



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 7, 2026 – 02:45 AM UTC

PDB ID : 3RED / pdb_00003red
Title : 3.0 A structure of the Prunus mume hydroxynitrile lyase isozyme-1
Authors : Cielo, C.B.C.; Yamane, T.; Asano, Y.; Watanabe, N.; Suzuki, A.; Fukuta, Y.
Deposited on : 2011-04-04
Resolution : 3.03 Å (reported)

This is a wwPDB X-ray Structure Validation Summary 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)
Xtrriage (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

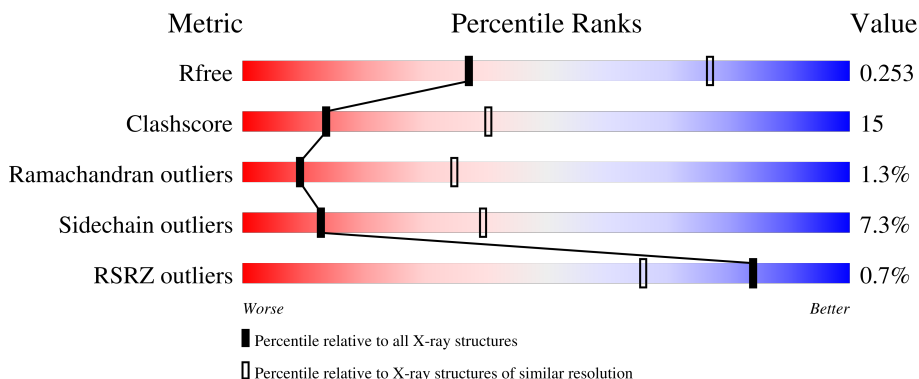
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.03 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	3685 (3.08-3.00)
Clashscore	190562	4007 (3.08-3.00)
Ramachandran outliers	187476	3834 (3.08-3.00)
Sidechain outliers	187428	3836 (3.08-3.00)
RSRZ outliers	180081	3684 (3.08-3.00)

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	521	 68% 29% ..
1	B	521	 69% 26% ..
1	C	521	 74% 22% ..
1	D	521	 64% 30% ..
1	E	521	 71% 25% ..

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Mol	Chain	Length	Quality of chain
1	F	521	 67% 30% ..
1	G	521	 67% 28% ..
1	H	521	 67% 28% 5%
1	I	521	 69% 26% ..
1	J	521	 69% 27% .
1	K	521	 68% 28% ..
1	L	521	 61% 35% ..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 48604 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 Hydroxynitrile lyase.

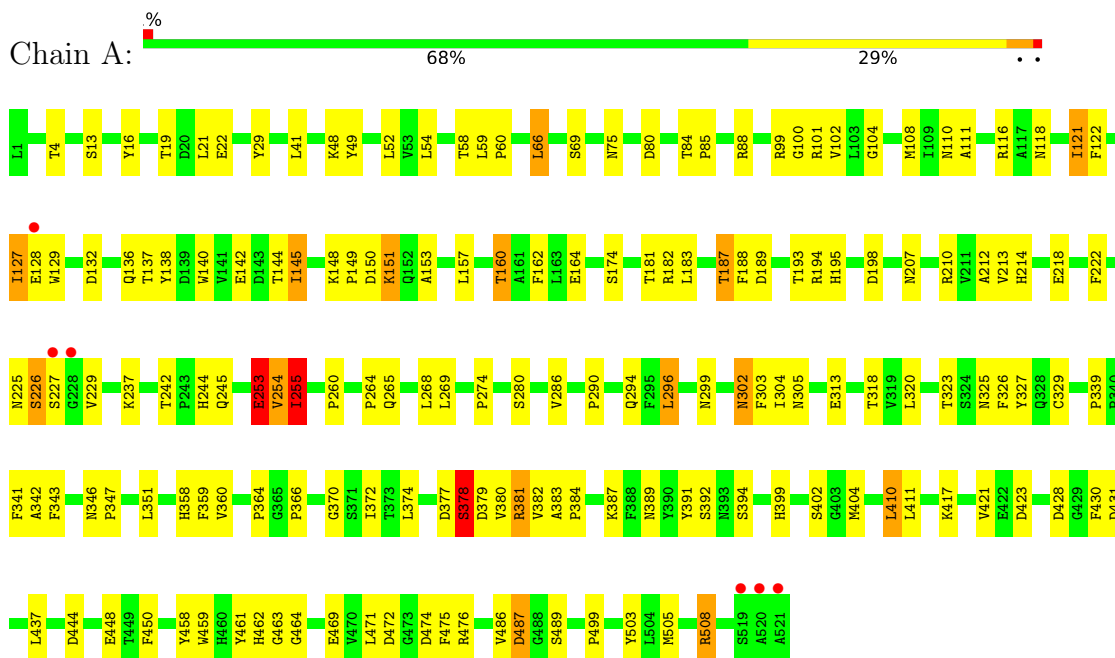
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	521	4001	2547	657	788	9	0	2	0
1	B	521	3999	2547	659	784	9	0	2	0
1	C	521	3993	2543	656	785	9	0	1	0
1	D	521	3993	2543	656	785	9	0	1	0
1	E	521	3993	2543	656	785	9	0	1	0
1	F	521	4001	2548	659	785	9	0	2	0
1	G	521	4001	2548	659	785	9	0	2	0
1	H	521	4001	2548	659	785	9	0	2	0
1	I	521	3993	2543	656	785	9	0	1	0
1	J	521	3991	2543	656	783	9	0	1	0
1	K	521	4001	2548	659	785	9	0	2	0
1	L	521	4001	2548	659	785	9	0	2	0

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

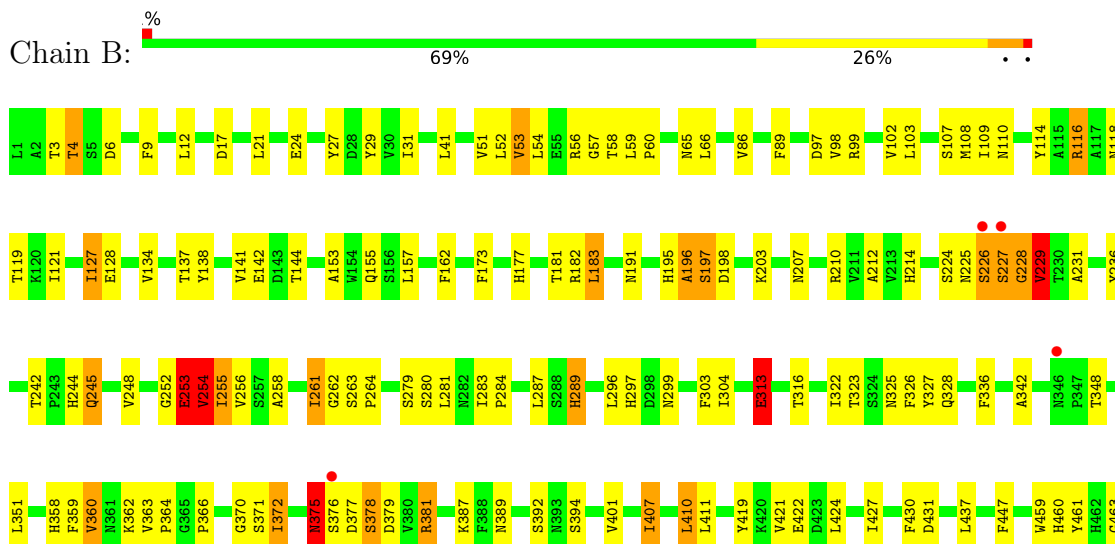
3 Residue-property plots [i](#)

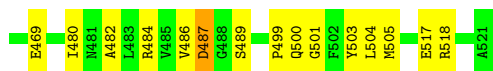
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Hydroxynitrile lyase

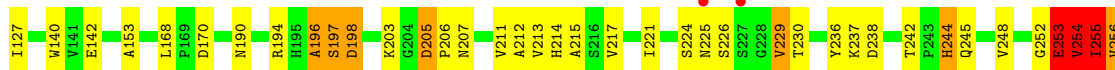
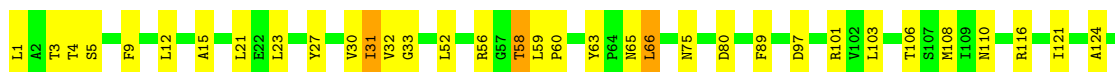
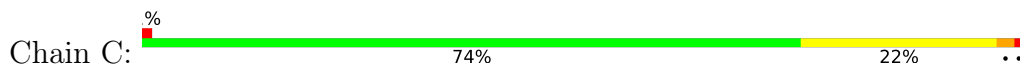


- Molecule 1: Hydroxynitrile lyase

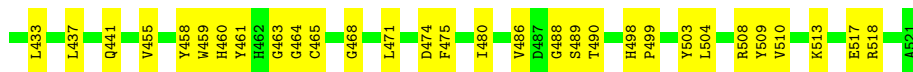
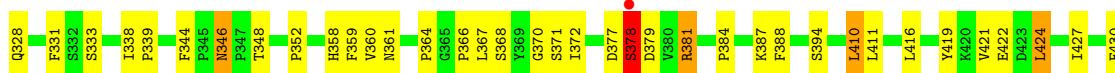




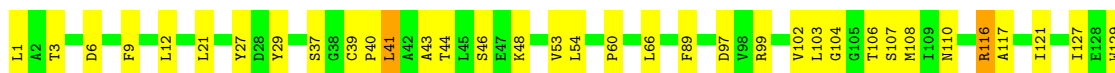
- Molecule 1: Hydroxynitrile lyase

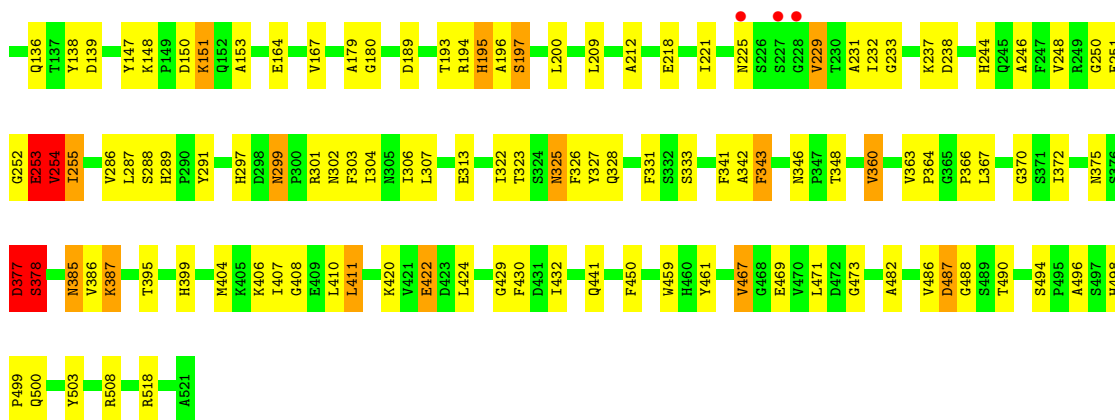


- Molecule 1: Hydroxynitrile lyase

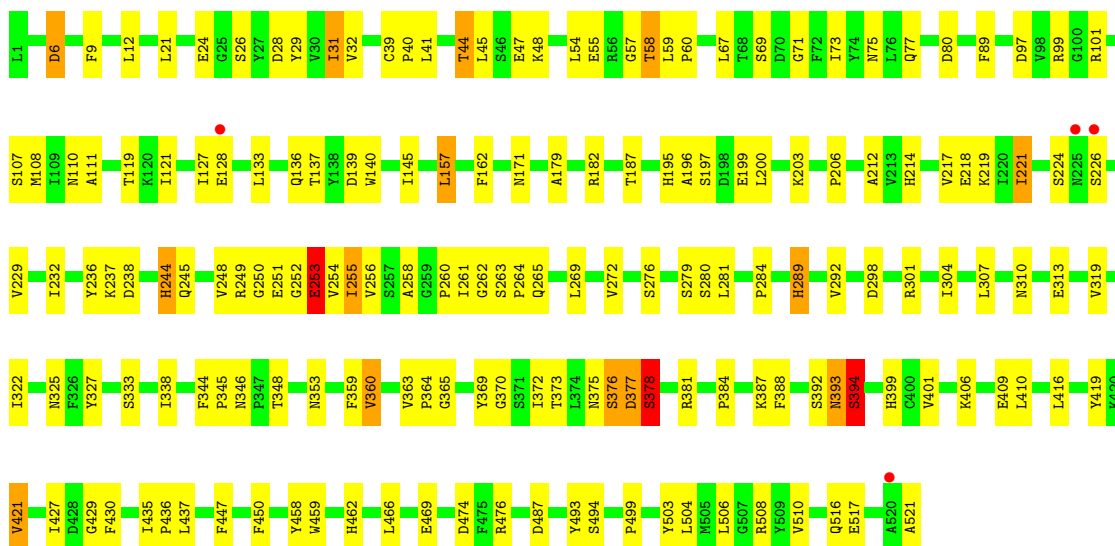


- Molecule 1: Hydroxynitrile lyase

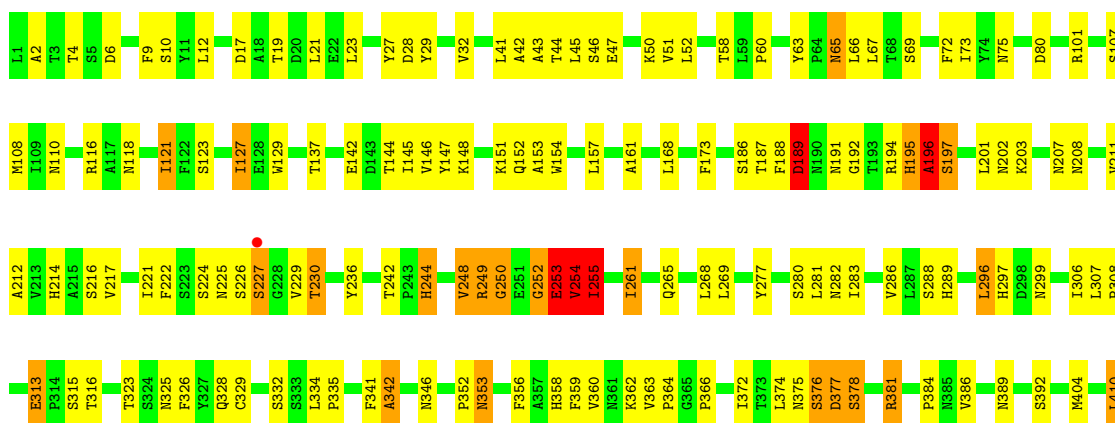




● Molecule 1: Hydroxynitrile lyase

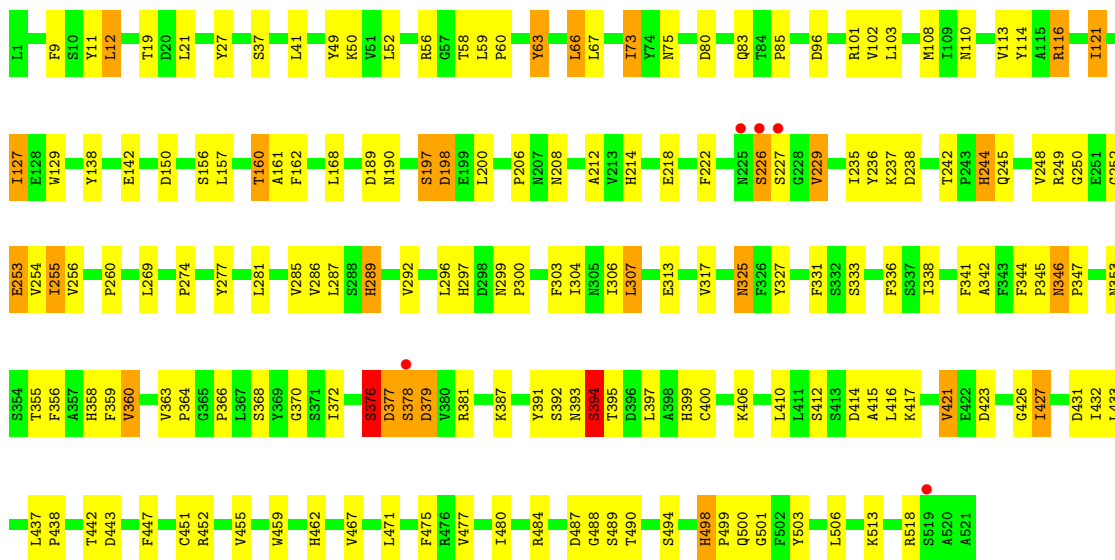


● Molecule 1: Hydroxynitrile lyase

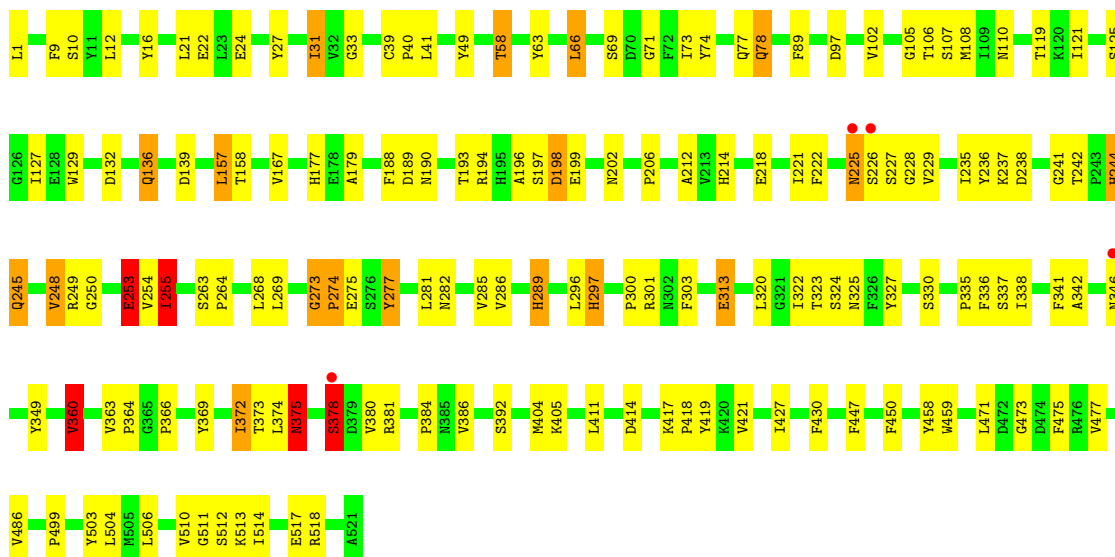




- Molecule 1: Hydroxynitrile lyase



- Molecule 1: Hydroxynitrile lyase



- Molecule 1: Hydroxynitrile lyase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	112.02Å 113.30Å 169.49Å 89.92° 79.13° 80.83°	Depositor
Resolution (Å)	10.97 – 3.03 10.97 – 3.03	Depositor EDS
% Data completeness (in resolution range)	96.0 (10.97-3.03) 94.1 (10.97-3.03)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.47 (at 3.01Å)	Xtrriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.191 , 0.253 0.195 , 0.253	Depositor DCC
R_{free} test set	7404 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å ²)	37.2	Xtrriage
Anisotropy	0.040	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 39.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	48604	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.46% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.91	13/4106 (0.3%)	1.07	16/5606 (0.3%)
1	B	0.88	9/4107 (0.2%)	1.10	20/5606 (0.4%)
1	C	0.87	6/4098 (0.1%)	1.08	19/5595 (0.3%)
1	D	1.01	16/4098 (0.4%)	1.15	26/5595 (0.5%)
1	E	0.90	12/4098 (0.3%)	1.09	24/5595 (0.4%)
1	F	0.91	7/4109 (0.2%)	1.10	19/5609 (0.3%)
1	G	0.95	13/4109 (0.3%)	1.10	20/5609 (0.4%)
1	H	0.94	13/4109 (0.3%)	1.11	24/5609 (0.4%)
1	I	0.91	10/4098 (0.2%)	1.08	18/5595 (0.3%)
1	J	0.89	8/4096 (0.2%)	1.06	17/5593 (0.3%)
1	K	0.93	11/4109 (0.3%)	1.07	12/5609 (0.2%)
1	L	0.95	12/4109 (0.3%)	1.07	21/5609 (0.4%)
All	All	0.92	130/49246 (0.3%)	1.09	236/67230 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	2
1	C	0	2
1	D	0	3
1	E	0	1
1	F	0	2
1	G	0	2
1	I	0	2
All	All	0	14

The worst 5 of 130 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	195	HIS	CA-C	-11.57	1.38	1.52
1	L	380	VAL	N-CA	-7.35	1.38	1.46
1	H	255	ILE	C-O	-7.21	1.16	1.24
1	L	254	VAL	CA-CB	-7.07	1.45	1.54
1	G	195	HIS	C-O	-6.98	1.15	1.23

The worst 5 of 236 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	195	HIS	N-CA-C	-13.90	86.24	108.90
1	L	255	ILE	N-CA-C	-8.82	95.32	108.46
1	L	254	VAL	N-CA-C	-8.76	95.56	108.87
1	J	307	LEU	CA-C-N	8.37	125.77	119.66
1	J	307	LEU	C-N-CA	8.37	125.77	119.66

There are no chirality outliers.

5 of 14 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	253	GLU	Peptide,Mainchain
1	C	253	GLU	Peptide
1	C	254	VAL	Peptide
1	D	194	ARG	Mainchain
1	D	253	GLU	Mainchain

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	4001	0	3847	104	0
1	B	3999	0	3853	112	0
1	C	3993	0	3844	90	0
1	D	3993	0	3844	137	0
1	E	3993	0	3844	95	0
1	F	4001	0	3857	114	0
1	G	4001	0	3857	124	0
1	H	4001	0	3857	123	0
1	I	3993	0	3844	120	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	J	3991	0	3838	115	0
1	K	4001	0	3857	110	0
1	L	4001	0	3857	146	0
2	A	53	0	31	5	0
2	B	53	0	31	4	0
2	C	53	0	31	6	0
2	D	53	0	31	12	0
2	E	53	0	31	6	0
2	F	53	0	31	5	0
2	G	53	0	31	4	0
2	H	53	0	31	7	0
2	I	53	0	31	5	0
2	J	53	0	31	7	0
2	K	53	0	31	6	0
2	L	53	0	31	5	0
All	All	48604	0	46571	1381	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 15.

The worst 5 of 1381 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:C:252:GLY:O	1:C:253:GLU:HG2	1.25	1.28
1:K:58:THR:HG22	1:K:214:HIS:CE1	1.70	1.26
1:B:375:ASN:N	1:B:376:SER:HB2	1.56	1.21
1:F:80:ASP:OD1	1:F:101:ARG:NH2	1.75	1.20
1:L:377:ASP:HB3	1:L:378:SER:O	1.42	1.19

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	521/521 (100%)	485 (93%)	31 (6%)	5 (1%)	12	41
1	B	521/521 (100%)	474 (91%)	36 (7%)	11 (2%)	5	24
1	C	520/521 (100%)	476 (92%)	39 (8%)	5 (1%)	12	41
1	D	520/521 (100%)	470 (90%)	42 (8%)	8 (2%)	8	32
1	E	520/521 (100%)	482 (93%)	34 (6%)	4 (1%)	16	46
1	F	521/521 (100%)	476 (91%)	37 (7%)	8 (2%)	8	32
1	G	521/521 (100%)	479 (92%)	32 (6%)	10 (2%)	6	27
1	H	521/521 (100%)	485 (93%)	30 (6%)	6 (1%)	10	37
1	I	520/521 (100%)	481 (92%)	33 (6%)	6 (1%)	10	37
1	J	520/521 (100%)	480 (92%)	35 (7%)	5 (1%)	12	41
1	K	521/521 (100%)	466 (89%)	45 (9%)	10 (2%)	6	27
1	L	521/521 (100%)	476 (91%)	38 (7%)	7 (1%)	9	35
All	All	6247/6252 (100%)	5730 (92%)	432 (7%)	85 (1%)	9	33

5 of 85 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	197	SER
1	B	228	GLY
1	B	229	VAL
1	B	280	SER
1	B	378	SER

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	442/440 (100%)	412 (93%)	30 (7%)	14	42
1	B	441/440 (100%)	410 (93%)	31 (7%)	14	41
1	C	441/440 (100%)	413 (94%)	28 (6%)	16	45
1	D	441/440 (100%)	405 (92%)	36 (8%)	10	35

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	441/440 (100%)	411 (93%)	30 (7%)	14	42
1	F	442/440 (100%)	408 (92%)	34 (8%)	12	37
1	G	442/440 (100%)	406 (92%)	36 (8%)	11	35
1	H	442/440 (100%)	407 (92%)	35 (8%)	11	36
1	I	441/440 (100%)	413 (94%)	28 (6%)	16	45
1	J	439/440 (100%)	414 (94%)	25 (6%)	18	49
1	K	442/440 (100%)	409 (92%)	33 (8%)	12	38
1	L	442/440 (100%)	400 (90%)	42 (10%)	8	29
All	All	5296/5280 (100%)	4908 (93%)	388 (7%)	13	39

5 of 388 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	157	LEU
1	I	512	SER
1	H	235	ILE
1	I	31	ILE
1	J	253	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 52 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	393	ASN
1	I	385	ASN
1	L	361	ASN
1	H	65	ASN
1	H	302	ASN

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](#)

12 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	I	773	-	58,58,58	1.14	6 (10%)	85,89,89	1.73	16 (18%)
2	FAD	E	773	-	58,58,58	1.28	6 (10%)	85,89,89	1.62	22 (25%)
2	FAD	D	773	-	58,58,58	1.15	7 (12%)	85,89,89	1.69	16 (18%)
2	FAD	C	773	-	58,58,58	1.16	5 (8%)	85,89,89	1.67	19 (22%)
2	FAD	J	773	-	58,58,58	1.14	7 (12%)	85,89,89	1.70	20 (23%)
2	FAD	L	773	-	58,58,58	1.23	8 (13%)	85,89,89	1.74	18 (21%)
2	FAD	H	773	-	58,58,58	1.19	5 (8%)	85,89,89	1.71	17 (20%)
2	FAD	G	773	-	58,58,58	1.19	7 (12%)	85,89,89	1.69	20 (23%)
2	FAD	K	773	-	58,58,58	1.07	5 (8%)	85,89,89	1.63	15 (17%)
2	FAD	A	773	-	58,58,58	1.27	7 (12%)	85,89,89	1.54	19 (22%)
2	FAD	F	773	-	58,58,58	1.17	6 (10%)	85,89,89	1.69	16 (18%)
2	FAD	B	773	-	58,58,58	1.25	8 (13%)	85,89,89	1.57	17 (20%)

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	I	773	-	-	3/34/50/50	0/6/6/6
2	FAD	E	773	-	-	6/34/50/50	0/6/6/6
2	FAD	D	773	-	-	3/34/50/50	0/6/6/6
2	FAD	C	773	-	-	8/34/50/50	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	J	773	-	-	3/34/50/50	0/6/6/6
2	FAD	L	773	-	-	5/34/50/50	0/6/6/6
2	FAD	H	773	-	-	5/34/50/50	0/6/6/6
2	FAD	G	773	-	-	9/34/50/50	0/6/6/6
2	FAD	K	773	-	-	9/34/50/50	0/6/6/6
2	FAD	A	773	-	-	12/34/50/50	0/6/6/6
2	FAD	F	773	-	-	5/34/50/50	0/6/6/6
2	FAD	B	773	-	-	10/34/50/50	0/6/6/6

The worst 5 of 77 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	773	FAD	C4X-N5	4.65	1.40	1.30
2	A	773	FAD	C4X-N5	4.13	1.39	1.30
2	C	773	FAD	C4X-N5	3.80	1.39	1.30
2	B	773	FAD	PA-O3P	3.71	1.63	1.59
2	A	773	FAD	PA-O3P	3.70	1.63	1.59

The worst 5 of 215 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	773	FAD	N3A-C2A-N1A	-6.23	119.15	128.58
2	F	773	FAD	N3A-C2A-N1A	-6.03	119.46	128.58
2	I	773	FAD	C5A-C4A-N3A	-5.78	118.75	126.72
2	J	773	FAD	N3A-C2A-N1A	-5.75	119.87	128.58
2	D	773	FAD	N3A-C2A-N1A	-5.68	119.98	128.58

There are no chirality outliers.

5 of 78 torsion outliers are listed below:

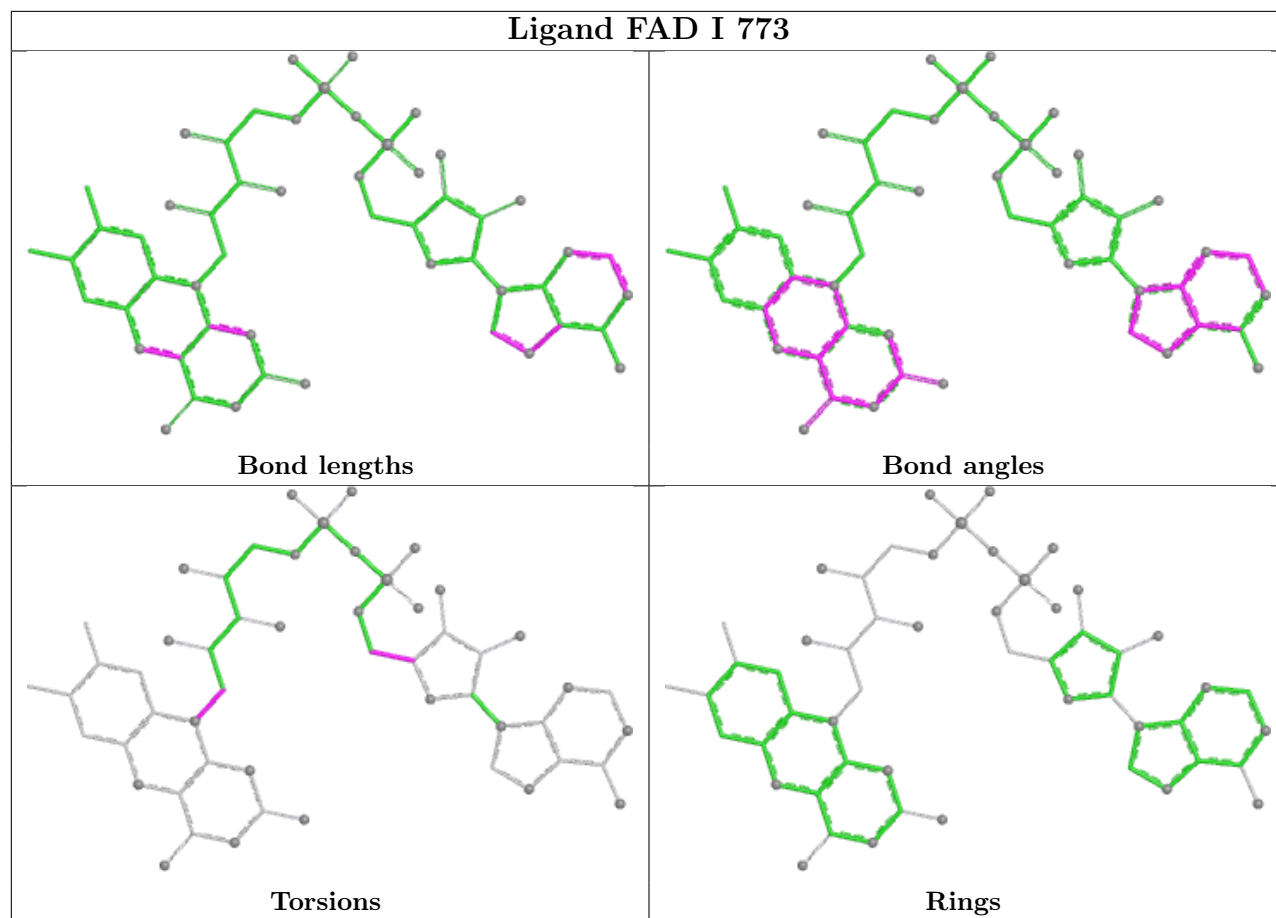
Mol	Chain	Res	Type	Atoms
2	A	773	FAD	N10-C1'-C2'-O2'
2	A	773	FAD	C3'-C4'-C5'-O5'
2	A	773	FAD	O4'-C4'-C5'-O5'
2	A	773	FAD	PA-O3P-P-O5'
2	B	773	FAD	N10-C1'-C2'-O2'

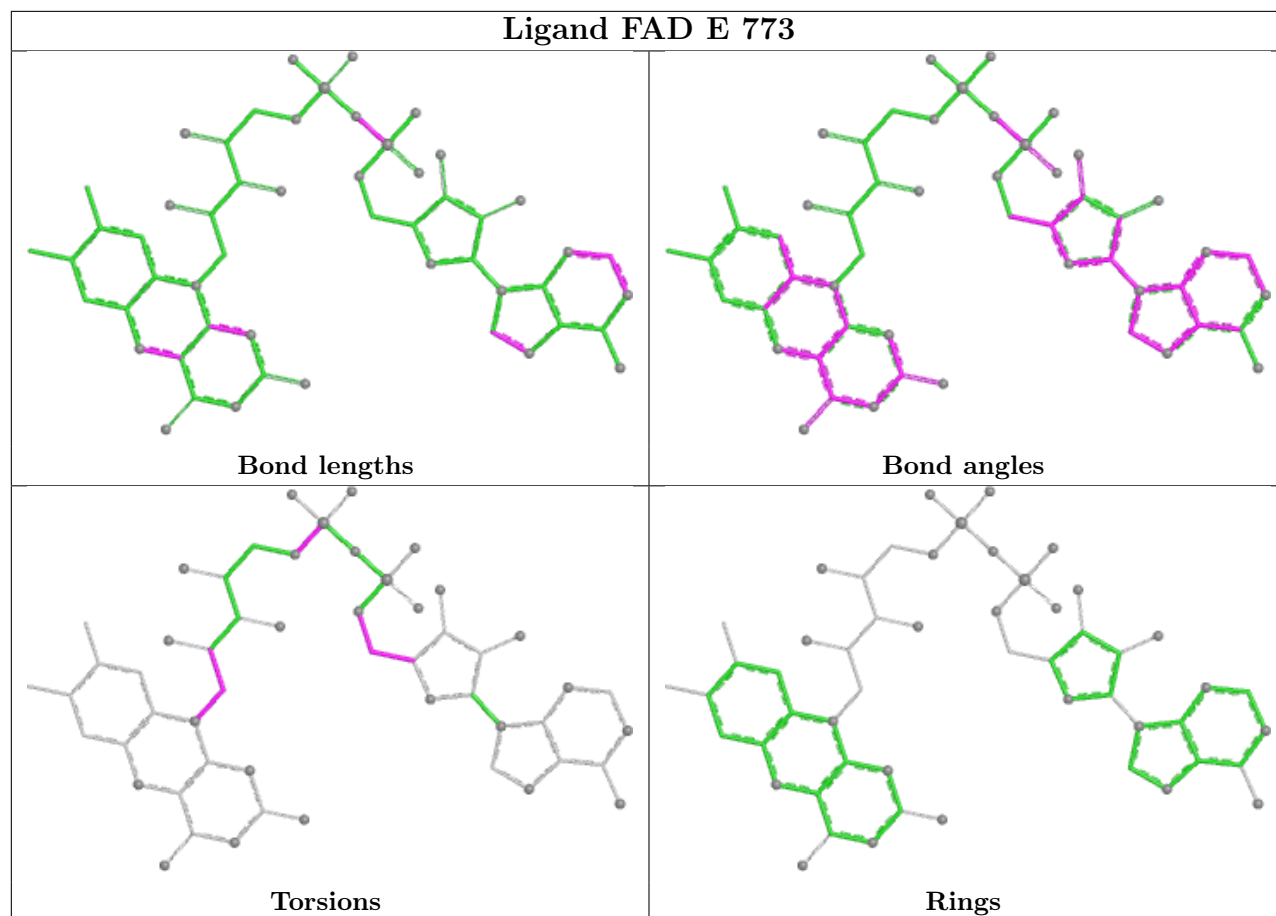
There are no ring outliers.

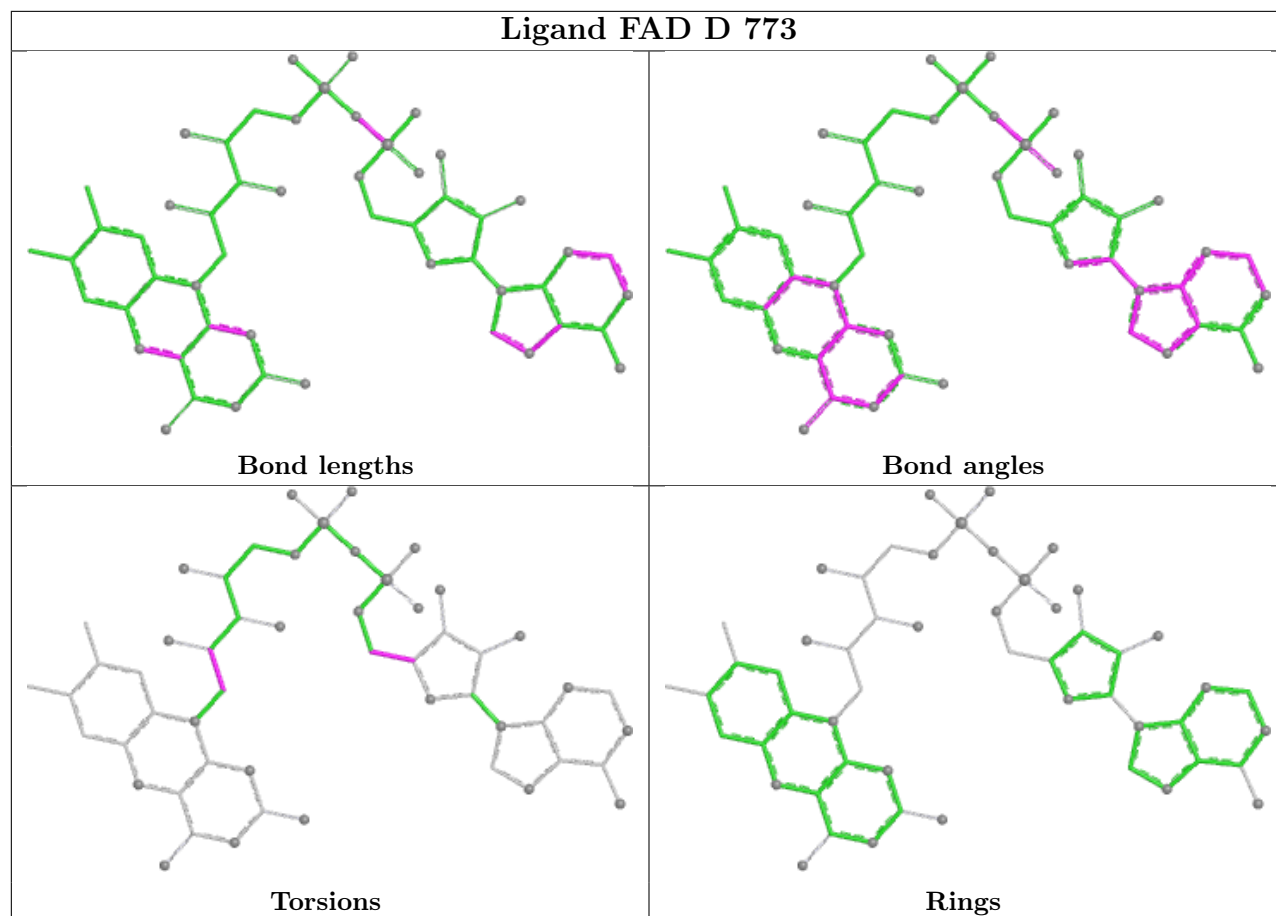
12 monomers are involved in 72 short contacts:

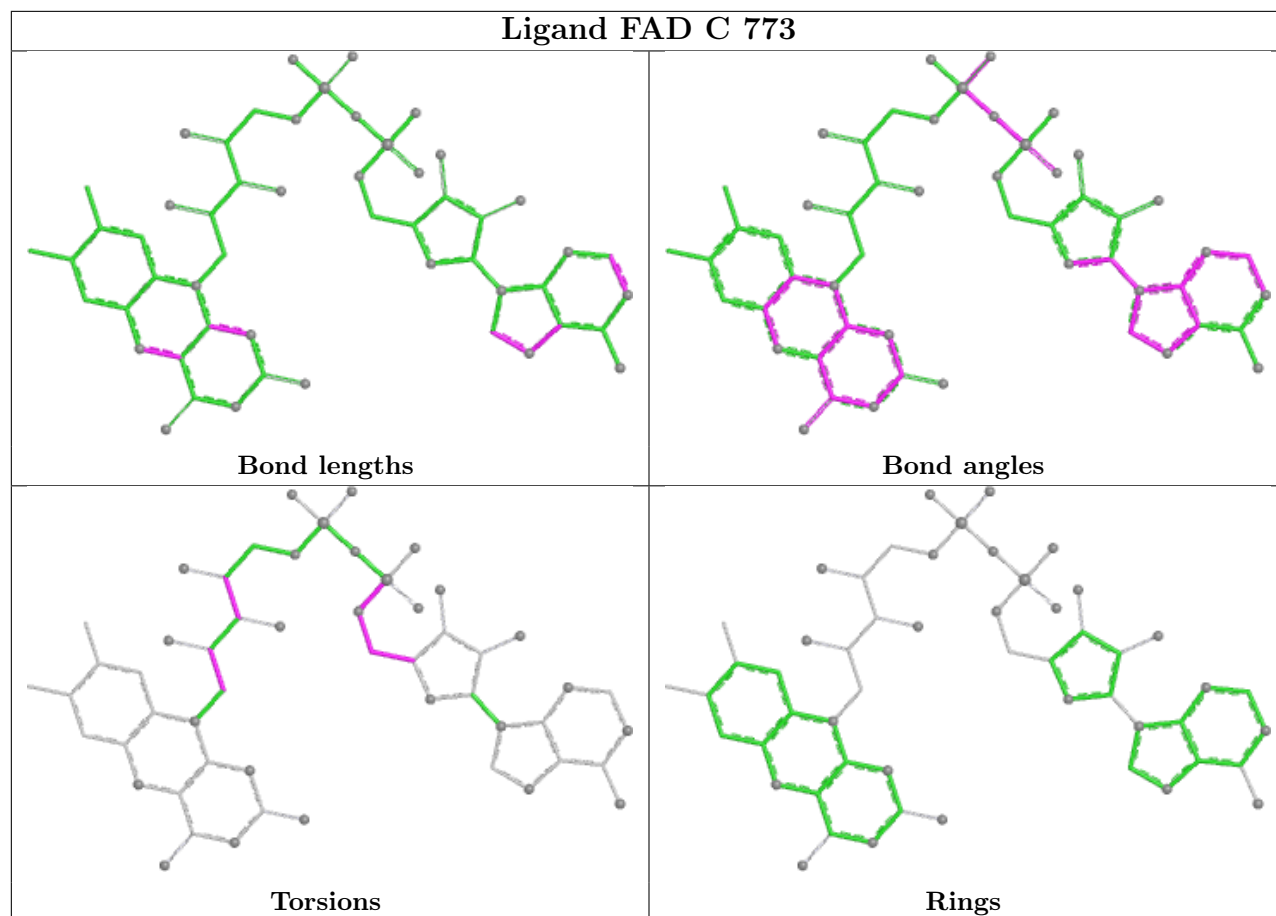
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	773	FAD	5	0
2	E	773	FAD	6	0
2	D	773	FAD	12	0
2	C	773	FAD	6	0
2	J	773	FAD	7	0
2	L	773	FAD	5	0
2	H	773	FAD	7	0
2	G	773	FAD	4	0
2	K	773	FAD	6	0
2	A	773	FAD	5	0
2	F	773	FAD	5	0
2	B	773	FAD	4	0

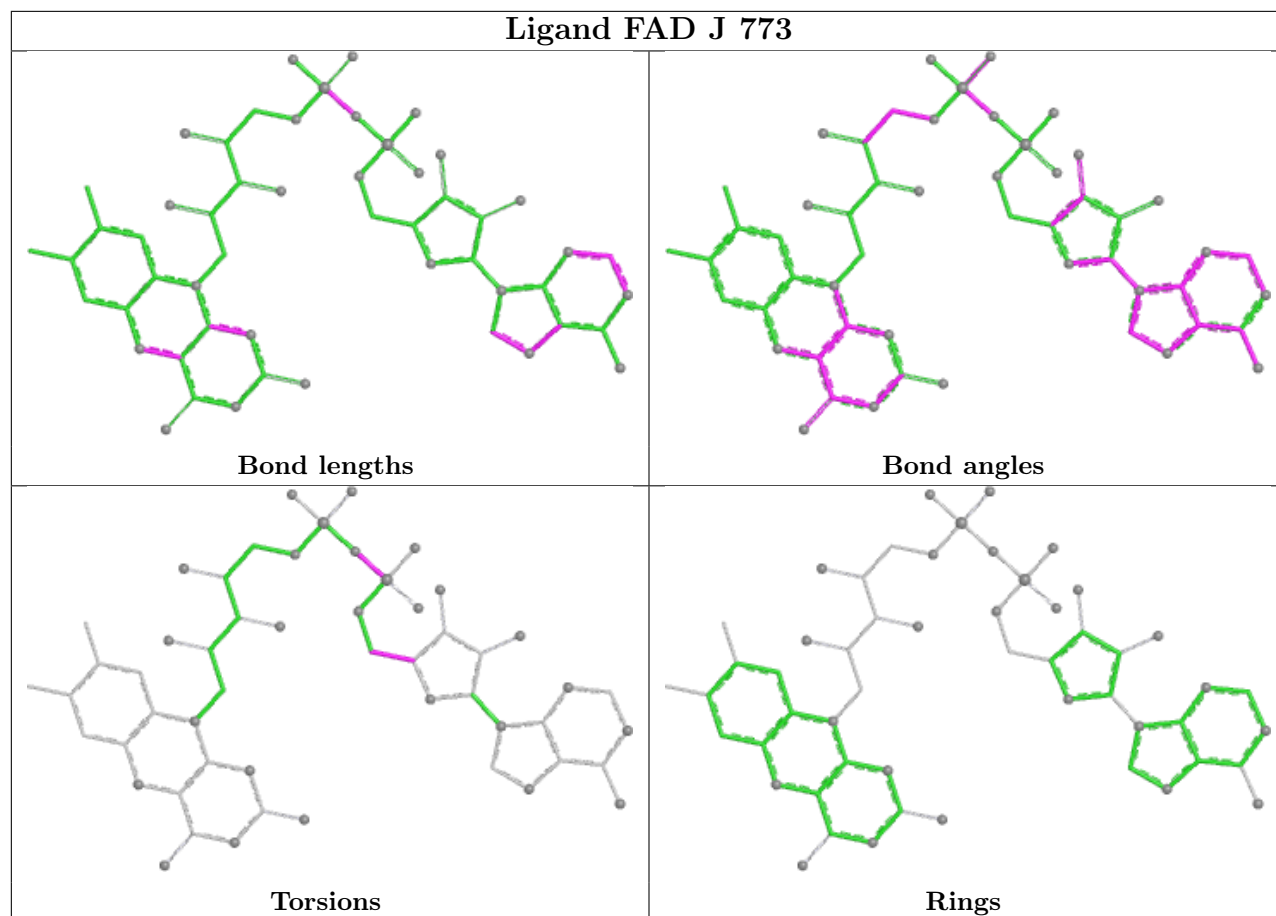
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

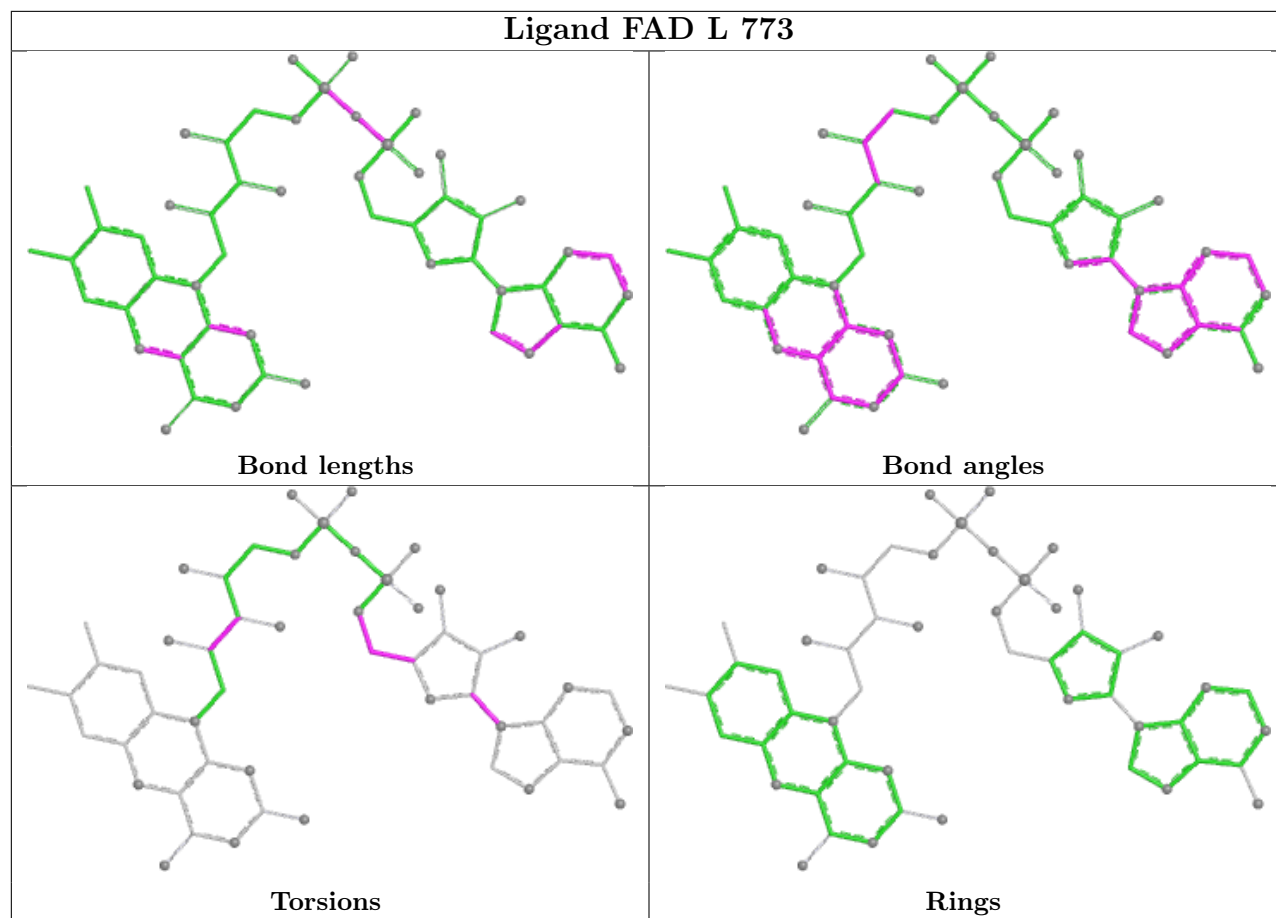


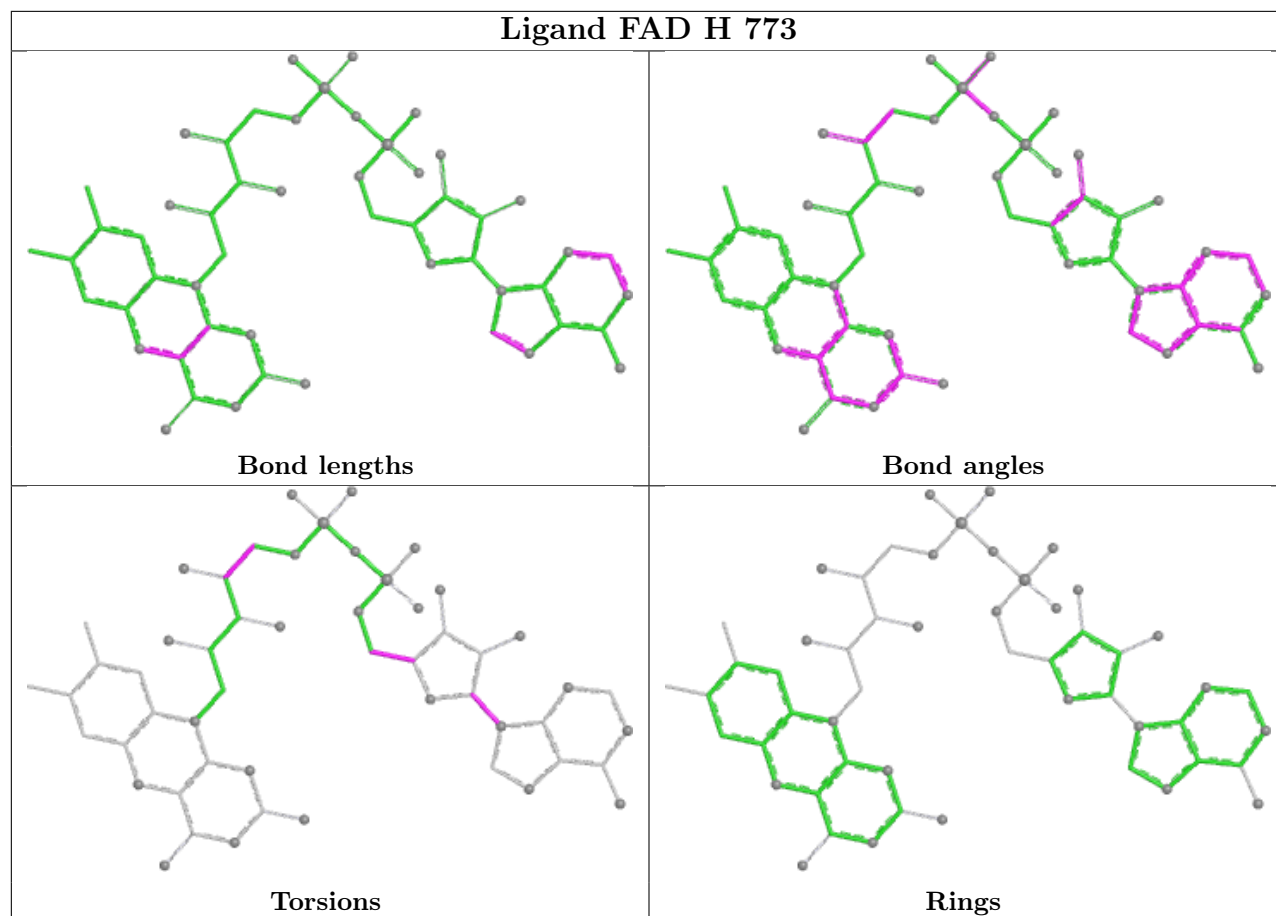


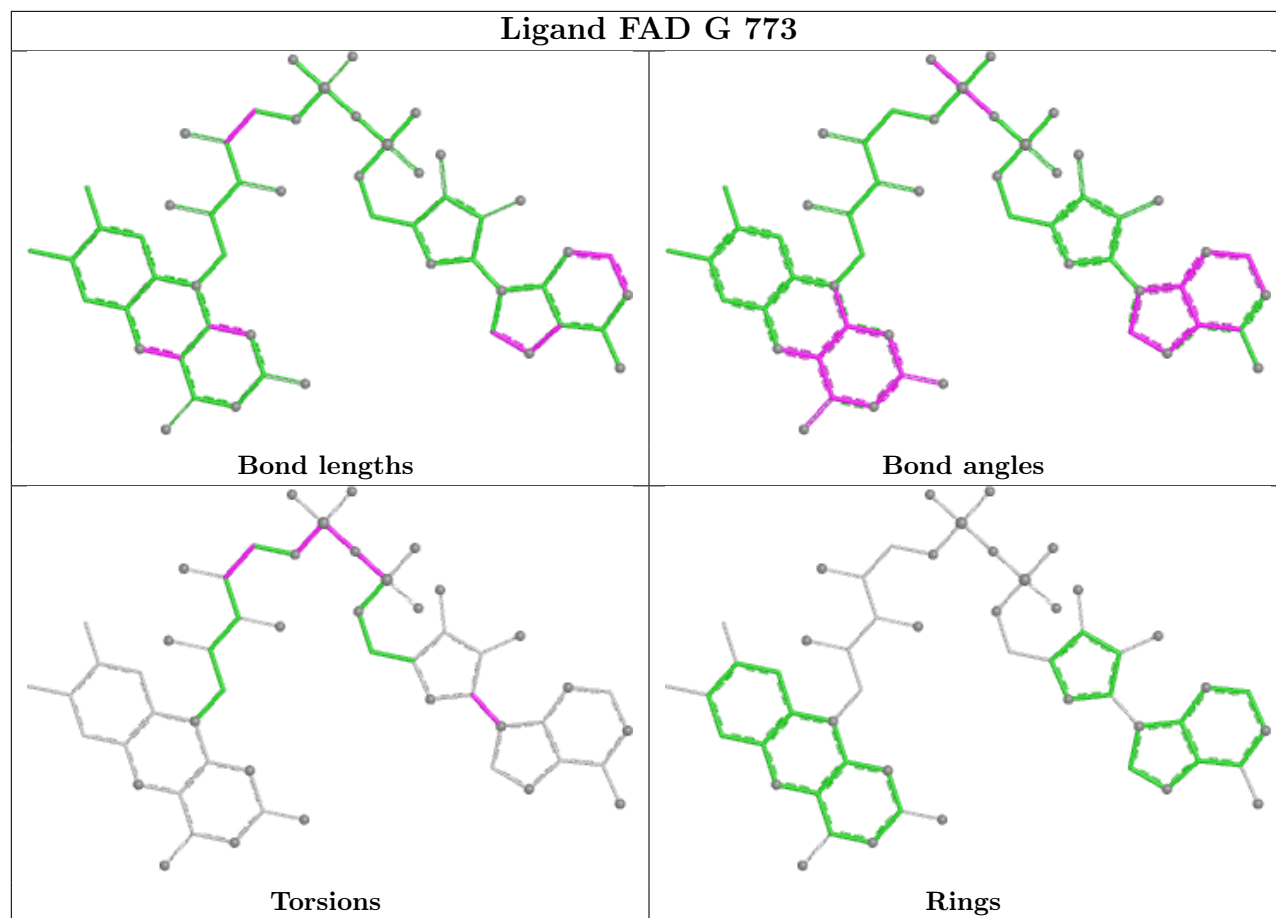


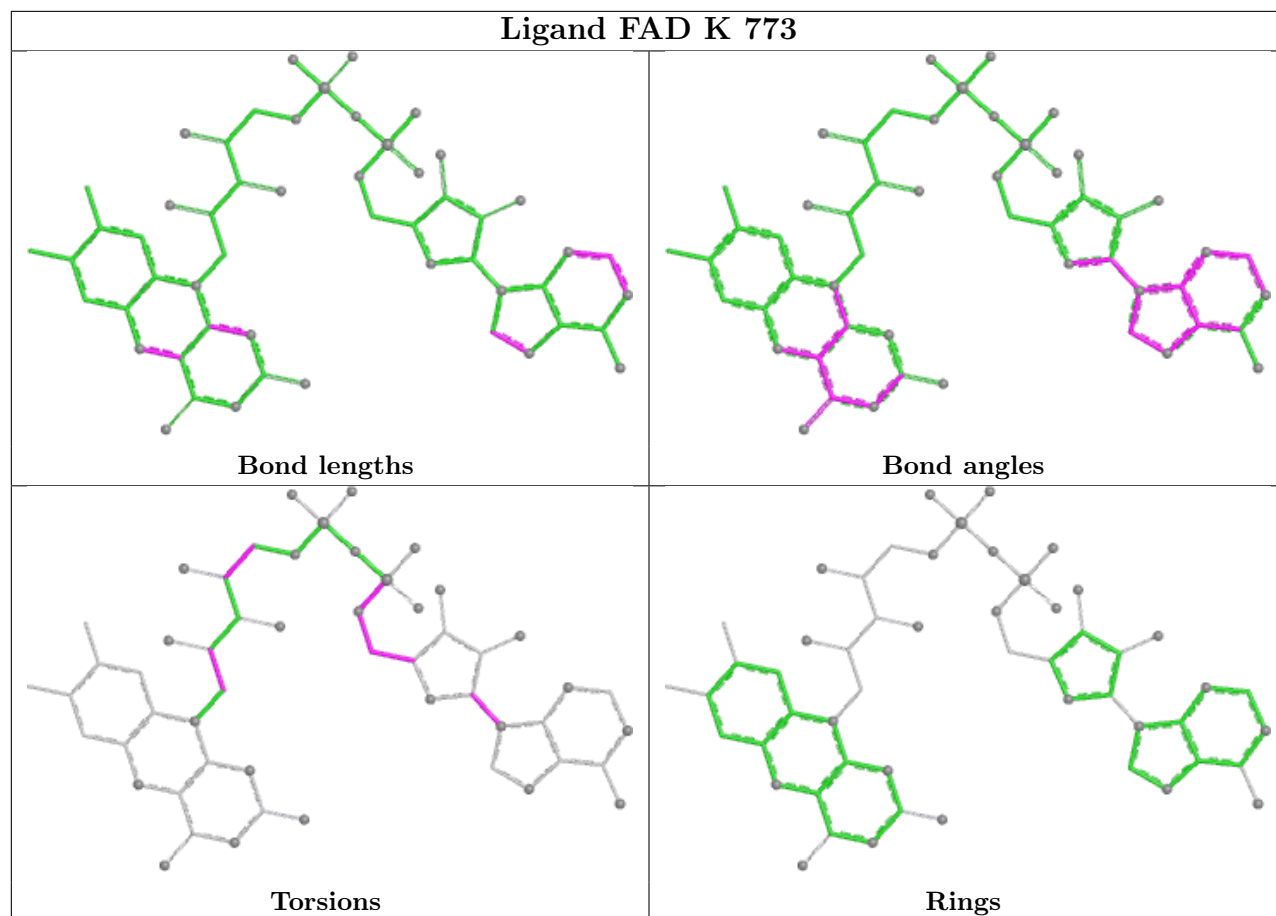


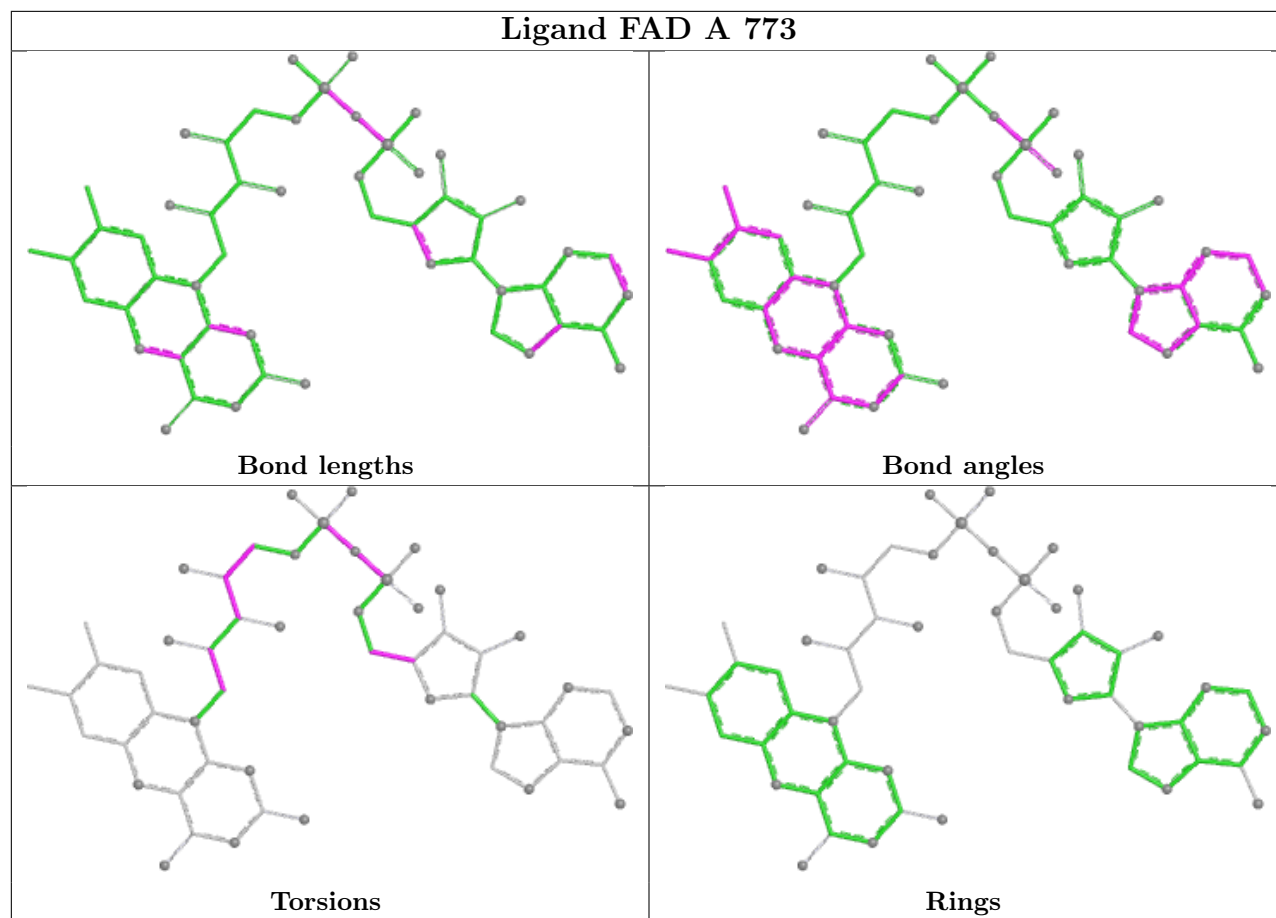


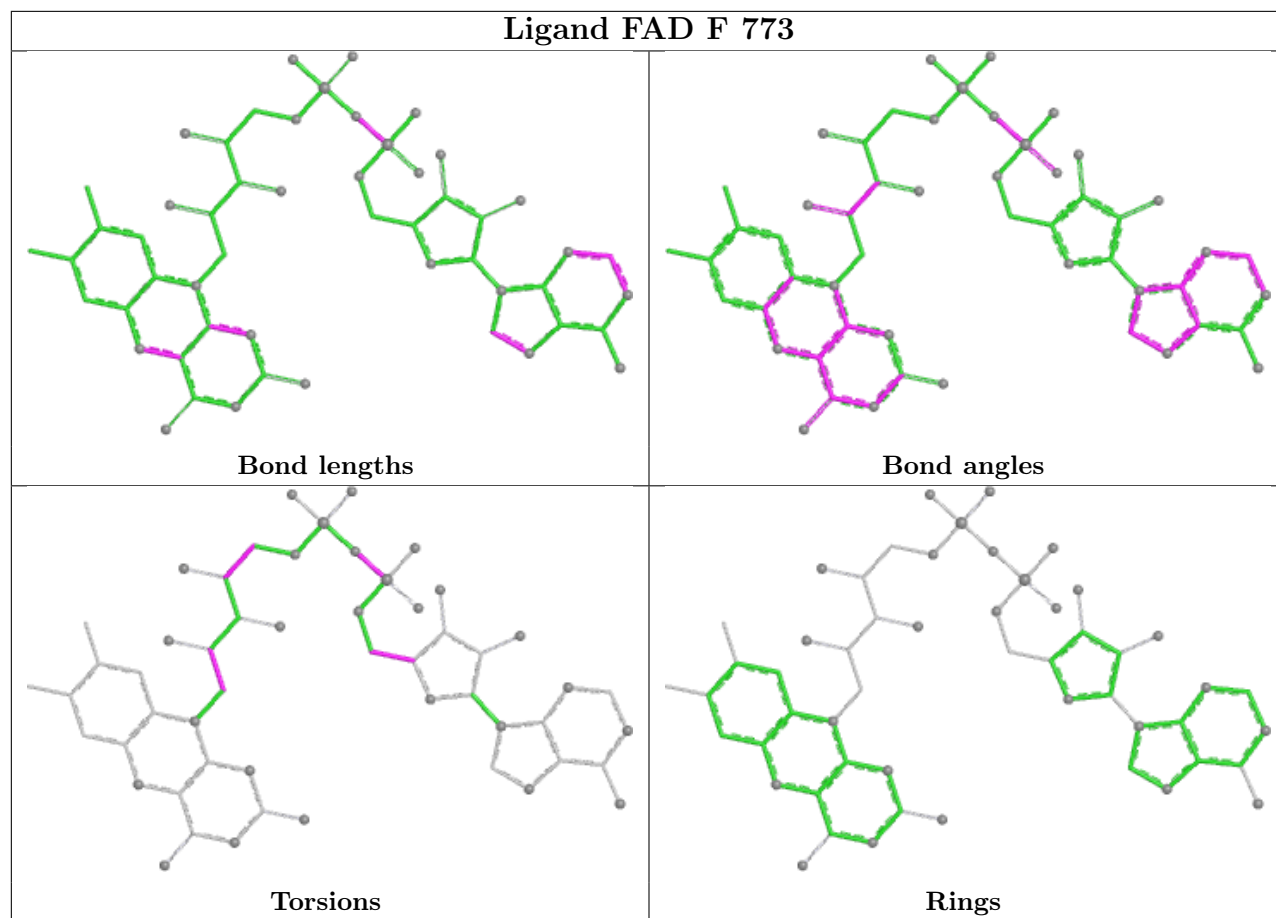


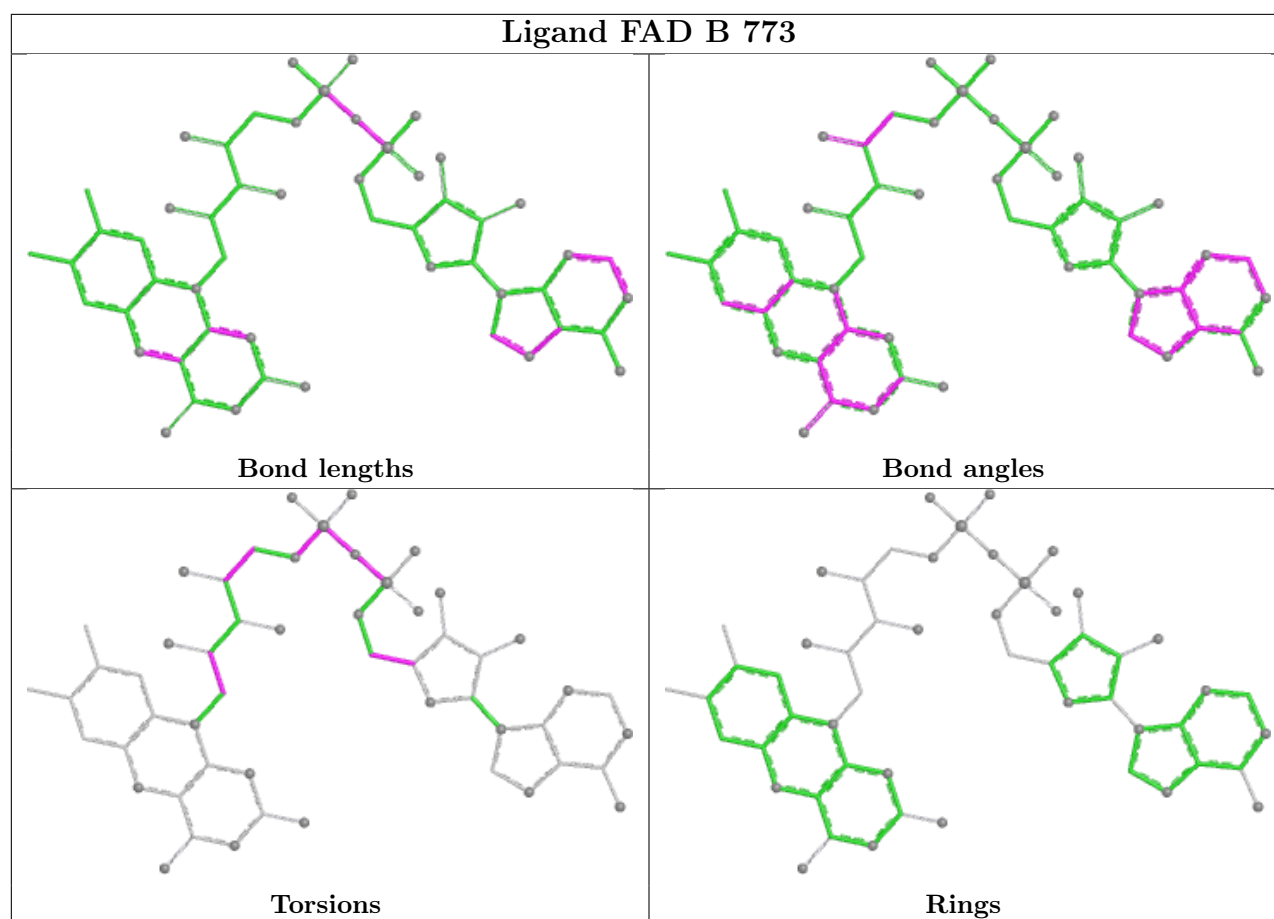












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	521/521 (100%)	-0.54	6 (1%) 76 54	9, 23, 38, 51	2 (0%)
1	B	521/521 (100%)	-0.54	4 (0%) 82 63	12, 23, 35, 53	2 (0%)
1	C	521/521 (100%)	-0.52	3 (0%) 85 69	10, 24, 37, 53	1 (0%)
1	D	521/521 (100%)	-0.52	5 (0%) 79 58	9, 23, 40, 53	1 (0%)
1	E	521/521 (100%)	-0.53	3 (0%) 85 69	10, 25, 39, 50	1 (0%)
1	F	521/521 (100%)	-0.53	4 (0%) 82 63	11, 23, 38, 51	2 (0%)
1	G	521/521 (100%)	-0.57	1 (0%) 91 83	12, 24, 37, 51	2 (0%)
1	H	521/521 (100%)	-0.49	5 (0%) 79 58	12, 26, 41, 50	2 (0%)
1	I	521/521 (100%)	-0.45	4 (0%) 82 63	12, 28, 44, 55	1 (0%)
1	J	521/521 (100%)	-0.46	3 (0%) 85 69	15, 28, 42, 54	1 (0%)
1	K	521/521 (100%)	-0.36	6 (1%) 76 54	13, 31, 46, 57	2 (0%)
1	L	521/521 (100%)	-0.27	1 (0%) 91 83	14, 35, 49, 55	2 (0%)
All	All	6252/6252 (100%)	-0.48	45 (0%) 84 66	9, 26, 43, 57	19 (0%)

The worst 5 of 45 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	226	SER	4.1
1	I	225	ASN	3.9
1	K	226	SER	3.8
1	G	227	SER	3.7
1	A	227	SER	3.6

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](#)

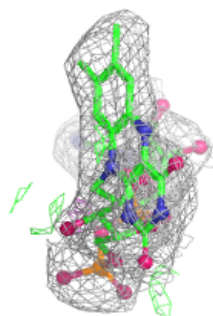
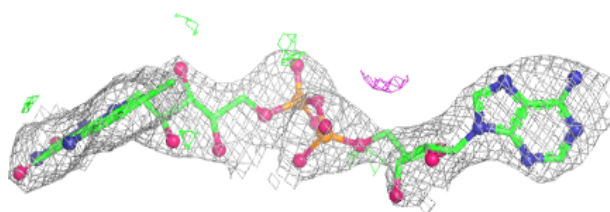
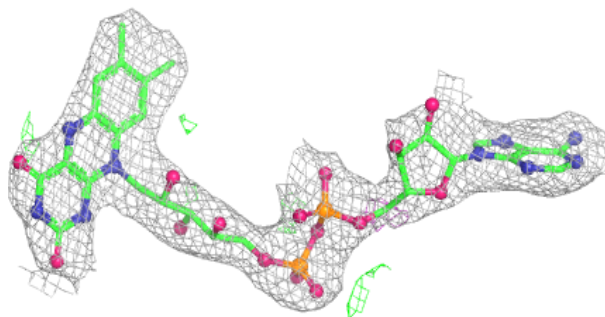
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	FAD	L	773	53/53	0.95	0.07	15,22,26,27	0
2	FAD	J	773	53/53	0.96	0.07	15,18,21,22	0
2	FAD	C	773	53/53	0.97	0.06	7,13,17,19	0
2	FAD	D	773	53/53	0.97	0.06	7,9,11,13	0
2	FAD	E	773	53/53	0.97	0.07	9,14,17,18	0
2	FAD	F	773	53/53	0.97	0.06	7,15,20,22	0
2	FAD	G	773	53/53	0.97	0.06	5,12,14,15	0
2	FAD	H	773	53/53	0.97	0.06	3,11,14,17	0
2	FAD	I	773	53/53	0.97	0.06	11,14,18,20	0
2	FAD	A	773	53/53	0.97	0.06	7,11,13,15	0
2	FAD	K	773	53/53	0.97	0.06	11,17,20,21	0
2	FAD	B	773	53/53	0.97	0.06	6,11,16,17	0

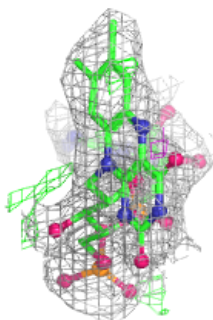
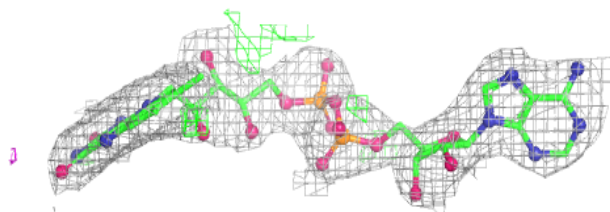
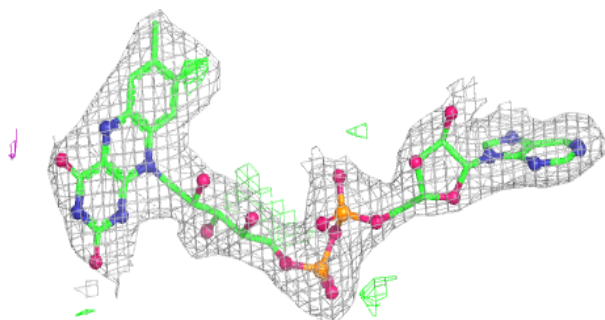
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FAD L 773:

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

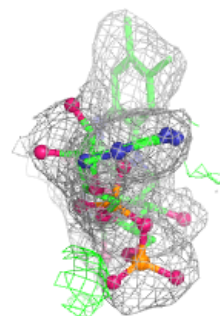
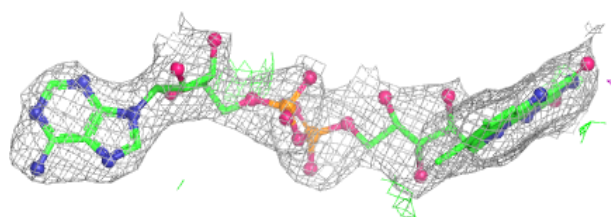
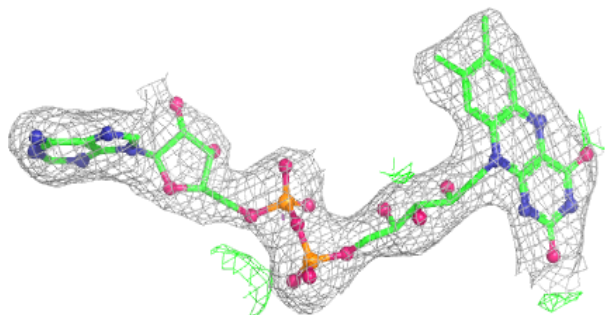
**Electron density around FAD J 773:**

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

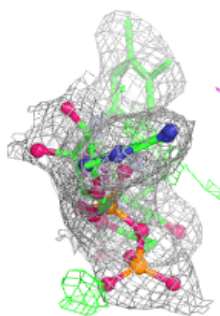
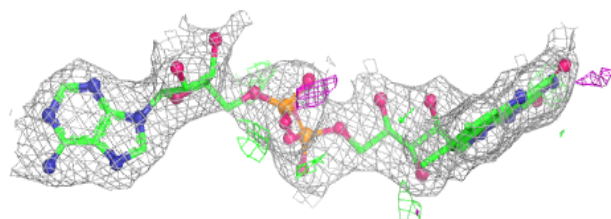
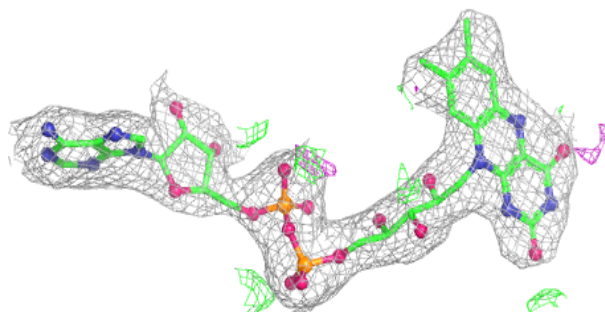


Electron density around FAD C 773:

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

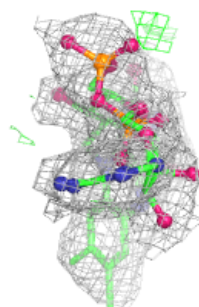
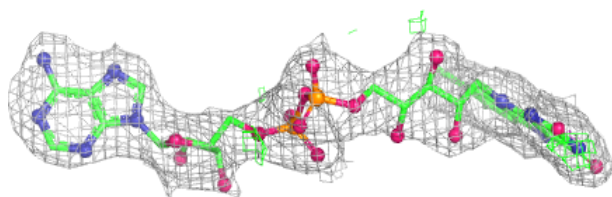
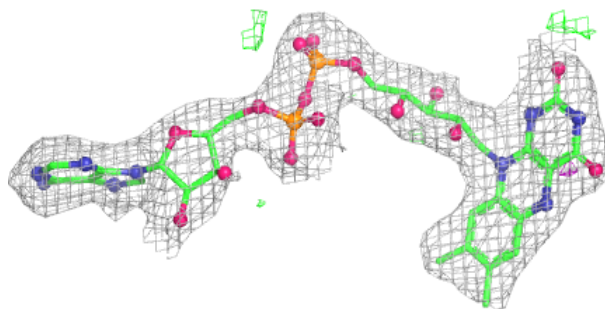
**Electron density around FAD D 773:**

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

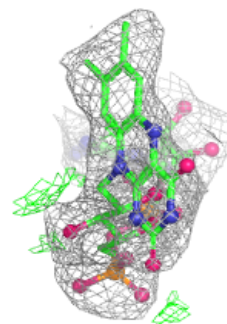
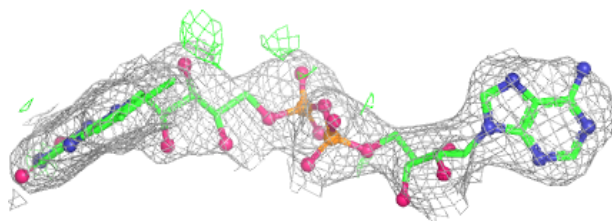
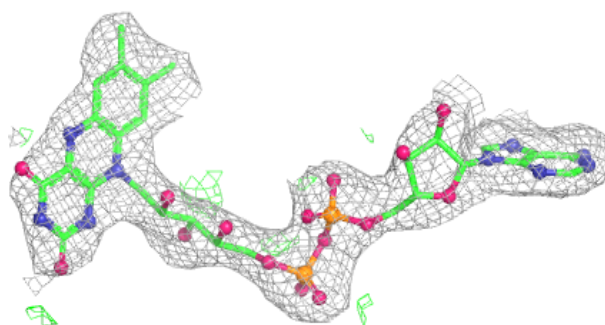


Electron density around FAD E 773:

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

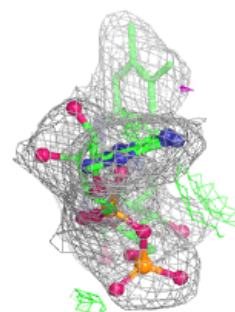
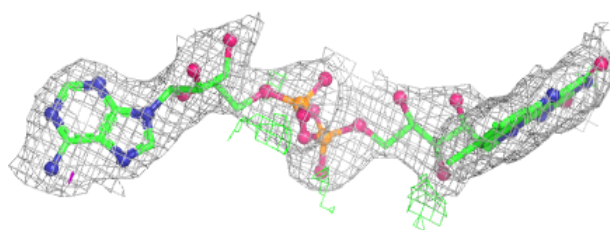
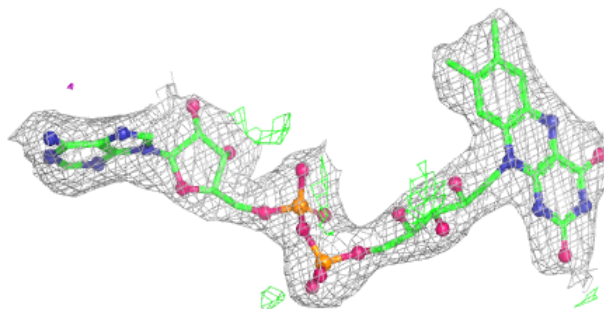
**Electron density around FAD F 773:**

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

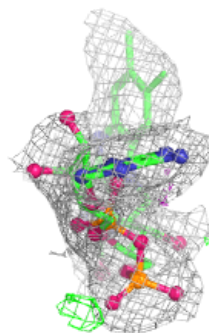
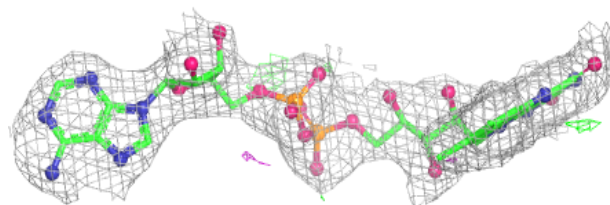
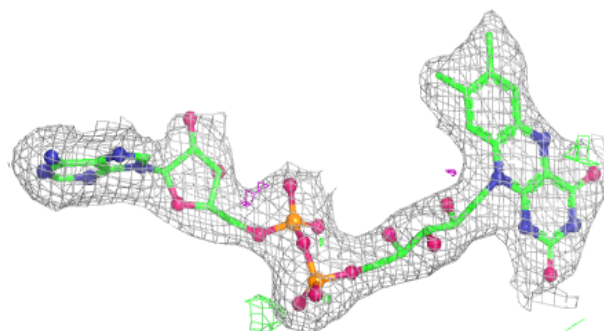


Electron density around FAD G 773:

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

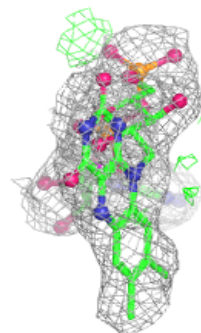
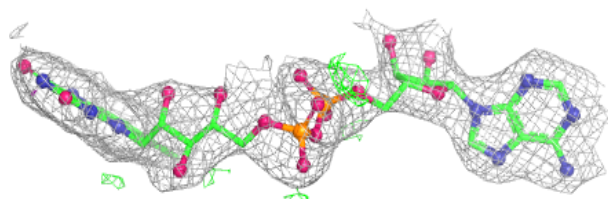
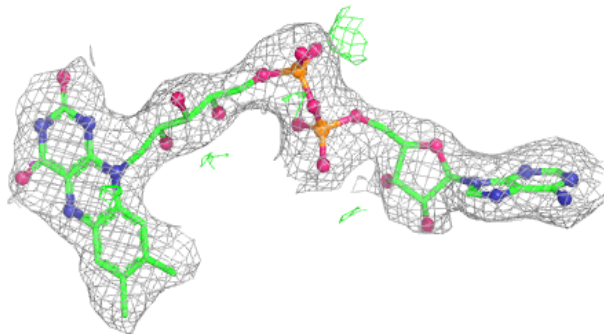
**Electron density around FAD H 773:**

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

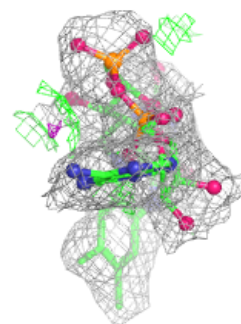
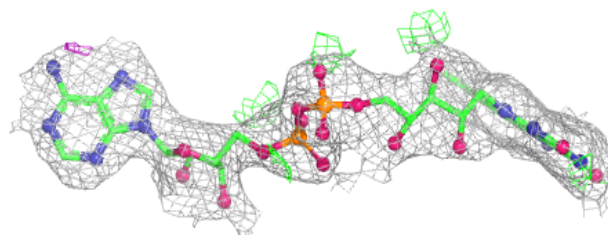
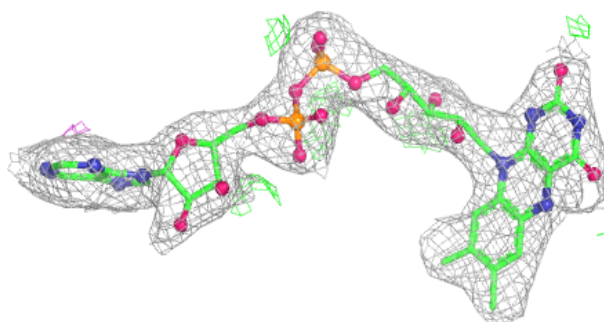


Electron density around FAD I 773:

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

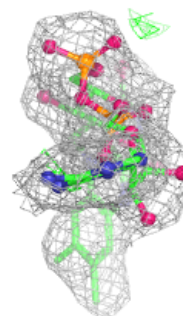
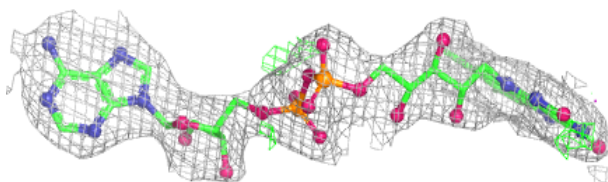
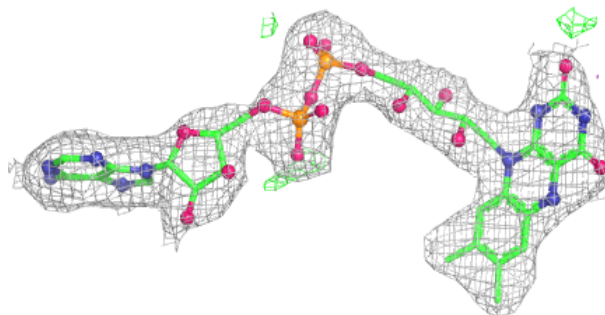
**Electron density around FAD A 773:**

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

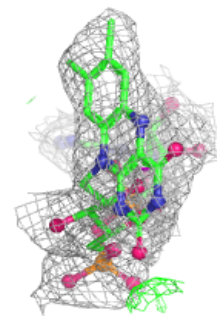
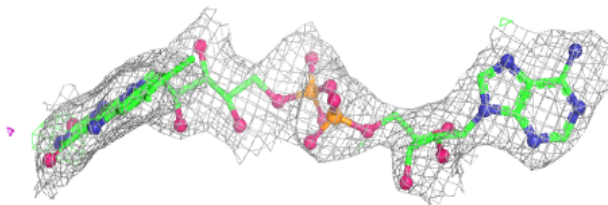
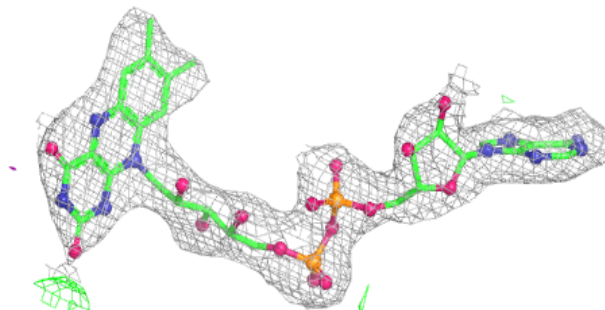


Electron density around FAD K 773:

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

**Electron density around FAD B 773:**

$2mF_o-DF_c$ (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.