



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 17, 2026 – 09:15 PM UTC

PDB ID : 2VTB / pdb_00002vtb
Title : Structure of cryptochrome 3 - DNA complex
Authors : Pokorny, R.; Klar, T.; Hennecke, U.; Carell, T.; Batschauer, A.; Essen, L.-O.
Deposited on : 2008-05-13
Resolution : 2.01 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)
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

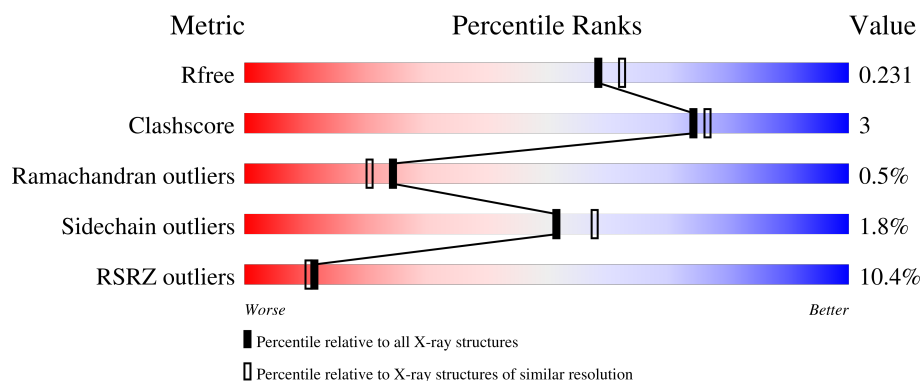
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

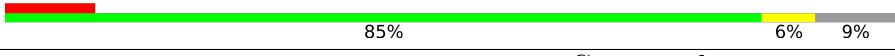
The reported resolution of this entry is 2.01 Å.

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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	526	
1	C	526	
1	D	526	
1	E	526	
1	F	526	

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Mol	Chain	Length	Quality of chain
2	B	525	13% 86% 7% 6%
3	G	5	20% 60% 20% 20%
3	H	5	20% 40% 20% 40%
3	I	5	60% 20% 20%
3	J	5	40% 20% 40%
3	K	5	40% 20% 20% 20%
3	L	5	60% 40% 20% 20%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 26329 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 CRYPTOCHROME DASH.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	500	Total	C	N	O	S	0	1	0
			4068	2603	707	738	20			
1	C	495	Total	C	N	O	S	0	1	0
			4042	2593	699	730	20			
1	D	484	Total	C	N	O	S	43	7	0
			3933	2523	674	715	21			
1	E	496	Total	C	N	O	S	0	0	0
			4042	2591	700	731	20			
1	F	480	Total	C	N	O	S	0	1	0
			3896	2503	667	705	21			

- Molecule 2 is a protein called CRYPTOCHROME DASH.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	491	Total	C	N	O	S	9	1	0
			3995	2564	688	723	20			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	353	ASN	GLN	conflict	UNP Q84KJ5

- Molecule 3 is a DNA chain called 5'-D(*DT*DT*DT*DT*DTP)-3'.

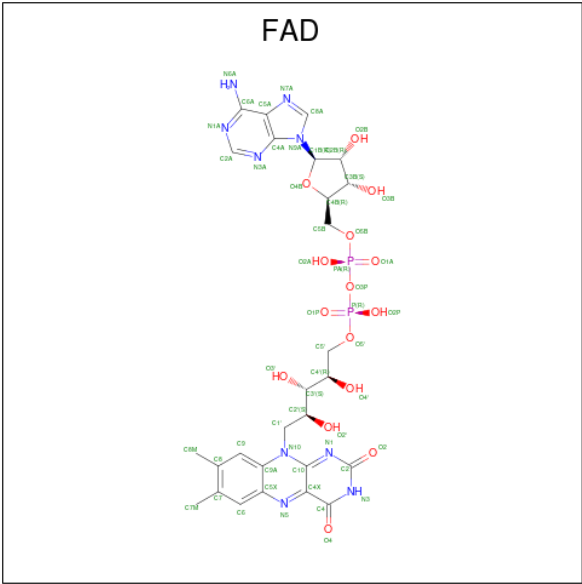
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	5	Total	C	N	O	P	0	0	0
			95	51	10	31	3			
3	H	5	Total	C	N	O	P	0	0	0
			95	51	10	31	3			
3	I	5	Total	C	N	O	P	0	0	0
			95	51	10	31	3			

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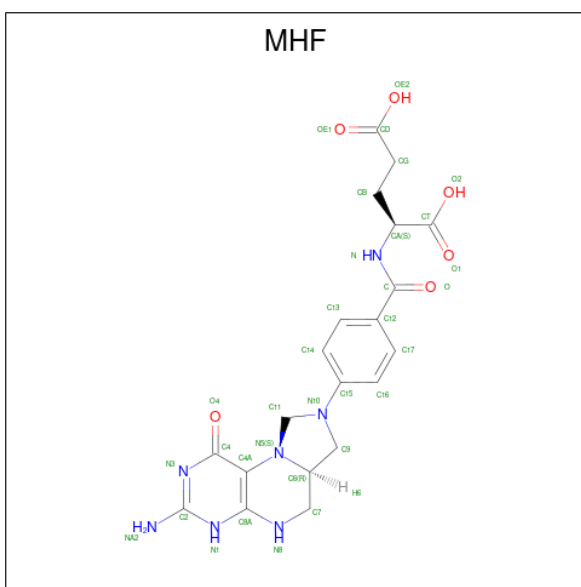
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	J	5	Total	C	N	O	P	9	0	0
			95	51	10	31	3			
3	K	4	Total	C	N	O	P	0	0	0
			78	41	8	26	3			
3	L	4	Total	C	N	O	P	0	0	0
			62	31	6	22	3			

- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



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

- Molecule 5 is 5,10-METHENYL-6,7,8-TRIHYDROFOLIC ACID (CCD ID: MHF) (formula: C₂₀H₂₃N₇O₆).

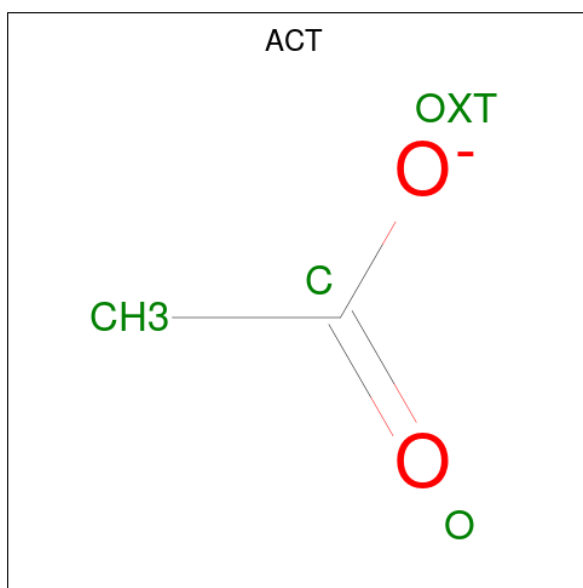


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total 33	C 20	N 7	O 6	0	0
5	B	1	Total 33	C 20	N 7	O 6	0	0
5	C	1	Total 33	C 20	N 7	O 6	0	0
5	D	1	Total 33	C 20	N 7	O 6	0	0
5	E	1	Total 33	C 20	N 7	O 6	0	0
5	F	1	Total 33	C 20	N 7	O 6	0	0

- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Cl 1 1	0	0
6	B	2	Total Cl 2 2	0	0
6	C	2	Total Cl 2 2	0	0
6	D	1	Total Cl 1 1	0	0
6	E	1	Total Cl 1 1	0	0
6	F	1	Total Cl 1 1	0	0

- Molecule 7 is ACETATE ION (CCD ID: ACT) (formula: $\text{C}_2\text{H}_3\text{O}_2$).



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

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	274	Total	O	0	0
			274	274		
8	B	178	Total	O	0	0
			178	178		
8	C	257	Total	O	0	0
			257	257		
8	D	209	Total	O	0	0
			209	209		
8	E	233	Total	O	0	0
			233	233		
8	F	120	Total	O	0	0
			120	120		
8	G	7	Total	O	0	0
			7	7		
8	H	4	Total	O	0	0
			4	4		
8	I	10	Total	O	0	0
			10	10		
8	J	5	Total	O	0	0
			5	5		

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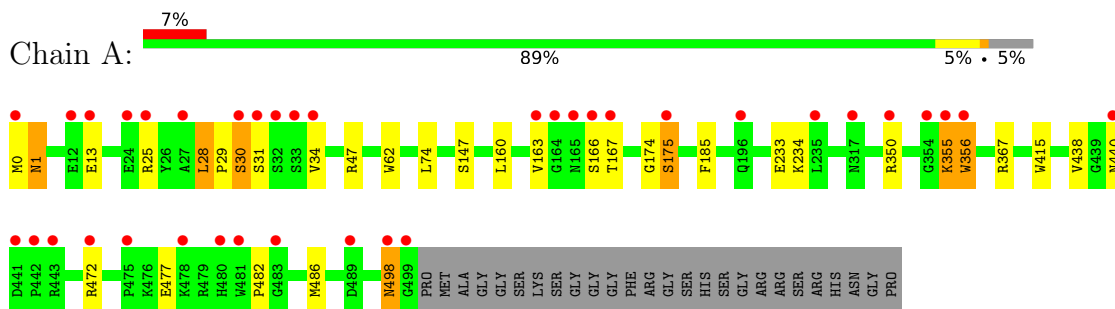
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	K	7	Total	O	0	0
			7	7		
8	L	1	Total	O	0	0
			1	1		

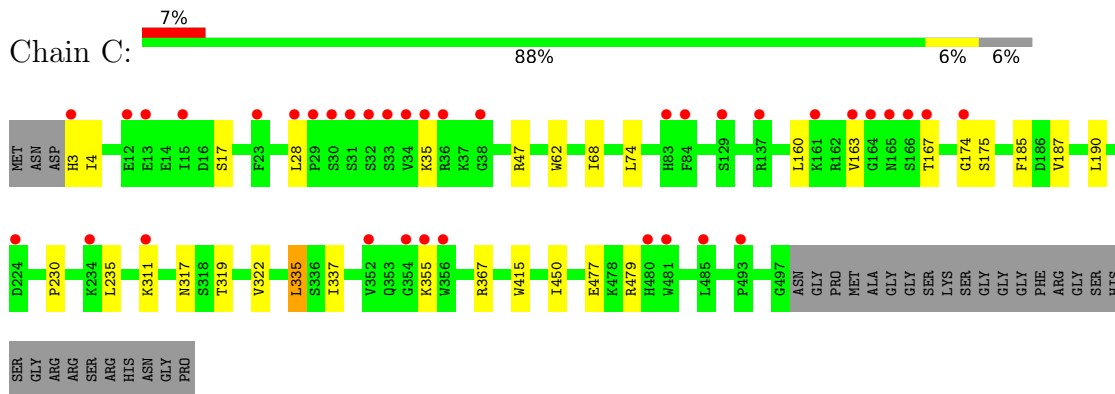
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

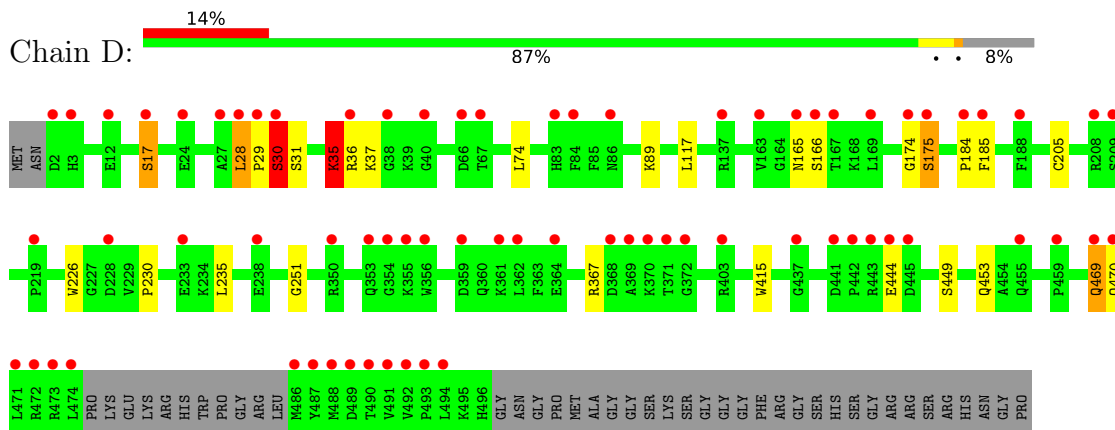
• Molecule 1: CRYPTOCHROME DASH



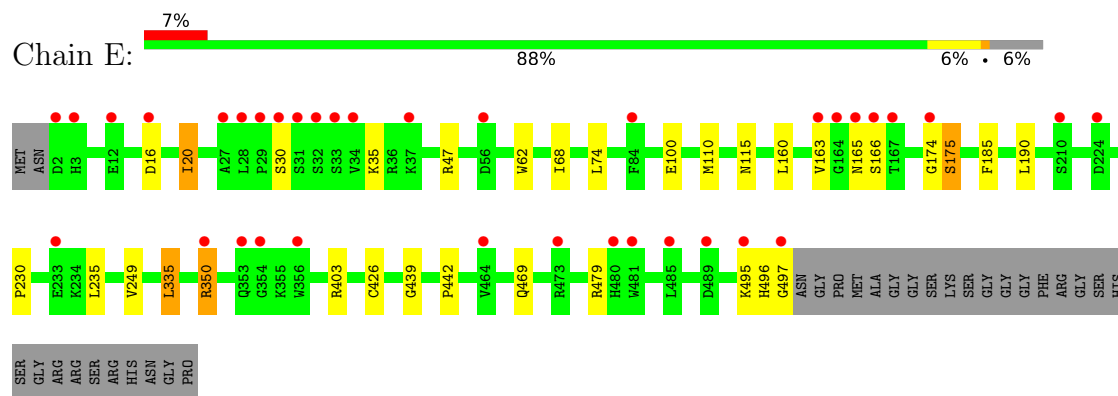
• Molecule 1: CRYPTOCHROME DASH



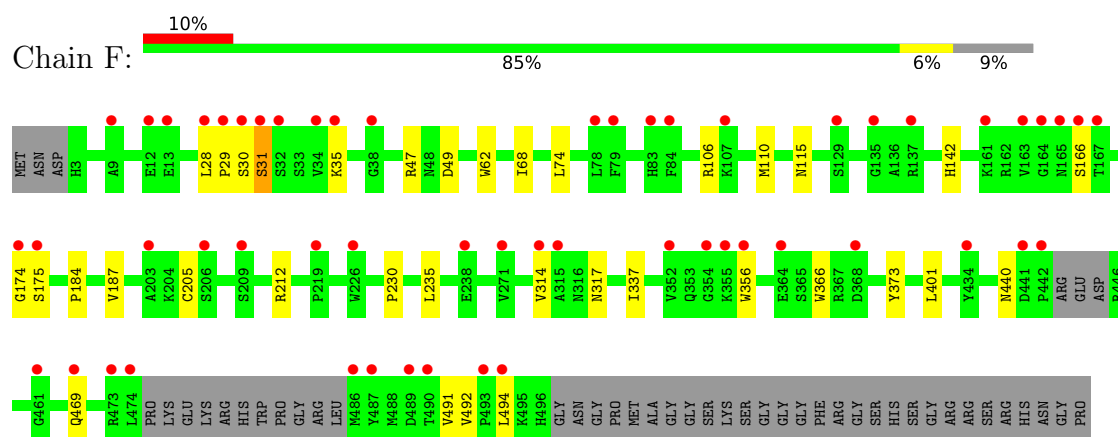
• Molecule 1: CRYPTOCHROME DASH



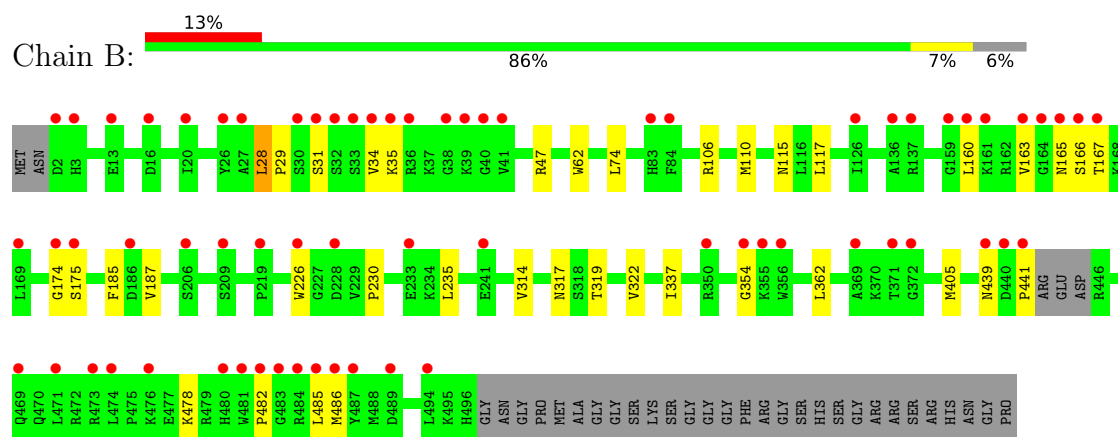
- Molecule 1: CRYPTOCHROME DASH



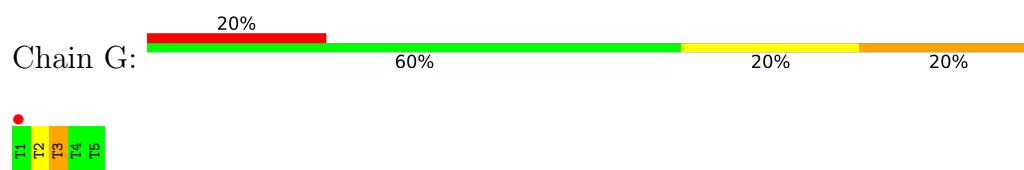
- Molecule 1: CRYPTOCHROME DASH



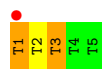
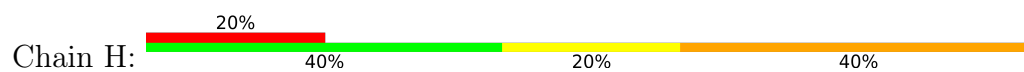
- Molecule 2: CRYPTOCHROME DASH



- Molecule 3: 5'-D(*DT*DT*DT*DT*DTP)-3'



- Molecule 3: 5'-D(*DT*DT*DT*DT*DTP)-3'



• Molecule 3: 5'-D(*DT*DT*DT*DT*DTP)-3'



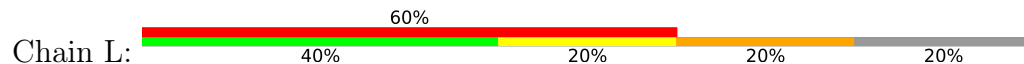
• Molecule 3: 5'-D(*DT*DT*DT*DT*DTP)-3'



• Molecule 3: 5'-D(*DT*DT*DT*DT*DTP)-3'



• Molecule 3: 5'-D(*DT*DT*DT*DT*DTP)-3'



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	120.73Å 136.08Å 211.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.03 – 2.01 15.03 – 2.01	Depositor EDS
% Data completeness (in resolution range)	99.2 (15.03-2.01) 99.2 (15.03-2.01)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.94 (at 2.01Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.184 , 0.222 0.195 , 0.231	Depositor DCC
R_{free} test set	1518 reflections (0.66%)	wwPDB-VP
Wilson B-factor (Å ²)	29.2	Xtrriage
Anisotropy	0.032	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 52.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	26329	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 37.07 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.5360e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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, CL, ACT, TCP, MHF

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	0.52	0/4181	0.73	0/5656
1	C	0.52	1/4157 (0.0%)	0.71	0/5625
1	D	0.80	4/4042 (0.1%)	0.94	10/5471 (0.2%)
1	E	0.52	0/4154	0.72	0/5622
1	F	0.46	0/4004	0.69	0/5419
2	B	0.50	0/4106	0.70	0/5561
3	G	0.27	0/83	0.96	0/124
3	H	0.26	0/83	1.23	1/124 (0.8%)
3	I	0.37	0/83	1.18	0/124
3	J	0.37	0/83	5.17	4/124 (3.2%)
3	K	0.32	0/64	1.17	0/94
3	L	0.29	0/46	0.88	0/67
All	All	0.56	5/25086 (0.0%)	0.82	15/34011 (0.0%)

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	D	0	2
3	J	1	0
All	All	1	2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	35[A]	LYS	C-N	-29.54	0.90	1.33
1	D	37[A]	LYS	C-N	-20.14	1.05	1.33
1	D	36	ARG	C-N	16.72	1.56	1.33
1	D	30	SER	C-N	8.75	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	450	ILE	CA-CB	5.00	1.57	1.54

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	1	DT	O4'-C1'-N1	41.76	171.04	108.40
1	D	30	SER	O-C-N	-38.22	71.76	122.59
3	J	1	DT	N1-C1'-C2'	-23.41	78.39	113.50
3	J	1	DT	C6-N1-C1'	-21.51	87.08	119.35
3	J	1	DT	C2-N1-C1'	20.34	149.86	119.35

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	J	1	DT	C1'

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	30	SER	Mainchain
1	D	35[A]	LYS	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	4068	0	3988	22	0
1	C	4042	0	3967	20	0
1	D	3933	0	3840	19	0
1	E	4042	0	3957	26	0
1	F	3896	0	3812	23	0
2	B	3995	0	3896	30	0
3	G	95	0	64	3	0
3	H	95	0	64	3	0
3	I	95	0	64	3	0
3	J	95	0	64	3	0
3	K	78	0	51	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	L	62	0	38	2	0
4	A	53	0	31	0	0
4	B	53	0	31	0	0
4	C	53	0	31	0	0
4	D	53	0	31	0	0
4	E	53	0	31	0	0
4	F	53	0	31	0	0
5	A	33	0	21	0	0
5	B	33	0	21	0	0
5	C	33	0	21	0	0
5	D	33	0	21	0	0
5	E	33	0	21	0	0
5	F	33	0	21	0	0
6	A	1	0	0	0	0
6	B	2	0	0	0	0
6	C	2	0	0	0	0
6	D	1	0	0	0	0
6	E	1	0	0	0	0
6	F	1	0	0	0	0
7	B	4	0	3	0	0
8	A	274	0	0	3	0
8	B	178	0	0	1	0
8	C	257	0	0	1	0
8	D	209	0	0	4	0
8	E	233	0	0	2	0
8	F	120	0	0	1	0
8	G	7	0	0	0	0
8	H	4	0	0	0	0
8	I	10	0	0	0	0
8	J	5	0	0	0	0
8	K	7	0	0	0	0
8	L	1	0	0	0	0
All	All	26329	0	24120	152	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

The worst 5 of 152 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:74:LEU:HD21	1:D:235:LEU:HD11	1.40	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:VAL:HG11	1:A:62:TRP:CH2	2.06	0.90
1:D:17:SER:CB	8:D:2004:HOH:O	2.21	0.89
2:B:74:LEU:HD21	2:B:235:LEU:HD11	1.55	0.88
2:B:160:LEU:HD22	2:B:167:THR:HG21	1.57	0.87

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	499/526 (95%)	479 (96%)	14 (3%)	6 (1%)	10	6
1	C	494/526 (94%)	475 (96%)	19 (4%)	0	100	100
1	D	481/526 (91%)	460 (96%)	19 (4%)	2 (0%)	30	27
1	E	494/526 (94%)	472 (96%)	20 (4%)	2 (0%)	30	27
1	F	475/526 (90%)	456 (96%)	16 (3%)	3 (1%)	21	17
2	B	487/525 (93%)	465 (96%)	19 (4%)	3 (1%)	21	17
All	All	2930/3155 (93%)	2807 (96%)	107 (4%)	16 (0%)	24	21

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1	ASN
1	A	30	SER
1	E	30	SER
1	A	355	LYS
1	A	356	TRP

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	440/459 (96%)	431 (98%)	9 (2%)	48	54
1	C	438/459 (95%)	428 (98%)	10 (2%)	44	49
1	D	426/459 (93%)	419 (98%)	7 (2%)	55	62
1	E	437/459 (95%)	428 (98%)	9 (2%)	47	52
1	F	422/459 (92%)	416 (99%)	6 (1%)	59	66
2	B	432/459 (94%)	426 (99%)	6 (1%)	59	66
All	All	2595/2754 (94%)	2548 (98%)	47 (2%)	51	58

5 of 47 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	35[A]	LYS
1	E	335	LEU
1	D	185	PHE
1	E	20	ILE
1	E	403	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	428	ASN
1	F	428	ASN
1	D	469	GLN
1	F	469	GLN
1	E	440	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 non-standard protein/DNA/RNA residues 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
3	TCP	K	3	3	19,19,19	0.93	1 (5%)	27,27,27	1.80	2 (7%)
3	TCP	G	3	3	19,19,19	0.95	1 (5%)	27,27,27	1.70	3 (11%)
3	TCP	L	3	3	19,19,19	0.94	1 (5%)	27,27,27	1.33	3 (11%)
3	TCP	J	3	3	19,19,19	0.96	1 (5%)	27,27,27	1.63	4 (14%)
3	TCP	I	3	3	19,19,19	0.98	1 (5%)	27,27,27	1.85	4 (14%)
3	TCP	H	3	3	19,19,19	0.96	1 (5%)	27,27,27	1.52	2 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	TCP	K	3	3	-	1/7/19/19	0/2/2/2
3	TCP	G	3	3	-	2/7/19/19	0/2/2/2
3	TCP	L	3	3	-	4/7/19/19	0/2/2/2
3	TCP	J	3	3	-	2/7/19/19	0/2/2/2
3	TCP	I	3	3	-	2/7/19/19	0/2/2/2
3	TCP	H	3	3	-	3/7/19/19	0/2/2/2

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	3	TCP	O5'-CP	3.68	1.60	1.42
3	L	3	TCP	O5'-CP	3.62	1.59	1.42
3	J	3	TCP	O5'-CP	3.62	1.59	1.42
3	H	3	TCP	O5'-CP	3.57	1.59	1.42
3	G	3	TCP	O5'-CP	3.55	1.59	1.42

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	3	TCP	O4'-C1'-N1	7.88	121.85	107.86
3	K	3	TCP	O4'-C1'-N1	7.61	121.37	107.86
3	G	3	TCP	O4'-C1'-N1	6.88	120.07	107.86
3	J	3	TCP	O4'-C1'-N1	6.74	119.83	107.86
3	H	3	TCP	O4'-C1'-N1	6.12	118.73	107.86

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	L	3	TCP	C2'-C1'-N1-C6
3	L	3	TCP	O4'-C1'-N1-C6
3	H	3	TCP	C2'-C1'-N1-C6
3	H	3	TCP	O4'-C1'-N1-C6
3	G	3	TCP	C2'-C1'-N1-C6

There are no ring outliers.

6 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	K	3	TCP	2	0
3	G	3	TCP	3	0
3	L	3	TCP	2	0
3	J	3	TCP	2	0
3	I	3	TCP	3	0
3	H	3	TCP	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 21 ligands modelled in this entry, 8 are monoatomic - leaving 13 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	MHF	A	999	-	35,36,36	1.20	3 (8%)	37,52,52	1.24	4 (10%)
5	MHF	C	999	-	35,36,36	1.32	3 (8%)	37,52,52	1.25	4 (10%)
7	ACT	B	1500	-	3,3,3	0.85	0	3,3,3	1.20	0
5	MHF	F	999	-	35,36,36	1.21	2 (5%)	37,52,52	1.21	3 (8%)
5	MHF	E	999	-	35,36,36	1.24	2 (5%)	37,52,52	1.16	3 (8%)
4	FAD	E	998	-	58,58,58	1.25	6 (10%)	85,89,89	1.54	16 (18%)
4	FAD	B	998	-	58,58,58	1.13	7 (12%)	85,89,89	1.56	17 (20%)
5	MHF	B	999	-	35,36,36	1.20	2 (5%)	37,52,52	1.32	3 (8%)
4	FAD	D	998	-	58,58,58	1.18	7 (12%)	85,89,89	1.52	14 (16%)
4	FAD	A	998	-	58,58,58	1.15	6 (10%)	85,89,89	1.51	13 (15%)
4	FAD	F	998	-	58,58,58	1.09	5 (8%)	85,89,89	1.50	14 (16%)
4	FAD	C	998	-	58,58,58	1.17	7 (12%)	85,89,89	1.42	11 (12%)
5	MHF	D	999	-	35,36,36	1.25	2 (5%)	37,52,52	1.23	3 (8%)

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
5	MHF	A	999	-	-	5/21/42/42	0/4/4/4
5	MHF	C	999	-	-	4/21/42/42	0/4/4/4
5	MHF	F	999	-	-	4/21/42/42	0/4/4/4
5	MHF	E	999	-	-	4/21/42/42	0/4/4/4
4	FAD	E	998	-	-	3/34/50/50	0/6/6/6
4	FAD	B	998	-	-	2/34/50/50	0/6/6/6
5	MHF	B	999	-	-	4/21/42/42	0/4/4/4
4	FAD	D	998	-	-	3/34/50/50	0/6/6/6
4	FAD	A	998	-	-	2/34/50/50	0/6/6/6
4	FAD	F	998	-	-	3/34/50/50	0/6/6/6
4	FAD	C	998	-	-	3/34/50/50	0/6/6/6
5	MHF	D	999	-	-	4/21/42/42	0/4/4/4

The worst 5 of 52 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	998	FAD	C4X-N5	4.14	1.39	1.30
5	C	999	MHF	C8A-N8	3.94	1.36	1.32
4	E	998	FAD	C4X-N5	3.93	1.39	1.30
4	B	998	FAD	C4X-N5	3.89	1.39	1.30
4	C	998	FAD	C4X-N5	3.83	1.39	1.30

The worst 5 of 105 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	998	FAD	N3A-C2A-N1A	-5.65	120.03	128.58
4	A	998	FAD	N3A-C2A-N1A	-5.54	120.20	128.58
4	D	998	FAD	N3A-C2A-N1A	-5.41	120.39	128.58
4	C	998	FAD	N3A-C2A-N1A	-5.34	120.50	128.58
4	E	998	FAD	N3A-C2A-N1A	-5.32	120.53	128.58

There are no chirality outliers.

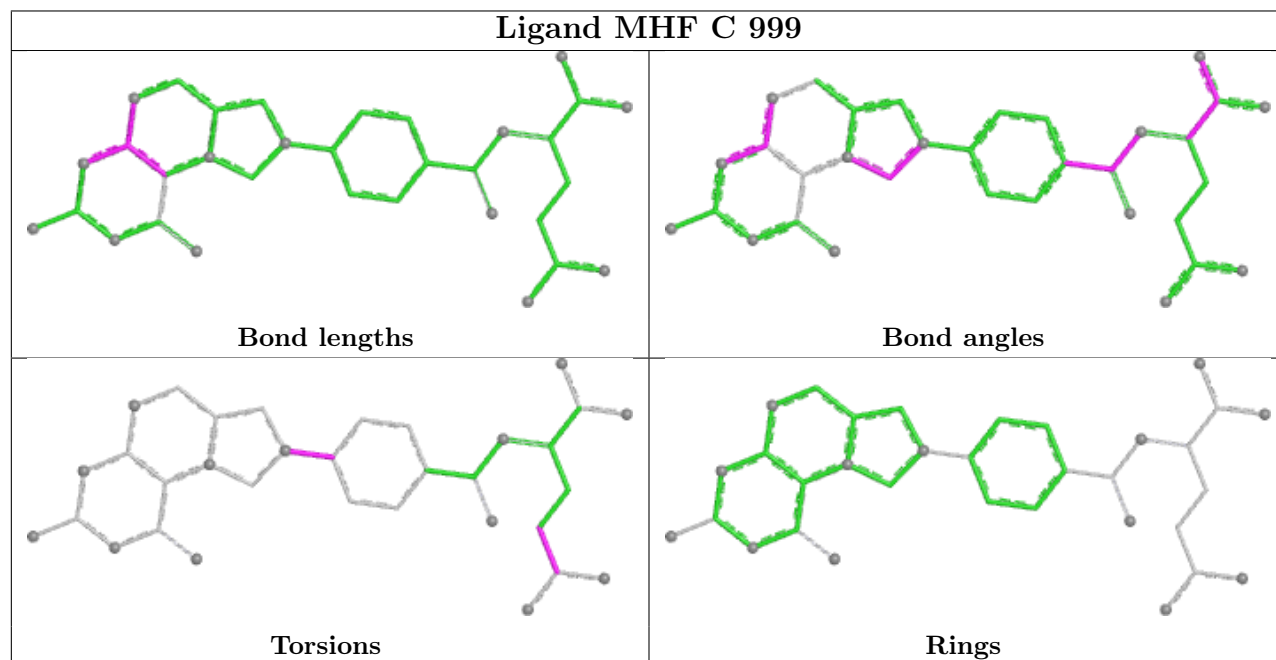
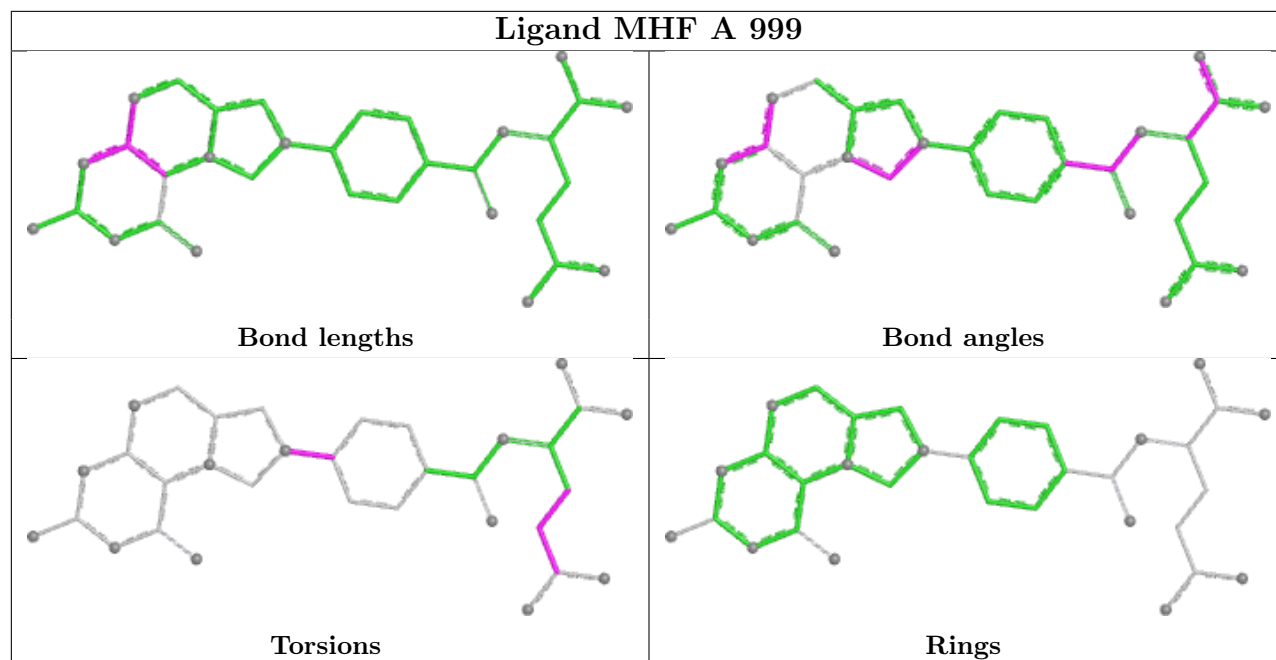
5 of 41 torsion outliers are listed below:

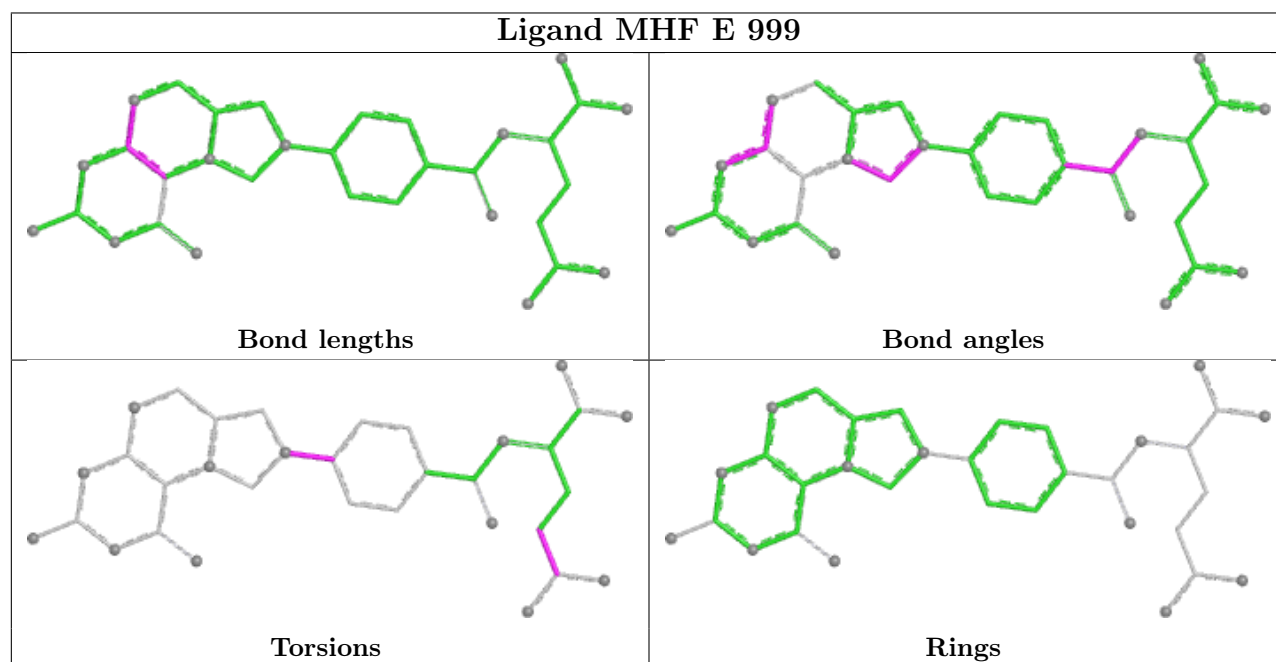
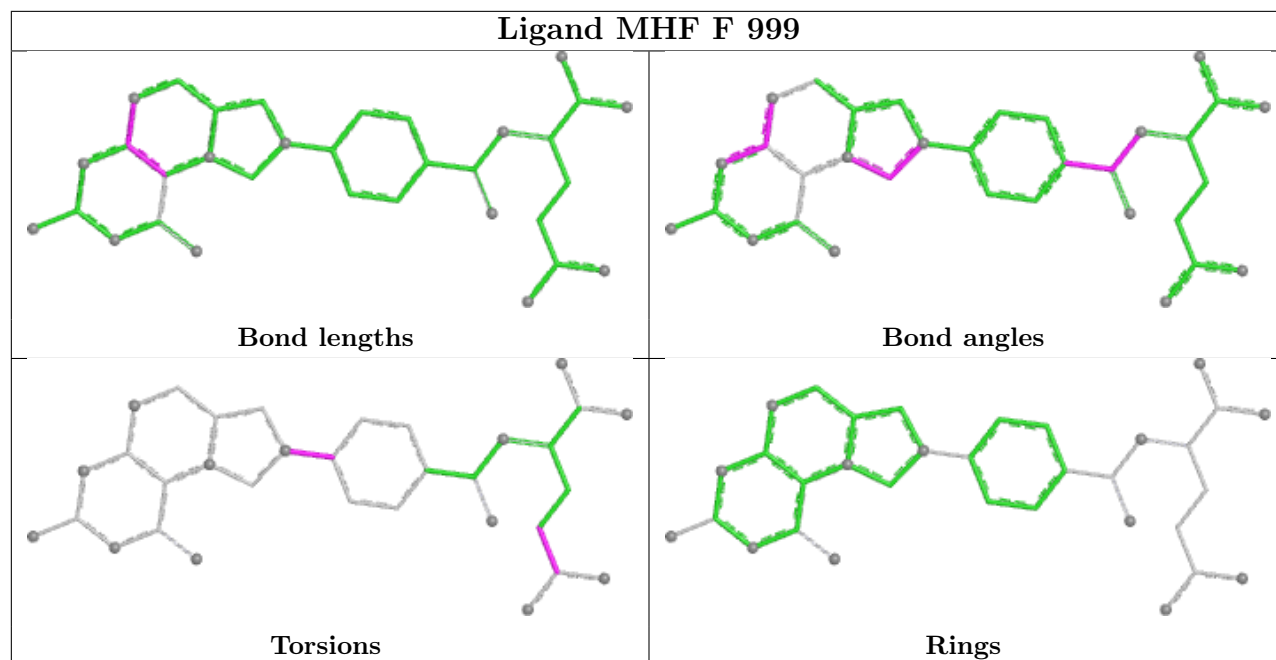
Mol	Chain	Res	Type	Atoms
5	A	999	MHF	C16-C15-N10-C9
5	C	999	MHF	C14-C15-N10-C9
5	F	999	MHF	C16-C15-N10-C9
5	A	999	MHF	C14-C15-N10-C9
5	B	999	MHF	C16-C15-N10-C9

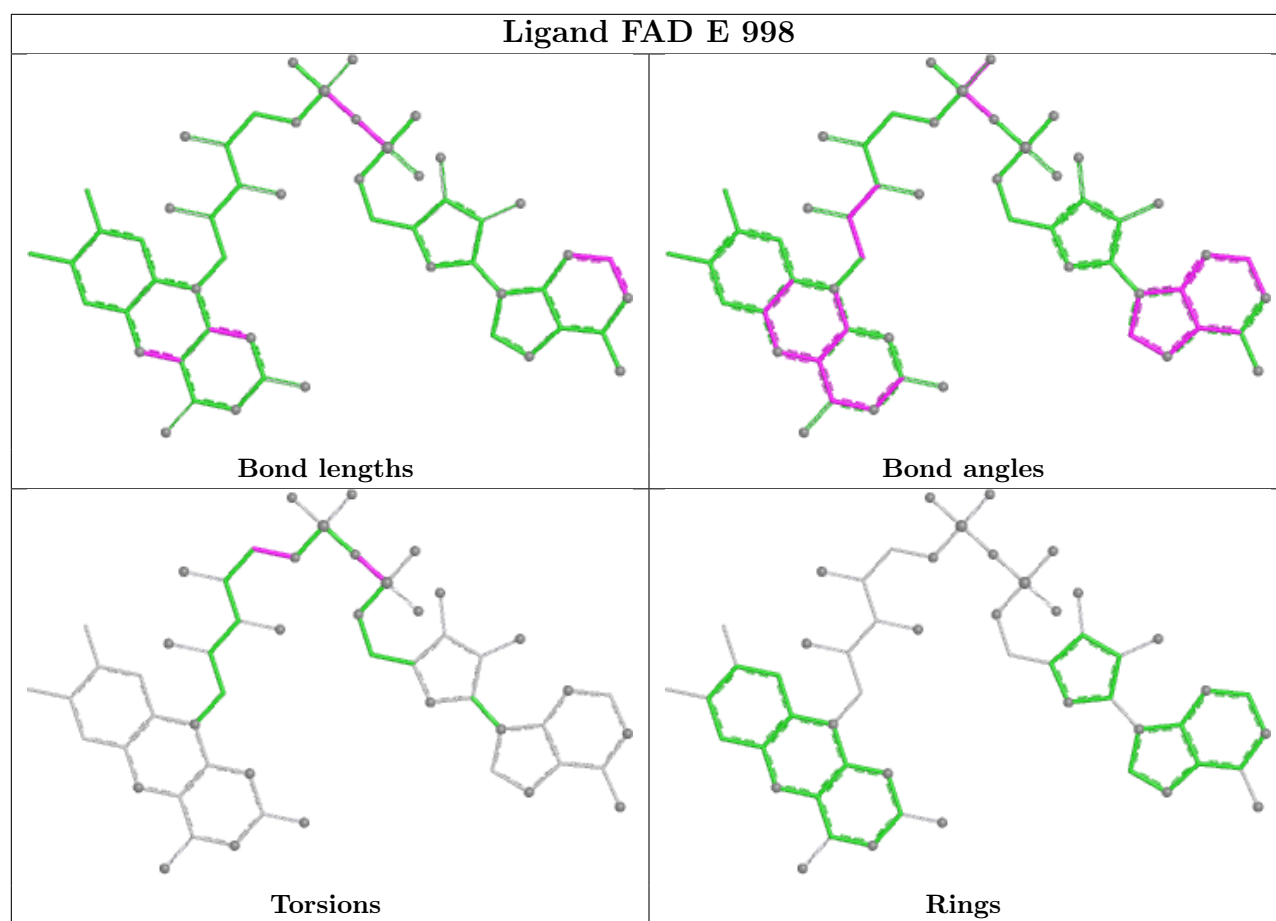
There are no ring outliers.

No monomer is involved in short contacts.

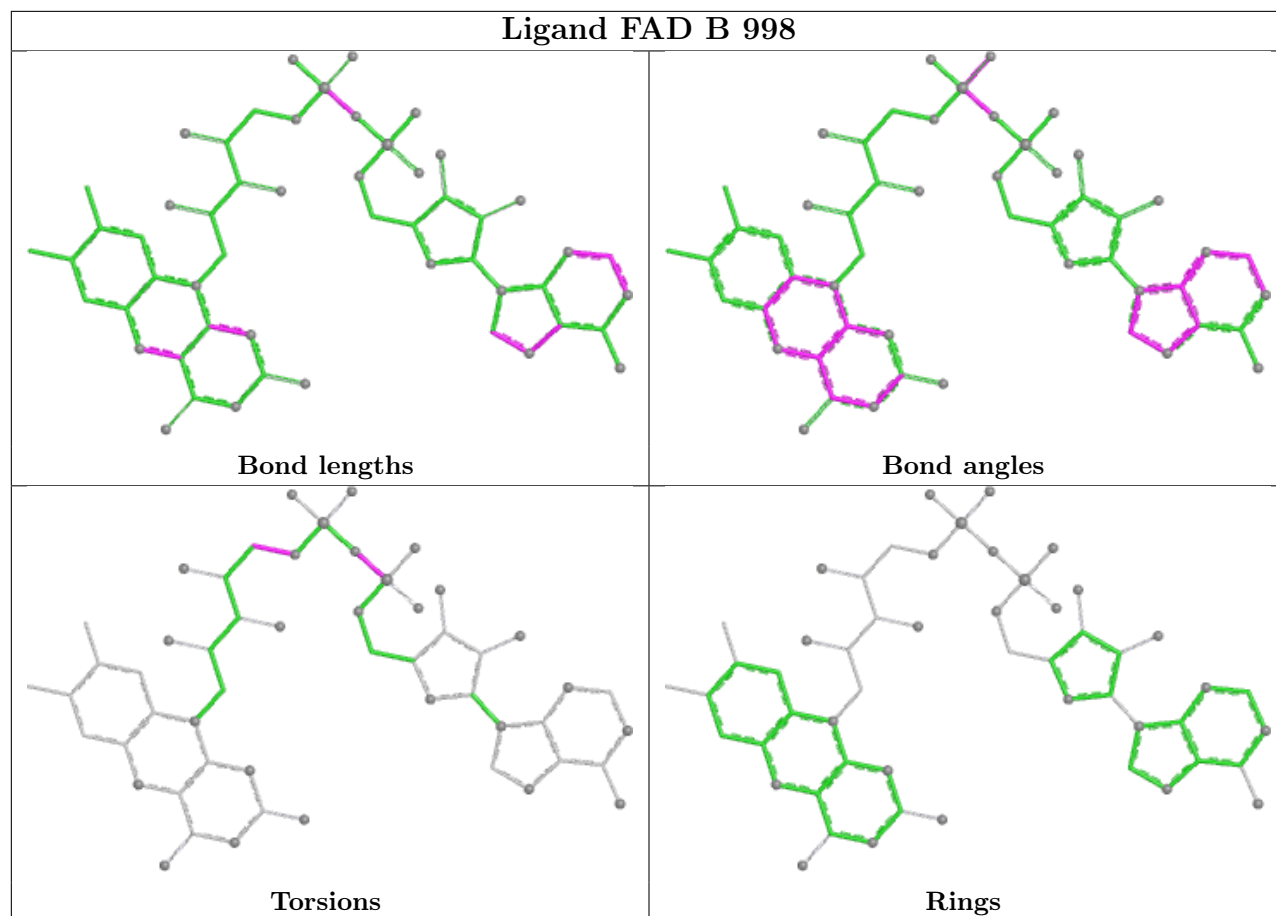
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



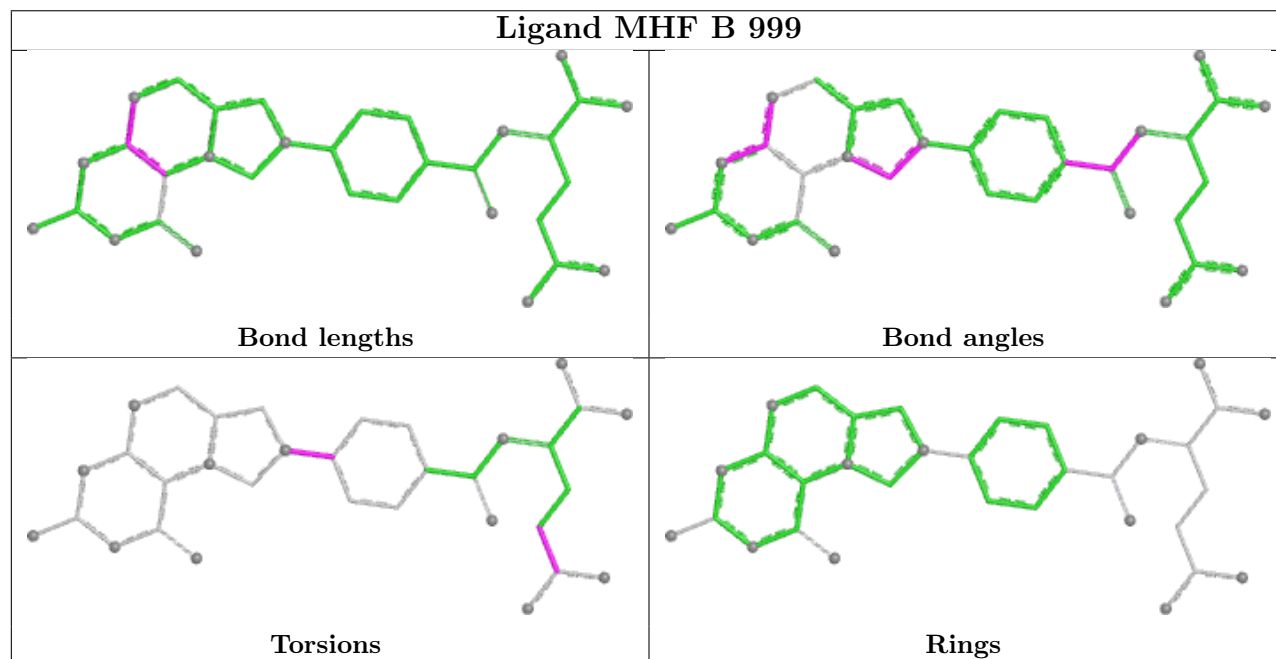


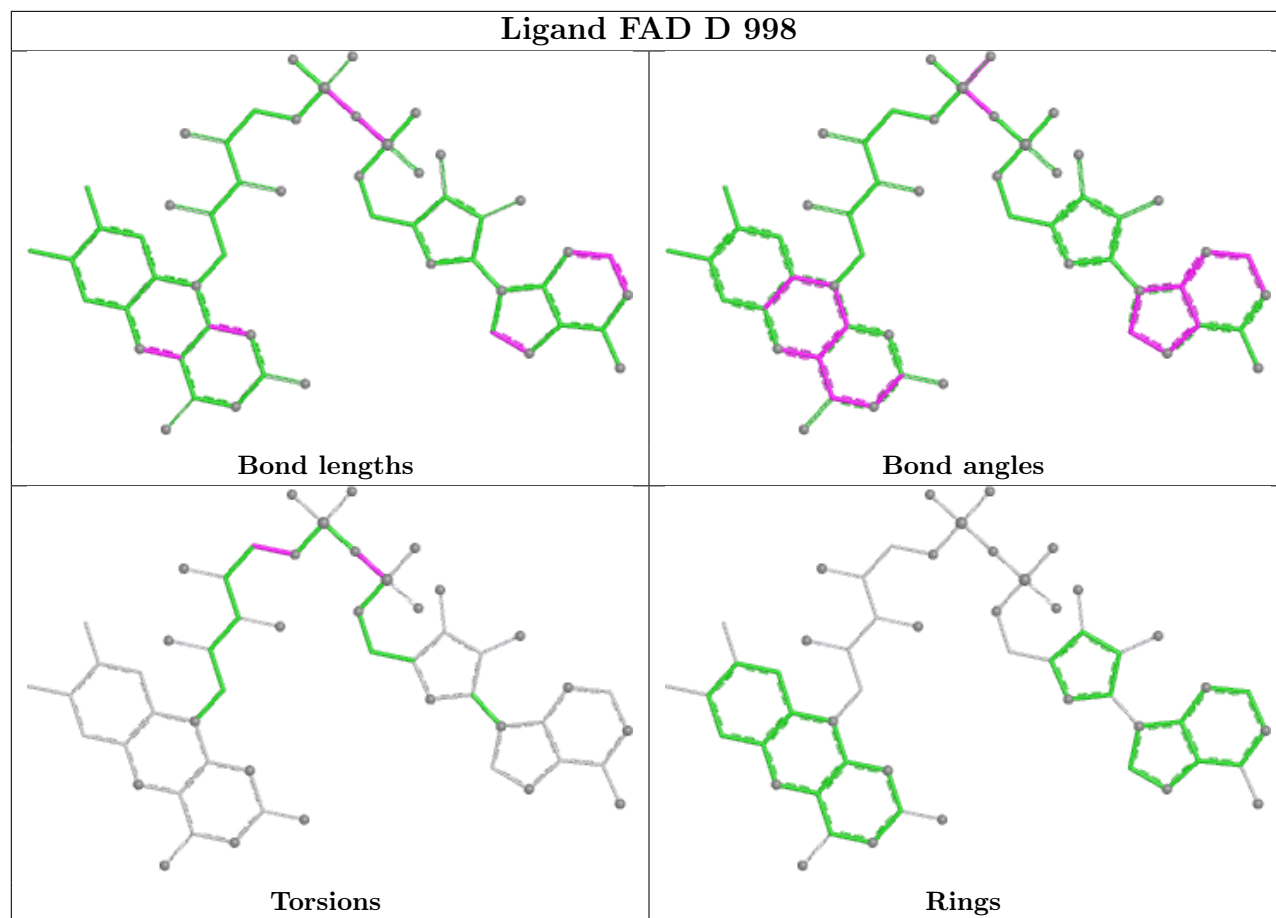


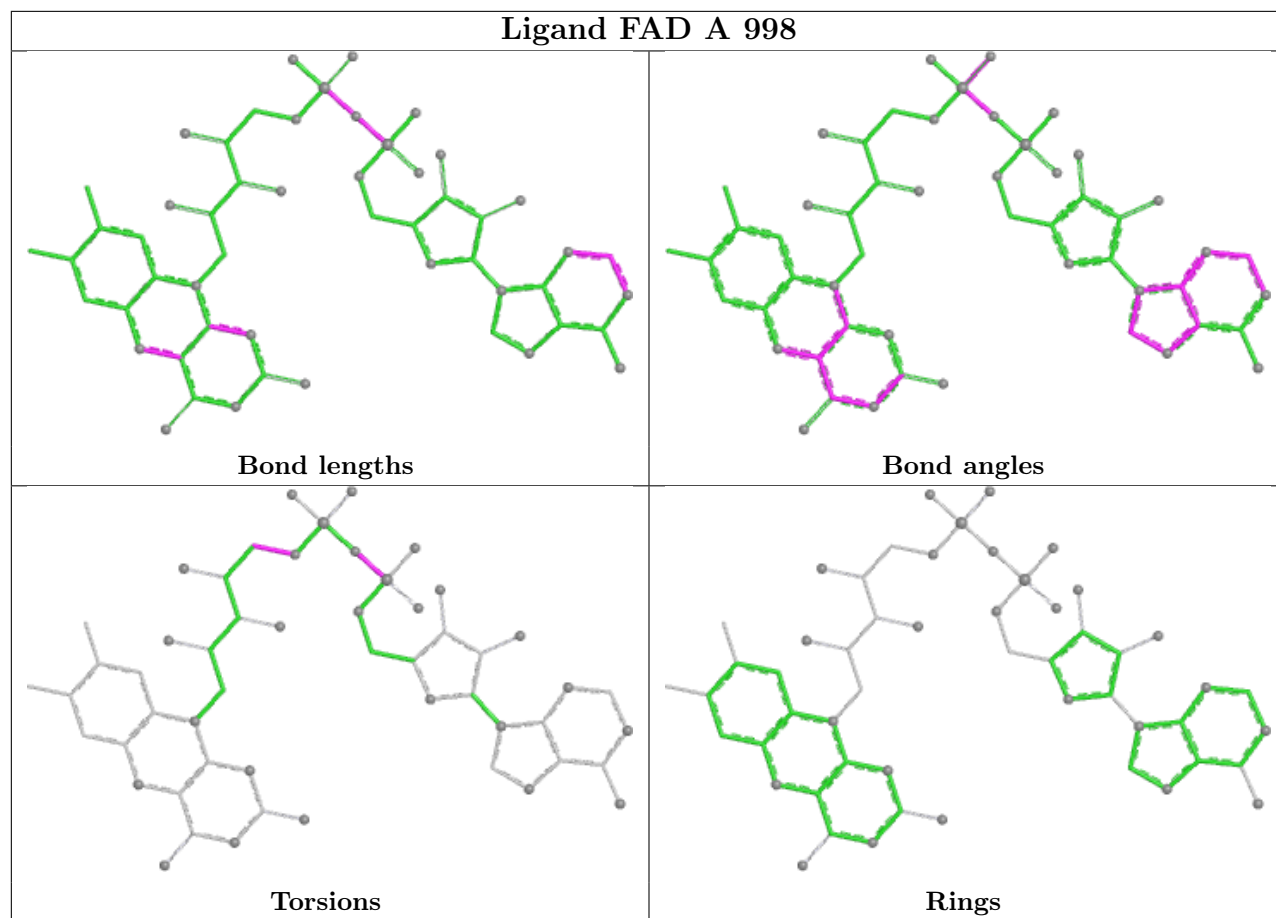
Ligand FAD B 998

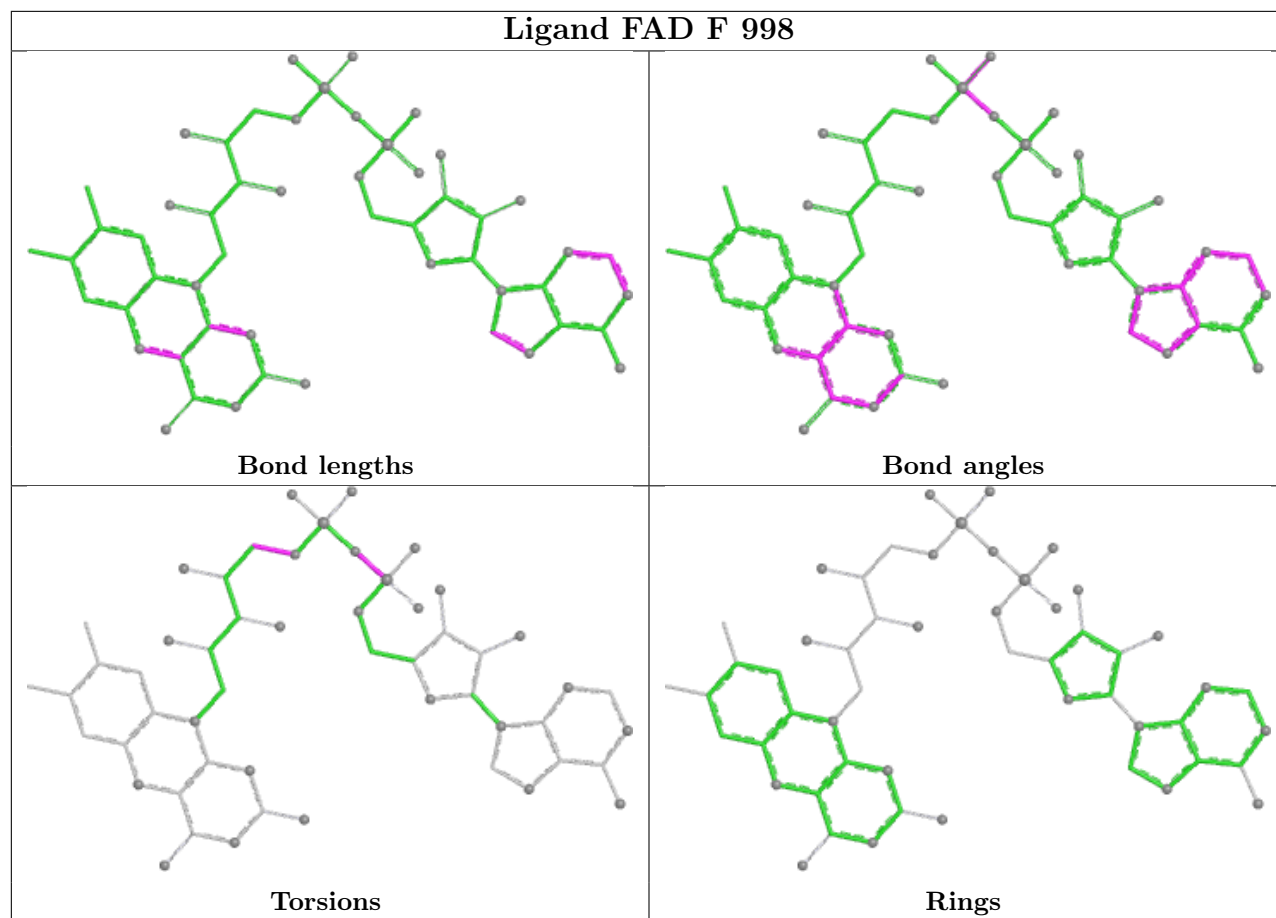


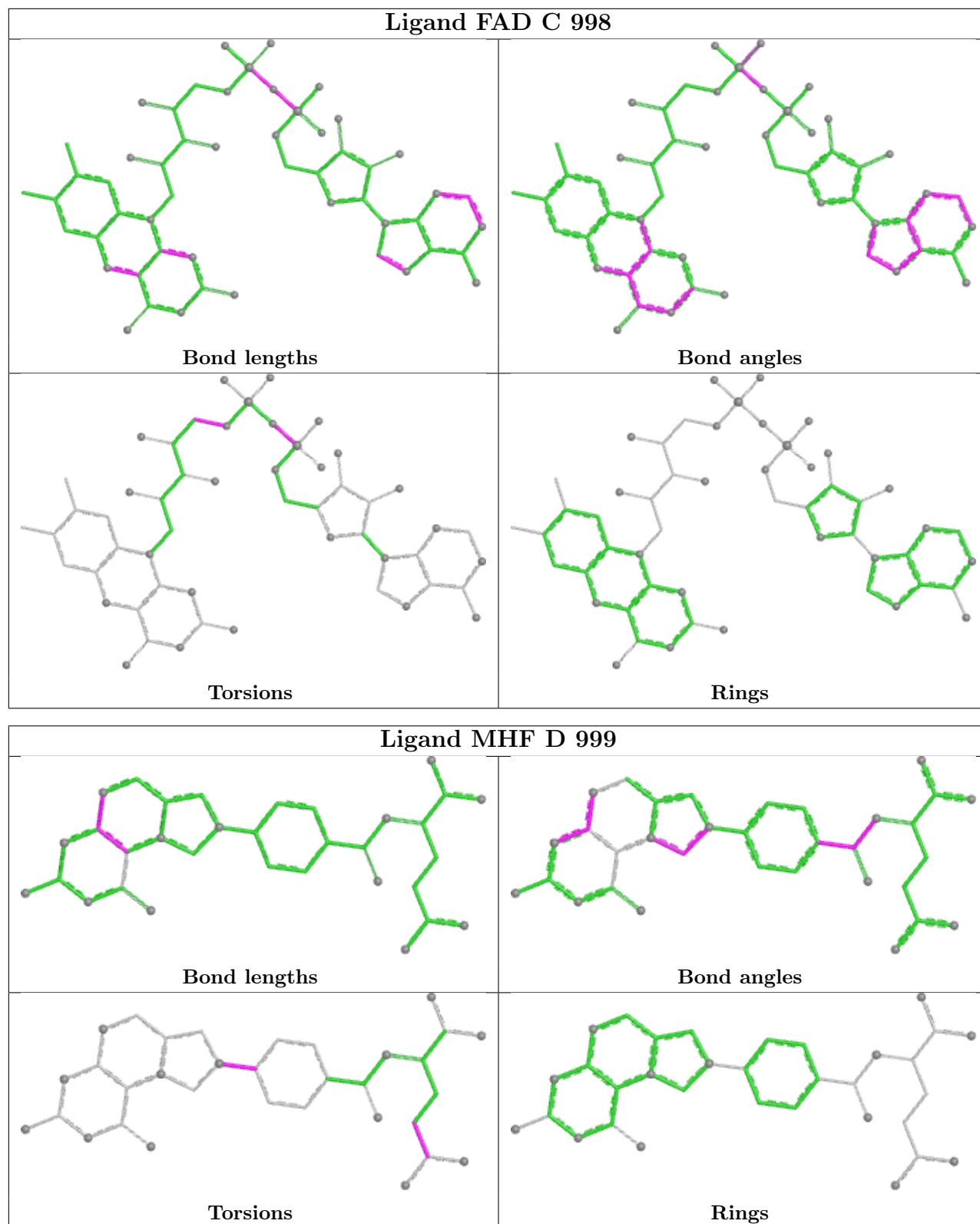
Ligand MHF B 999











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	D	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	37[A]:LYS	C	38:GLY	N	1.05
1	D	35[A]:LYS	C	36:ARG	N	0.90

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	500/526 (95%)	0.41	37 (7%) 20 19	27, 41, 59, 67	1 (0%)
1	C	495/526 (94%)	0.58	37 (7%) 20 19	24, 41, 57, 68	1 (0%)
1	D	478/526 (90%)	0.94	72 (15%) 5 5	30, 41, 57, 64	1 (0%)
1	E	496/526 (94%)	0.49	36 (7%) 21 19	35, 41, 59, 69	0
1	F	480/526 (91%)	0.93	55 (11%) 9 8	30, 41, 56, 65	1 (0%)
2	B	491/525 (93%)	0.86	67 (13%) 7 6	22, 41, 58, 69	1 (0%)
3	G	4/5 (80%)	0.71	1 (25%) 2 1	40, 45, 47, 52	0
3	H	4/5 (80%)	1.50	1 (25%) 2 1	50, 59, 61, 62	0
3	I	4/5 (80%)	0.26	0 100 100	34, 36, 44, 45	0
3	J	4/5 (80%)	0.94	0 100 100	26, 47, 61, 66	1 (25%)
3	K	3/5 (60%)	0.45	0 100 100	40, 40, 40, 49	0
3	L	3/5 (60%)	2.36	3 (100%) 0 0	70, 70, 74, 76	0
All	All	2962/3185 (92%)	0.70	309 (10%) 11 10	22, 41, 58, 76	6 (0%)

The worst 5 of 309 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	442	PRO	7.4
1	A	166	SER	7.3
1	F	30	SER	6.6
1	E	164	GLY	6.5
2	B	483	GLY	6.4

6.2 Non-standard residues in protein, DNA, RNA chains [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	TCP	L	3	18/18	0.71	0.20	72,73,73,73	0
3	TCP	J	3	18/18	0.86	0.13	45,46,50,51	0
3	TCP	H	3	18/18	0.86	0.12	45,46,51,52	0
3	TCP	G	3	18/18	0.92	0.11	37,39,42,43	0
3	TCP	K	3	18/18	0.93	0.10	37,38,39,41	0
3	TCP	I	3	18/18	0.93	0.09	33,34,35,38	0

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.

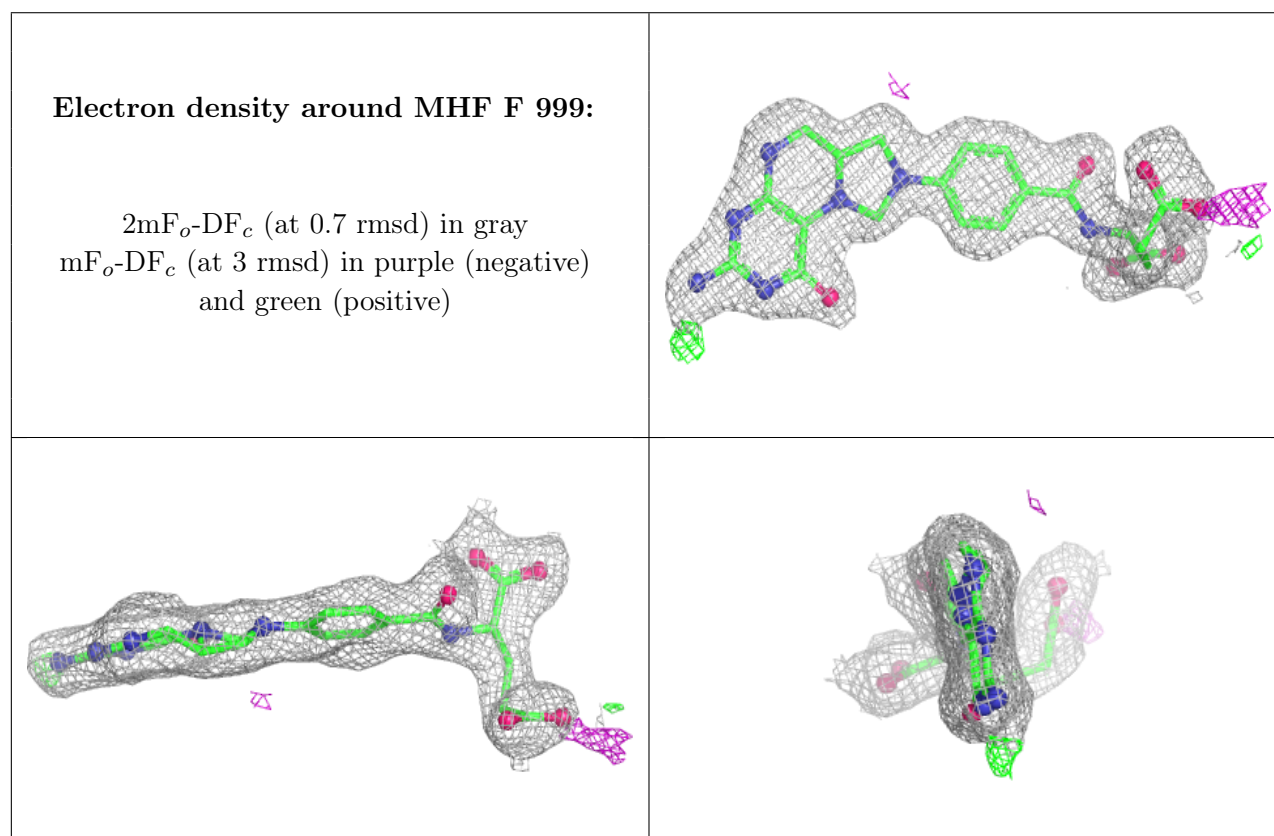
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	ACT	B	1500	4/4	0.65	0.18	63,64,64,64	0
5	MHF	F	999	33/33	0.90	0.09	35,36,44,47	0
6	CL	F	1498	1/1	0.91	0.11	69,69,69,69	0
5	MHF	E	999	33/33	0.91	0.09	35,36,45,48	0
5	MHF	B	999	33/33	0.92	0.09	35,37,44,48	0
5	MHF	D	999	33/33	0.92	0.08	35,37,44,47	0
5	MHF	A	999	33/33	0.93	0.08	35,36,44,47	0
6	CL	B	1499	1/1	0.93	0.10	70,70,70,70	0
4	FAD	F	998	53/53	0.95	0.08	34,34,36,37	0
5	MHF	C	999	33/33	0.95	0.07	34,37,45,49	0
4	FAD	D	998	53/53	0.96	0.07	34,34,36,37	0
4	FAD	B	998	53/53	0.96	0.07	34,35,36,36	0
6	CL	B	1498	1/1	0.96	0.12	52,52,52,52	0
4	FAD	E	998	53/53	0.97	0.06	34,35,37,37	0
4	FAD	C	998	53/53	0.97	0.06	34,35,37,38	0
4	FAD	A	998	53/53	0.97	0.06	34,35,36,37	0
6	CL	C	1500	1/1	0.98	0.14	53,53,53,53	0
6	CL	D	1498	1/1	0.98	0.12	47,47,47,47	0
6	CL	E	1499	1/1	0.99	0.10	44,44,44,44	0
6	CL	A	1501	1/1	0.99	0.12	46,46,46,46	0

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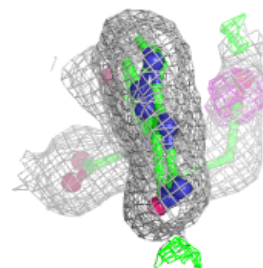
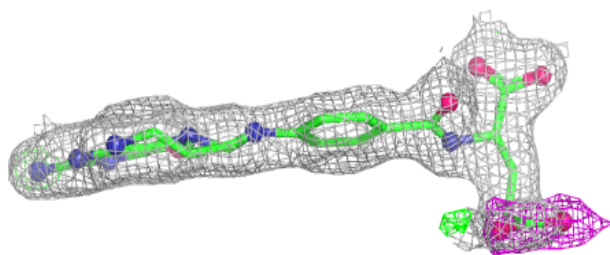
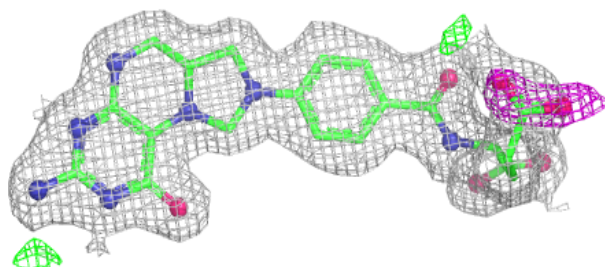
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	CL	C	1499	1/1	0.99	0.10	48,48,48,48	0

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.

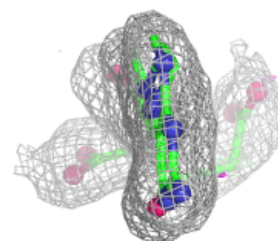
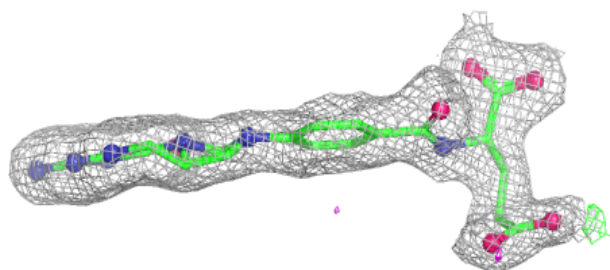
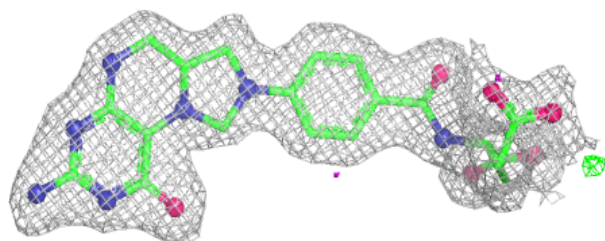


Electron density around MHF E 999:

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

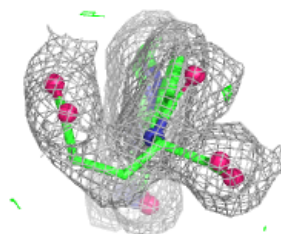
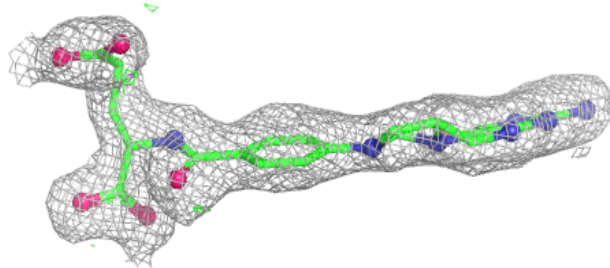
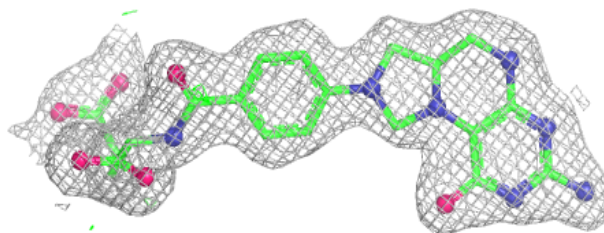
**Electron density around MHF B 999:**

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

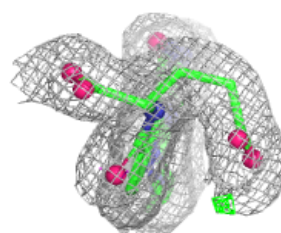
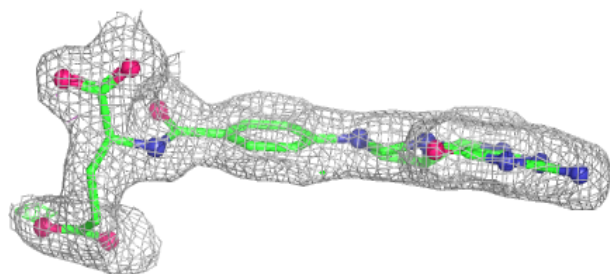
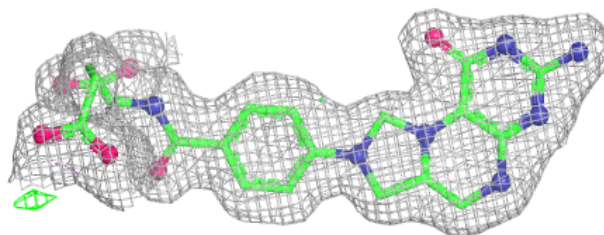


Electron density around MHF D 999:

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

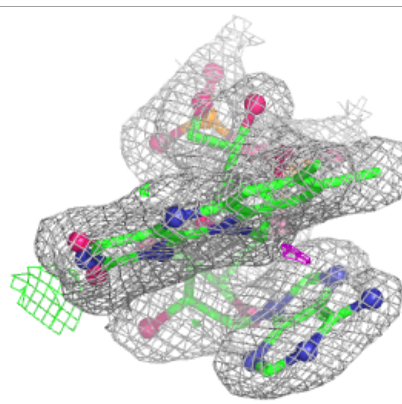
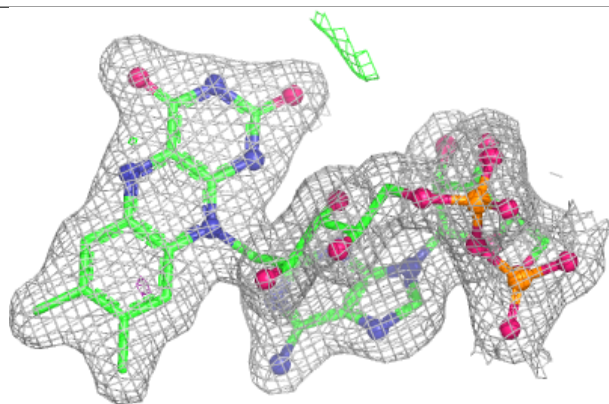
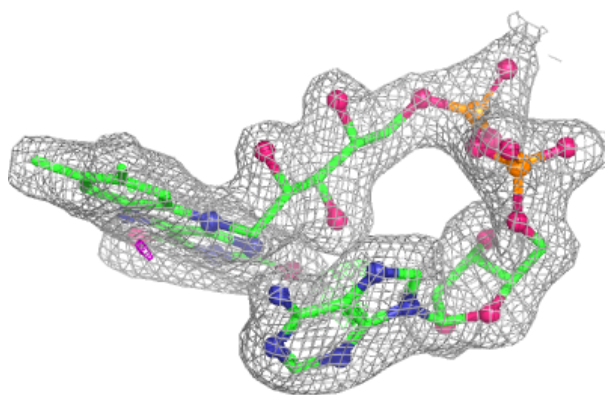
**Electron density around MHF A 999:**

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

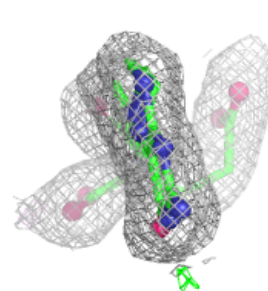
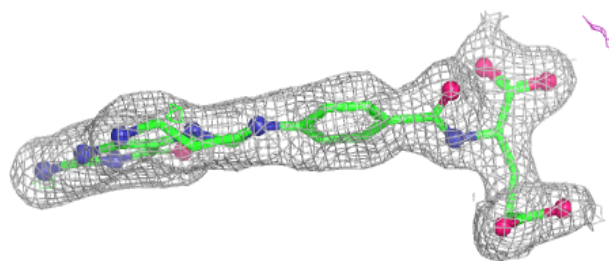
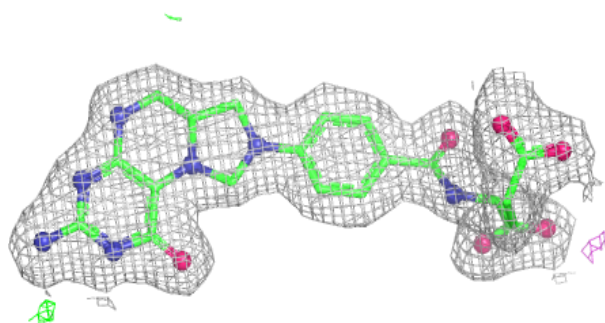


Electron density around FAD F 998:

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

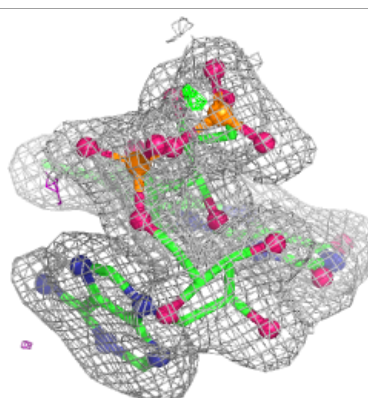
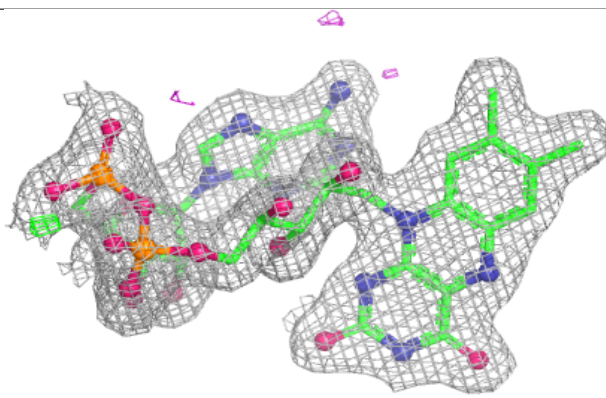
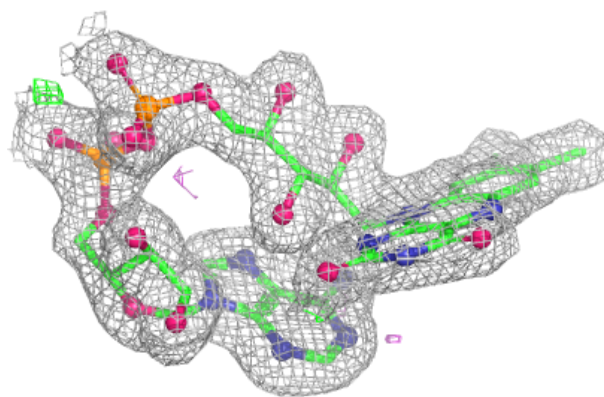
**Electron density around MHF C 999:**

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

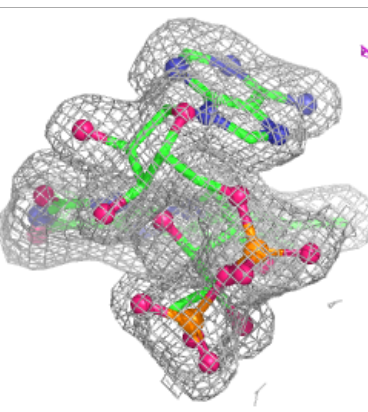
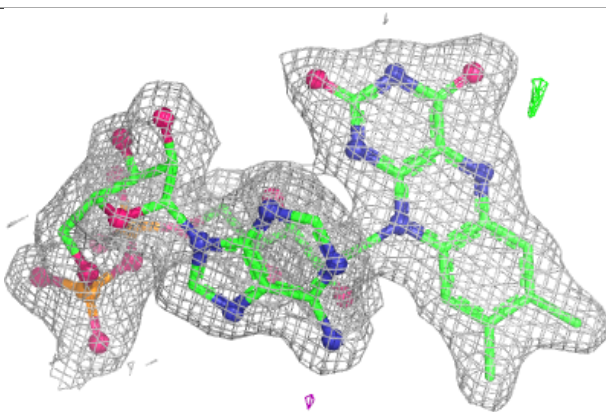
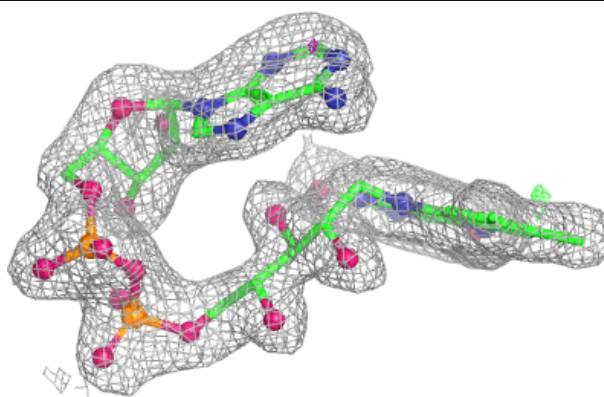


Electron density around FAD D 998:

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

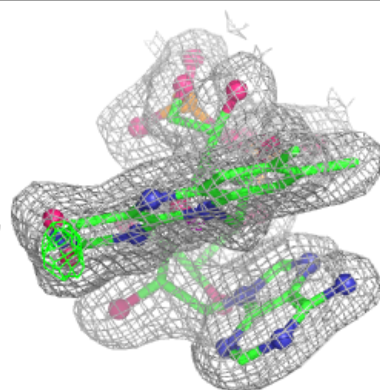
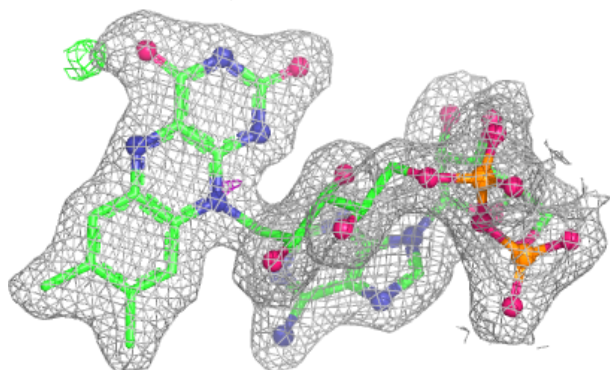
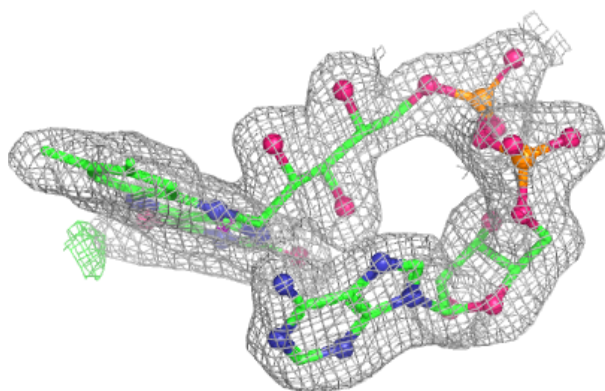
**Electron density around FAD B 998:**

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

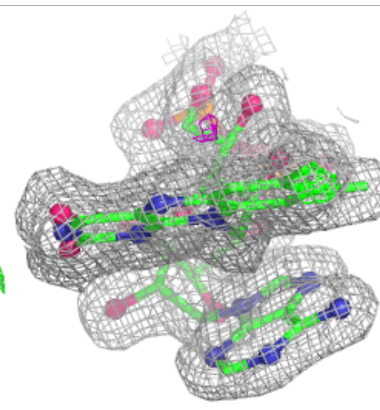
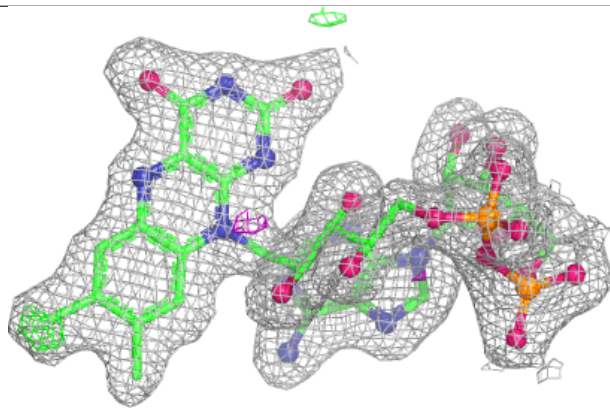
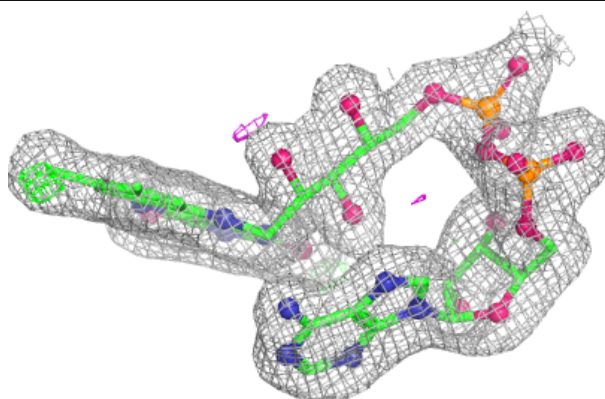


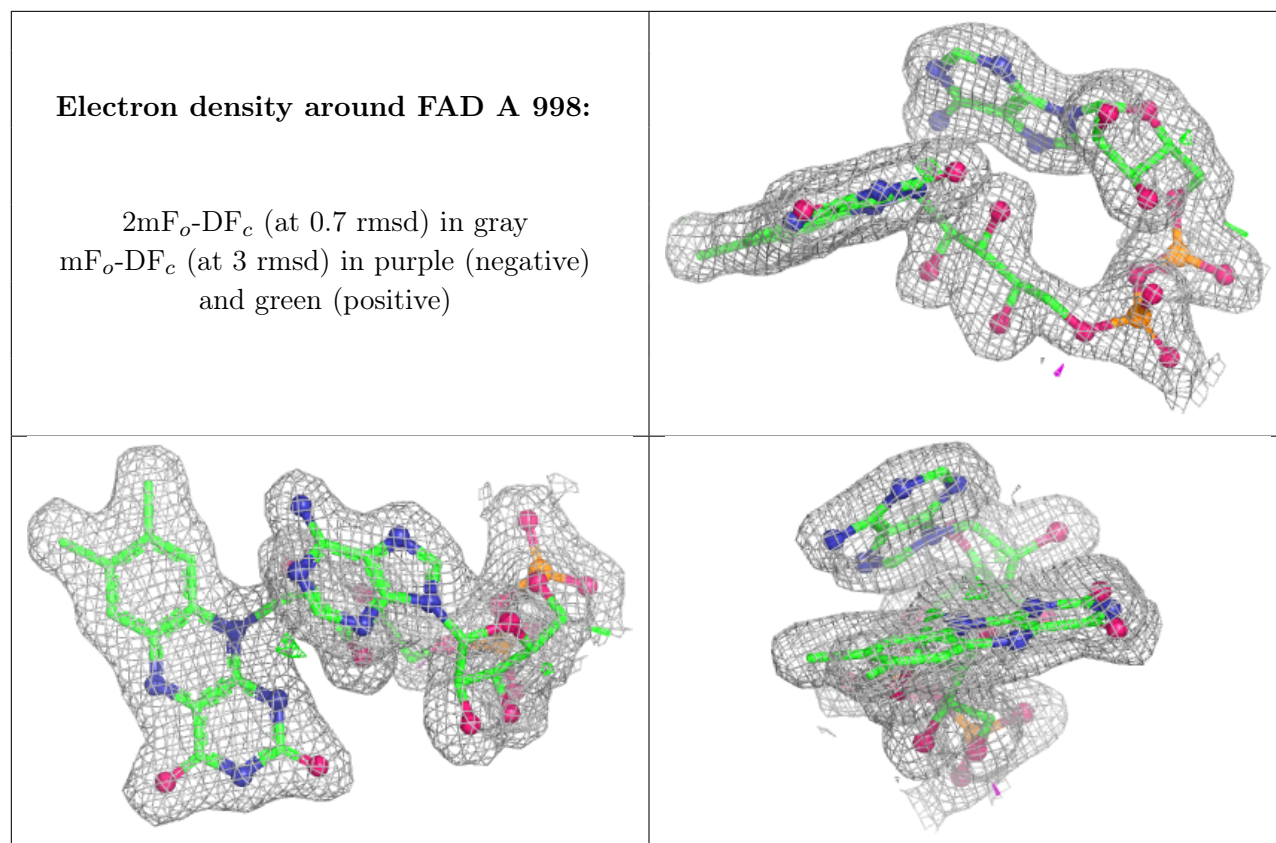
Electron density around FAD E 998:

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

**Electron density around FAD C 998:**

$2mF_o-DF_c$ (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.