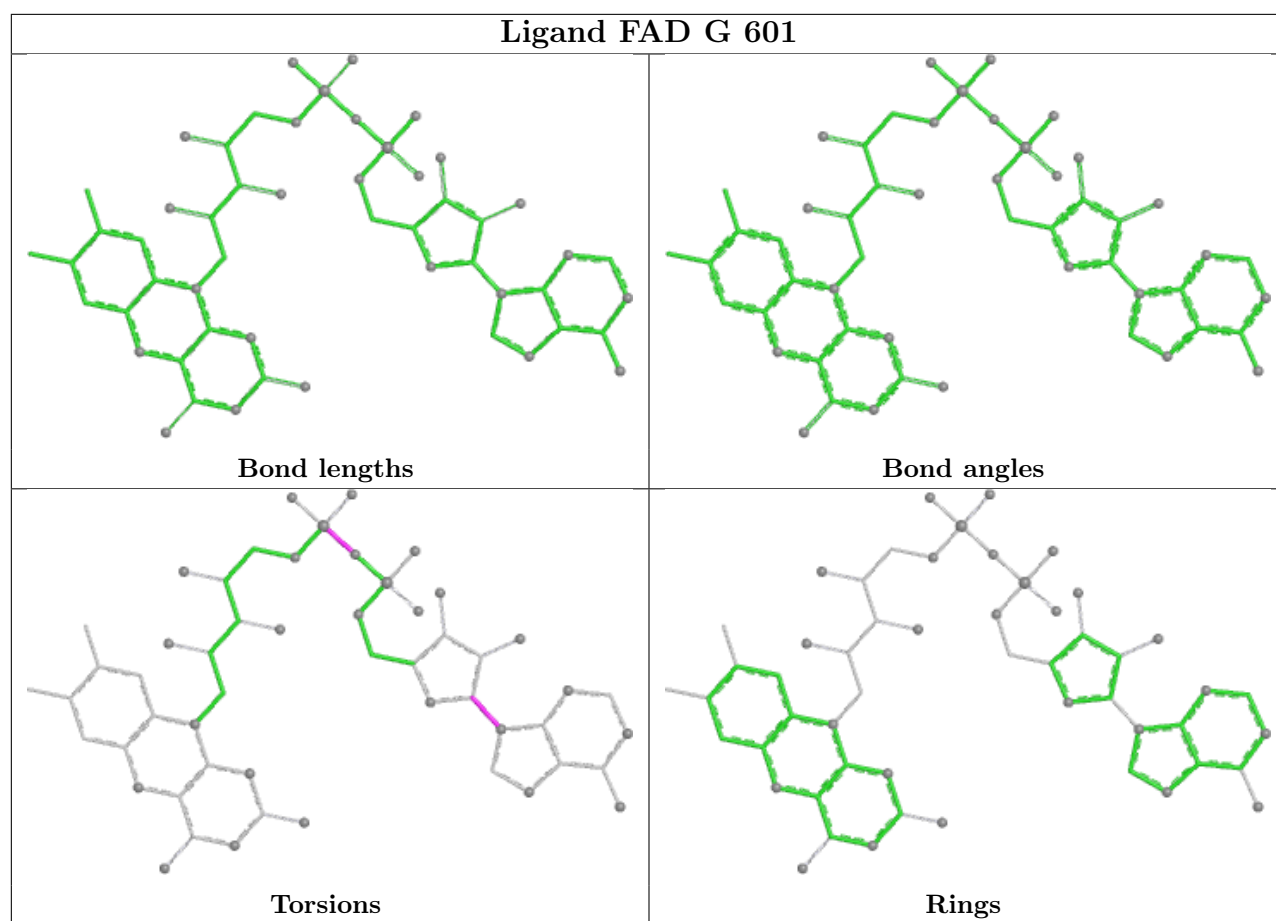


Ligand E6A E 602

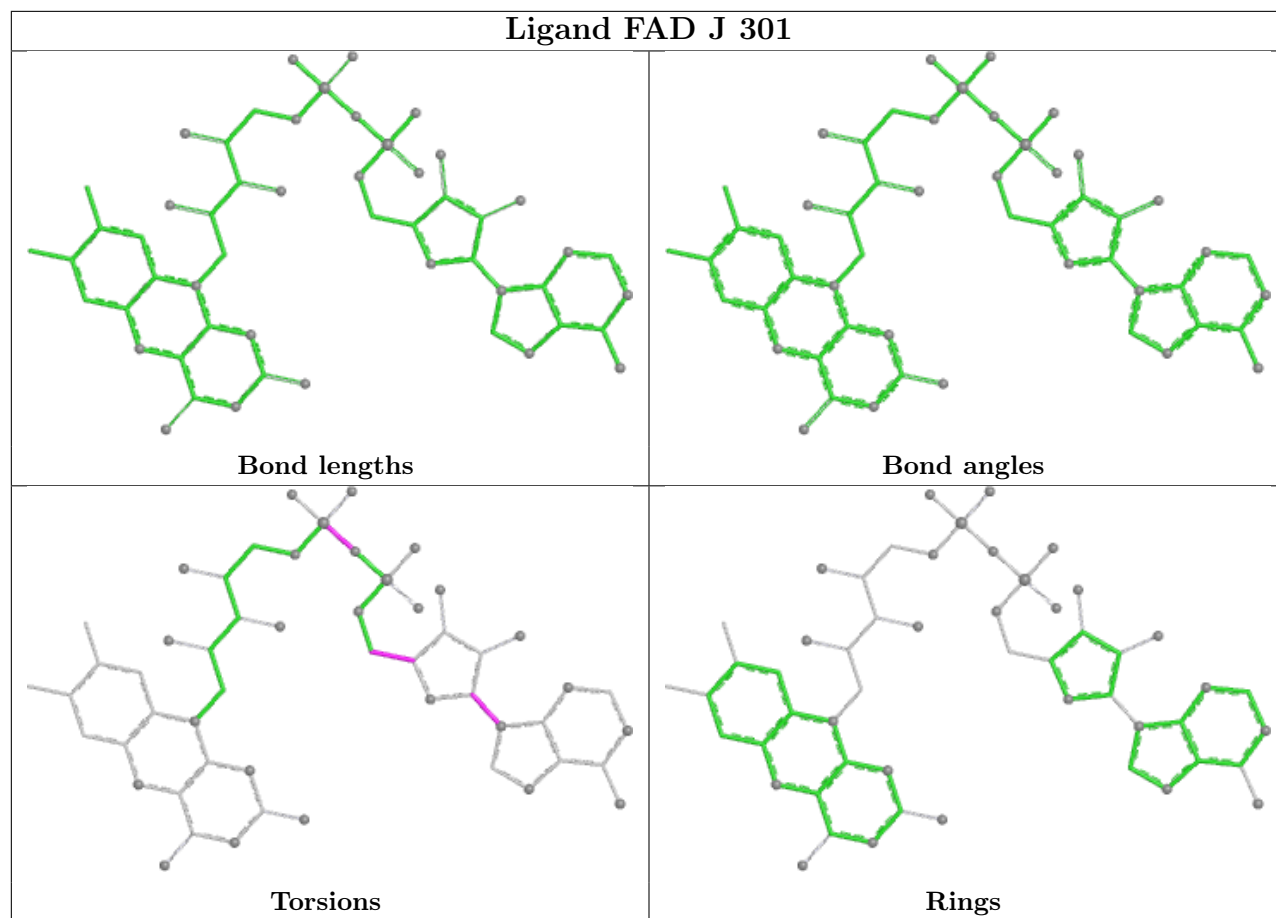


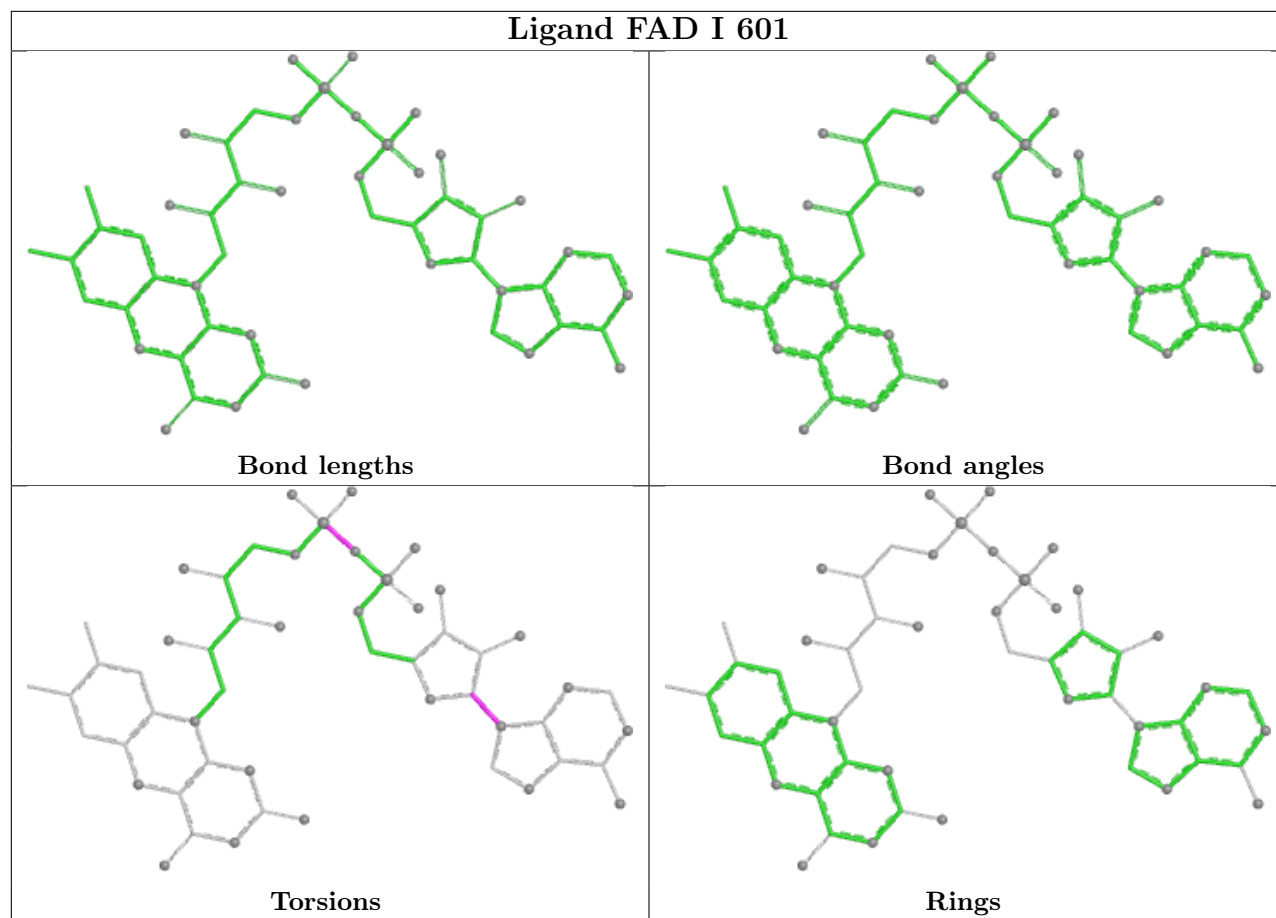






Ligand FAD J 301





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	270/277 (97%)	-0.32	1 (0%) 88 85	37, 64, 90, 104	13 (4%)
1	B	269/277 (97%)	-0.15	2 (0%) 84 79	34, 72, 99, 114	17 (6%)
1	C	271/277 (97%)	-0.38	1 (0%) 88 85	31, 60, 84, 109	13 (4%)
1	D	271/277 (97%)	-0.23	0 100 100	44, 67, 96, 113	16 (5%)
1	E	271/277 (97%)	-0.28	3 (1%) 78 71	29, 60, 90, 109	16 (5%)
1	F	270/277 (97%)	-0.19	3 (1%) 78 71	33, 68, 95, 108	14 (5%)
1	G	272/277 (98%)	-0.12	4 (1%) 72 64	31, 75, 101, 134	21 (7%)
1	H	271/277 (97%)	-0.20	0 100 100	34, 69, 97, 112	23 (8%)
1	I	272/277 (98%)	-0.29	0 100 100	30, 66, 91, 102	9 (3%)
1	J	270/277 (97%)	-0.28	2 (0%) 84 79	28, 66, 92, 102	14 (5%)
1	K	271/277 (97%)	-0.18	1 (0%) 88 85	30, 73, 100, 110	20 (7%)
1	L	272/277 (98%)	-0.18	3 (1%) 78 71	34, 70, 99, 117	17 (6%)
1	M	272/277 (98%)	-0.07	1 (0%) 88 85	34, 76, 100, 119	19 (6%)
1	N	271/277 (97%)	-0.17	0 100 100	41, 73, 102, 112	15 (5%)
All	All	3793/3878 (97%)	-0.22	21 (0%) 85 81	28, 69, 97, 134	227 (5%)

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	2	GLY	2.9
1	J	3	ARG	2.9
1	B	76	LYS	2.8
1	F	233	GLN	2.8
1	G	79	HIS	2.8
1	E	194	HIS	2.7
1	B	3	ARG	2.6
1	F	3	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	G	198	ASP	2.5
1	E	272	ARG	2.4
1	E	2	GLY	2.3
1	A	194	HIS	2.2
1	F	245	GLU	2.2
1	G	232	PHE	2.2
1	L	232	PHE	2.2
1	G	233	GLN	2.1
1	K	127	THR	2.1
1	L	248	ASN	2.1
1	C	128	TYR	2.1
1	J	2	GLY	2.1
1	M	128	TYR	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.

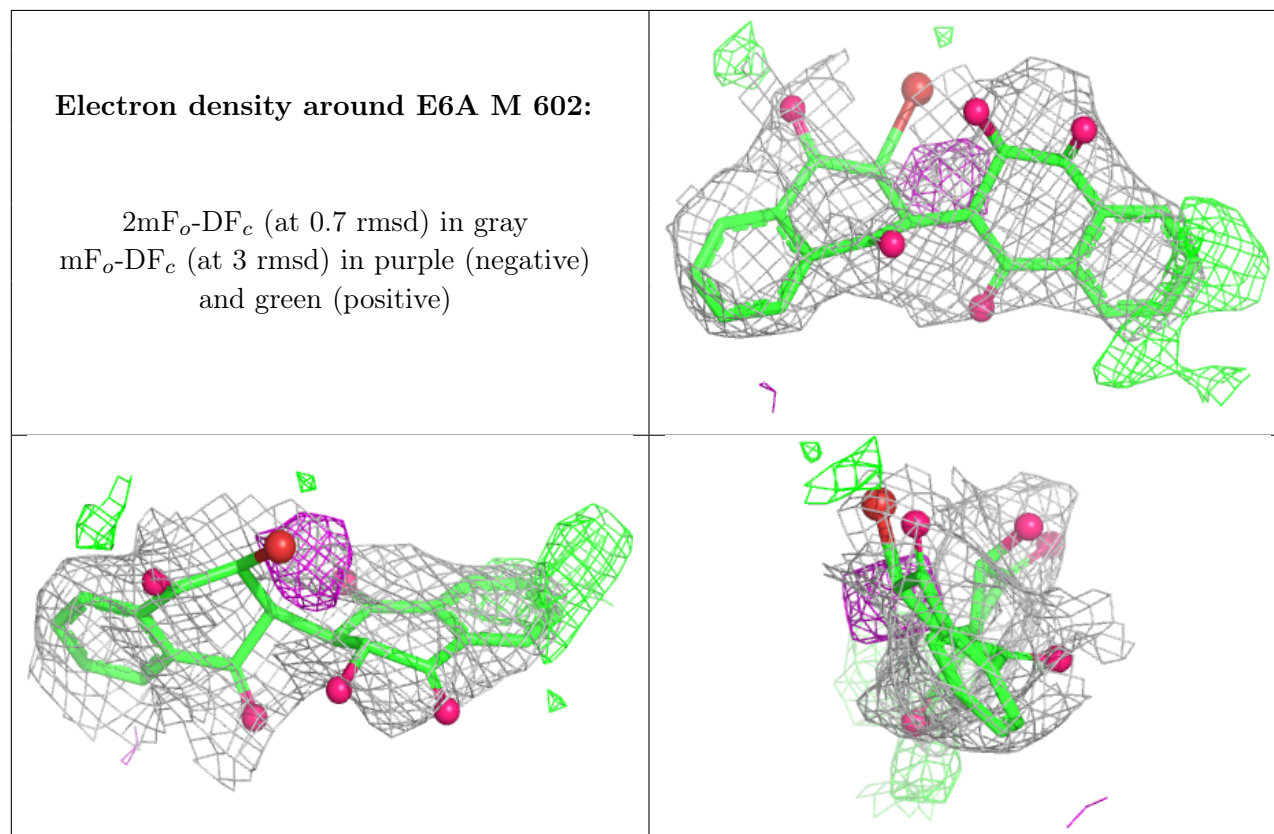
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	E6A	M	602	26/26	0.85	0.17	98,111,115,126	4
3	E6A	B	302	26/26	0.87	0.15	90,98,109,120	4
3	E6A	E	602	26/26	0.90	0.14	74,87,99,106	4
3	E6A	H	302	26/26	0.92	0.12	81,87,97,104	4
2	FAD	B	301	53/53	0.93	0.09	48,75,107,110	0
3	E6A	K	602	26/26	0.94	0.11	81,94,99,108	4
2	FAD	M	601	53/53	0.94	0.08	57,76,102,106	0
2	FAD	H	301	53/53	0.95	0.07	59,69,79,81	0
2	FAD	I	601	53/53	0.95	0.07	56,70,85,86	0
2	FAD	K	601	53/53	0.95	0.07	56,75,89,97	0

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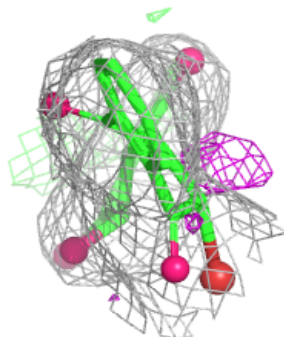
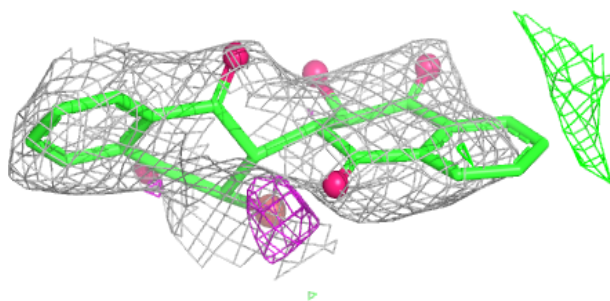
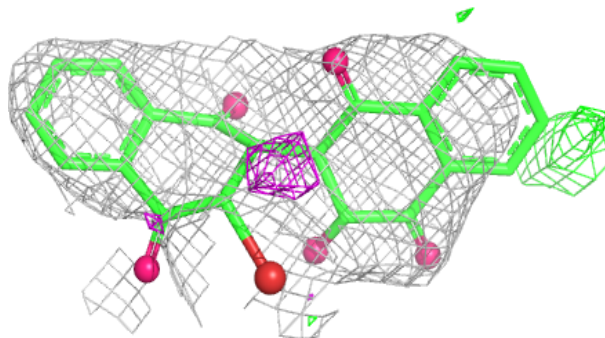
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FAD	G	601	53/53	0.95	0.07	49,67,90,95	0
2	FAD	N	301	53/53	0.95	0.07	61,69,79,80	0
2	FAD	D	301	53/53	0.96	0.07	41,63,103,103	0
2	FAD	E	601	53/53	0.96	0.06	47,62,86,87	0
2	FAD	J	301	53/53	0.96	0.07	52,67,84,90	0
2	FAD	F	301	53/53	0.96	0.07	50,60,88,93	0
2	FAD	L	301	53/53	0.96	0.07	50,69,94,101	0
2	FAD	A	601	53/53	0.96	0.07	56,68,91,92	0
2	FAD	C	601	53/53	0.97	0.07	50,59,84,93	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.

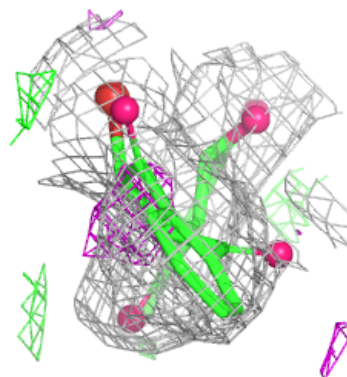
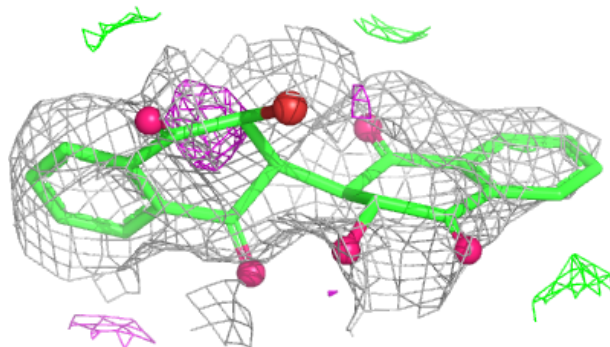
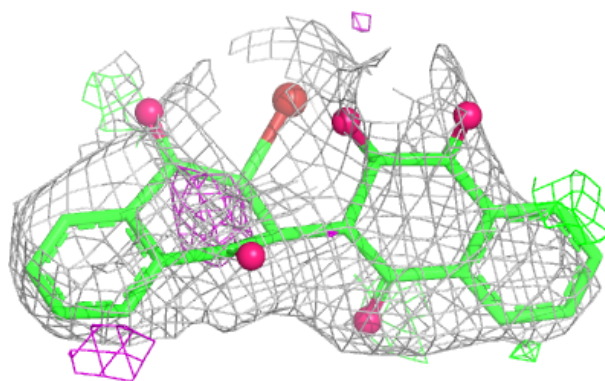


Electron density around E6A B 302:

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

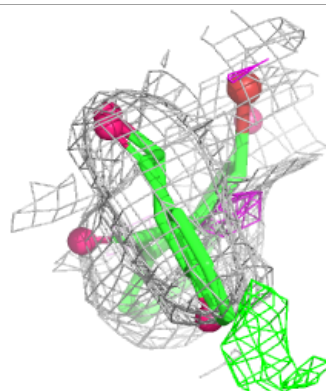
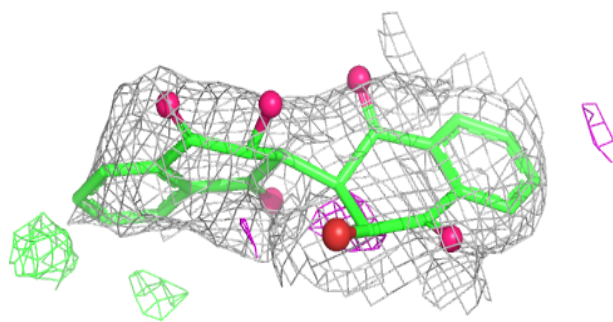
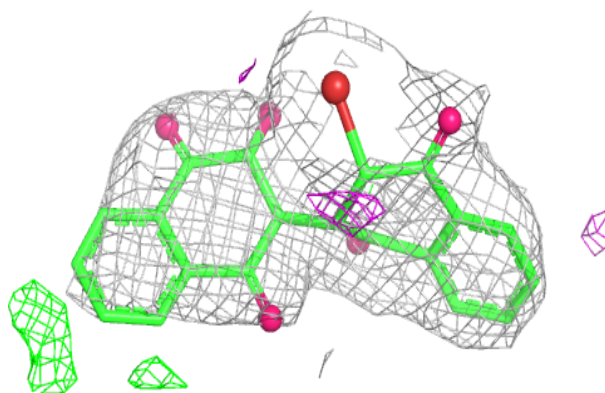
**Electron density around E6A E 602:**

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

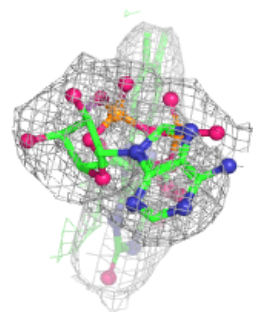
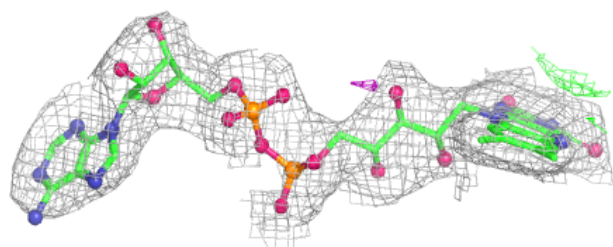
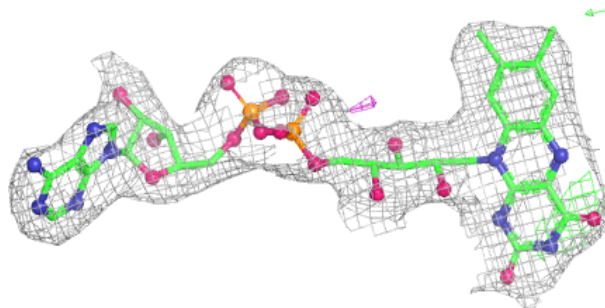


Electron density around E6A H 302:

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

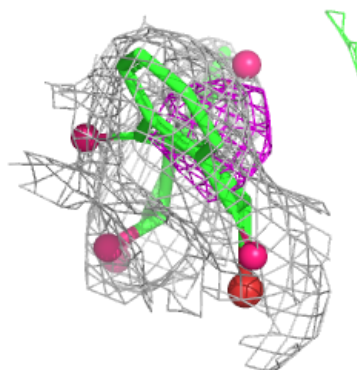
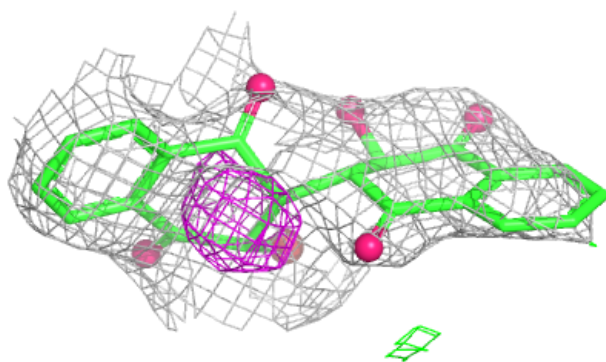
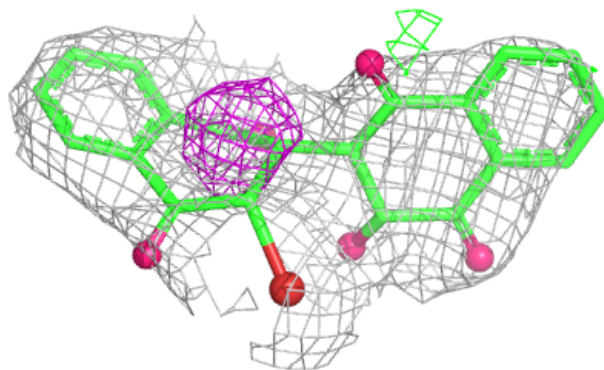
**Electron density around FAD B 301:**

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and green (positive)

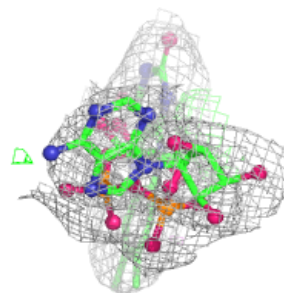
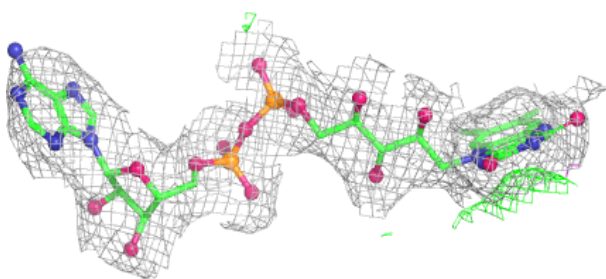
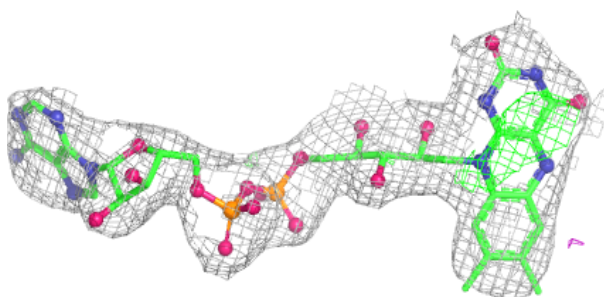


Electron density around E6A K 602:

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

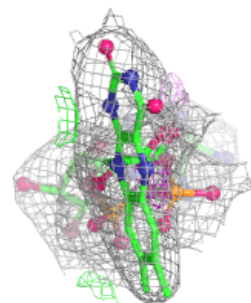
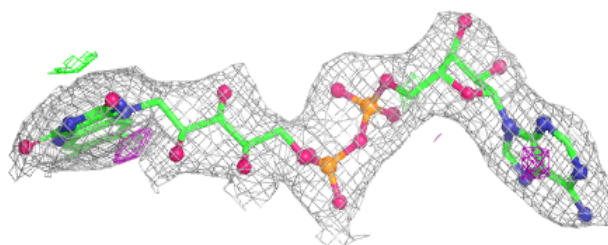
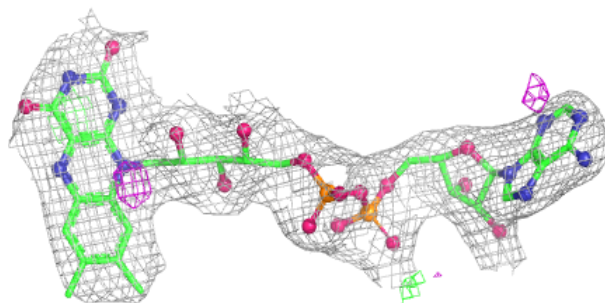
**Electron density around FAD M 601:**

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

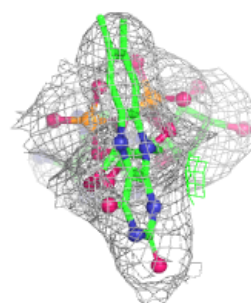
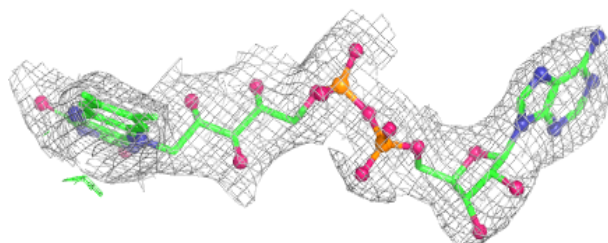
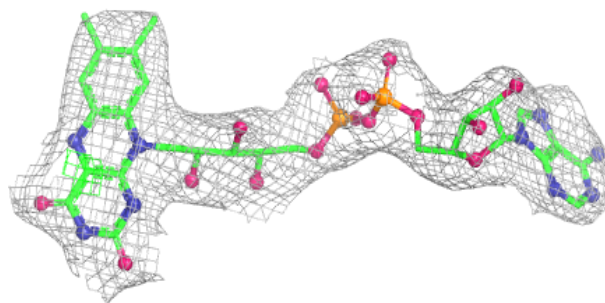


Electron density around FAD H 301:

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

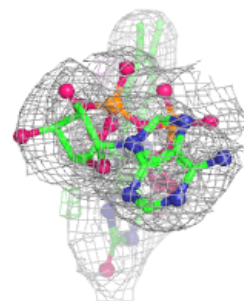
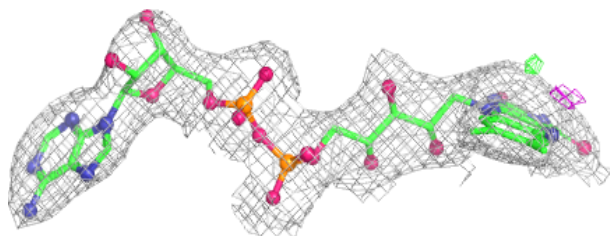
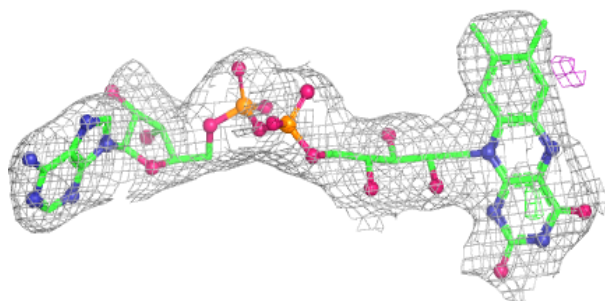
**Electron density around FAD I 601:**

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and green (positive)

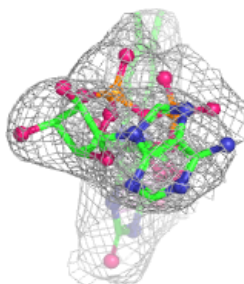
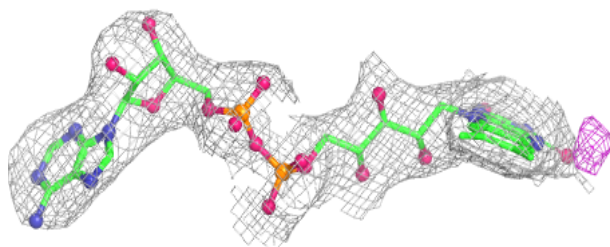
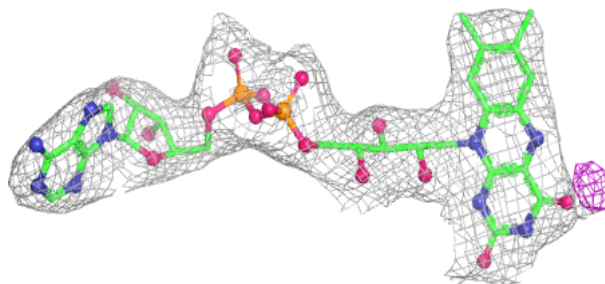


Electron density around FAD K 601:

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

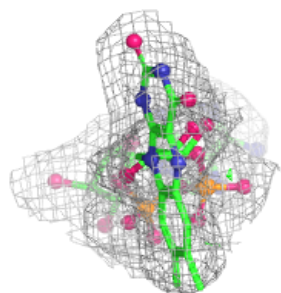
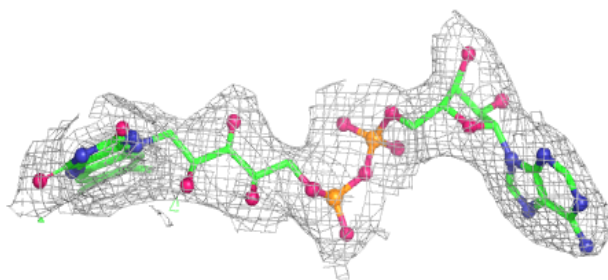
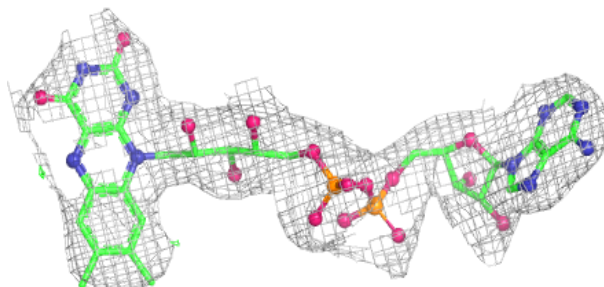
**Electron density around FAD G 601:**

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

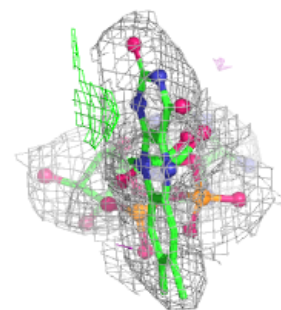
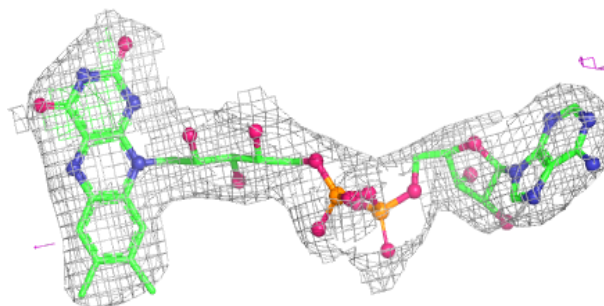


Electron density around FAD N 301:

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

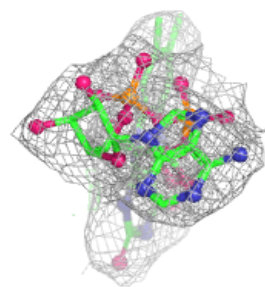
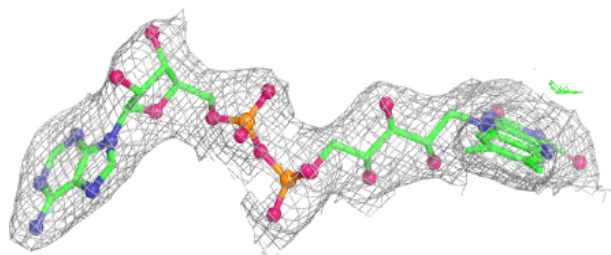
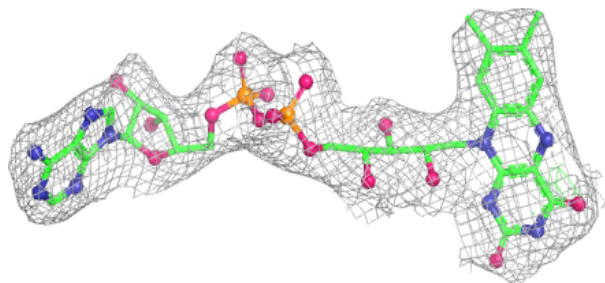
**Electron density around FAD D 301:**

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

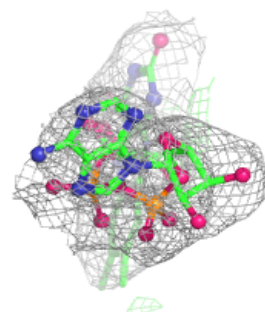
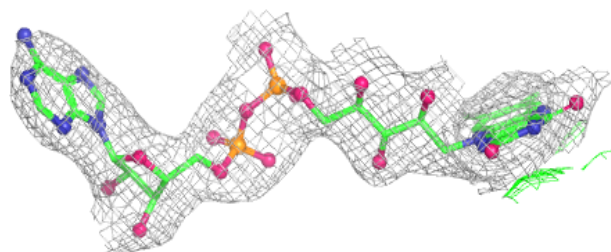
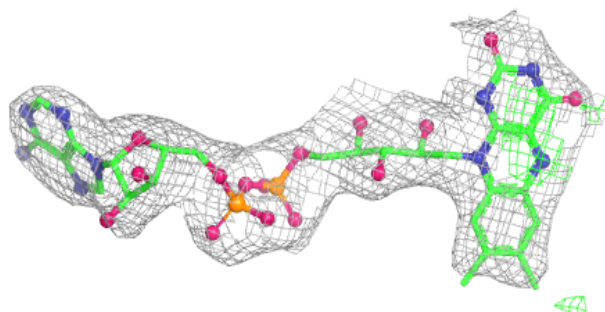


Electron density around FAD E 601:

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

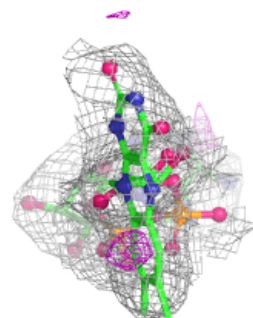
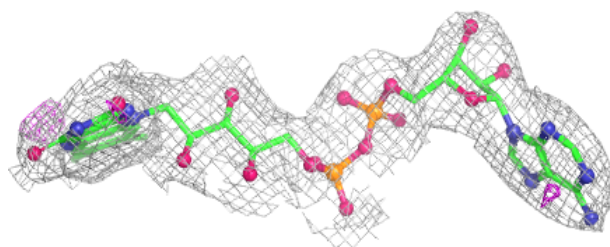
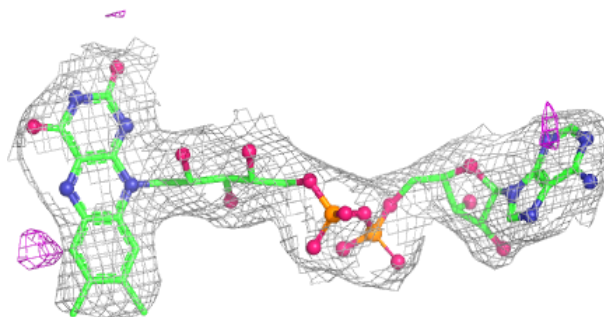
**Electron density around FAD J 301:**

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

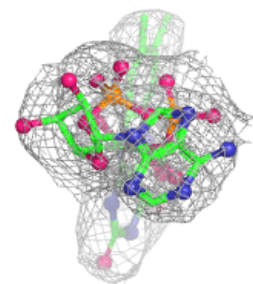
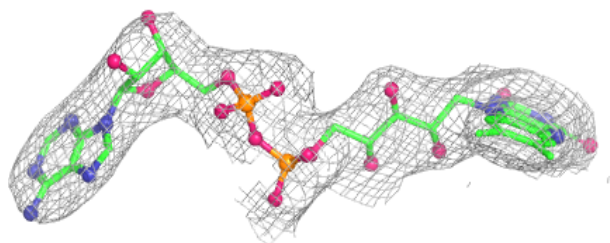
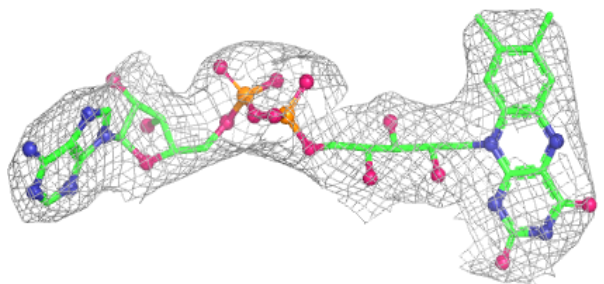


Electron density around FAD F 301:

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

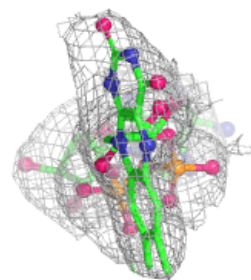
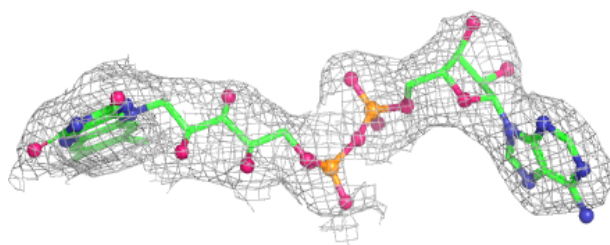
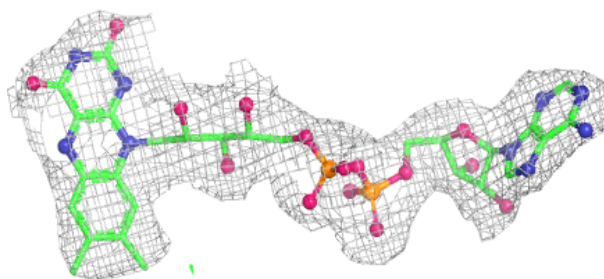
**Electron density around FAD L 301:**

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

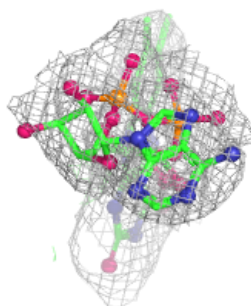
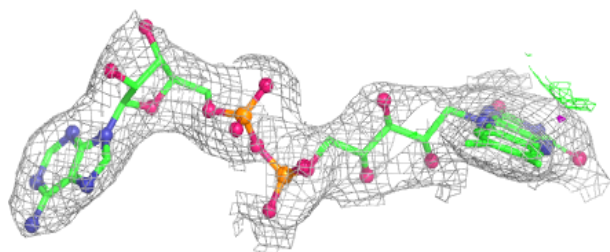
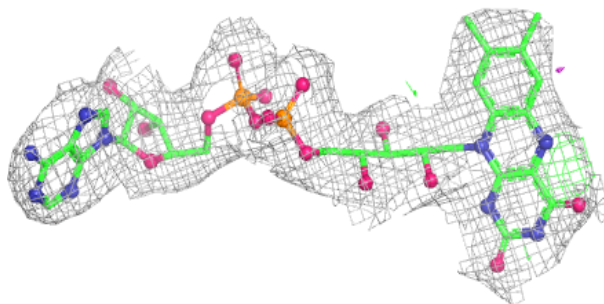


Electron density around FAD A 601:

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

**Electron density around 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.