Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 09:18 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 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:

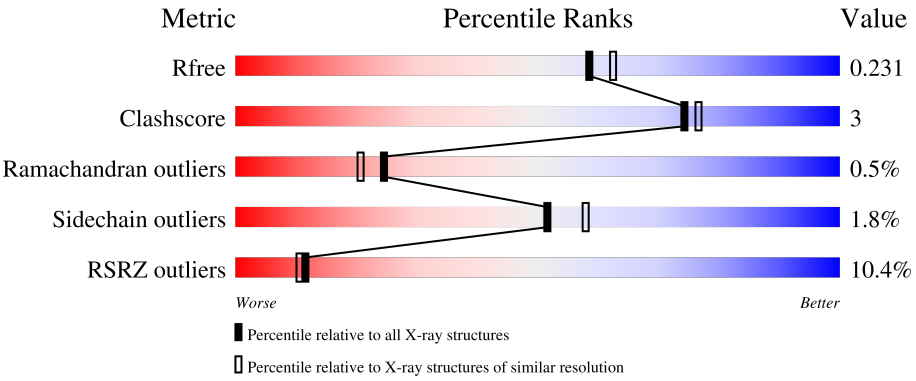
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 (i)

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 <=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	7% 89% 5% • 5%
1	C	526	7% 88% 6% 6%
1	D	526	14% 87% • • 8%
1	E	526	7% 88% 6% • 6%
1	F	526	10% 85% 6% 9%

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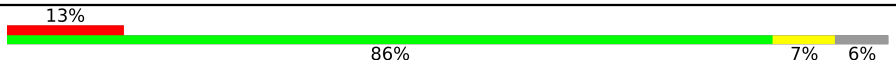
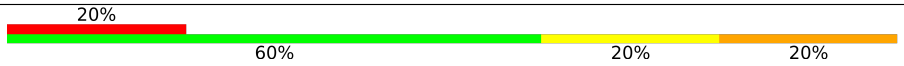
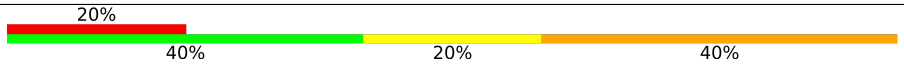
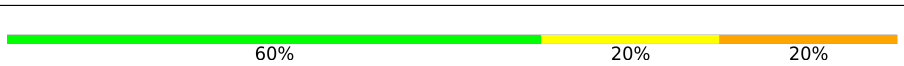
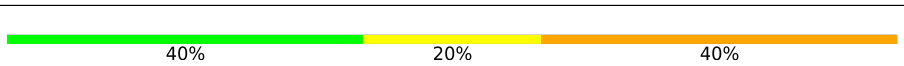
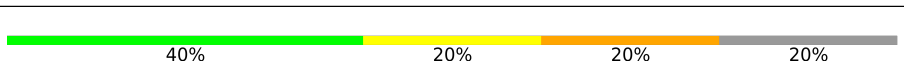
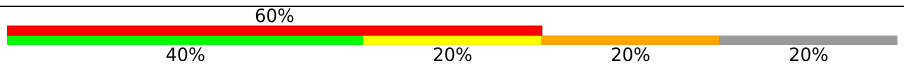
Mol	Chain	Length	Quality of chain
2	B	525	
3	G	5	
3	H	5	
3	I	5	
3	J	5	
3	K	5	
3	L	5	

2 Entry composition (i)

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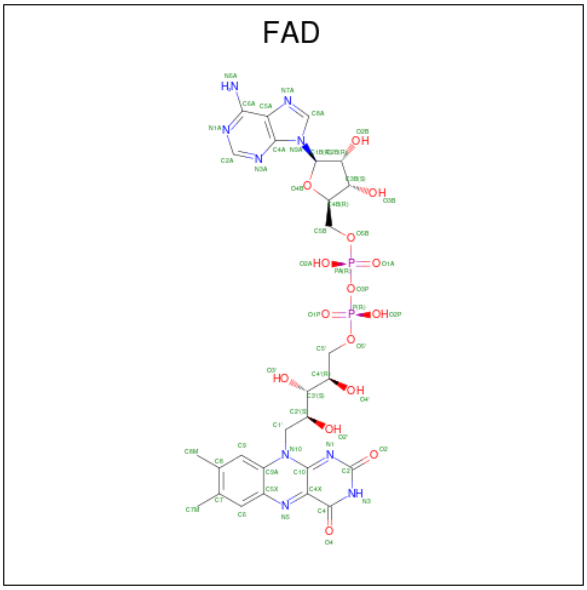
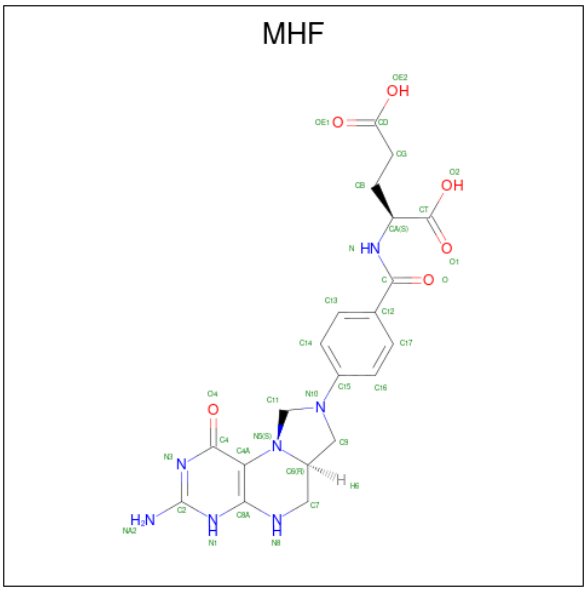
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	J	5	Total	C	N	O	P	9	0	0
			95	51	10	31	3			
3	K	4	Total	C	N	O	P	0	0	0
			78	41	8	26	3			
3	L	4	Total	C	N	O	P	0	0	0
			62	31	6	22	3			

- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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: $C_{20}H_{23}N_7O_6$).

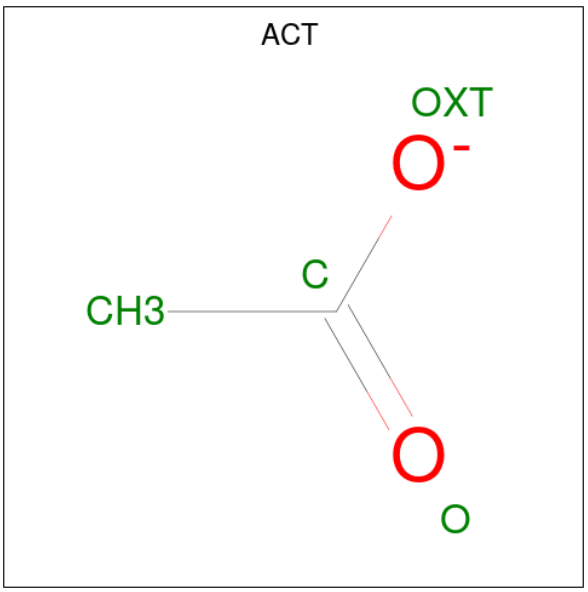


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O 33 20 7 6	0	0
5	B	1	Total C N O 33 20 7 6	0	0
5	C	1	Total C N O 33 20 7 6	0	0
5	D	1	Total C N O 33 20 7 6	0	0
5	E	1	Total C N O 33 20 7 6	0	0
5	F	1	Total C N O 33 20 7 6	0	0

- 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: $C_2H_3O_2$).



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

- Molecule 8 is water.

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

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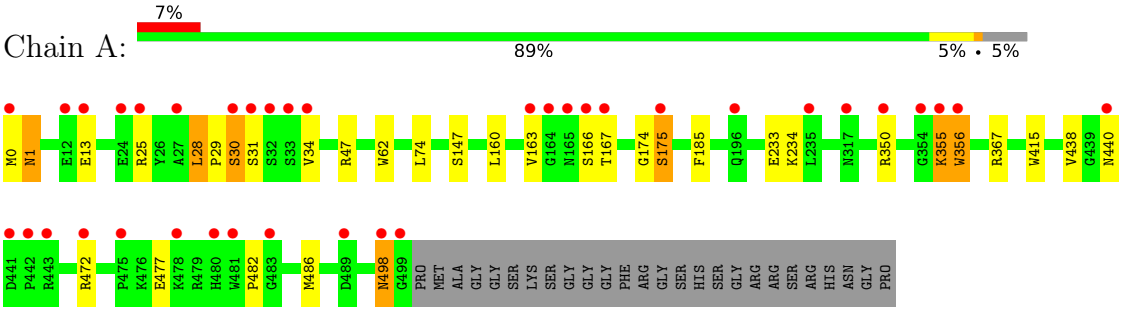
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	K	7	Total O 7 7	0	0
8	L	1	Total O 1 1	0	0

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.

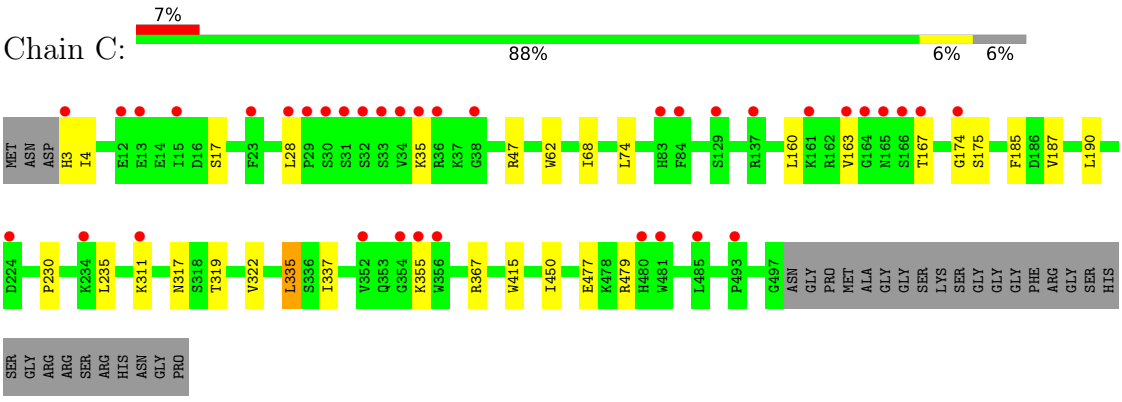
• Molecule 1: CRYPTOCHROME DASH

Chain A:



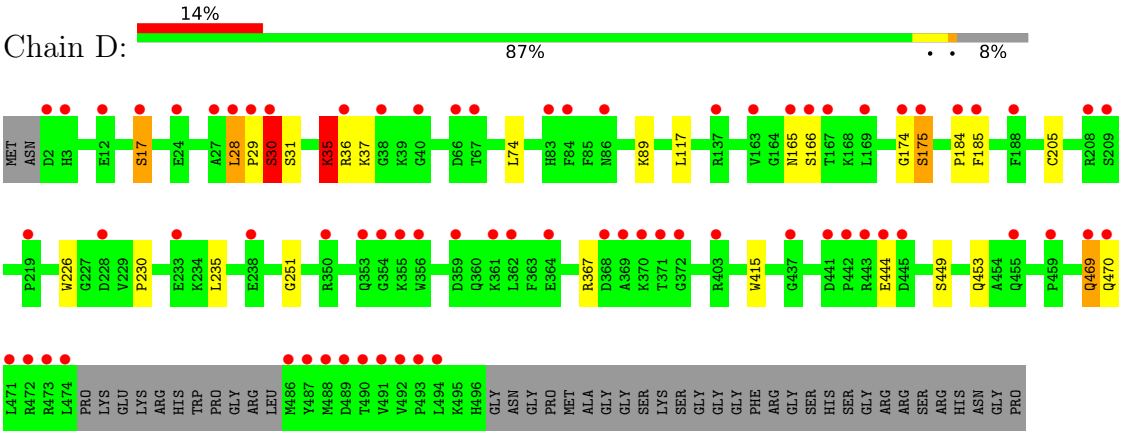
• Molecule 1: CRYPTOCHROME DASH

Chain C:



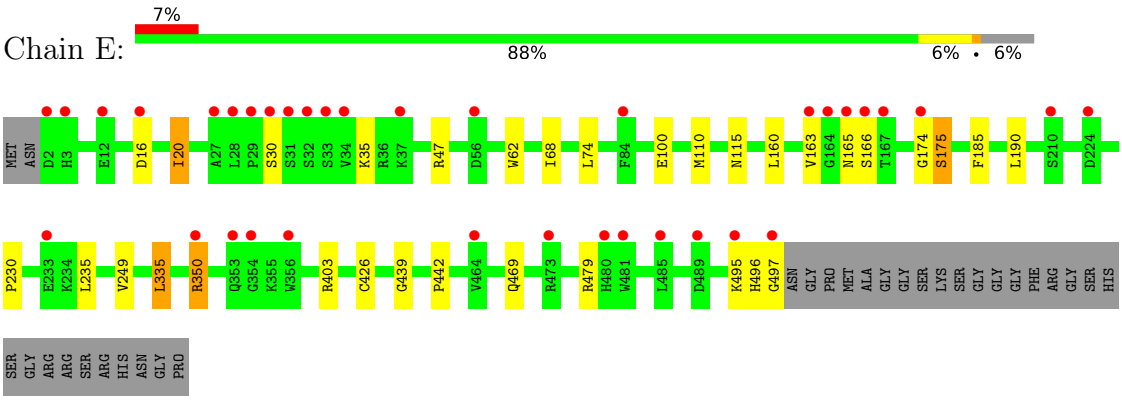
• Molecule 1: CRYPTOCHROME DASH

Chain D:



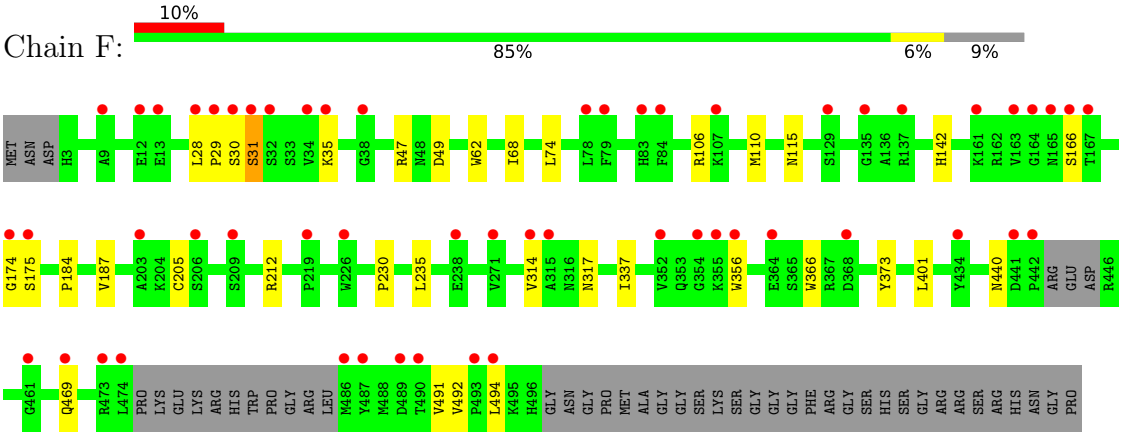
• Molecule 1: CRYPTOCHROME DASH

Chain E:



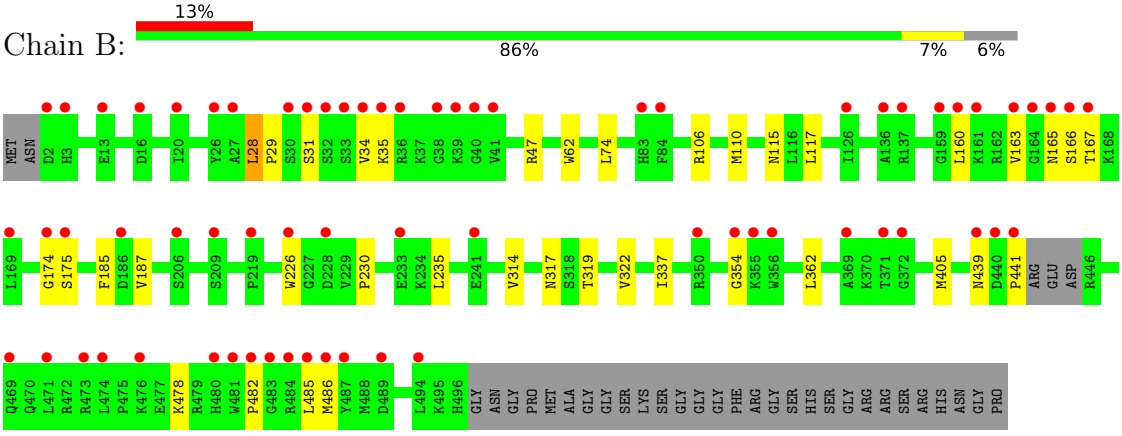
• Molecule 1: CRYPTOCHROME DASH

Chain F:



• Molecule 2: CRYPTOCHROME DASH

Chain B:

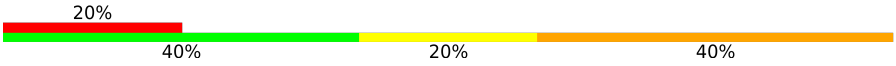


• Molecule 3: 5'-D(*DT*DT*DT*DT*DTP)-3'

Chain G:

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

Chain H:

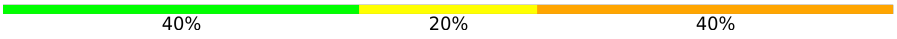


• Molecule 3: 5'-D(*DT*DT*DT*DT*DTP)-3'

Chain I:

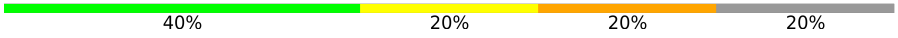
• Molecule 3: 5'-D(*DT*DT*DT*DT*DTP)-3'

Chain J:



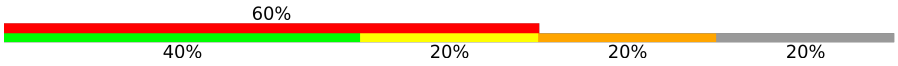
• Molecule 3: 5'-D(*DT*DT*DT*DT*DTP)-3'

Chain K:



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

Chain L:



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	1.94 (at 2.01Å)	Xtriage
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	Xtriage
Anisotropy	0.032	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 52.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
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

Xtriage'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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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
1	D	36	ARG	CA-C-N	12.24	143.14	121.97
1	D	36	ARG	C-N-CA	12.24	143.14	121.97
1	D	36	ARG	O-C-N	-11.07	106.00	122.28
1	D	30	SER	CA-C-N	-8.64	105.03	121.54
1	D	30	SER	C-N-CA	-8.64	105.03	121.54
3	H	1	DT	P-O3'-C3'	7.32	131.18	120.20
1	D	35[A]	LYS	O-C-N	7.14	131.36	123.22
1	D	37[A]	LYS	CA-C-N	5.44	132.24	121.53
1	D	37[A]	LYS	C-N-CA	5.44	132.24	121.53
1	D	251	GLY	N-CA-C	5.23	116.92	111.95

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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.

All (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
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
2:B:47:ARG:HD3	8:B:2049:HOH:O	1.75	0.86
1:D:74:LEU:HD23	1:D:235:LEU:HD21	1.56	0.85
1:E:190:LEU:HD23	1:E:335:LEU:HD13	1.60	0.84
1:C:74:LEU:HD21	1:C:235:LEU:HD11	1.59	0.82
1:D:17:SER:OG	8:D:2004:HOH:O	1.98	0.80
1:F:74:LEU:HD21	1:F:235:LEU:HD11	1.61	0.80
1:E:350:ARG:CZ	1:E:350:ARG:HB2	2.12	0.79
1:C:74:LEU:HD23	1:C:235:LEU:HD21	1.64	0.79
1:E:74:LEU:HD21	1:E:235:LEU:HD11	1.63	0.79
1:D:17:SER:HB3	8:D:2004:HOH:O	1.83	0.78
1:F:110:MET:HE2	1:F:115:ASN:HD21	1.50	0.76
1:C:74:LEU:HD22	1:C:230:PRO:HG3	1.69	0.75
3:I:2:DT:H72	3:I:3:TCP:H71	1.67	0.75
1:F:110:MET:HE2	1:F:115:ASN:ND2	2.01	0.75
1:E:47:ARG:HD3	8:E:2070:HOH:O	1.87	0.73
2:B:28:LEU:HD23	2:B:29:PRO:HD2	1.73	0.71
2:B:160:LEU:HD22	2:B:167:THR:CG2	2.20	0.71
3:J:2:DT:H72	3:J:3:TCP:H71	1.75	0.69
1:F:74:LEU:HD22	1:F:230:PRO:HG3	1.75	0.68
1:A:482:PRO:O	1:A:486:MET:CE	2.42	0.68
2:B:74:LEU:HD22	2:B:230:PRO:HG3	1.77	0.67
2:B:74:LEU:HD22	2:B:230:PRO:CG	2.26	0.67
1:C:74:LEU:CD2	1:C:235:LEU:HD21	2.27	0.65
2:B:439:ASN:HD22	2:B:441:PRO:HD2	1.62	0.65
1:C:74:LEU:HD22	1:C:230:PRO:CG	2.28	0.64
1:F:174:GLY:O	1:F:175:SER:OG	2.16	0.63
2:B:74:LEU:HD23	2:B:235:LEU:HD21	1.79	0.63
1:F:106:ARG:CG	1:F:110:MET:HE3	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:74:LEU:HD21	1:D:235:LEU:CD1	2.24	0.62
1:C:74:LEU:HD21	1:C:235:LEU:CD1	2.29	0.62
2:B:74:LEU:HD21	2:B:235:LEU:CD1	2.29	0.61
1:A:31:SER:O	1:A:34:VAL:HG12	2.01	0.61
1:C:3:HIS:CG	1:C:4:ILE:H	2.19	0.60
1:F:373:TYR:CE1	1:F:494:LEU:HD21	2.36	0.60
1:A:47:ARG:HD3	8:A:2087:HOH:O	2.01	0.60
1:E:74:LEU:HD23	1:E:235:LEU:HD21	1.83	0.60
1:E:190:LEU:CD2	1:E:335:LEU:HD13	2.31	0.59
1:A:160:LEU:HD22	1:A:167:THR:HG21	1.84	0.59
2:B:106:ARG:CG	2:B:110:MET:HE3	2.33	0.59
1:C:47:ARG:HD3	8:C:2070:HOH:O	2.02	0.58
3:G:2:DT:H72	3:G:3:TCP:H72	1.85	0.58
1:F:74:LEU:CD2	1:F:235:LEU:HD21	2.34	0.58
1:E:174:GLY:O	1:E:175:SER:OG	2.17	0.58
1:A:498:ASN:HD22	1:A:498:ASN:N	2.01	0.57
1:F:74:LEU:HD22	1:F:230:PRO:CG	2.32	0.57
1:E:74:LEU:HD22	1:E:230:PRO:CG	2.33	0.57
1:E:350:ARG:CZ	1:E:350:ARG:CB	2.83	0.57
1:A:28:LEU:HD23	1:A:29:PRO:HD2	1.86	0.56
1:A:438:VAL:O	8:A:2243:HOH:O	2.17	0.56
1:D:165:ASN:O	1:D:166:SER:OG	2.13	0.56
1:F:47:ARG:HD3	8:F:2021:HOH:O	2.04	0.56
3:H:2:DT:H72	3:H:3:TCP:H72	1.89	0.55
1:F:74:LEU:HD23	1:F:235:LEU:HD21	1.88	0.54
1:D:174:GLY:O	1:D:175:SER:OG	2.24	0.54
1:C:190:LEU:HD23	1:C:335:LEU:HD13	1.90	0.53
1:E:74:LEU:CD2	1:E:235:LEU:HD21	2.38	0.53
1:F:106:ARG:HG3	1:F:110:MET:HE3	1.90	0.53
1:F:184:PRO:HD3	1:F:205[A]:CYS:SG	2.49	0.53
1:E:160:LEU:O	1:E:163:VAL:HG22	2.09	0.52
1:F:28:LEU:HD23	1:F:29:PRO:HD2	1.91	0.52
2:B:174:GLY:O	2:B:175:SER:OG	2.21	0.52
1:F:74:LEU:HD21	1:F:235:LEU:CD1	2.35	0.52
2:B:160:LEU:O	2:B:163:VAL:HG22	2.10	0.52
2:B:478:LYS:CG	2:B:486:MET:HE1	2.41	0.51
1:F:62:TRP:HA	1:F:68:ILE:HD11	1.90	0.51
3:I:2:DT:H72	3:I:3:TCP:C5M	2.38	0.51
2:B:106:ARG:HG2	2:B:110:MET:HE3	1.92	0.51
1:E:74:LEU:HD22	1:E:230:PRO:HG3	1.91	0.51
1:A:482:PRO:O	1:A:486:MET:HE2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:0:MET:O	1:A:1:ASN:CB	2.59	0.50
1:E:350:ARG:NH2	1:E:439:GLY:O	2.44	0.50
1:D:74:LEU:CD2	1:D:235:LEU:HD21	2.34	0.50
1:E:74:LEU:HD21	1:E:235:LEU:CD1	2.39	0.50
3:K:2:DT:C5	3:K:3:TCP:C5	2.95	0.50
1:E:496:HIS:O	1:E:497:GLY:C	2.54	0.50
1:C:311:LYS:CE	1:E:249:VAL:HG13	2.43	0.49
1:C:311:LYS:HZ3	1:E:100:GLU:CD	2.21	0.49
3:K:2:DT:H72	3:K:3:TCP:H71	1.95	0.48
1:F:49:ASP:OD2	1:F:142:HIS:HD2	1.96	0.48
1:D:74:LEU:CD2	1:D:235:LEU:HD11	2.29	0.48
1:A:482:PRO:O	1:A:486:MET:HE3	2.12	0.47
1:A:147:SER:OG	8:A:2094:HOH:O	2.20	0.47
1:D:367:ARG:HG3	1:D:415:TRP:CE2	2.50	0.47
2:B:439:ASN:ND2	2:B:441:PRO:HD2	2.27	0.47
1:C:160:LEU:O	1:C:163:VAL:HG22	2.15	0.47
1:E:16:ASP:O	1:E:20:ILE:HD13	2.14	0.47
1:A:355:LYS:HG3	1:A:356:TRP:N	2.30	0.46
3:L:2:DT:H72	3:L:3:TCP:H72	1.97	0.46
1:A:160:LEU:HD22	1:A:167:THR:CG2	2.45	0.46
2:B:319:THR:O	2:B:322:VAL:HG12	2.15	0.46
1:D:184:PRO:HD3	1:D:205[A]:CYS:SG	2.56	0.46
1:D:444:GLU:OE1	3:J:1:DT:H1'	2.15	0.46
1:C:367:ARG:HG3	1:C:415:TRP:CE2	2.51	0.46
1:E:174:GLY:O	1:E:175:SER:CB	2.64	0.46
1:E:190:LEU:HD23	1:E:335:LEU:CD1	2.38	0.46
2:B:362:LEU:HD22	2:B:405:MET:HE2	1.98	0.46
1:C:62:TRP:HA	1:C:68:ILE:HD11	1.97	0.45
1:F:28:LEU:HD22	1:F:30:SER:O	2.16	0.45
1:A:367:ARG:HG3	1:A:415:TRP:CE2	2.51	0.45
2:B:74:LEU:CD2	2:B:235:LEU:HD21	2.46	0.45
1:C:311:LYS:NZ	1:E:249:VAL:HG13	2.32	0.45
1:A:74:LEU:C	1:A:74:LEU:HD13	2.42	0.44
1:F:366:TRP:CD2	1:F:401:LEU:HD12	2.52	0.44
1:C:319:THR:O	1:C:322:VAL:HG12	2.17	0.44
1:A:160:LEU:O	1:A:163:VAL:HG22	2.17	0.44
2:B:74:LEU:HD22	2:B:230:PRO:HG2	1.97	0.44
1:F:187:VAL:HG21	1:F:337:ILE:HG21	2.00	0.44
2:B:478:LYS:CD	2:B:486:MET:HE1	2.47	0.44
3:G:2:DT:H72	3:G:3:TCP:C5M	2.47	0.44
2:B:28:LEU:HD23	2:B:29:PRO:CD	2.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:117:LEU:HD12	2:B:226:TRP:HA	2.00	0.43
3:I:2:DT:C5	3:I:3:TCP:C5	3.01	0.43
2:B:34:VAL:HG13	2:B:34:VAL:O	2.17	0.43
1:C:174:GLY:O	1:C:175:SER:OG	2.32	0.43
1:C:187:VAL:HG21	1:C:337:ILE:HG21	2.00	0.43
1:A:174:GLY:O	1:A:175:SER:HB2	2.19	0.43
3:J:2:DT:H72	3:J:3:TCP:C5M	2.47	0.43
1:D:469:GLN:HE21	1:D:469:GLN:HB3	1.71	0.43
1:C:190:LEU:HD23	1:C:335:LEU:CD1	2.49	0.43
1:D:74:LEU:HD22	1:D:230:PRO:CG	2.48	0.43
1:E:350:ARG:CZ	1:E:442:PRO:HG3	2.48	0.43
1:A:350:ARG:HB3	1:A:440:ASN:OD1	2.18	0.43
1:F:491:VAL:HG13	1:F:492:VAL:HG22	2.00	0.43
3:L:2:DT:H72	3:L:3:TCP:C5M	2.49	0.43
1:A:34:VAL:HG13	1:A:34:VAL:O	2.19	0.42
2:B:110:MET:HE2	2:B:115:ASN:ND2	2.34	0.42
1:E:165:ASN:O	1:E:166:SER:OG	2.22	0.42
2:B:165:ASN:O	2:B:166:SER:OG	2.29	0.42
1:F:28:LEU:HD23	1:F:29:PRO:CD	2.49	0.42
3:G:2:DT:C7	3:G:3:TCP:H72	2.50	0.42
3:H:2:DT:H72	3:H:3:TCP:C5M	2.49	0.42
1:A:29:PRO:O	1:A:30:SER:O	2.38	0.41
1:E:110:MET:HE2	1:E:115:ASN:ND2	2.35	0.41
1:E:426:CYS:SG	8:E:2210:HOH:O	2.62	0.41
2:B:34:VAL:HG11	2:B:62:TRP:CZ3	2.56	0.41
1:C:3:HIS:CG	1:C:4:ILE:N	2.85	0.41
2:B:187:VAL:HG21	2:B:337:ILE:HG21	2.03	0.41
1:E:62:TRP:HA	1:E:68:ILE:HD11	2.02	0.41
1:A:355:LYS:CG	1:A:356:TRP:N	2.83	0.41
1:D:28:LEU:HD23	1:D:29:PRO:HD2	2.03	0.41
1:F:30:SER:OG	1:F:31:SER:N	2.54	0.41
1:D:449:SER:O	1:D:453:GLN:HG2	2.20	0.41
2:B:439:ASN:ND2	2:B:441:PRO:HG2	2.36	0.40
1:D:117:LEU:HD12	1:D:226:TRP:HA	2.03	0.40
1:D:89:LYS:NZ	8:D:2038:HOH:O	2.54	0.40
2:B:115:ASN:HB3	2:B:226:TRP:CZ3	2.56	0.40
3:H:1:DT:H4'	3:H:2:DT:OP2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	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

All (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
2	B	31	SER
1	D	30	SER
2	B	482	PRO
1	E	175	SER
1	F	31	SER
1	A	175	SER
2	B	354	GLY
1	F	356	TRP
1	A	166	SER
1	D	175	SER
1	F	166	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	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

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

Mol	Chain	Res	Type
1	A	13	GLU
1	A	25	ARG
1	A	28	LEU
1	A	185	PHE
1	A	233	GLU
1	A	234	LYS
1	A	472	ARG
1	A	477	GLU
1	A	498	ASN
2	B	28	LEU
2	B	35	LYS
2	B	185	PHE
2	B	314	VAL
2	B	317	ASN
2	B	485	LEU
1	C	17	SER
1	C	28	LEU
1	C	35	LYS
1	C	167	THR
1	C	185	PHE
1	C	317	ASN
1	C	335	LEU

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Mol	Chain	Res	Type
1	C	355	LYS
1	C	477	GLU
1	C	479	ARG
1	D	17	SER
1	D	28	LEU
1	D	31[A]	SER
1	D	35[A]	LYS
1	D	185	PHE
1	D	469	GLN
1	D	470	GLN
1	E	20	ILE
1	E	35	LYS
1	E	185	PHE
1	E	335	LEU
1	E	350	ARG
1	E	403	ARG
1	E	469	GLN
1	E	479	ARG
1	E	495	LYS
1	F	35	LYS
1	F	212	ARG
1	F	314	VAL
1	F	317	ASN
1	F	440	ASN
1	F	469	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	240	GLN
1	A	428	ASN
1	A	498	ASN
2	B	428	ASN
2	B	456	ASN
1	C	428	ASN
1	C	480	HIS
1	D	428	ASN
1	D	469	GLN
1	E	157	ASN
1	E	428	ASN
1	E	440	ASN
1	F	142	HIS

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Mol	Chain	Res	Type
1	F	428	ASN
1	F	469	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	TCP	H	3	3	-	3/7/19/19	0/2/2/2

All (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
3	K	3	TCP	O5'-CP	3.51	1.59	1.42

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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
3	L	3	TCP	O4'-C1'-N1	4.69	116.19	107.86
3	K	3	TCP	C4'-O4'-C1'	-2.99	102.41	109.51
3	I	3	TCP	O4-C4-C5	-2.67	121.87	124.92
3	I	3	TCP	C4'-O4'-C1'	-2.55	103.45	109.51
3	J	3	TCP	C4'-O4'-C1'	-2.43	103.73	109.51
3	G	3	TCP	C4'-O4'-C1'	-2.33	103.97	109.51
3	L	3	TCP	O4-C4-C5	-2.31	122.28	124.92
3	H	3	TCP	C4'-O4'-C1'	-2.23	104.21	109.51
3	I	3	TCP	O4'-C1'-C2'	-2.12	102.28	106.25
3	J	3	TCP	O4-C4-C5	-2.12	122.49	124.92
3	J	3	TCP	O4'-C1'-C2'	-2.12	102.28	106.25
3	G	3	TCP	O4-C4-C5	-2.06	122.56	124.92
3	L	3	TCP	C4'-O4'-C1'	-2.01	104.74	109.51

There are no chirality outliers.

All (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

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Mol	Chain	Res	Type	Atoms
3	H	3	TCP	O4'-C1'-N1-C6
3	G	3	TCP	C2'-C1'-N1-C6
3	G	3	TCP	O4'-C1'-N1-C6
3	J	3	TCP	O4'-C1'-N1-C6
3	J	3	TCP	C2'-C1'-N1-C6
3	L	3	TCP	C2'-C1'-N1-C2
3	L	3	TCP	O4'-C1'-N1-C2
3	I	3	TCP	O4'-C1'-N1-C6
3	H	3	TCP	O4'-C1'-N1-C2
3	I	3	TCP	C2'-C1'-N1-C6
3	K	3	TCP	O4'-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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
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

All (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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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
5	D	999	MHF	C8A-N8	3.79	1.36	1.32
4	A	998	FAD	C4X-N5	3.77	1.38	1.30
4	F	998	FAD	C4X-N5	3.70	1.38	1.30
5	E	999	MHF	C8A-N8	3.55	1.36	1.32
5	A	999	MHF	C4A-C8A	3.42	1.48	1.37
5	F	999	MHF	C8A-N8	3.41	1.35	1.32
5	C	999	MHF	C4A-C8A	3.38	1.48	1.37
5	B	999	MHF	C8A-N8	3.38	1.35	1.32
4	E	998	FAD	P-O3P	3.23	1.63	1.59
5	B	999	MHF	C4A-C8A	3.23	1.48	1.37
5	E	999	MHF	C4A-C8A	3.20	1.48	1.37
5	F	999	MHF	C4A-C8A	3.20	1.48	1.37
5	D	999	MHF	C4A-C8A	3.11	1.47	1.37
5	A	999	MHF	C8A-N8	3.09	1.35	1.32
4	E	998	FAD	C2A-N3A	2.88	1.39	1.33
4	B	998	FAD	C10-N1	2.87	1.39	1.33
4	E	998	FAD	PA-O3P	2.83	1.62	1.59
4	C	998	FAD	C2A-N3A	2.80	1.38	1.33
4	E	998	FAD	C10-N1	2.79	1.38	1.33
4	D	998	FAD	C10-N1	2.72	1.38	1.33
4	C	998	FAD	C2A-N1A	2.70	1.38	1.33
4	E	998	FAD	C2A-N1A	2.69	1.38	1.33
4	A	998	FAD	P-O3P	2.69	1.62	1.59
4	F	998	FAD	C2A-N1A	2.62	1.38	1.33
4	D	998	FAD	PA-O3P	2.61	1.62	1.59
4	A	998	FAD	C2A-N3A	2.58	1.38	1.33
4	B	998	FAD	C2A-N1A	2.56	1.38	1.33
4	F	998	FAD	C2A-N3A	2.55	1.38	1.33
4	C	998	FAD	C10-N1	2.50	1.38	1.33
4	C	998	FAD	P-O3P	2.49	1.62	1.59
4	D	998	FAD	P-O3P	2.46	1.62	1.59
4	A	998	FAD	C10-N1	2.46	1.38	1.33
4	F	998	FAD	C10-N1	2.43	1.38	1.33
4	F	998	FAD	C8A-N7A	2.33	1.36	1.31
4	D	998	FAD	C2A-N1A	2.33	1.38	1.33
4	D	998	FAD	C2A-N3A	2.30	1.38	1.33
4	A	998	FAD	PA-O3P	2.30	1.62	1.59
5	A	999	MHF	C8A-N1	-2.29	1.33	1.37
4	A	998	FAD	C2A-N1A	2.29	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	998	FAD	C2A-N3A	2.22	1.37	1.33
4	B	998	FAD	P-O3P	2.19	1.61	1.59
4	D	998	FAD	C8A-N7A	2.19	1.35	1.31
4	C	998	FAD	C8A-N7A	2.14	1.35	1.31
4	C	998	FAD	PA-O3P	2.13	1.61	1.59
4	B	998	FAD	C8A-N7A	2.10	1.35	1.31
5	C	999	MHF	C8A-N1	-2.09	1.33	1.37
4	B	998	FAD	C5A-N7A	-2.03	1.35	1.39

All (105) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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
4	F	998	FAD	N3A-C2A-N1A	-5.22	120.69	128.58
4	E	998	FAD	C5A-C4A-N3A	-4.62	120.36	126.72
5	B	999	MHF	N5-C11-N10	-4.58	96.89	103.37
5	F	999	MHF	N5-C11-N10	-4.54	96.95	103.37
4	B	998	FAD	N9A-C8A-N7A	-4.20	107.98	113.94
5	E	999	MHF	N5-C11-N10	-4.15	97.50	103.37
5	D	999	MHF	N5-C11-N10	-4.08	97.60	103.37
4	A	998	FAD	C5A-C4A-N3A	-4.03	121.17	126.72
5	A	999	MHF	N5-C11-N10	-3.99	97.72	103.37
4	F	998	FAD	C5A-C4A-N3A	-3.96	121.26	126.72
4	D	998	FAD	C5A-C4A-N3A	-3.94	121.29	126.72
4	F	998	FAD	N9A-C8A-N7A	-3.92	108.38	113.94
5	C	999	MHF	N5-C11-N10	-3.88	97.87	103.37
4	B	998	FAD	C5A-C4A-N3A	-3.82	121.45	126.72
4	A	998	FAD	C4X-C10-N10	3.73	121.82	116.48
4	D	998	FAD	C4X-C10-N10	3.65	121.70	116.48
4	F	998	FAD	C4X-C10-N10	3.64	121.70	116.48
4	A	998	FAD	N9A-C8A-N7A	-3.60	108.83	113.94
4	C	998	FAD	C5A-C4A-N3A	-3.55	121.83	126.72
4	E	998	FAD	N9A-C8A-N7A	-3.45	109.05	113.94
4	B	998	FAD	C4-N3-C2	-3.42	119.57	125.64
4	D	998	FAD	N9A-C8A-N7A	-3.41	109.09	113.94
4	E	998	FAD	C5A-N7A-C8A	3.37	108.75	103.45
4	F	998	FAD	C4-N3-C2	-3.34	119.71	125.64
4	D	998	FAD	C4-N3-C2	-3.32	119.74	125.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	998	FAD	C5A-N7A-C8A	3.30	108.64	103.45
4	E	998	FAD	C2A-N3A-C4A	3.28	119.85	111.83
4	C	998	FAD	C4X-C10-N10	3.28	121.18	116.48
4	E	998	FAD	C4-N3-C2	-3.24	119.88	125.64
4	A	998	FAD	C5A-N7A-C8A	3.23	108.52	103.45
4	E	998	FAD	C4X-C10-N10	3.22	121.09	116.48
4	F	998	FAD	C5A-N7A-C8A	3.21	108.50	103.45
4	B	998	FAD	C2A-N3A-C4A	3.11	119.43	111.83
4	D	998	FAD	C5A-N7A-C8A	3.11	108.34	103.45
4	A	998	FAD	C2A-N3A-C4A	3.09	119.39	111.83
4	A	998	FAD	C4-N3-C2	-3.08	120.17	125.64
4	C	998	FAD	O2P-P-O3P	3.08	115.59	107.27
4	B	998	FAD	C4X-C10-N10	3.06	120.86	116.48
4	D	998	FAD	C2A-N3A-C4A	3.05	119.28	111.83
4	C	998	FAD	N9A-C8A-N7A	-3.03	109.64	113.94
4	F	998	FAD	C2A-N3A-C4A	3.01	119.19	111.83
4	D	998	FAD	C4X-C4-N3	3.00	120.88	113.25
4	B	998	FAD	C4X-C4-N3	2.91	120.67	113.25
5	A	999	MHF	C12-C-N	2.88	122.38	117.04
5	B	999	MHF	C12-C-N	2.87	122.36	117.04
4	D	998	FAD	C4-C4X-N5	2.84	122.14	118.21
4	A	998	FAD	C10-C4X-N5	-2.82	119.05	124.81
4	B	998	FAD	O2P-P-O3P	2.80	114.85	107.27
4	F	998	FAD	C10-C4X-N5	-2.80	119.09	124.81
4	E	998	FAD	C4A-C5A-N7A	-2.77	107.42	110.58
4	E	998	FAD	C10-C4X-N5	-2.76	119.17	124.81
4	E	998	FAD	N3A-C4A-N9A	2.76	131.86	127.17
5	C	999	MHF	C12-C-N	2.74	122.12	117.04
4	C	998	FAD	C5A-N7A-C8A	2.67	107.64	103.45
4	C	998	FAD	C2A-N3A-C4A	2.67	118.34	111.83
5	D	999	MHF	N1-C8A-N8	2.65	122.25	117.28
4	D	998	FAD	C10-C4X-N5	-2.65	119.40	124.81
4	C	998	FAD	C4-N3-C2	-2.64	120.95	125.64
4	E	998	FAD	C4X-C4-N3	2.63	119.96	113.25
4	E	998	FAD	O2P-P-O3P	2.63	114.39	107.27
4	B	998	FAD	C10-C4X-N5	-2.62	119.46	124.81
4	F	998	FAD	C4X-C4-N3	2.61	119.89	113.25
5	D	999	MHF	C12-C-N	2.59	121.84	117.04
4	B	998	FAD	N3A-C4A-N9A	2.56	131.52	127.17
4	C	998	FAD	C10-C4X-N5	-2.54	119.62	124.81
5	E	999	MHF	C12-C-N	2.53	121.73	117.04
4	A	998	FAD	N3A-C4A-N9A	2.53	131.47	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	998	FAD	C4A-C5A-N7A	-2.46	107.76	110.58
4	D	998	FAD	C4A-C5A-N7A	-2.46	107.77	110.58
4	A	998	FAD	C4X-C4-N3	2.46	119.51	113.25
4	F	998	FAD	O2P-P-O3P	2.46	113.92	107.27
4	B	998	FAD	C4A-N9A-C8A	2.42	108.28	105.74
4	A	998	FAD	C4-C4X-N5	2.35	121.45	118.21
4	F	998	FAD	N3A-C4A-N9A	2.35	131.16	127.17
5	B	999	MHF	N1-C8A-N8	2.34	121.67	117.28
4	C	998	FAD	C4X-C4-N3	2.31	119.14	113.25
5	F	999	MHF	N1-C8A-N8	2.29	121.58	117.28
5	F	999	MHF	C12-C-N	2.29	121.28	117.04
4	B	998	FAD	C4-C4X-N5	2.28	121.35	118.21
4	F	998	FAD	C4A-C5A-N7A	-2.25	108.00	110.58
4	B	998	FAD	C9A-C5X-N5	-2.25	120.06	122.45
4	F	998	FAD	C4-C4X-N5	2.25	121.32	118.21
4	D	998	FAD	O2P-P-O3P	2.24	113.34	107.27
5	C	999	MHF	N1-C8A-N8	2.24	121.48	117.28
4	E	998	FAD	C6A-C5A-C4A	2.23	120.23	117.18
4	B	998	FAD	C4A-C5A-N7A	-2.20	108.07	110.58
4	D	998	FAD	N3A-C4A-N9A	2.19	130.89	127.17
4	E	998	FAD	C4-C4X-N5	2.18	121.21	118.21
4	C	998	FAD	C4A-C5A-N7A	-2.17	108.10	110.58
5	A	999	MHF	O2-CT-CA	2.17	120.85	113.51
4	A	998	FAD	O2P-P-O3P	2.15	113.10	107.27
4	F	998	FAD	C4X-C10-N1	-2.15	119.31	124.59
5	E	999	MHF	N1-C8A-N8	2.13	121.29	117.28
4	B	998	FAD	C4X-C10-N1	-2.13	119.36	124.59
5	C	999	MHF	O2-CT-CA	2.11	120.66	113.51
5	A	999	MHF	N1-C8A-N8	2.11	121.24	117.28
4	E	998	FAD	C9A-C5X-N5	-2.08	120.25	122.45
4	B	998	FAD	C5X-C9A-N10	2.04	119.81	117.97
4	E	998	FAD	C1'-C2'-C3'	2.03	115.17	109.66
4	D	998	FAD	C5X-C9A-N10	2.03	119.80	117.97

There are no chirality outliers.

All (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

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Mol	Chain	Res	Type	Atoms
5	B	999	MHF	C16-C15-N10-C9
5	D	999	MHF	C14-C15-N10-C9
5	D	999	MHF	C16-C15-N10-C9
5	F	999	MHF	C14-C15-N10-C9
5	B	999	MHF	C14-C15-N10-C9
5	C	999	MHF	C16-C15-N10-C9
5	E	999	MHF	C14-C15-N10-C9
5	E	999	MHF	C16-C15-N10-C9
4	D	998	FAD	P-O3P-PA-O1A
5	E	999	MHF	OE1-CD-CG-CB
5	A	999	MHF	OE1-CD-CG-CB
5	F	999	MHF	OE2-CD-CG-CB
5	F	999	MHF	OE1-CD-CG-CB
5	D	999	MHF	OE1-CD-CG-CB
4	A	998	FAD	C4'-C5'-O5'-P
4	E	998	FAD	C4'-C5'-O5'-P
5	B	999	MHF	OE1-CD-CG-CB
5	C	999	MHF	OE1-CD-CG-CB
5	E	999	MHF	OE2-CD-CG-CB
5	A	999	MHF	OE2-CD-CG-CB
5	D	999	MHF	OE2-CD-CG-CB
5	C	999	MHF	OE2-CD-CG-CB
4	B	998	FAD	P-O3P-PA-O1A
4	B	998	FAD	C4'-C5'-O5'-P
4	C	998	FAD	C4'-C5'-O5'-P
4	D	998	FAD	C4'-C5'-O5'-P
4	F	998	FAD	C4'-C5'-O5'-P
5	B	999	MHF	OE2-CD-CG-CB
5	A	999	MHF	CA-CB-CG-CD
4	A	998	FAD	P-O3P-PA-O2A
4	E	998	FAD	P-O3P-PA-O1A
4	F	998	FAD	P-O3P-PA-O1A
4	C	998	FAD	P-O3P-PA-O1A
4	C	998	FAD	P-O3P-PA-O2A
4	D	998	FAD	P-O3P-PA-O2A
4	E	998	FAD	P-O3P-PA-O2A
4	F	998	FAD	P-O3P-PA-O2A

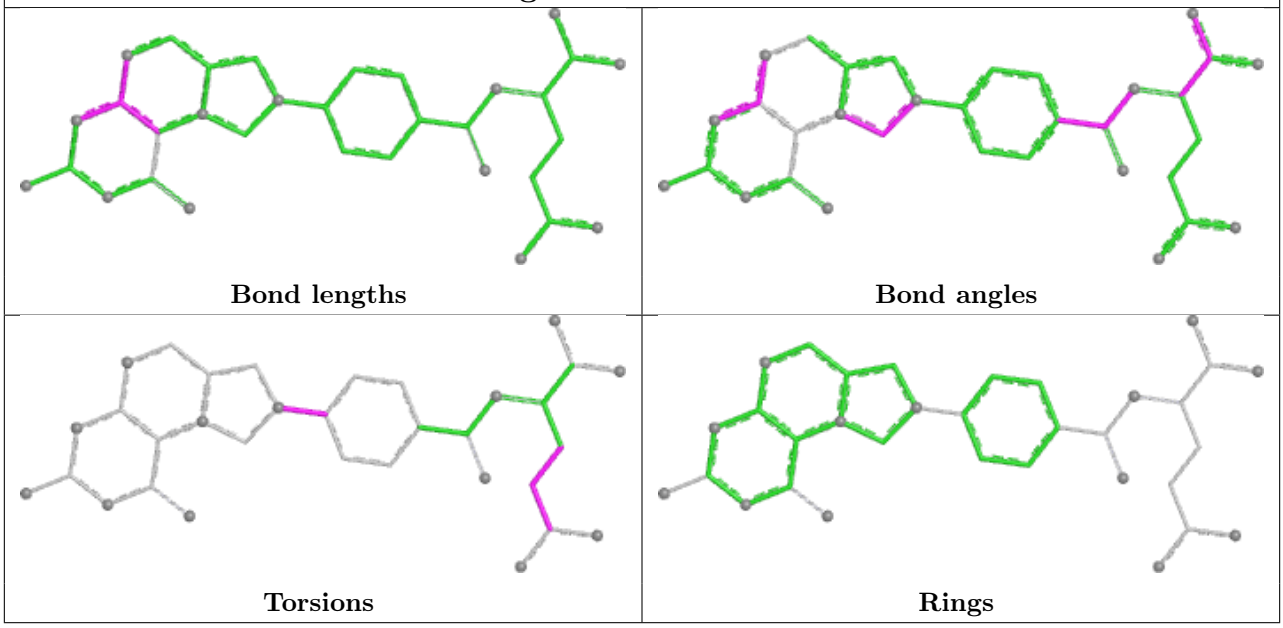
There are no ring outliers.

No monomer is involved in short contacts.

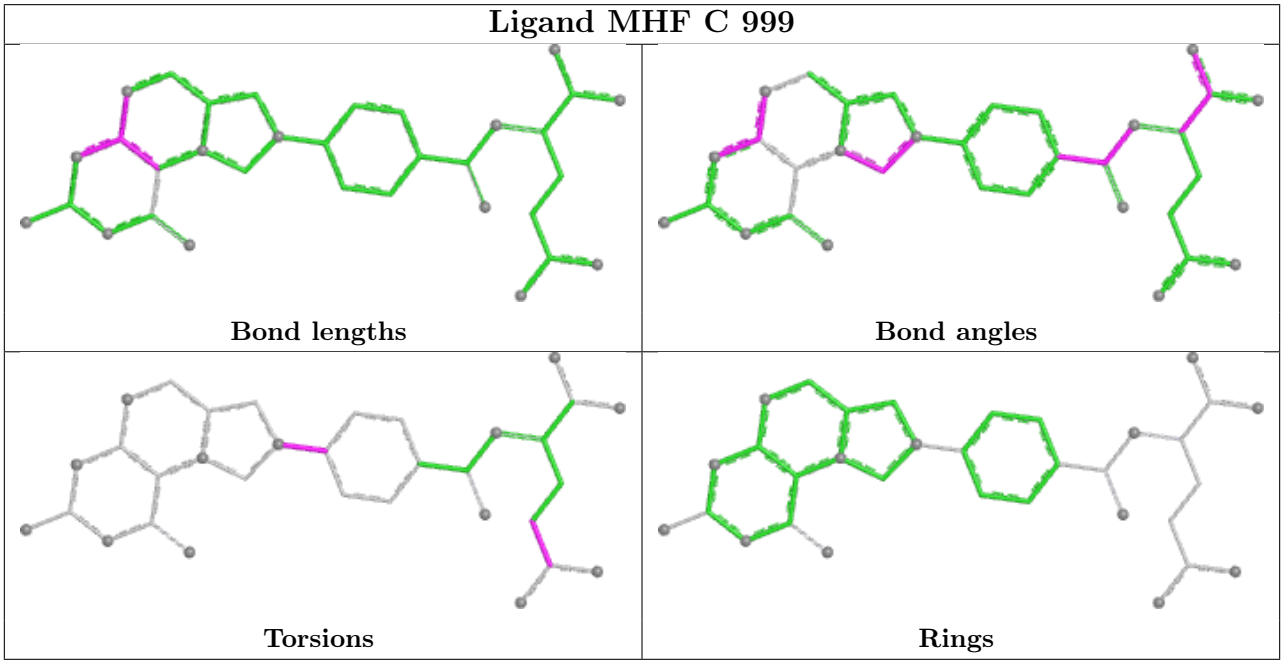
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.

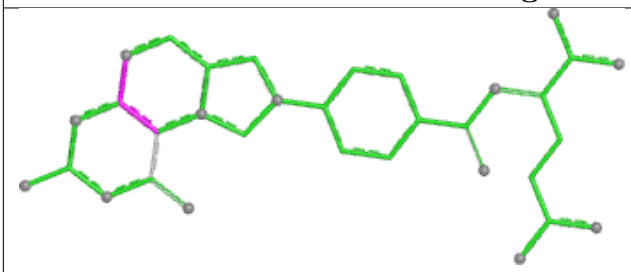
Ligand MHF A 999



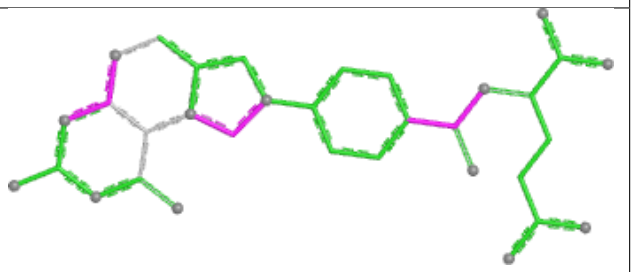
Ligand MHF C 999



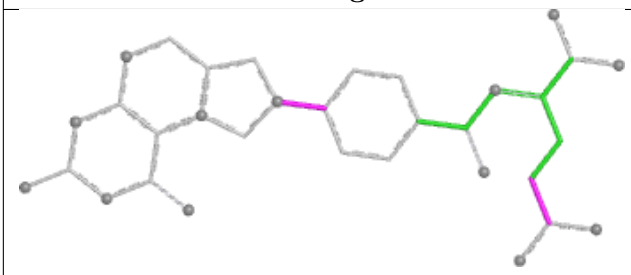
Ligand MHF F 999



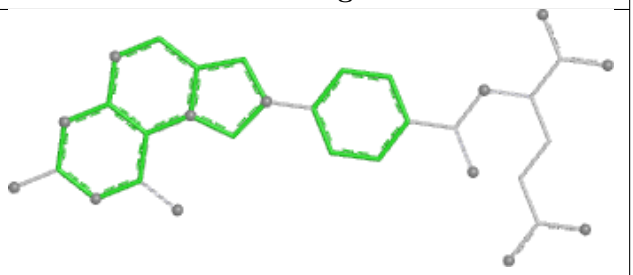
Bond lengths



Bond angles

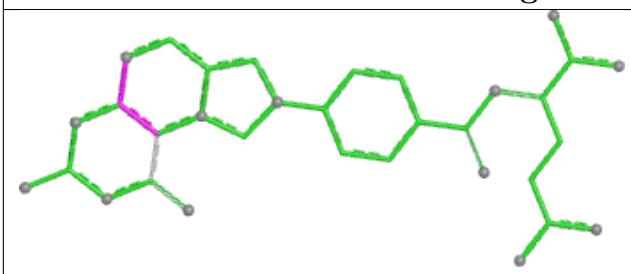


Torsions

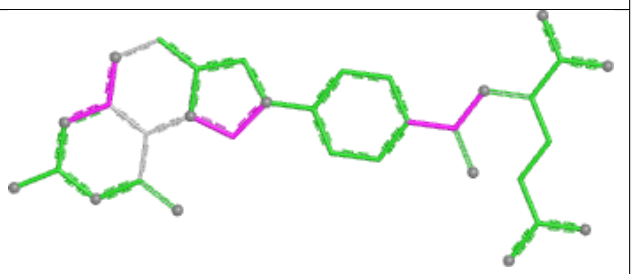


Rings

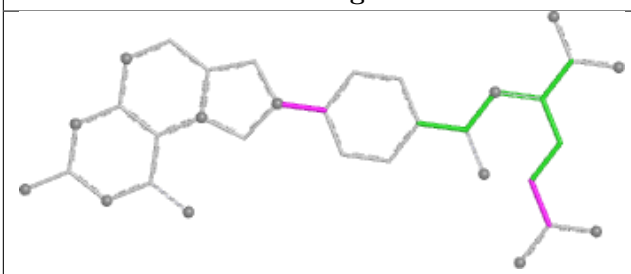
Ligand MHF E 999



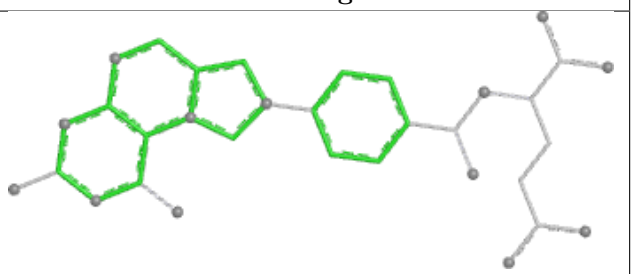
Bond lengths



Bond angles

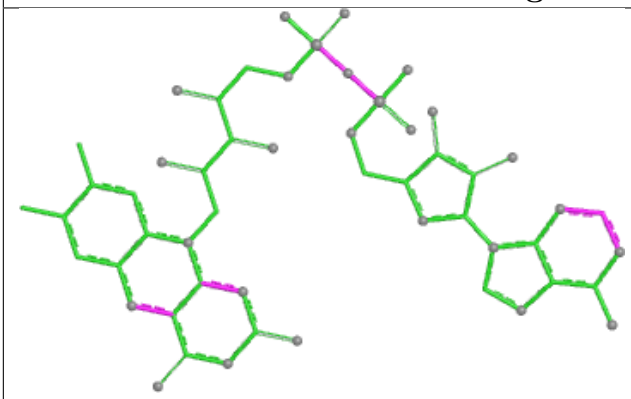


Torsions

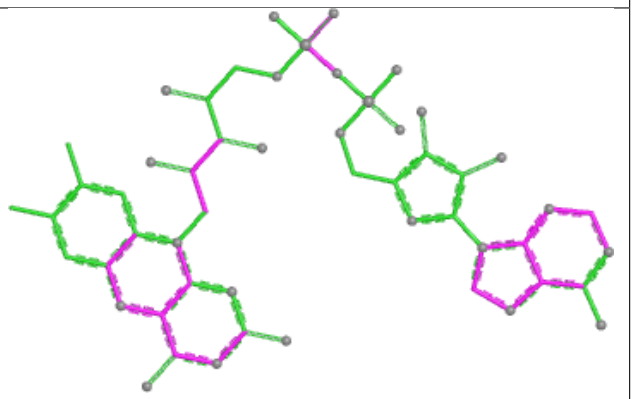


Rings

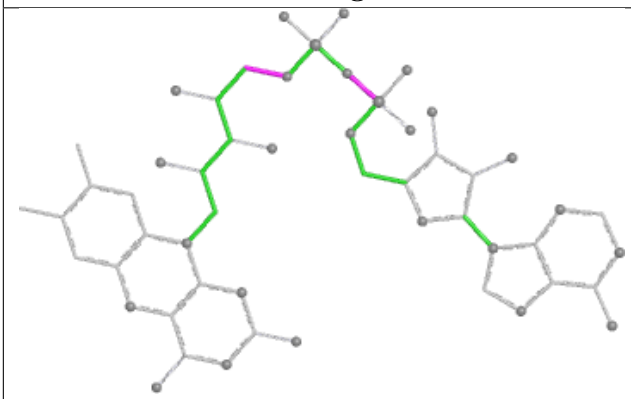
Ligand FAD E 998



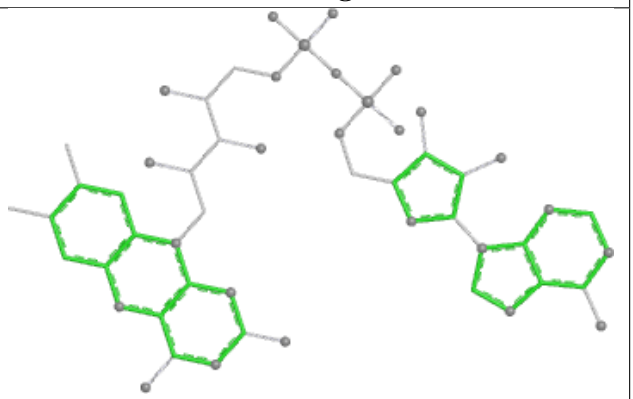
Bond lengths



Bond angles

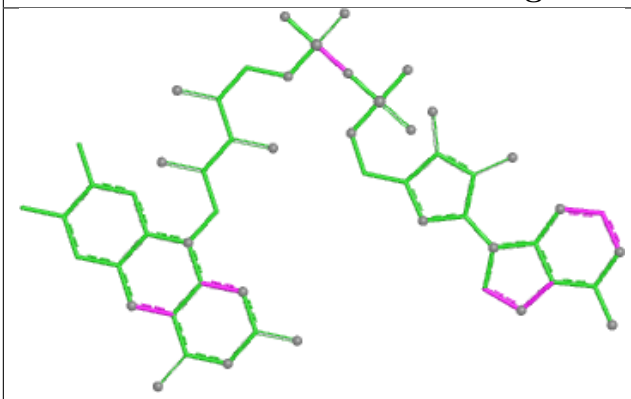


Torsions

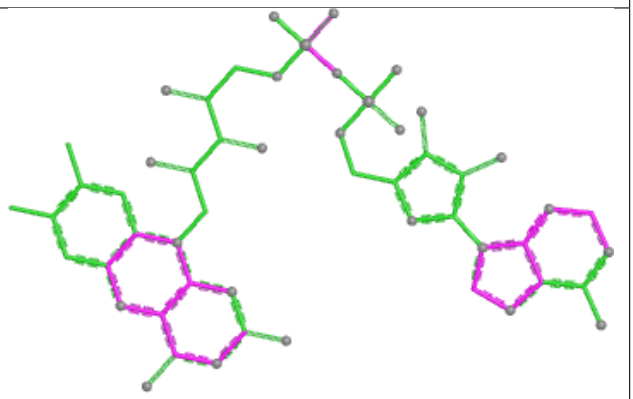


Rings

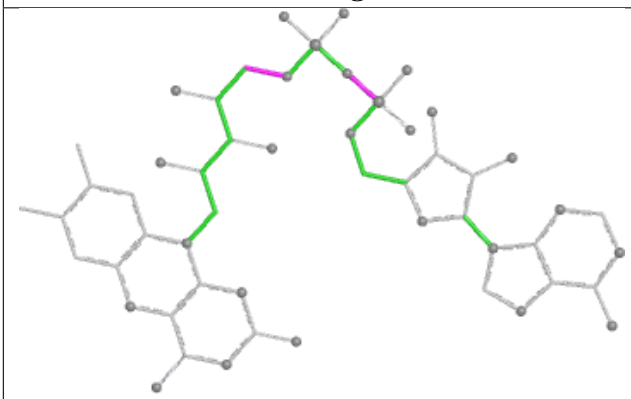
Ligand FAD B 998



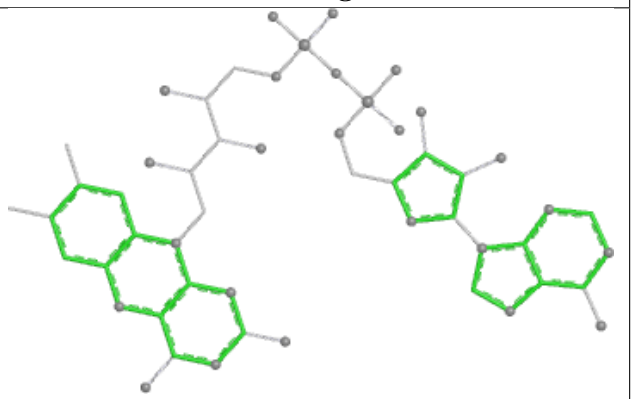
Bond lengths



Bond angles

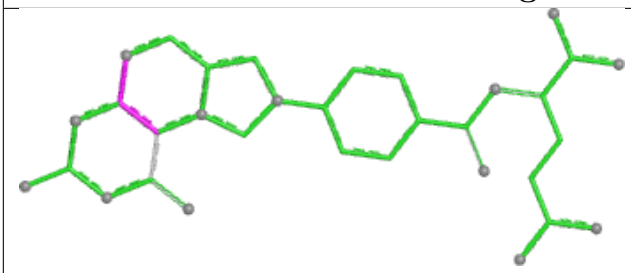


Torsions



Rings

Ligand MHF B 999



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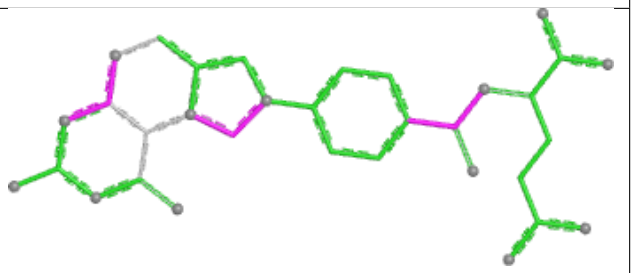
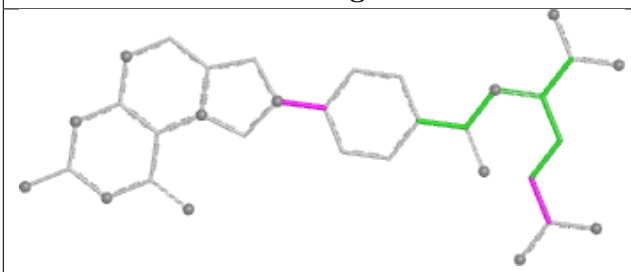


Bond angles



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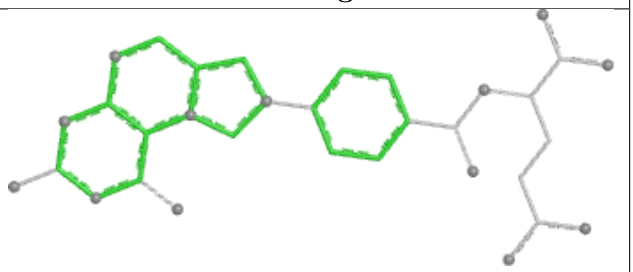
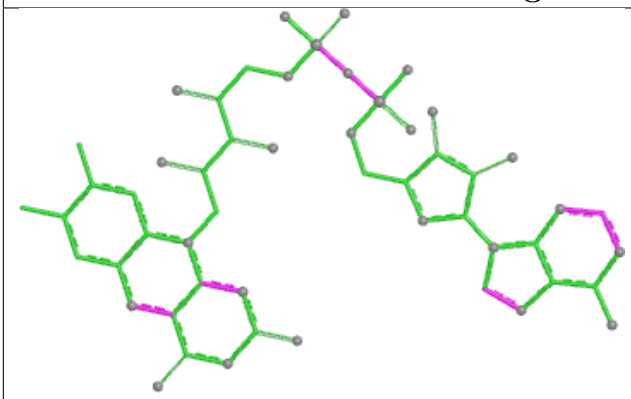
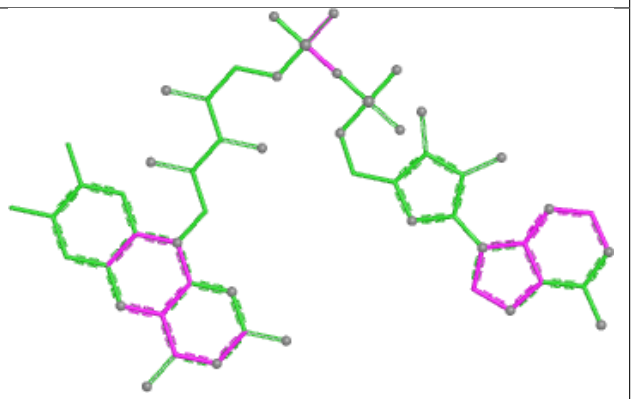


Rings

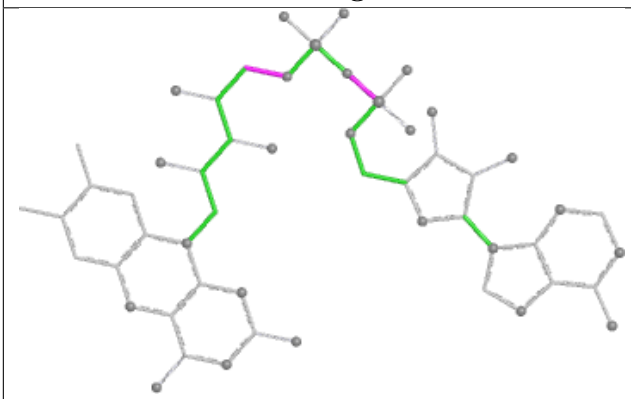
Ligand FAD D 998



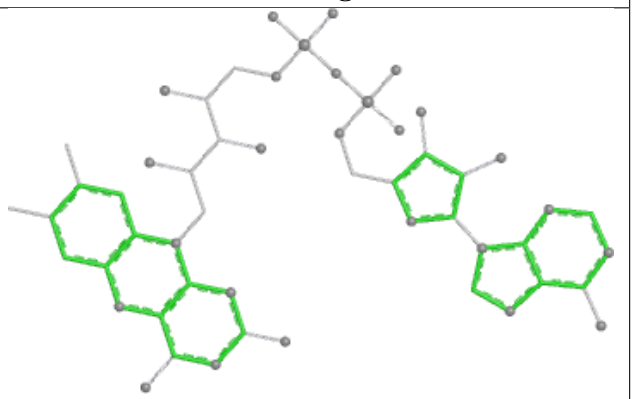
Bond lengths



Bond angles

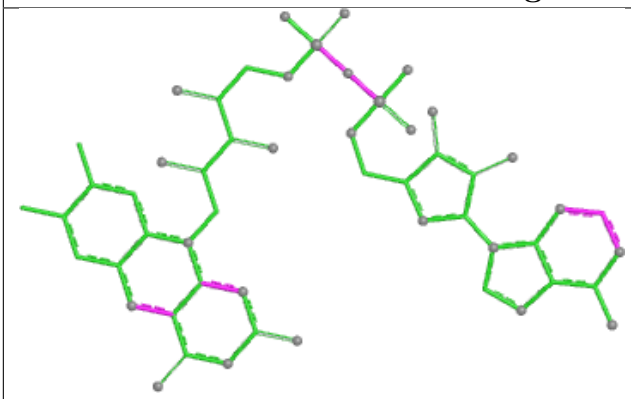


Torsions



Rings

Ligand FAD A 998



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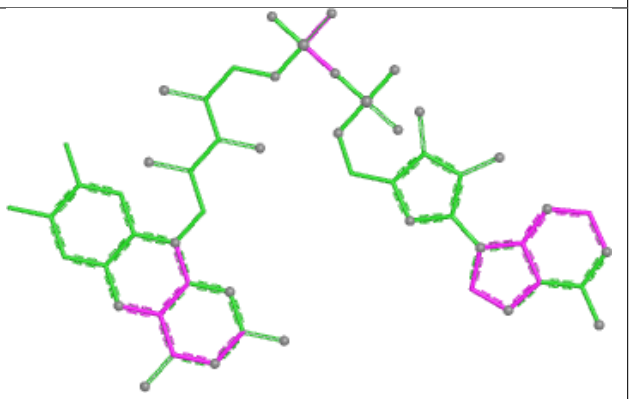
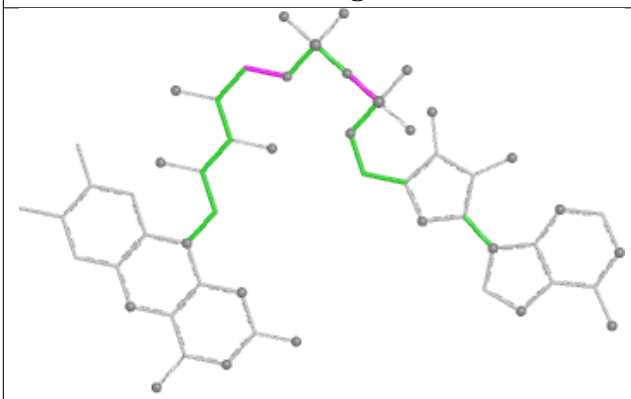
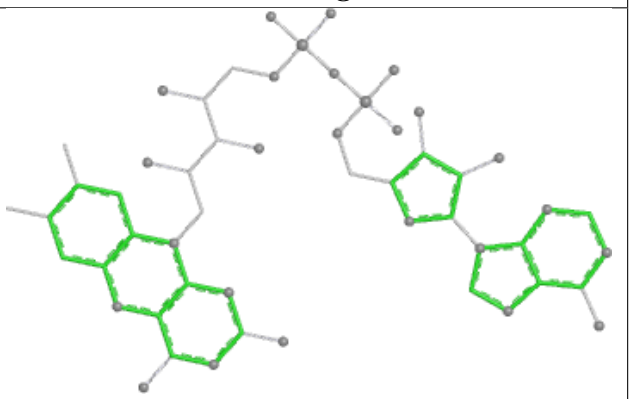


Bond angles



Torsions



Rings

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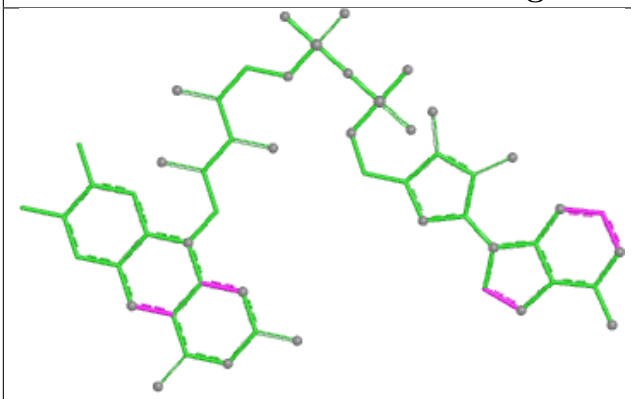
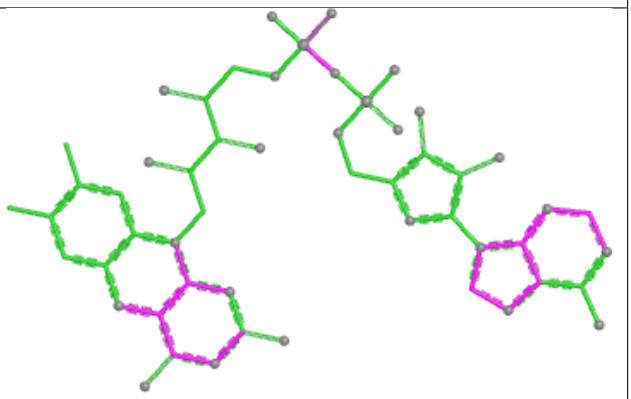
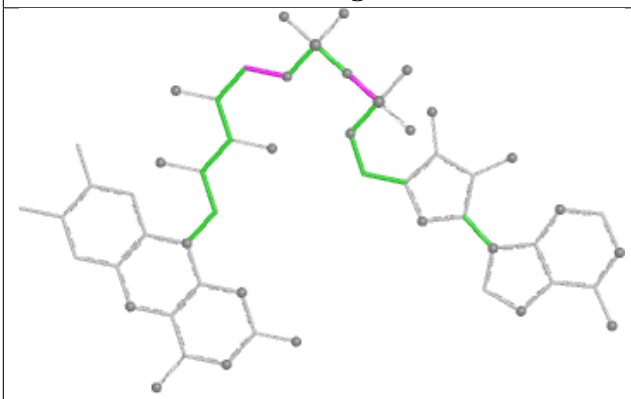


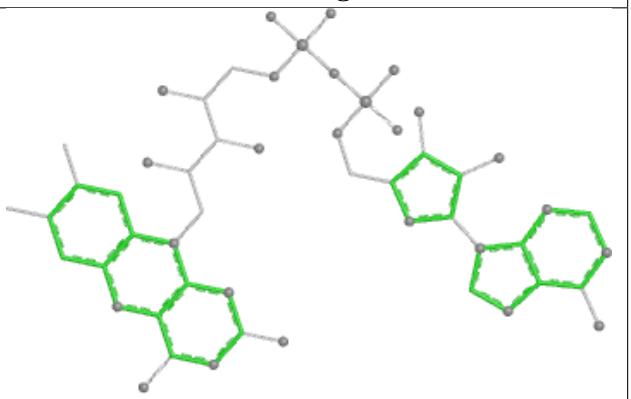
Bond lengths



Bond angles

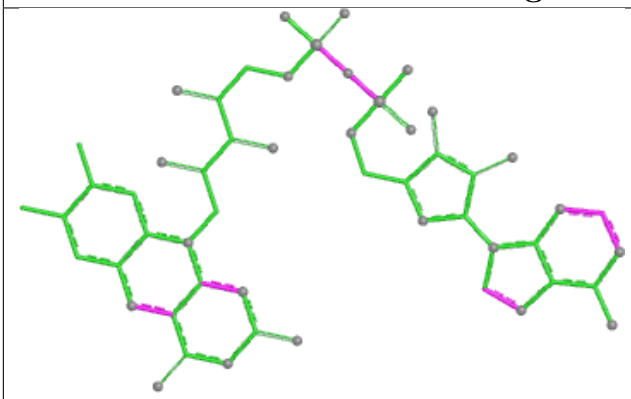


Torsions

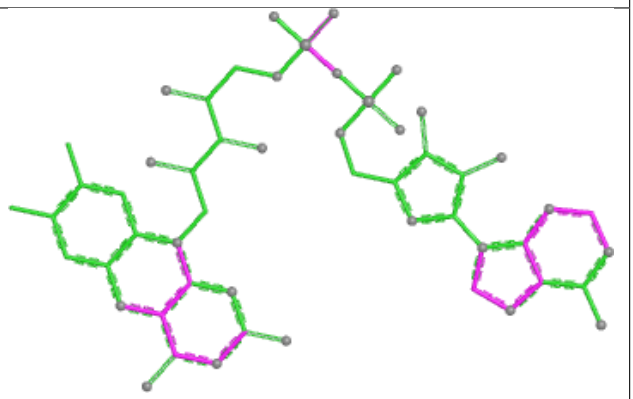


Rings

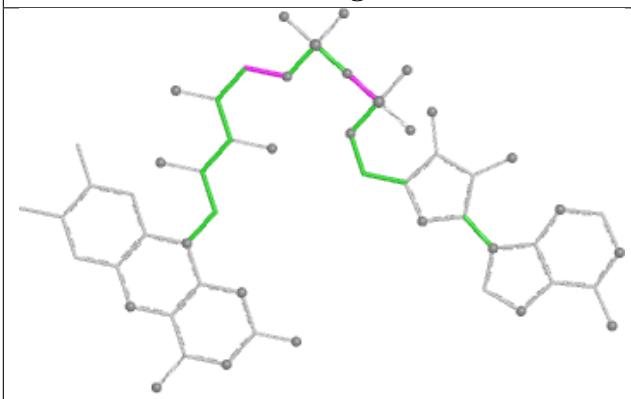
Ligand FAD C 998



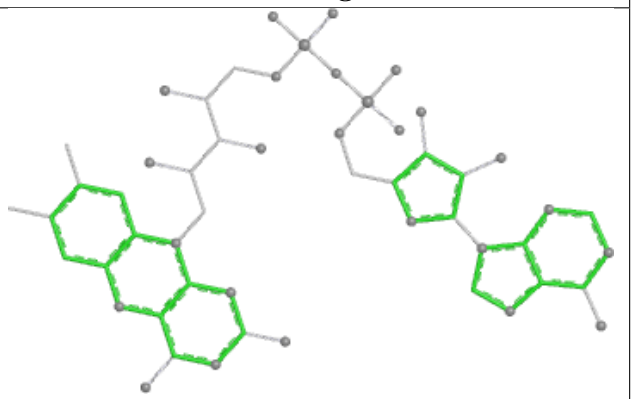
Bond lengths



Bond angles

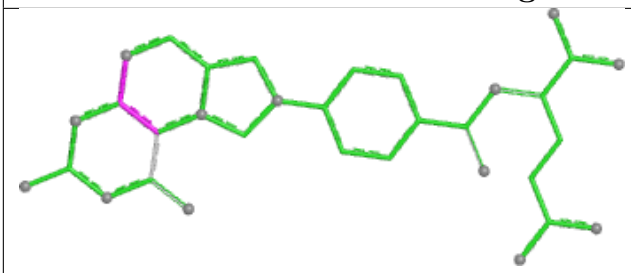


Torsions



Rings

Ligand MHF D 999



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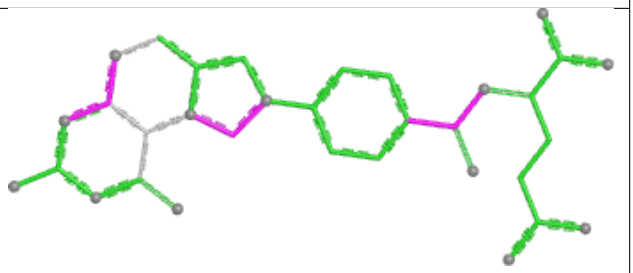
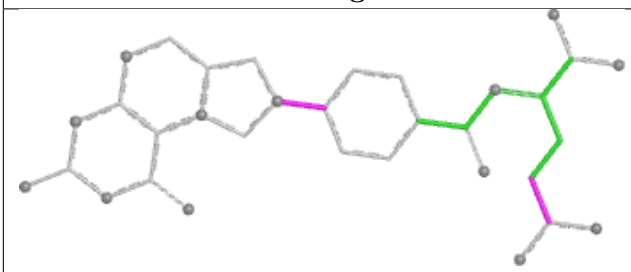
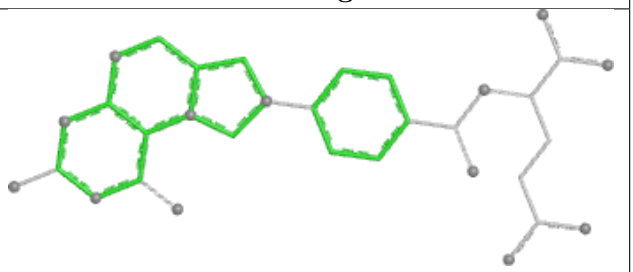


Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

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

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, 95^{th} 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%)

All (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
2	B	32	SER	6.4
1	F	166	SER	6.3
1	E	32	SER	5.8
1	C	32	SER	5.6
1	A	164	GLY	5.5
2	B	31	SER	5.3

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Mol	Chain	Res	Type	RSRZ
1	C	38	GLY	5.3
1	C	163	VAL	5.2
1	D	474	LEU	5.2
1	E	33	SER	5.1
1	E	31	SER	5.0
2	B	30	SER	4.9
1	F	31	SER	4.9
1	C	29	PRO	4.8
1	C	31	SER	4.8
1	F	174	GLY	4.7
1	D	486	MET	4.7
1	C	481	TRP	4.6
1	E	30	SER	4.6
1	F	13	GLU	4.6
1	C	34	VAL	4.6
1	C	33	SER	4.6
2	B	166	SER	4.6
1	D	487	TYR	4.5
1	D	469	GLN	4.5
1	D	38	GLY	4.4
1	D	356	TRP	4.4
1	D	473	ARG	4.2
2	B	439	ASN	4.2
1	F	34	VAL	4.1
2	B	485	LEU	4.1
1	A	0	MET	4.0
1	A	354	GLY	4.0
2	B	34	VAL	4.0
1	D	174	GLY	4.0
1	C	30	SER	4.0
1	A	31	SER	3.9
2	B	441	PRO	3.9
1	D	489	ASP	3.8
1	F	355	LYS	3.8
2	B	355	LYS	3.8
1	A	499	GLY	3.7
1	A	356	TRP	3.7
3	H	1	DT	3.7
1	E	350	ARG	3.7
1	D	30	SER	3.7
2	B	489	ASP	3.7
1	D	471	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
1	E	163	VAL	3.6
1	A	498	ASN	3.6
1	A	443	ARG	3.6
1	E	166	SER	3.6
1	F	12	GLU	3.6
1	D	29	PRO	3.5
2	B	33	SER	3.5
1	E	481	TRP	3.5
1	F	473	ARG	3.5
1	A	33	SER	3.5
1	D	163	VAL	3.5
1	E	473	ARG	3.5
2	B	473	ARG	3.5
2	B	163	VAL	3.5
1	F	356	TRP	3.4
1	D	28	LEU	3.4
1	D	166	SER	3.4
1	F	32	SER	3.4
1	A	165	ASN	3.4
2	B	164	GLY	3.4
1	E	2	ASP	3.4
1	D	372	GLY	3.4
1	E	174	GLY	3.4
1	C	23	PHE	3.4
2	B	484	ARG	3.4
2	B	161	LYS	3.4
1	F	434	TYR	3.3
1	A	442	PRO	3.3
1	F	354	GLY	3.3
1	F	442	PRO	3.3
1	F	494	LEU	3.3
1	A	163	VAL	3.3
1	C	165	ASN	3.3
1	A	481	TRP	3.3
1	D	445	ASP	3.3
1	A	30	SER	3.3
1	E	29	PRO	3.2
1	A	34	VAL	3.2
1	E	34	VAL	3.2
1	E	489	ASP	3.2
2	B	2	ASP	3.2
1	A	32	SER	3.2

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Mol	Chain	Res	Type	RSRZ
2	B	174	GLY	3.2
2	B	175	SER	3.2
1	E	356	TRP	3.2
1	A	480	HIS	3.2
1	F	28	LEU	3.1
1	D	472	ARG	3.1
1	C	224	ASP	3.1
1	D	238	GLU	3.1
1	C	355	LYS	3.1
1	D	40	GLY	3.1
2	B	40	GLY	3.1
2	B	486	MET	3.1
1	D	492	VAL	3.1
2	B	356	TRP	3.0
1	E	480	HIS	3.0
1	F	175	SER	3.0
1	C	164	GLY	3.0
1	D	36	ARG	3.0
2	B	481[A]	TRP	3.0
1	D	2	ASP	3.0
2	B	228	ASP	3.0
1	C	3	HIS	3.0
1	C	311	LYS	3.0
1	D	165	ASN	2.9
2	B	469	GLN	2.9
2	B	13	GLU	2.9
2	B	16	ASP	2.9
1	D	364	GLU	2.9
1	C	174	GLY	2.9
1	C	480	HIS	2.9
1	D	359	ASP	2.9
1	F	469	GLN	2.8
1	C	166	SER	2.8
1	E	165	ASN	2.8
2	B	84	PHE	2.8
2	B	487	TYR	2.8
1	A	235	LEU	2.8
1	C	35	LYS	2.8
1	E	495	LYS	2.8
1	F	161	LYS	2.8
1	E	210	SER	2.8
1	C	12	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	F	364	GLU	2.8
2	B	482	PRO	2.8
1	F	35	LYS	2.8
1	D	175	SER	2.8
1	D	443	ARG	2.8
1	A	13	GLU	2.8
1	C	13	GLU	2.8
1	C	84	PHE	2.8
1	F	84	PHE	2.8
2	B	372	GLY	2.8
2	B	494	LEU	2.8
1	D	355	LYS	2.8
1	E	12	GLU	2.7
1	F	164	GLY	2.7
1	D	27	ALA	2.7
1	D	169	LEU	2.7
2	B	36	ARG	2.7
1	C	137	ARG	2.7
1	F	474	LEU	2.7
2	B	167	THR	2.7
1	F	487	TYR	2.7
1	D	3	HIS	2.7
1	F	441	ASP	2.7
1	C	161	LYS	2.7
1	D	84	PHE	2.7
2	B	27	ALA	2.7
1	D	209	SER	2.7
1	D	491	VAL	2.7
1	E	353	GLN	2.6
1	C	167	THR	2.6
1	A	440	ASN	2.6
2	B	480	HIS	2.6
3	L	2	DT	2.6
1	A	475	PRO	2.6
1	A	355	LYS	2.6
1	D	17	SER	2.6
2	B	186	ASP	2.6
1	D	354	GLY	2.6
2	B	241	GLU	2.6
1	D	86	ASN	2.6
1	F	490	THR	2.6
1	A	478	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	441	ASP	2.6
1	A	167	THR	2.6
1	F	167	THR	2.6
1	A	489	ASP	2.6
1	D	368	ASP	2.6
1	D	455	GLN	2.5
1	E	37	LYS	2.5
1	D	228	ASP	2.5
1	D	188	PHE	2.5
1	E	497	GLY	2.5
1	F	135	GLY	2.5
2	B	354	GLY	2.5
1	A	472	ARG	2.5
1	D	371	THR	2.5
1	D	362	LEU	2.5
1	E	84	PHE	2.5
1	D	493	PRO	2.5
1	F	219	PRO	2.5
2	B	369	ALA	2.5
1	C	28	LEU	2.5
1	D	370	LYS	2.5
2	B	41	VAL	2.4
1	E	354	GLY	2.4
1	A	12	GLU	2.4
1	C	356	TRP	2.4
2	B	440	ASP	2.4
2	B	219	PRO	2.4
2	B	159	GLY	2.4
1	F	163	VAL	2.4
1	C	36	ARG	2.4
1	A	196	GLN	2.4
1	F	209	SER	2.4
1	E	167	THR	2.4
1	D	219	PRO	2.4
1	A	24	GLU	2.3
1	D	444	GLU	2.3
2	B	38	GLY	2.3
1	D	350	ARG	2.3
2	B	371	THR	2.3
1	E	28	LEU	2.3
2	B	169	LEU	2.3
1	D	66	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	56	ASP	2.3
1	D	67	THR	2.3
1	F	315	ALA	2.3
1	C	354	GLY	2.3
1	D	208	ARG	2.3
1	E	16	ASP	2.3
1	F	38	GLY	2.3
2	B	350	ARG	2.3
1	C	234	LYS	2.3
3	L	5	DT	2.3
2	B	206	SER	2.3
2	B	126	ILE	2.3
1	A	25	ARG	2.3
1	F	368	ASP	2.3
2	B	35	LYS	2.3
1	E	233	GLU	2.2
1	C	129	SER	2.2
2	B	20	ILE	2.2
1	C	485	LEU	2.2
1	D	167	THR	2.2
1	D	24	GLU	2.2
1	E	485	LEU	2.2
1	E	3	HIS	2.2
1	F	107	LYS	2.2
2	B	165	ASN	2.2
1	D	488	MET	2.2
3	L	4	DT	2.2
1	E	27	ALA	2.2
1	F	203	ALA	2.2
2	B	136	ALA	2.2
2	B	3	HIS	2.2
2	B	474	LEU	2.2
1	A	175	SER	2.2
2	B	209	SER	2.2
2	B	26	TYR	2.2
2	B	476	LYS	2.2
1	A	317	ASN	2.2
1	F	165	ASN	2.2
1	C	15	ILE	2.1
1	D	12	GLU	2.1
1	F	238	GLU	2.1
1	C	352	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	464	VAL	2.1
1	F	314	VAL	2.1
1	F	352	VAL	2.1
1	A	483	GLY	2.1
1	F	83	HIS	2.1
2	B	83	HIS	2.1
1	D	369	ALA	2.1
1	F	137	ARG	2.1
2	B	471	LEU	2.1
1	F	206	SER	2.1
1	D	361	LYS	2.1
2	B	39	LYS	2.1
1	A	441	ASP	2.1
1	D	184	PRO	2.1
1	D	185	PHE	2.1
1	C	83	HIS	2.1
1	D	83	HIS	2.1
1	A	27	ALA	2.1
2	B	160	LEU	2.1
1	D	459	PRO	2.1
1	D	470	GLN	2.1
1	F	29	PRO	2.1
1	A	350	ARG	2.1
1	D	137	ARG	2.1
1	F	226	TRP	2.1
1	F	9	ALA	2.1
1	D	494	LEU	2.1
1	F	78	LEU	2.1
1	D	353	GLN	2.1
1	C	493	PRO	2.1
1	D	490	THR	2.1
1	F	79	PHE	2.1
2	B	226	TRP	2.1
1	D	233	GLU	2.0
1	F	129	SER	2.1
1	F	461	GLY	2.0
1	F	271	VAL	2.0
2	B	233	GLU	2.0
1	F	486	MET	2.0
1	E	224	ASP	2.0
1	F	489	ASP	2.0
1	D	403	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
2	B	137	ARG	2.0
3	G	1	DT	2.0
1	F	493	PRO	2.0
1	D	437	GLY	2.0

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, 95^{th} 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, 95^{th} 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

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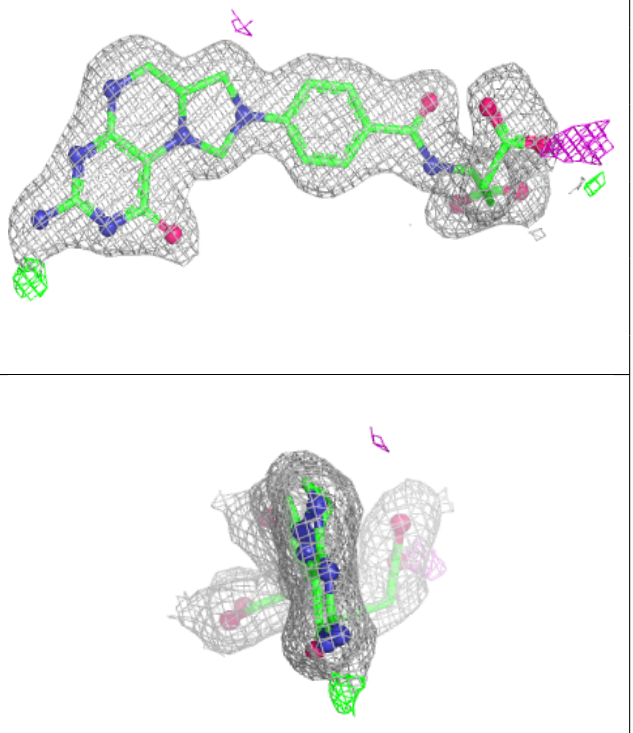
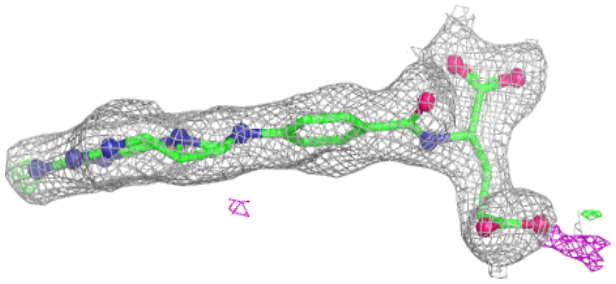
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	FAD	F	998	53/53	0.95	0.08	34,34,36,37	0
5	MHF	C	999	33/33	0.95	0.07	34,37,45,49	0
4	FAD	D	998	53/53	0.96	0.07	34,34,36,37	0
4	FAD	B	998	53/53	0.96	0.07	34,35,36,36	0
6	CL	B	1498	1/1	0.96	0.12	52,52,52,52	0
4	FAD	E	998	53/53	0.97	0.06	34,35,37,37	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
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 F 999:

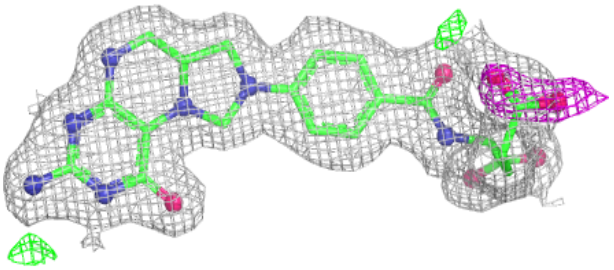
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

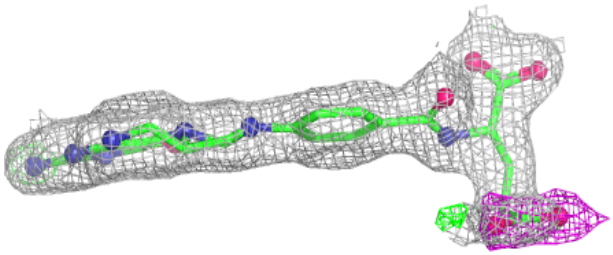


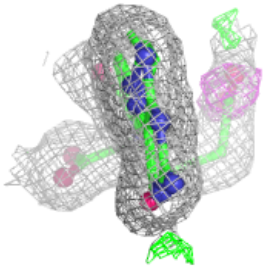


Electron density around MHF E 999:

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

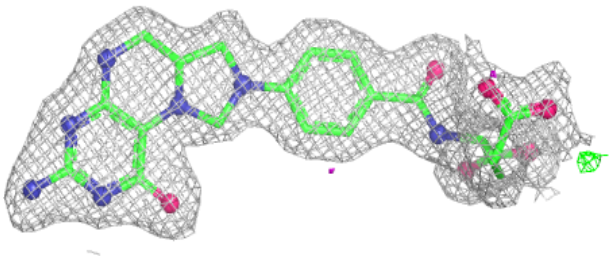


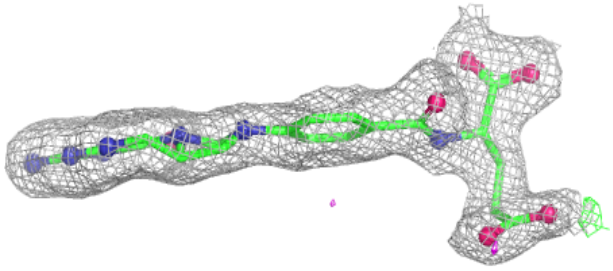


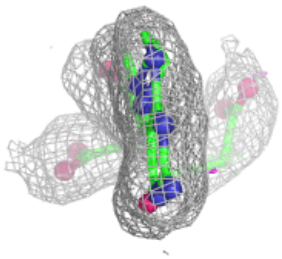


Electron density around MHF B 999:

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

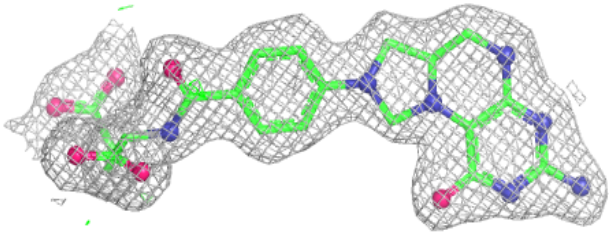


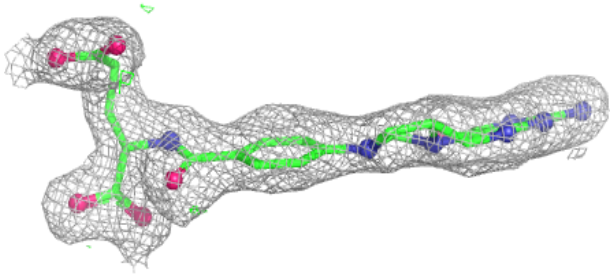


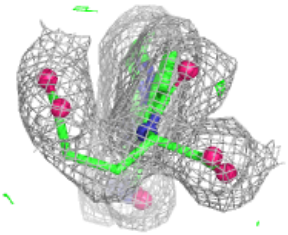


Electron density around MHF D 999:

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

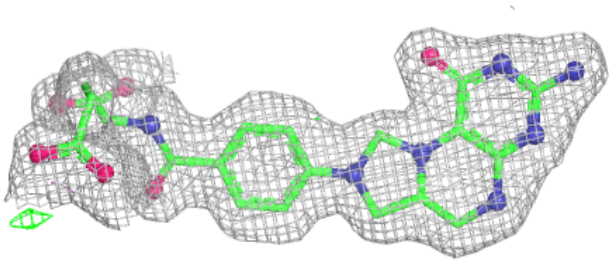


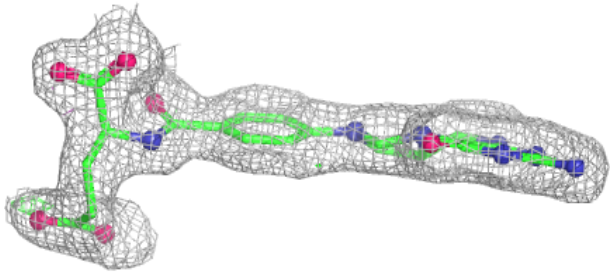


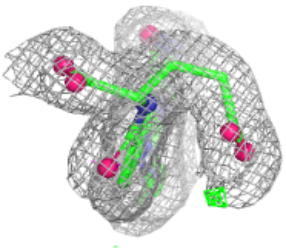


Electron density around MHF A 999:

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

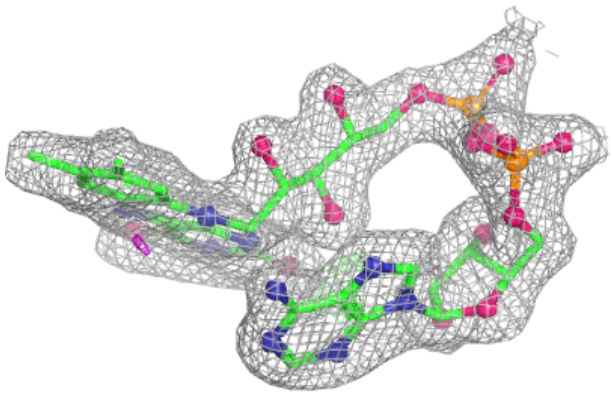


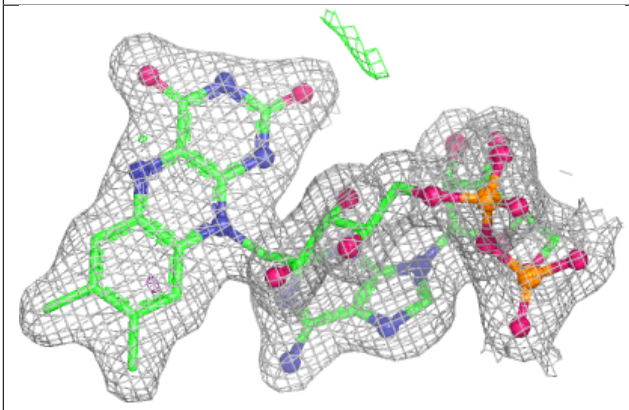


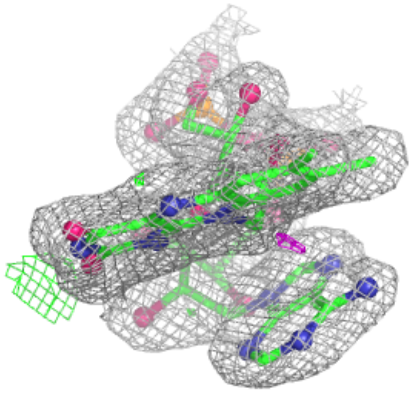


Electron density around FAD F 998:

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

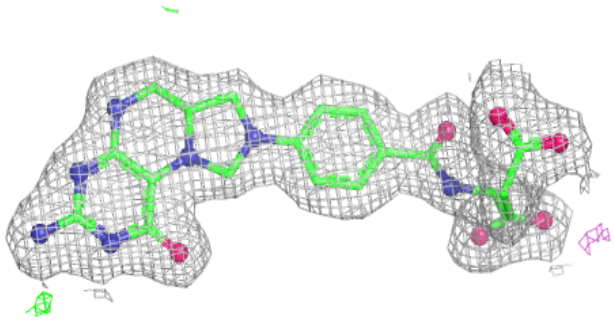


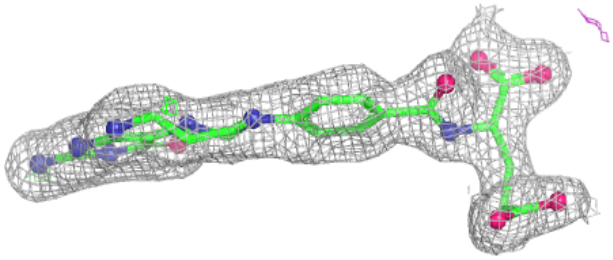


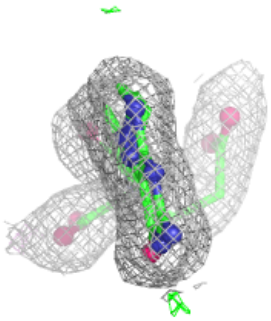


Electron density around MHF C 999:

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

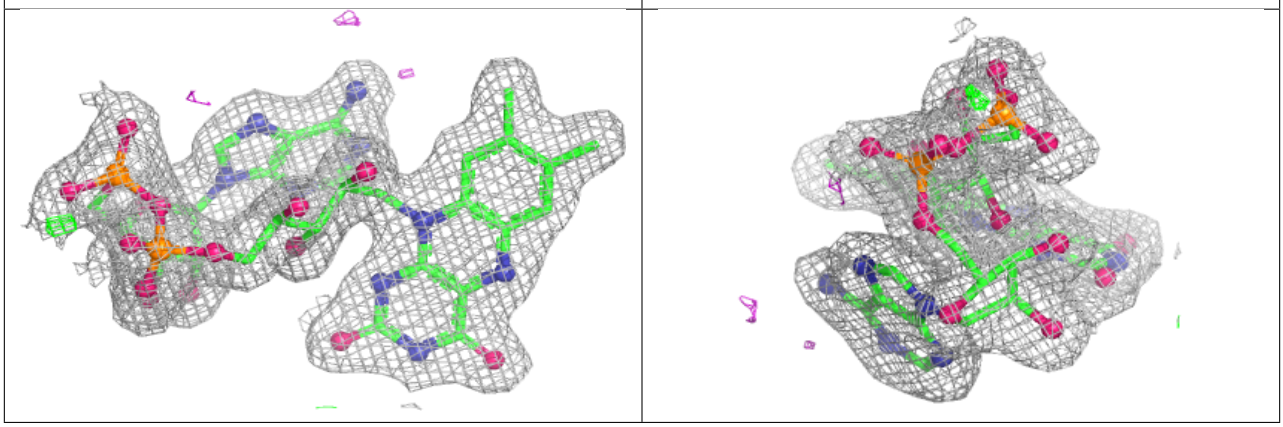






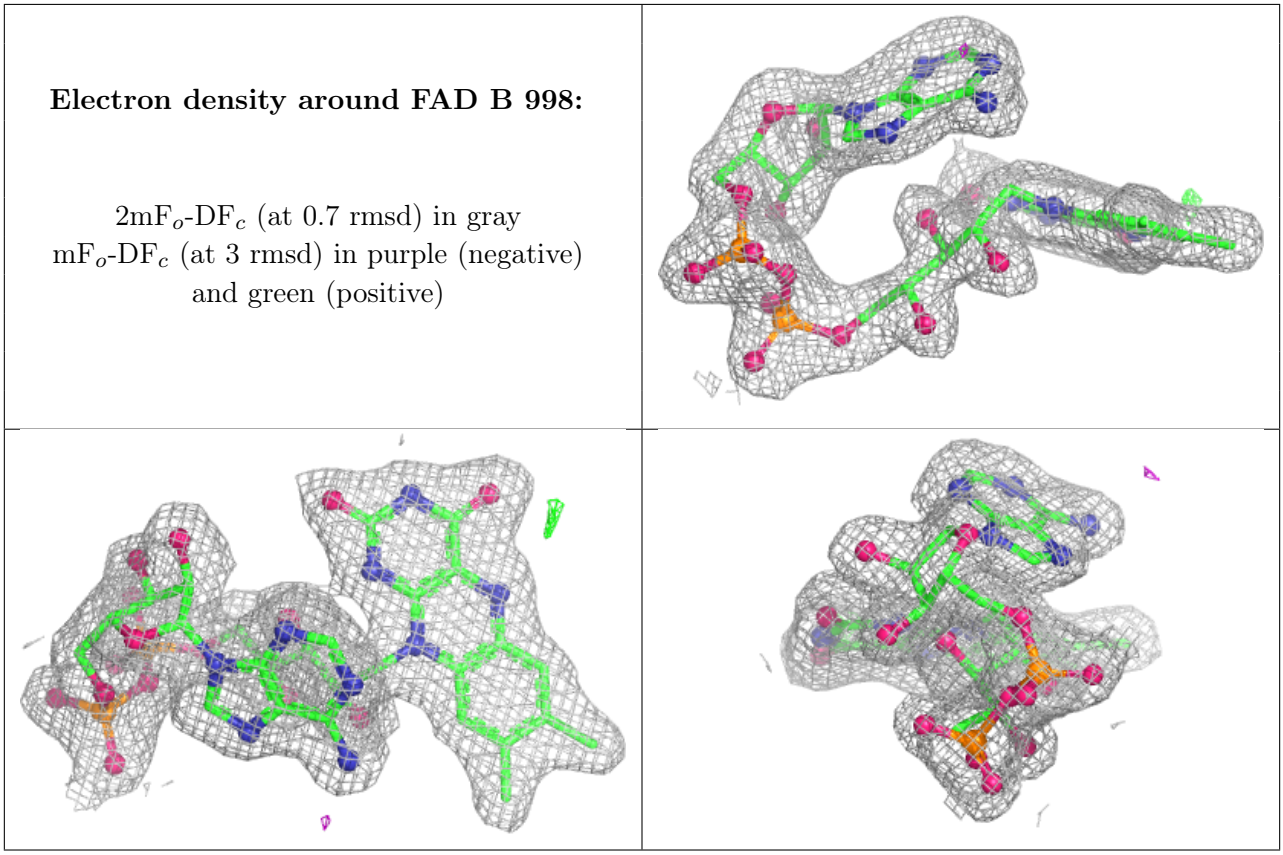
Electron density around FAD D 998:

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



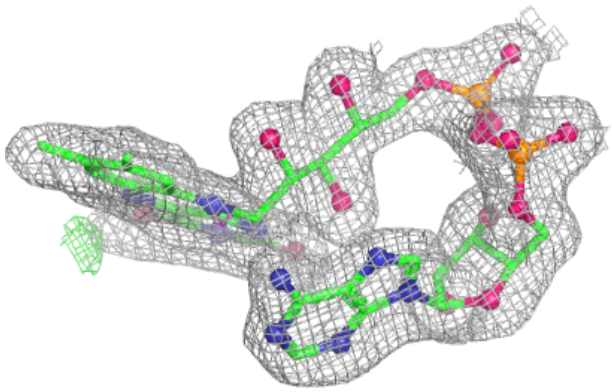
Electron density around FAD B 998:

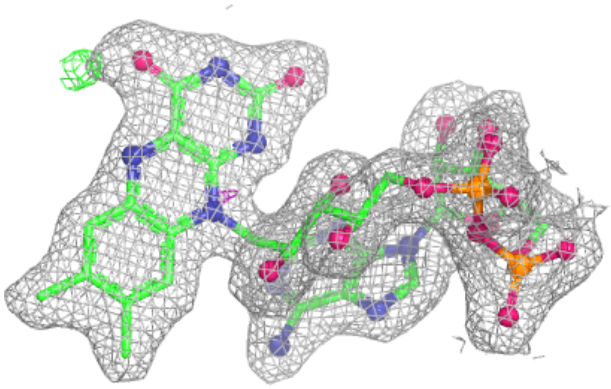
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

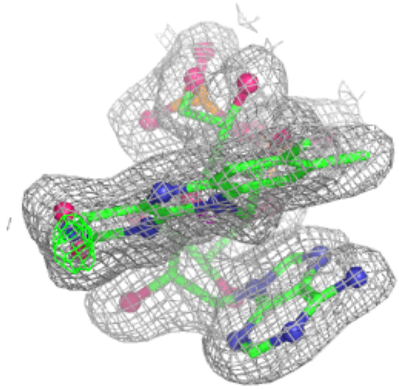


Electron density around FAD E 998:

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

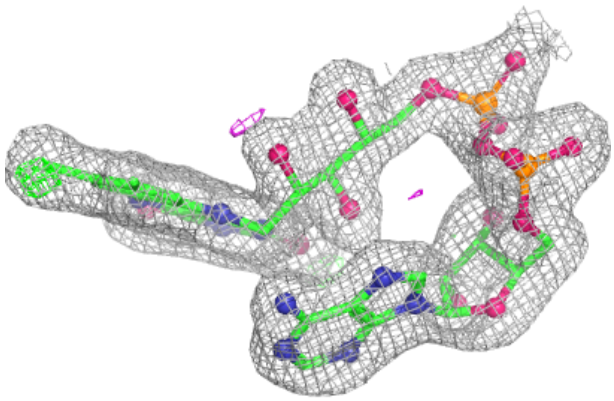


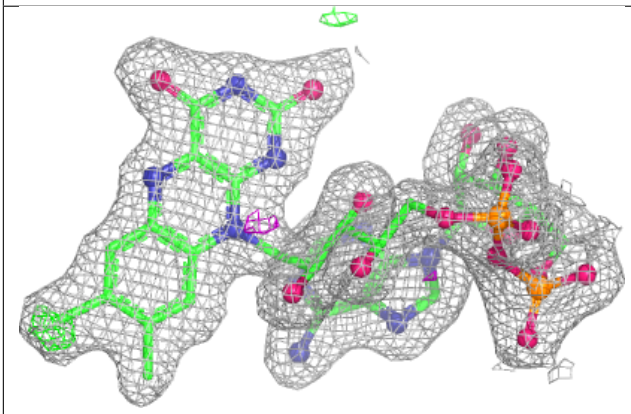


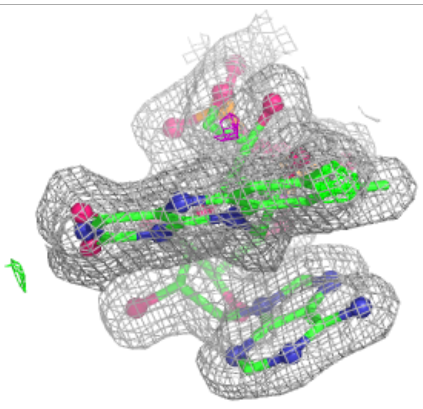


Electron density around FAD C 998:

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

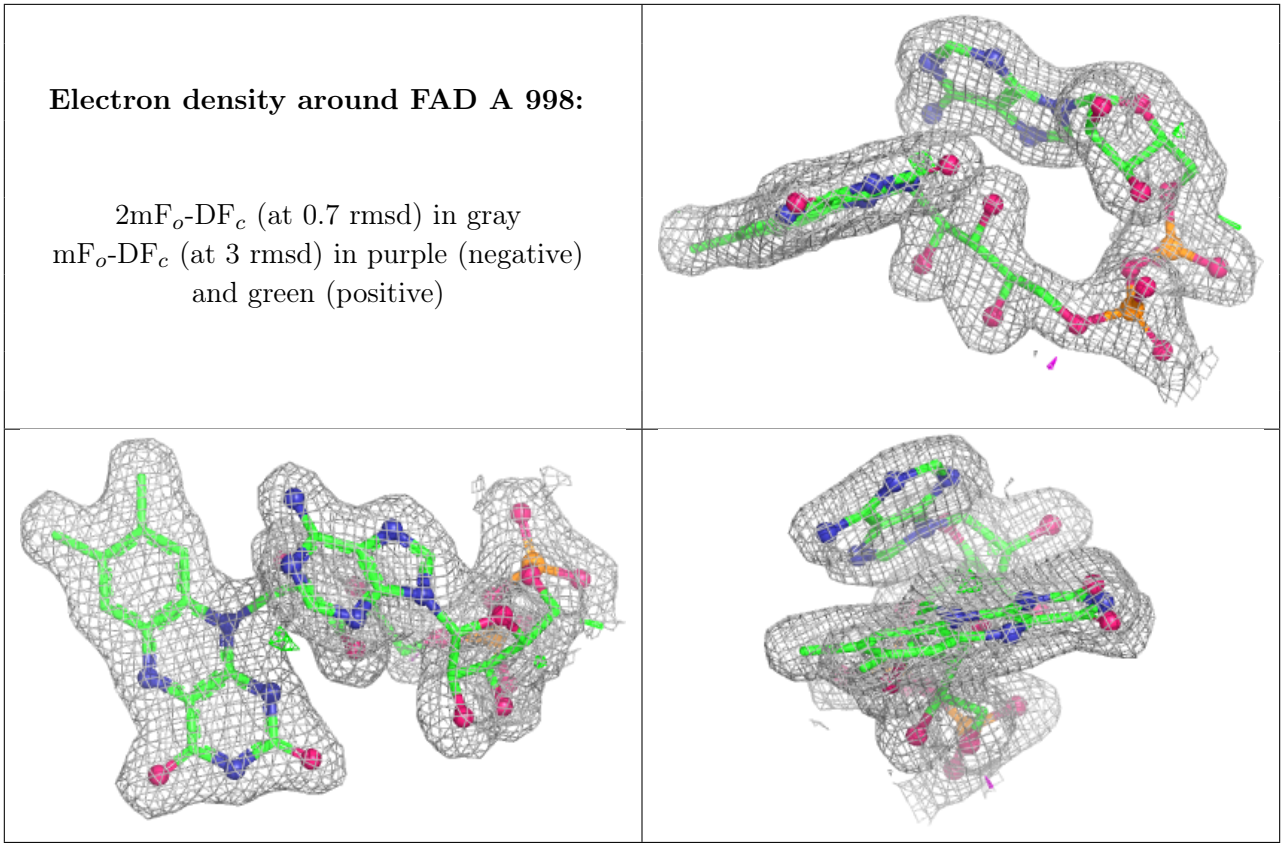






Electron density around FAD A 998:

$2mF_o$-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.