



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 02:18 AM EDT

PDB ID : 1TEZ / pdb_00001tez
Title : COMPLEX BETWEEN DNA AND THE DNA PHOTOLYASE FROM ANA-CYSTIS NIDULANS
Authors : Essen, L.-O.; Carell, T.; Mees, A.; Klar, T.
Deposited on : 2004-05-26
Resolution : 1.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

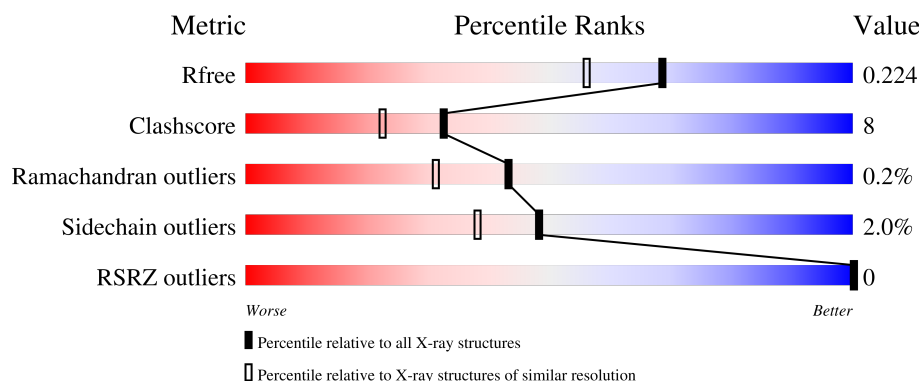
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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.



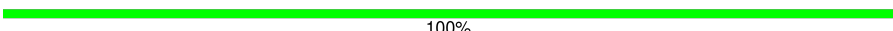
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	I	11	64% 36%
1	K	11	64% 36%
2	J	9	56% 44%
2	L	9	44% 56%
3	M	4	100%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	O	4	 50% 50%
4	N	5	 100%
4	P	5	 60% 40%
5	A	474	 83% 16% .
5	B	474	 83% 16% .
5	C	474	 83% 16% .
5	D	474	 85% 14% .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	HDF	A	5486	X	-	-	-
8	HDF	B	6486	X	-	-	-
8	HDF	C	7486	X	-	-	-
8	HDF	D	8486	X	-	-	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 18206 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 DNA chain called 5'-D(*AP*TP*CP*GP*GP*CP*T*(TCP)P*CP*GP*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	I	11	Total	C	N	O	P	0	0	0
			218	107	38	64	9			
1	K	11	Total	C	N	O	P	0	0	0
			218	107	38	64	9			

- Molecule 2 is a DNA chain called 5'-D(P*CP*GP*AP*AP*GP*CP*CP*GP*A)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	J	9	Total	C	N	O	P	0	0	0
			186	87	39	51	9			
2	L	9	Total	C	N	O	P	0	0	0
			186	87	39	51	9			

- Molecule 3 is a DNA chain called 5'-D(*TP*CP*GP*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	4	Total	C	N	O	P	1	0	0
			77	38	13	23	3			
3	O	4	Total	C	N	O	P	0	0	0
			77	38	13	23	3			

- Molecule 4 is a DNA chain called 5'-D(P*GP*CP*CP*GP*A)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	N	5	Total	C	N	O	P	0	0	0
			103	48	21	29	5			
4	P	5	Total	C	N	O	P	0	0	0
			103	48	21	29	5			

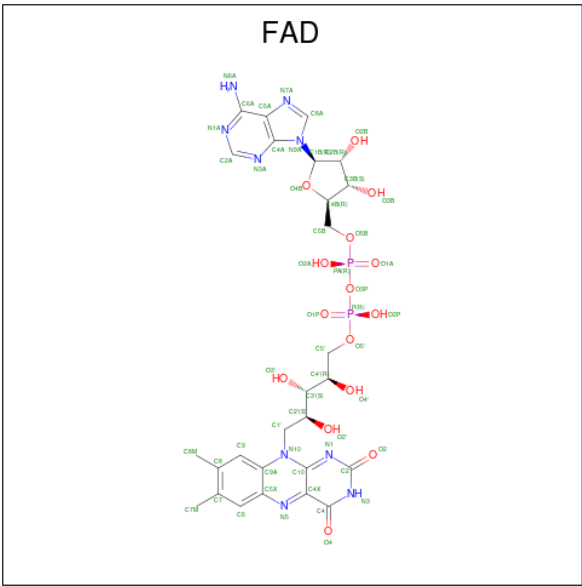
- Molecule 5 is a protein called Deoxyribodipyrimidine photo-lyase type I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	A	474	Total	C	N	O	S	2	0	0
			3774	2411	674	679	10			
5	B	474	Total	C	N	O	S	6	0	0
			3782	2414	678	680	10			
5	C	474	Total	C	N	O	S	0	0	0
			3773	2409	674	680	10			
5	D	474	Total	C	N	O	S	6	0	0
			3777	2412	675	680	10			

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

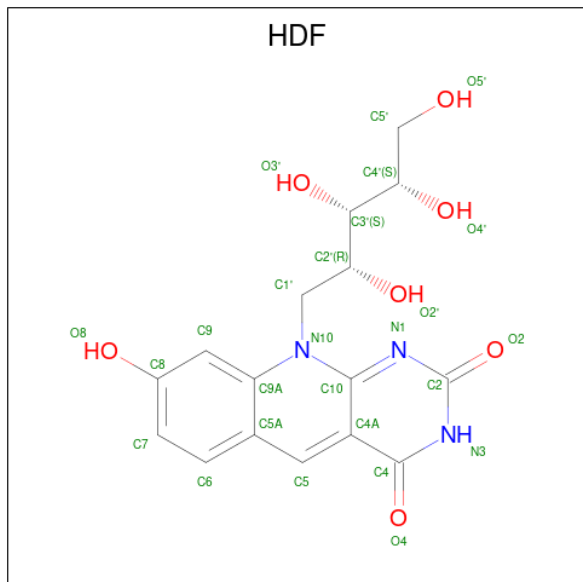
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Mg	0	0
			1	1		
6	B	1	Total	Mg	0	0
			1	1		

- Molecule 7 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



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

- Molecule 8 is 8-HYDROXY-10-(D-RIBO-2,3,4,5-TETRAHYDROXYPENTYL)-5-DEAZAISOALLOXAZINE (CCD ID: HDF) (formula: $C_{16}H_{17}N_3O_7$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	O	0	0
			26	16	3	7		
8	B	1	Total	C	N	O	0	0
			26	16	3	7		
8	C	1	Total	C	N	O	0	0
			26	16	3	7		
8	D	1	Total	C	N	O	0	0
			26	16	3	7		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	I	10	Total	O	0	0
			10	10		
9	J	11	Total	O	0	0
			11	11		
9	K	8	Total	O	0	0
			8	8		
9	L	9	Total	O	0	0
			9	9		
9	M	14	Total	O	0	0
			14	14		
9	N	10	Total	O	0	0
			10	10		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	P	5	Total 5	O 5	0	0
9	A	409	Total 409	O 409	0	0
9	B	404	Total 404	O 404	0	0
9	C	374	Total 374	O 374	0	0
9	D	360	Total 360	O 360	0	0

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.

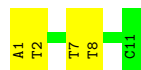
- Molecule 1: 5'-D(*AP*TP*CP*GP*GP*CP*T*(TCP)P*CP*GP*C)-3'

Chain I: 



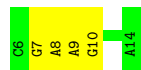
- Molecule 1: 5'-D(*AP*TP*CP*GP*GP*CP*T*(TCP)P*CP*GP*C)-3'

Chain K: 

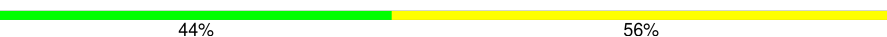


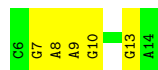
- Molecule 2: 5'-D(P*CP*GP*AP*AP*GP*CP*CP*GP*A)-3'

Chain J: 

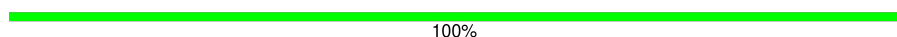


- Molecule 2: 5'-D(P*CP*GP*AP*AP*GP*CP*CP*GP*A)-3'

Chain L: 



- Molecule 3: 5'-D(*TP*CP*GP*C)-3'

Chain M: 

There are no outlier residues recorded for this chain.

- Molecule 3: 5'-D(*TP*CP*GP*C)-3'

Chain O: 



- Molecule 4: 5'-D(P*GP*CP*CP*GP*A)-3'

Chain N: 100%

There are no outlier residues recorded for this chain.

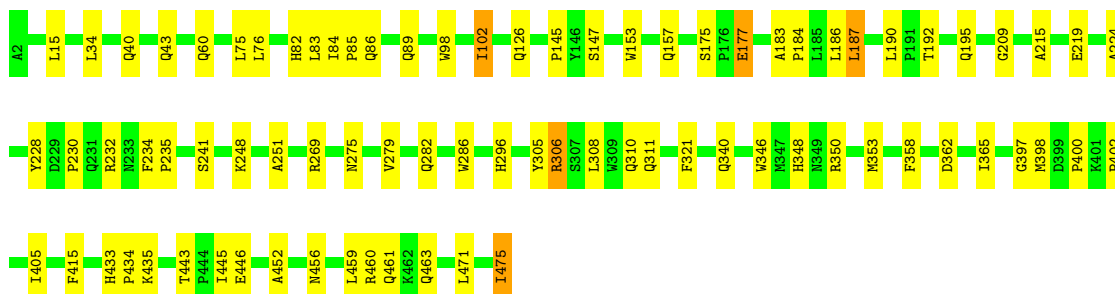
- Molecule 4: 5'-D(P*GP*CP*CP*GP*A)-3'

Chain P: 60% 40%



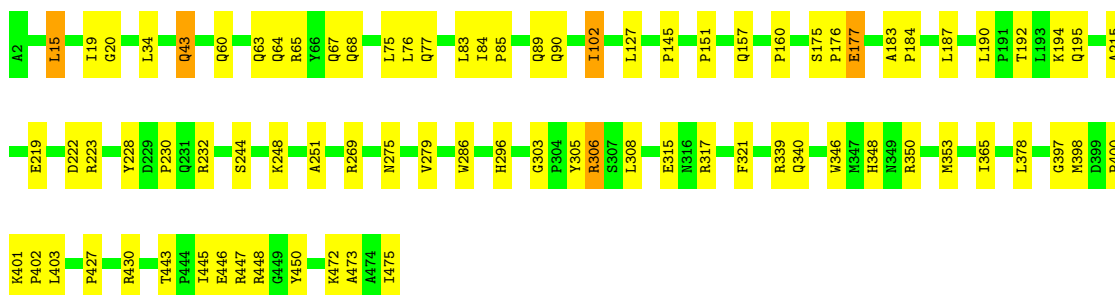
- Molecule 5: Deoxyribodipyrimidine photo-lyase type I

Chain A: 83% 16%



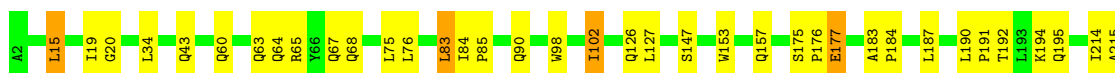
- Molecule 5: Deoxyribodipyrimidine photo-lyase type I

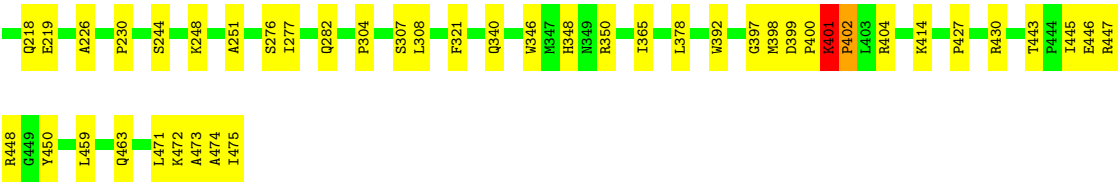
Chain B: 83% 16%



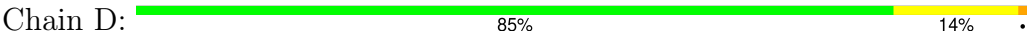
- Molecule 5: Deoxyribodipyrimidine photo-lyase type I

Chain C: 83% 16%





• Molecule 5: Deoxyribodipyrimidine photo-lyase type I



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	173.81Å 88.50Å 161.62Å 90.00° 90.11° 90.00°	Depositor
Resolution (Å)	29.92 – 1.80 29.92 – 1.80	Depositor EDS
% Data completeness (in resolution range)	96.1 (29.92-1.80) 95.8 (29.92-1.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.83 (at 1.80Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.205 , 0.226 0.203 , 0.224	Depositor DCC
R_{free} test set	7425 reflections (3.40%)	wwPDB-VP
Wilson B-factor (Å ²)	24.7	Xtriage
Anisotropy	0.348	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 36.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.417 for -h,-k,l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	18206	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.06% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	I	0.24	0/222	0.57	0/338
1	K	0.24	0/222	0.58	0/338
2	J	0.34	0/209	0.60	0/320
2	L	0.34	0/209	0.59	0/320
3	M	0.27	0/85	0.80	0/129
3	O	0.25	0/85	0.79	0/129
4	N	0.40	0/115	0.57	0/175
4	P	0.39	0/115	0.60	0/175
5	A	0.37	0/3883	0.84	9/5292 (0.2%)
5	B	0.37	0/3891	0.85	7/5302 (0.1%)
5	C	0.37	0/3882	0.85	6/5292 (0.1%)
5	D	0.38	0/3886	0.85	9/5296 (0.2%)
All	All	0.37	0/16804	0.83	31/23106 (0.1%)

There are no bond length outliers.

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	251	ALA	N-CA-C	-6.26	105.13	112.89
5	B	303	GLY	CA-C-N	6.25	127.65	119.84
5	B	303	GLY	C-N-CA	6.25	127.65	119.84
5	B	251	ALA	N-CA-C	-6.10	105.09	112.54
5	D	403	LEU	N-CA-C	-6.02	102.73	110.19
5	C	83	LEU	N-CA-C	6.02	117.92	111.36
5	A	209	GLY	N-CA-C	5.99	118.99	112.29
5	D	251	ALA	N-CA-C	-5.91	105.56	112.89
5	B	83	LEU	N-CA-C	5.82	117.70	111.36
5	C	251	ALA	N-CA-C	-5.79	105.47	112.54
5	C	307	SER	N-CA-C	5.72	117.98	111.11
5	B	187	LEU	N-CA-C	-5.56	100.62	109.96

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	186	LEU	N-CA-C	5.46	118.88	110.42
5	D	209	GLY	N-CA-C	5.46	118.40	112.29
5	D	187	LEU	N-CA-C	-5.44	100.82	109.96
5	D	241	SER	N-CA-C	5.41	118.09	111.82
5	A	187	LEU	N-CA-C	-5.38	100.93	109.96
5	B	378	LEU	N-CA-C	5.38	117.49	109.59
5	C	187	LEU	N-CA-C	-5.36	100.96	109.96
5	B	19	ILE	N-CA-C	5.28	115.72	110.23
5	C	19	ILE	N-CA-C	5.27	115.71	110.23
5	A	452	ALA	N-CA-C	-5.20	102.58	110.39
5	A	241	SER	N-CA-C	5.20	117.85	111.82
5	D	224	ALA	N-CA-C	5.17	118.36	111.75
5	A	147	SER	N-CA-C	-5.16	106.95	114.12
5	A	186	LEU	N-CA-C	5.14	118.39	110.42
5	D	452	ALA	N-CA-C	-5.10	102.74	110.39
5	A	224	ALA	N-CA-C	5.09	118.27	111.75
5	A	415	PHE	N-CA-C	5.09	119.58	113.17
5	C	378	LEU	N-CA-C	5.03	117.50	109.96
5	D	19	ILE	N-CA-C	5.01	115.44	110.23

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	I	218	0	128	9	0
1	K	218	0	128	9	0
2	J	186	0	100	5	0
2	L	186	0	100	5	0
3	M	77	0	47	0	0
3	O	77	0	47	1	0
4	N	103	0	56	0	0
4	P	103	0	56	1	0
5	A	3774	0	3681	60	0
5	B	3782	0	3694	61	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	3773	0	3674	66	0
5	D	3777	0	3685	57	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
7	A	53	0	31	0	0
7	B	53	0	31	1	0
7	C	53	0	31	1	0
7	D	53	0	31	1	0
8	A	26	0	15	0	0
8	B	26	0	16	0	0
8	C	26	0	15	0	0
8	D	26	0	15	0	0
9	A	409	0	0	5	0
9	B	404	0	0	7	0
9	C	374	0	0	9	0
9	D	360	0	0	9	0
9	I	10	0	0	0	0
9	J	11	0	0	0	0
9	K	8	0	0	0	0
9	L	9	0	0	0	0
9	M	14	0	0	0	0
9	N	10	0	0	0	0
9	P	5	0	0	0	0
All	All	18206	0	15581	254	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 8.

All (254) 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)
5:C:401:LYS:HB2	5:C:402:PRO:HD2	1.33	1.07
5:C:401:LYS:HG2	5:C:404:ARG:HH21	1.29	0.98
5:C:401:LYS:HG2	5:C:404:ARG:NH2	1.88	0.88
5:D:199:ASP:HB2	9:D:8744:HOH:O	1.75	0.85
5:C:226:ALA:HA	9:C:7764:HOH:O	1.78	0.84
5:D:403:LEU:O	5:D:404:ARG:HB2	1.79	0.82
5:A:306:ARG:NH2	5:A:400:PRO:HG3	1.94	0.82
5:C:277:ILE:HG13	9:C:7764:HOH:O	1.80	0.81
5:C:401:LYS:CG	5:C:404:ARG:HH21	1.98	0.77
1:I:1:DA:H2''	1:I:2:DT:C5	2.23	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:86:GLN:HE21	5:C:195:GLN:HG2	1.54	0.73
5:A:459:LEU:O	5:A:463:GLN:HG3	1.89	0.72
2:J:9:DA:C2	5:A:402:PRO:HD3	2.25	0.72
1:K:1:DA:H2''	1:K:2:DT:C5	2.25	0.71
5:B:60:GLN:NE2	9:B:9389:HOH:O	2.25	0.70
5:A:84:ILE:HB	5:A:85:PRO:HD3	1.74	0.70
5:B:195:GLN:HG2	5:D:86:GLN:HE21	1.55	0.69
5:D:84:ILE:HB	5:D:85:PRO:HD3	1.75	0.69
5:A:269:ARG:NH2	5:B:219:GLU:HA	2.09	0.68
5:B:64:GLN:O	5:B:68:GLN:HG3	1.94	0.68
5:B:306:ARG:NH2	5:B:400:PRO:HG3	2.09	0.67
5:A:34:LEU:CD1	5:A:76:LEU:HD13	2.25	0.67
5:C:401:LYS:HB2	5:C:402:PRO:CD	2.20	0.66
5:D:34:LEU:CD1	5:D:76:LEU:HD13	2.26	0.66
5:D:404:ARG:NH2	5:D:465:LYS:NZ	2.44	0.66
5:A:102:ILE:HD13	5:A:102:ILE:H	1.62	0.65
5:A:215:ALA:O	5:A:219:GLU:HG3	1.97	0.65
5:C:192:THR:OG1	5:C:195:GLN:HG3	1.96	0.64
5:C:471:LEU:HD12	9:C:7770:HOH:O	1.96	0.64
5:D:102:ILE:HD13	5:D:102:ILE:H	1.63	0.64
5:D:215:ALA:O	5:D:219:GLU:HG3	1.98	0.64
5:B:102:ILE:HD13	5:B:102:ILE:H	1.62	0.63
5:D:400:PRO:O	5:D:401:LYS:HG3	1.97	0.63
5:B:77:GLN:NE2	9:B:9386:HOH:O	2.32	0.62
5:C:84:ILE:HB	5:C:85:PRO:HD3	1.80	0.62
5:C:102:ILE:HD13	5:C:102:ILE:H	1.65	0.62
5:B:84:ILE:HB	5:B:85:PRO:HD3	1.81	0.62
5:B:215:ALA:O	5:B:219:GLU:HG3	1.99	0.61
5:D:398:MET:HE3	5:D:398:MET:HA	1.82	0.61
5:C:215:ALA:O	5:C:219:GLU:HG3	2.00	0.61
5:A:228:TYR:CE2	5:A:232:ARG:HD2	2.36	0.61
5:C:248:LYS:HD3	5:C:248:LYS:C	2.26	0.61
5:C:392:TRP:O	5:C:404:ARG:NH1	2.34	0.60
5:B:248:LYS:HD3	5:B:248:LYS:C	2.27	0.59
5:D:348:HIS:CD2	5:D:350:ARG:H	2.21	0.59
5:D:403:LEU:O	5:D:404:ARG:CB	2.47	0.59
5:B:192:THR:OG1	5:B:195:GLN:HG3	2.02	0.59
5:A:275:ASN:O	5:A:279:VAL:HG23	2.03	0.58
5:C:348:HIS:CD2	5:C:350:ARG:H	2.20	0.58
5:B:60:GLN:HG2	5:B:190:LEU:HD23	1.84	0.58
5:A:348:HIS:CD2	5:A:350:ARG:H	2.20	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:348:HIS:HD2	5:C:350:ARG:H	1.51	0.58
5:B:308:LEU:C	5:B:308:LEU:HD23	2.29	0.58
5:D:399:ASP:N	5:D:400:PRO:HD3	2.19	0.58
1:K:7:DT:H72	5:B:286:TRP:CD2	2.39	0.58
5:C:60:GLN:HG2	5:C:190:LEU:HD23	1.86	0.57
5:B:160:PRO:HG2	9:B:9119:HOH:O	2.04	0.57
5:C:399:ASP:N	5:C:400:PRO:HD3	2.19	0.57
5:B:348:HIS:CD2	5:B:350:ARG:H	2.21	0.57
5:A:269:ARG:HH21	5:B:219:GLU:HA	1.67	0.57
5:C:308:LEU:C	5:C:308:LEU:HD23	2.30	0.57
5:D:348:HIS:HD2	5:D:350:ARG:H	1.51	0.57
5:C:276:SER:HB2	9:C:7764:HOH:O	2.03	0.57
5:A:192:THR:OG1	5:A:195:GLN:HG3	2.05	0.57
5:B:75:LEU:C	5:B:76:LEU:HD12	2.30	0.56
5:C:34:LEU:CD1	5:C:76:LEU:HD13	2.35	0.56
5:B:348:HIS:HD2	5:B:350:ARG:H	1.53	0.56
5:D:192:THR:OG1	5:D:195:GLN:HG3	2.05	0.56
5:D:248:LYS:HD3	5:D:248:LYS:C	2.29	0.56
5:C:321:PHE:HB2	5:C:365:ILE:HD13	1.86	0.56
5:C:473:ALA:C	5:C:475:ILE:H	2.14	0.56
5:C:75:LEU:C	5:C:76:LEU:HD12	2.31	0.56
5:C:400:PRO:O	5:C:401:LYS:HB3	2.06	0.56
5:D:405:ILE:HD12	5:D:461:GLN:HG3	1.86	0.56
5:B:427:PRO:HA	5:B:430:ARG:NE	2.21	0.55
5:C:427:PRO:HA	5:C:430:ARG:NE	2.22	0.55
5:A:43:GLN:NE2	5:C:43:GLN:O	2.40	0.54
5:C:15:LEU:HD22	5:C:65:ARG:HB3	1.89	0.54
5:A:305:TYR:CE1	5:A:398:MET:HG2	2.42	0.54
5:D:308:LEU:C	5:D:308:LEU:HD23	2.32	0.54
5:A:348:HIS:HD2	5:A:350:ARG:H	1.54	0.54
5:D:147:SER:O	5:D:399:ASP:N	2.40	0.54
1:K:7:DT:H72	5:B:286:TRP:CE3	2.43	0.54
5:C:401:LYS:CB	5:C:402:PRO:HD2	2.17	0.54
5:A:306:ARG:CZ	5:A:400:PRO:HG3	2.38	0.53
5:A:308:LEU:HD23	5:A:308:LEU:C	2.33	0.53
5:C:401:LYS:CD	5:C:404:ARG:HH21	2.21	0.53
5:D:321:PHE:HB2	5:D:365:ILE:HD13	1.91	0.53
2:L:9:DA:C2	5:B:402:PRO:HD3	2.43	0.53
5:A:248:LYS:HD3	5:A:248:LYS:C	2.33	0.53
5:D:75:LEU:C	5:D:76:LEU:HD12	2.34	0.53
5:D:472:LYS:O	5:D:475:ILE:HG22	2.09	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:160:PRO:HG2	9:D:8603:HOH:O	2.08	0.52
5:B:228:TYR:CE2	5:B:232:ARG:HD2	2.44	0.52
5:B:34:LEU:CD1	5:B:76:LEU:HD13	2.39	0.52
5:A:75:LEU:C	5:A:76:LEU:HD12	2.35	0.52
5:A:321:PHE:HB2	5:A:365:ILE:HD13	1.92	0.52
5:D:232:ARG:HD2	9:D:8648:HOH:O	2.10	0.52
5:D:404:ARG:NH2	5:D:465:LYS:HZ3	2.07	0.51
5:C:447:ARG:HB2	5:C:450:TYR:HB3	1.91	0.51
5:A:86:GLN:HE21	5:C:195:GLN:CG	2.21	0.51
5:A:306:ARG:HB2	5:A:397:GLY:O	2.09	0.51
5:D:147:SER:HB2	5:D:398:MET:HE2	1.93	0.51
5:C:64:GLN:O	5:C:68:GLN:HG3	2.11	0.50
1:I:7:DT:H72	5:A:286:TRP:CD2	2.47	0.50
5:A:177:GLU:CD	5:A:177:GLU:H	2.20	0.50
5:A:311:GLN:CD	5:A:475:ILE:HD11	2.36	0.50
5:B:447:ARG:HB2	5:B:450:TYR:HB3	1.92	0.50
5:C:445:ILE:HD12	5:C:446:GLU:N	2.26	0.50
5:D:34:LEU:HD21	5:D:84:ILE:CD1	2.42	0.49
5:A:445:ILE:HG13	9:A:9409:HOH:O	2.11	0.49
5:D:459:LEU:HG	5:D:463:GLN:HE21	1.76	0.49
5:A:40:GLN:HG2	9:A:9283:HOH:O	2.12	0.49
5:B:445:ILE:HD12	5:B:446:GLU:N	2.27	0.49
5:A:269:ARG:NH2	5:B:219:GLU:HG2	2.27	0.49
9:A:9218:HOH:O	5:B:269:ARG:HG2	2.12	0.49
5:A:34:LEU:HD21	5:A:84:ILE:CD1	2.43	0.49
5:A:98:TRP:CE2	5:A:126:GLN:HG2	2.47	0.49
5:B:43:GLN:O	5:D:43:GLN:NE2	2.42	0.49
5:B:401:LYS:HE3	9:B:9267:HOH:O	2.12	0.49
5:A:175:SER:OG	5:A:177:GLU:HG2	2.13	0.49
5:B:306:ARG:HB2	5:B:397:GLY:O	2.13	0.49
5:D:405:ILE:CD1	5:D:461:GLN:HG3	2.41	0.49
5:A:340:GLN:HG2	5:A:346:TRP:O	2.12	0.48
1:K:8:TCP:C6	5:B:353:MET:SD	3.01	0.48
1:I:8:TCP:C6	5:A:353:MET:SD	3.02	0.48
1:K:7:DT:H2''	1:K:8:TCP:O5'	2.12	0.48
5:B:177:GLU:CD	5:B:177:GLU:H	2.21	0.48
5:D:85:PRO:O	5:D:89:GLN:HG3	2.14	0.48
5:B:473:ALA:C	5:B:475:ILE:H	2.22	0.48
1:I:7:DT:H73	1:I:8:TCP:H71	1.96	0.48
5:B:321:PHE:HB2	5:B:365:ILE:HD13	1.95	0.48
5:D:340:GLN:HG2	5:D:346:TRP:O	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:414:LYS:HG3	9:D:8833:HOH:O	2.13	0.48
2:L:7:DG:H1'	2:L:8:DA:O5'	2.14	0.48
1:I:7:DT:H2''	1:I:8:TCP:O5'	2.14	0.47
5:B:60:GLN:HG2	5:B:190:LEU:CD2	2.44	0.47
1:I:1:DA:H2''	1:I:2:DT:C6	2.49	0.47
5:B:60:GLN:O	5:B:64:GLN:HG3	2.14	0.47
5:D:183:ALA:N	5:D:184:PRO:HD2	2.28	0.47
5:C:60:GLN:HG2	5:C:190:LEU:CD2	2.44	0.47
5:C:397:GLY:O	5:C:400:PRO:HG3	2.15	0.47
5:B:472:LYS:O	5:B:475:ILE:HG22	2.14	0.47
5:D:153:TRP:CH2	5:D:282:GLN:HG2	2.50	0.47
5:D:404:ARG:HH21	5:D:465:LYS:HZ3	1.63	0.47
5:B:427:PRO:HB3	5:B:430:ARG:CZ	2.44	0.47
5:D:275:ASN:O	5:D:279:VAL:HG23	2.15	0.47
5:C:414:LYS:NZ	9:C:7849:HOH:O	2.41	0.47
5:B:222:ASP:O	5:B:223:ARG:HD3	2.16	0.46
5:C:447:ARG:O	5:C:448:ARG:C	2.58	0.46
5:B:176:PRO:HD2	5:B:177:GLU:OE2	2.16	0.46
5:C:153:TRP:CH2	5:C:282:GLN:HG2	2.50	0.46
5:C:472:LYS:O	5:C:475:ILE:HG22	2.15	0.46
5:A:183:ALA:HB3	5:A:184:PRO:HD3	1.97	0.46
5:B:339:ARG:HD3	9:B:9357:HOH:O	2.16	0.46
5:D:404:ARG:NH2	5:D:465:LYS:HZ1	2.14	0.46
5:B:63:GLN:O	5:B:67:GLN:HG3	2.15	0.46
5:D:98:TRP:CE2	5:D:126:GLN:HG2	2.50	0.46
5:A:82:HIS:ND1	5:C:194:LYS:NZ	2.51	0.46
5:A:145:PRO:HB3	5:A:296:HIS:CD2	2.51	0.46
5:B:15:LEU:HD22	5:B:65:ARG:HB3	1.97	0.46
5:C:20:GLY:HA2	5:C:127:LEU:HD12	1.97	0.46
5:C:177:GLU:H	5:C:177:GLU:CD	2.23	0.46
5:D:445:ILE:HG13	9:D:8837:HOH:O	2.16	0.46
1:K:1:DA:H2''	1:K:2:DT:C6	2.50	0.45
1:K:1:DA:H2''	1:K:2:DT:H72	1.99	0.45
5:A:153:TRP:CH2	5:A:282:GLN:HG2	2.51	0.45
5:B:447:ARG:O	5:B:448:ARG:C	2.59	0.45
2:J:7:DG:H1'	2:J:8:DA:O5'	2.15	0.45
5:A:305:TYR:CD1	5:A:398:MET:HG2	2.51	0.45
5:C:401:LYS:CG	5:C:404:ARG:NH2	2.67	0.45
5:C:443:THR:HG23	9:C:7767:HOH:O	2.16	0.45
1:I:7:DT:H72	5:A:286:TRP:CE3	2.52	0.45
5:C:401:LYS:HD2	5:C:404:ARG:HE	1.80	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:183:ALA:HB3	5:B:184:PRO:HD3	1.97	0.45
5:D:404:ARG:NH1	5:D:461:GLN:OE1	2.49	0.45
5:A:348:HIS:HE1	9:A:9025:HOH:O	2.00	0.45
1:I:1:DA:H2''	1:I:2:DT:H72	1.98	0.44
5:D:404:ARG:HD3	5:D:405:ILE:N	2.31	0.44
5:A:234:PHE:HA	5:A:235:PRO:HD2	1.94	0.44
5:B:175:SER:OG	5:B:177:GLU:HG2	2.17	0.44
5:C:340:GLN:HG2	5:C:346:TRP:O	2.16	0.44
5:C:63:GLN:O	5:C:67:GLN:HG3	2.18	0.44
5:A:435:LYS:HB2	5:A:435:LYS:HE3	1.85	0.44
5:B:43:GLN:OE1	5:B:43:GLN:HA	2.14	0.44
2:J:8:DA:H2''	5:A:402:PRO:HG3	1.99	0.44
5:B:306:ARG:CZ	5:B:400:PRO:HG3	2.48	0.44
5:C:98:TRP:CE2	5:C:126:GLN:HG2	2.52	0.44
5:C:244:SER:HB3	7:C:7485:FAD:C5'	2.47	0.43
2:J:7:DG:H2''	2:J:8:DA:O5'	2.18	0.43
5:C:176:PRO:HD2	5:C:177:GLU:OE2	2.18	0.43
5:D:456:ASN:O	5:D:460:ARG:HG2	2.18	0.43
5:B:194:LYS:NZ	5:D:82:HIS:ND1	2.53	0.43
5:C:401:LYS:HB3	5:C:401:LYS:NZ	2.33	0.43
5:C:459:LEU:O	5:C:463:GLN:HG3	2.18	0.43
1:I:1:DA:H2''	1:I:2:DT:C7	2.48	0.43
5:B:64:GLN:HB3	9:B:9210:HOH:O	2.18	0.43
5:D:404:ARG:HH22	5:D:465:LYS:HZ1	1.67	0.43
5:B:340:GLN:HG2	5:B:346:TRP:O	2.17	0.43
5:D:244:SER:HB3	7:D:8485:FAD:C5'	2.48	0.43
5:A:405:ILE:HG21	5:A:461:GLN:HG3	2.00	0.43
5:A:471:LEU:O	5:A:475:ILE:HB	2.19	0.43
5:B:315:GLU:HG2	5:B:317:ARG:HG3	2.01	0.43
5:C:64:GLN:HB3	9:C:7727:HOH:O	2.17	0.43
1:K:7:DT:H73	1:K:8:TCP:H71	2.00	0.43
5:B:275:ASN:O	5:B:279:VAL:HG23	2.19	0.43
5:B:305:TYR:CD1	5:B:398:MET:HB3	2.53	0.43
5:C:83:LEU:HD22	9:C:7779:HOH:O	2.18	0.43
5:C:401:LYS:CG	5:C:404:ARG:HE	2.32	0.43
5:D:158:ALA:HB3	9:D:8776:HOH:O	2.19	0.43
1:K:1:DA:H2''	1:K:2:DT:C7	2.49	0.43
5:B:244:SER:HB3	7:B:6485:FAD:C5'	2.49	0.43
3:O:9:DC:H2''	3:O:10:DG:OP2	2.17	0.42
5:C:183:ALA:N	5:C:184:PRO:HD2	2.34	0.42
5:C:214:ILE:O	5:C:218:GLN:HG3	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:194:LYS:CD	9:D:8744:HOH:O	2.66	0.42
5:D:459:LEU:O	5:D:463:GLN:HG3	2.19	0.42
5:A:76:LEU:HD23	5:A:83:LEU:HB3	2.00	0.42
5:A:60:GLN:HG2	5:A:190:LEU:HD23	2.01	0.42
5:A:305:TYR:O	5:A:310:GLN:NE2	2.52	0.42
5:A:433:HIS:ND1	5:A:434:PRO:HD2	2.34	0.42
2:L:9:DA:H2''	2:L:10:DG:O5'	2.19	0.42
2:L:13:DG:C5'	5:B:151:PRO:HG2	2.49	0.42
5:D:5:ILE:HD12	5:D:28:SER:HB3	2.02	0.42
5:D:219:GLU:HG3	9:D:8642:HOH:O	2.19	0.42
5:A:85:PRO:O	5:A:89:GLN:HG3	2.20	0.42
5:A:475:ILE:OXT	5:A:475:ILE:HG23	2.19	0.42
5:A:471:LEU:HD11	5:A:475:ILE:HD12	2.02	0.42
5:D:187:LEU:HD12	5:D:187:LEU:HA	1.95	0.42
4:P:11:DC:H2''	4:P:12:DC:C5	2.55	0.42
5:C:34:LEU:HD21	5:C:84:ILE:CD1	2.49	0.42
5:C:147:SER:O	5:C:399:ASP:N	2.50	0.42
5:D:34:LEU:HD21	5:D:84:ILE:HD12	2.00	0.42
5:D:404:ARG:HD3	5:D:405:ILE:H	1.84	0.42
2:L:7:DG:H2''	2:L:8:DA:O5'	2.20	0.41
5:C:392:TRP:HD1	9:C:7668:HOH:O	2.03	0.41
5:D:473:ALA:C	5:D:475:ILE:H	2.28	0.41
5:A:219:GLU:HG3	9:A:9159:HOH:O	2.20	0.41
5:C:427:PRO:HB3	5:C:430:ARG:CZ	2.50	0.41
5:A:306:ARG:HH22	5:A:308:LEU:HD13	1.85	0.41
5:B:85:PRO:O	5:B:89:GLN:HG3	2.21	0.41
5:A:443:THR:OG1	5:A:446:GLU:HG3	2.21	0.41
5:A:456:ASN:O	5:A:460:ARG:HG2	2.21	0.41
5:C:34:LEU:HD21	5:C:84:ILE:HD12	2.03	0.41
5:C:190:LEU:HD12	5:C:191:PRO:HD2	2.03	0.40
2:J:9:DA:H2''	2:J:10:DG:O5'	2.21	0.40
5:B:20:GLY:HA2	5:B:127:LEU:HD12	2.03	0.40
5:B:145:PRO:HB3	5:B:296:HIS:CD2	2.56	0.40
5:D:145:PRO:HB3	5:D:296:HIS:CD2	2.55	0.40
5:A:187:LEU:HD12	5:A:187:LEU:HA	1.96	0.40
5:D:126:GLN:NE2	9:D:8518:HOH:O	2.55	0.40
5:A:358:PHE:O	5:A:362:ASP:HB2	2.22	0.40
5:B:443:THR:HG23	9:B:9276:HOH:O	2.21	0.40
5:C:175:SER:OG	5:C:177:GLU:HG2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	A	472/474 (100%)	457 (97%)	15 (3%)	0	100	100
5	B	472/474 (100%)	458 (97%)	14 (3%)	0	100	100
5	C	472/474 (100%)	454 (96%)	15 (3%)	3 (1%)	21	11
5	D	472/474 (100%)	453 (96%)	18 (4%)	1 (0%)	43	31
All	All	1888/1896 (100%)	1822 (96%)	62 (3%)	4 (0%)	43	31

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	D	404	ARG
5	C	474	ALA
5	C	402	PRO
5	C	401	LYS

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	
5	A	383/385 (100%)	376 (98%)	7 (2%)	51	43
5	B	385/385 (100%)	376 (98%)	9 (2%)	44	33
5	C	383/385 (100%)	374 (98%)	9 (2%)	44	33
5	D	384/385 (100%)	378 (98%)	6 (2%)	55	47
All	All	1535/1540 (100%)	1504 (98%)	31 (2%)	48	38

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	A	15	LEU
5	A	102	ILE
5	A	157	GLN
5	A	177	GLU
5	A	230	PRO
5	A	306	ARG
5	A	475	ILE
5	B	15	LEU
5	B	43	GLN
5	B	90	GLN
5	B	102	ILE
5	B	157	GLN
5	B	177	GLU
5	B	230	PRO
5	B	306	ARG
5	B	403	LEU
5	C	15	LEU
5	C	90	GLN
5	C	102	ILE
5	C	157	GLN
5	C	177	GLU
5	C	230	PRO
5	C	304	PRO
5	C	398	MET
5	C	401	LYS
5	D	15	LEU
5	D	102	ILE
5	D	157	GLN
5	D	230	PRO
5	D	398	MET
5	D	404	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
5	A	63	GLN
5	A	86	GLN
5	A	126	GLN
5	A	157	GLN
5	A	259	GLN
5	A	282	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	A	310	GLN
5	A	348	HIS
5	A	376	GLN
5	A	386	ASN
5	A	463	GLN
5	B	63	GLN
5	B	90	GLN
5	B	112	GLN
5	B	126	GLN
5	B	144	ASN
5	B	157	GLN
5	B	311	GLN
5	B	348	HIS
5	B	372	GLN
5	B	376	GLN
5	B	386	ASN
5	C	40	GLN
5	C	63	GLN
5	C	68	GLN
5	C	77	GLN
5	C	90	GLN
5	C	112	GLN
5	C	126	GLN
5	C	157	GLN
5	C	159	GLN
5	C	282	GLN
5	C	348	HIS
5	C	376	GLN
5	C	386	ASN
5	C	391	GLN
5	C	461	GLN
5	D	63	GLN
5	D	81	GLN
5	D	86	GLN
5	D	126	GLN
5	D	157	GLN
5	D	282	GLN
5	D	348	HIS
5	D	376	GLN
5	D	386	ASN
5	D	463	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 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	$\# Z > 2$
1	TCP	I	8	1	19,19,19	0.25	0	27,27,27	0.61	0
1	TCP	K	8	1	19,19,19	0.28	0	27,27,27	0.63	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	TCP	I	8	1	-	4/7/19/19	0/2/2/2
1	TCP	K	8	1	-	4/7/19/19	0/2/2/2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	I	8	TCP	C2'-C1'-N1-C6
1	K	8	TCP	C2'-C1'-N1-C6
1	I	8	TCP	O4'-C1'-N1-C6
1	K	8	TCP	O4'-C1'-N1-C6
1	I	8	TCP	C2'-C1'-N1-C2
1	K	8	TCP	C2'-C1'-N1-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	I	8	TCP	O4'-C1'-N1-C2
1	K	8	TCP	O4'-C1'-N1-C2

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	I	8	TCP	3	0
1	K	8	TCP	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 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
8	HDF	C	7486	-	28,28,28	1.55	4 (14%)	38,41,41	2.80	10 (26%)
7	FAD	C	7485	-	58,58,58	1.21	5 (8%)	85,89,89	0.99	4 (4%)
8	HDF	B	6486	-	28,28,28	1.55	5 (17%)	38,41,41	2.78	10 (26%)
7	FAD	D	8485	-	58,58,58	1.21	5 (8%)	85,89,89	0.97	4 (4%)
8	HDF	D	8486	-	28,28,28	1.60	5 (17%)	38,41,41	2.76	11 (28%)
7	FAD	A	5485	-	58,58,58	1.18	5 (8%)	85,89,89	0.95	4 (4%)
8	HDF	A	5486	-	28,28,28	1.56	6 (21%)	38,41,41	2.76	10 (26%)
7	FAD	B	6485	-	58,58,58	1.25	4 (6%)	85,89,89	0.98	4 (4%)

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
7	FAD	B	6485	-	-	4/34/50/50	0/6/6/6
8	HDF	C	7486	-	2/2/3/3	5/14/14/14	0/3/3/3
7	FAD	C	7485	-	-	4/34/50/50	0/6/6/6
7	FAD	D	8485	-	-	5/34/50/50	0/6/6/6
8	HDF	D	8486	-	2/2/3/3	5/14/14/14	0/3/3/3
8	HDF	B	6486	-	2/2/3/3	5/14/14/14	0/3/3/3
8	HDF	A	5486	-	2/2/3/3	5/14/14/14	0/3/3/3
7	FAD	A	5485	-	-	5/34/50/50	0/6/6/6

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	8485	FAD	C4X-N5	4.42	1.40	1.30
7	B	6485	FAD	C4X-N5	4.41	1.40	1.30
7	A	5485	FAD	C4X-N5	4.36	1.40	1.30
8	D	8486	HDF	C1'-N10	-4.26	1.37	1.47
8	A	5486	HDF	C1'-N10	-4.18	1.37	1.47
8	B	6486	HDF	C1'-C2'	-4.03	1.47	1.52
7	C	7485	FAD	C4X-N5	4.02	1.39	1.30
8	C	7486	HDF	C1'-N10	-3.96	1.38	1.47
8	D	8486	HDF	C1'-C2'	-3.94	1.47	1.52
8	C	7486	HDF	C1'-C2'	-3.86	1.47	1.52
8	B	6486	HDF	C1'-N10	-3.83	1.38	1.47
8	A	5486	HDF	C1'-C2'	-3.79	1.47	1.52
8	D	8486	HDF	C10-N1	3.35	1.40	1.33
8	A	5486	HDF	C10-N1	3.22	1.39	1.33
7	B	6485	FAD	P-O3P	-3.18	1.56	1.59
8	C	7486	HDF	C10-N1	3.10	1.39	1.33
8	B	6486	HDF	C10-N1	3.04	1.39	1.33
7	C	7485	FAD	PA-O3P	2.99	1.62	1.59
7	A	5485	FAD	C9A-C5X	2.80	1.45	1.41
7	C	7485	FAD	C9A-C5X	2.67	1.45	1.41
7	D	8485	FAD	C9A-C5X	2.61	1.45	1.41
7	B	6485	FAD	C9A-C5X	2.56	1.45	1.41
8	B	6486	HDF	C5A-C5	-2.50	1.38	1.43
8	C	7486	HDF	C5A-C5	-2.45	1.38	1.43
7	A	5485	FAD	PA-O3P	2.34	1.62	1.59
7	C	7485	FAD	P-O3P	-2.30	1.57	1.59
7	C	7485	FAD	C2A-N1A	2.25	1.37	1.33
8	D	8486	HDF	C5A-C5	-2.23	1.39	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	8485	FAD	C10-N1	2.23	1.37	1.33
8	B	6486	HDF	C5-C4A	2.23	1.40	1.35
8	A	5486	HDF	C5A-C5	-2.19	1.39	1.43
7	D	8485	FAD	C2A-N1A	2.17	1.37	1.33
8	A	5486	HDF	C6-C5A	-2.15	1.37	1.41
7	B	6485	FAD	C10-N1	2.15	1.37	1.33
7	A	5485	FAD	C10-N1	2.14	1.37	1.33
7	A	5485	FAD	C2A-N1A	2.11	1.37	1.33
7	D	8485	FAD	PA-O3P	2.07	1.61	1.59
8	D	8486	HDF	C6-C5A	-2.06	1.37	1.41
8	A	5486	HDF	C5-C4A	2.04	1.40	1.35

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	7486	HDF	C4-C4A-C10	12.59	124.08	117.48
8	A	5486	HDF	C4-C4A-C10	12.53	124.05	117.48
8	D	8486	HDF	C4-C4A-C10	12.46	124.01	117.48
8	B	6486	HDF	C4-C4A-C10	12.44	124.00	117.48
8	C	7486	HDF	C10-N1-C2	5.44	128.63	116.85
8	B	6486	HDF	C10-N1-C2	5.43	128.60	116.85
8	D	8486	HDF	C10-N1-C2	5.42	128.59	116.85
8	A	5486	HDF	C10-N1-C2	5.31	128.34	116.85
8	D	8486	HDF	C1'-C2'-C3'	4.42	121.65	109.66
8	B	6486	HDF	C1'-C2'-C3'	4.42	121.64	109.66
8	C	7486	HDF	C1'-C2'-C3'	4.39	121.58	109.66
8	A	5486	HDF	C1'-C2'-C3'	4.37	121.52	109.66
8	C	7486	HDF	O3'-C3'-C2'	3.45	116.76	108.93
8	B	6486	HDF	O3'-C3'-C2'	3.38	116.60	108.93
8	C	7486	HDF	C5A-C9A-N10	3.33	122.63	118.72
8	B	6486	HDF	C5A-C9A-N10	3.25	122.54	118.72
8	D	8486	HDF	C5A-C9A-N10	3.19	122.46	118.72
8	A	5486	HDF	C5A-C9A-N10	3.17	122.45	118.72
8	D	8486	HDF	O3'-C3'-C2'	3.16	116.12	108.93
8	A	5486	HDF	O3'-C3'-C2'	3.12	116.02	108.93
7	D	8485	FAD	C9A-C5X-N5	-2.95	119.32	122.45
7	B	6485	FAD	C9A-C5X-N5	-2.90	119.38	122.45
7	A	5485	FAD	C9A-C5X-N5	-2.81	119.47	122.45
7	C	7485	FAD	C9A-C5X-N5	-2.76	119.53	122.45
8	B	6486	HDF	C9A-N10-C10	-2.74	116.57	120.75
8	C	7486	HDF	C9A-N10-C10	-2.72	116.60	120.75
8	D	8486	HDF	C9A-N10-C10	-2.70	116.63	120.75

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	5486	HDF	C9A-N10-C10	-2.66	116.69	120.75
7	C	7485	FAD	C4-C4X-N5	2.59	121.78	118.21
7	A	5485	FAD	C4-C4X-N5	2.52	121.68	118.21
7	D	8485	FAD	C4-C4X-N5	2.49	121.65	118.21
8	A	5486	HDF	C4'-C3'-C2'	2.42	117.60	113.57
8	C	7486	HDF	C4'-C3'-C2'	2.40	117.56	113.57
8	D	8486	HDF	N3-C2-N1	-2.37	114.47	119.50
7	B	6485	FAD	C4-C4X-N5	2.34	121.44	118.21
8	B	6486	HDF	N3-C2-N1	-2.32	114.57	119.50
8	C	7486	HDF	N3-C2-N1	-2.32	114.58	119.50
7	C	7485	FAD	C10-C4X-N5	-2.31	120.10	124.81
8	A	5486	HDF	N3-C2-N1	-2.30	114.61	119.50
8	D	8486	HDF	C4'-C3'-C2'	2.29	117.39	113.57
8	C	7486	HDF	C9-C9A-N10	-2.28	118.79	121.85
8	B	6486	HDF	C9-C9A-N10	-2.25	118.82	121.85
8	B	6486	HDF	C4'-C3'-C2'	2.25	117.32	113.57
8	C	7486	HDF	O2-C2-N3	2.18	122.76	118.58
7	D	8485	FAD	C10-C4X-N5	-2.17	120.38	124.81
7	B	6485	FAD	C10-C4X-N5	-2.15	120.41	124.81
7	D	8485	FAD	N3A-C2A-N1A	-2.14	125.34	128.58
8	B	6486	HDF	O2-C2-N3	2.14	122.69	118.58
7	A	5485	FAD	N3A-C2A-N1A	-2.14	125.35	128.58
7	B	6485	FAD	N3A-C2A-N1A	-2.13	125.35	128.58
8	D	8486	HDF	O2-C2-N3	2.12	122.66	118.58
7	A	5485	FAD	C10-C4X-N5	-2.12	120.49	124.81
7	C	7485	FAD	N3A-C2A-N1A	-2.11	125.39	128.58
8	D	8486	HDF	C9-C9A-N10	-2.10	119.03	121.85
8	A	5486	HDF	C9-C9A-N10	-2.10	119.03	121.85
8	D	8486	HDF	N10-C10-N1	2.04	124.52	118.51
8	A	5486	HDF	N10-C10-N1	2.00	124.41	118.51

All (8) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
8	A	5486	HDF	C4'
8	A	5486	HDF	C2'
8	B	6486	HDF	C4'
8	B	6486	HDF	C2'
8	C	7486	HDF	C4'
8	C	7486	HDF	C2'
8	D	8486	HDF	C4'
8	D	8486	HDF	C2'

All (38) torsion outliers are listed below:

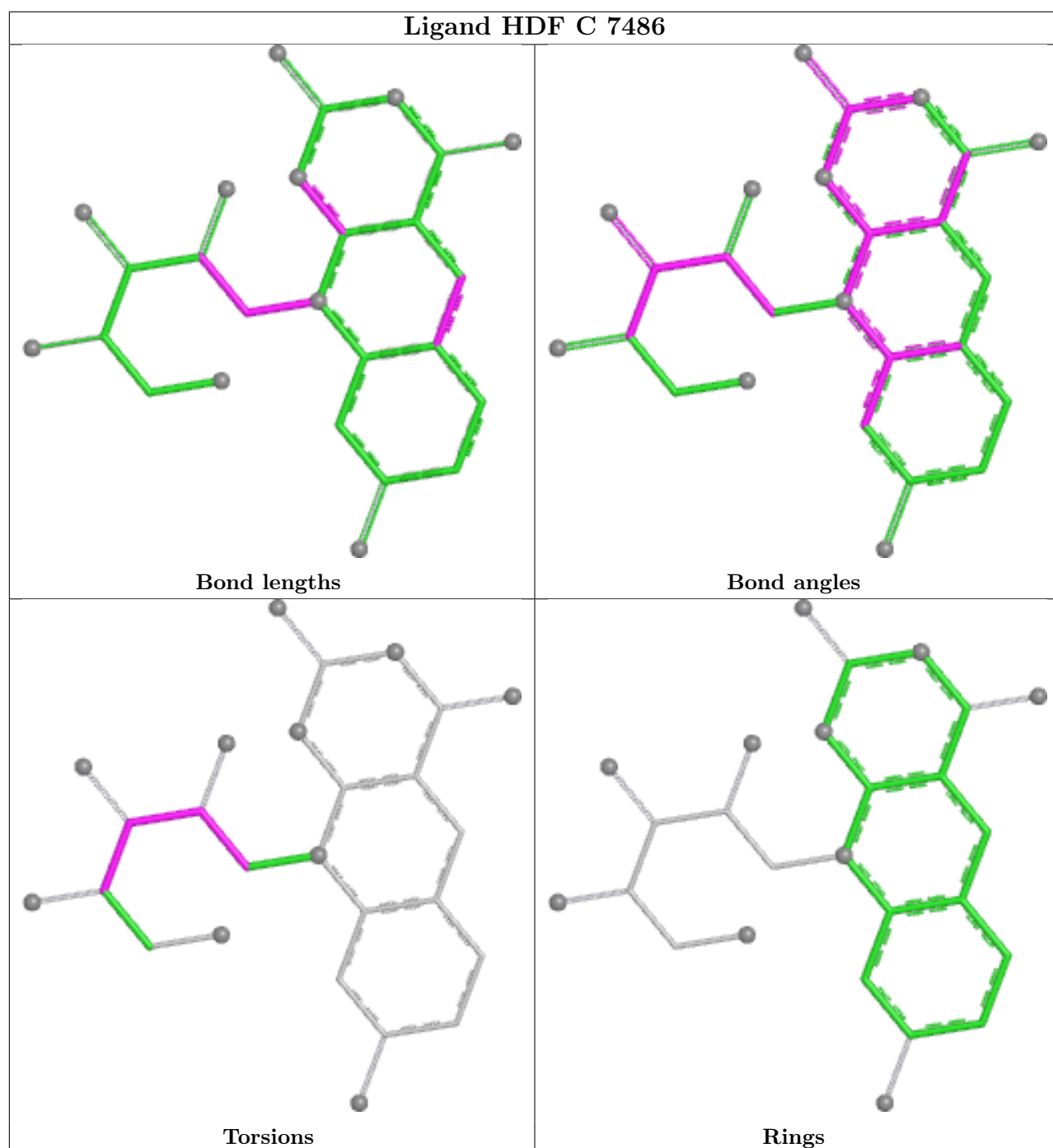
Mol	Chain	Res	Type	Atoms
7	A	5485	FAD	C5B-O5B-PA-O1A
7	B	6485	FAD	C5B-O5B-PA-O1A
7	C	7485	FAD	C5B-O5B-PA-O1A
8	A	5486	HDF	N10-C1'-C2'-O2'
8	A	5486	HDF	N10-C1'-C2'-C3'
8	A	5486	HDF	O2'-C2'-C3'-O3'
8	A	5486	HDF	O2'-C2'-C3'-C4'
8	B	6486	HDF	N10-C1'-C2'-O2'
8	B	6486	HDF	N10-C1'-C2'-C3'
8	B	6486	HDF	O2'-C2'-C3'-O3'
8	B	6486	HDF	O2'-C2'-C3'-C4'
8	C	7486	HDF	N10-C1'-C2'-O2'
8	C	7486	HDF	N10-C1'-C2'-C3'
8	C	7486	HDF	O2'-C2'-C3'-O3'
8	C	7486	HDF	O2'-C2'-C3'-C4'
8	D	8486	HDF	N10-C1'-C2'-O2'
8	D	8486	HDF	N10-C1'-C2'-C3'
8	D	8486	HDF	O2'-C2'-C3'-O3'
8	D	8486	HDF	O2'-C2'-C3'-C4'
8	C	7486	HDF	C2'-C3'-C4'-O4'
8	B	6486	HDF	C2'-C3'-C4'-O4'
7	B	6485	FAD	P-O3P-PA-O1A
7	C	7485	FAD	P-O3P-PA-O1A
7	D	8485	FAD	P-O3P-PA-O1A
7	A	5485	FAD	C5'-O5'-P-O1P
7	B	6485	FAD	C5'-O5'-P-O1P
7	C	7485	FAD	C5'-O5'-P-O1P
7	D	8485	FAD	C5B-O5B-PA-O1A
7	D	8485	FAD	C5'-O5'-P-O1P
7	C	7485	FAD	C4'-C5'-O5'-P
7	A	5485	FAD	P-O3P-PA-O1A
7	B	6485	FAD	C4'-C5'-O5'-P
7	A	5485	FAD	C4'-C5'-O5'-P
7	D	8485	FAD	C4'-C5'-O5'-P
8	A	5486	HDF	C2'-C3'-C4'-O4'
8	D	8486	HDF	C2'-C3'-C4'-O4'
7	A	5485	FAD	P-O3P-PA-O2A
7	D	8485	FAD	P-O3P-PA-O2A

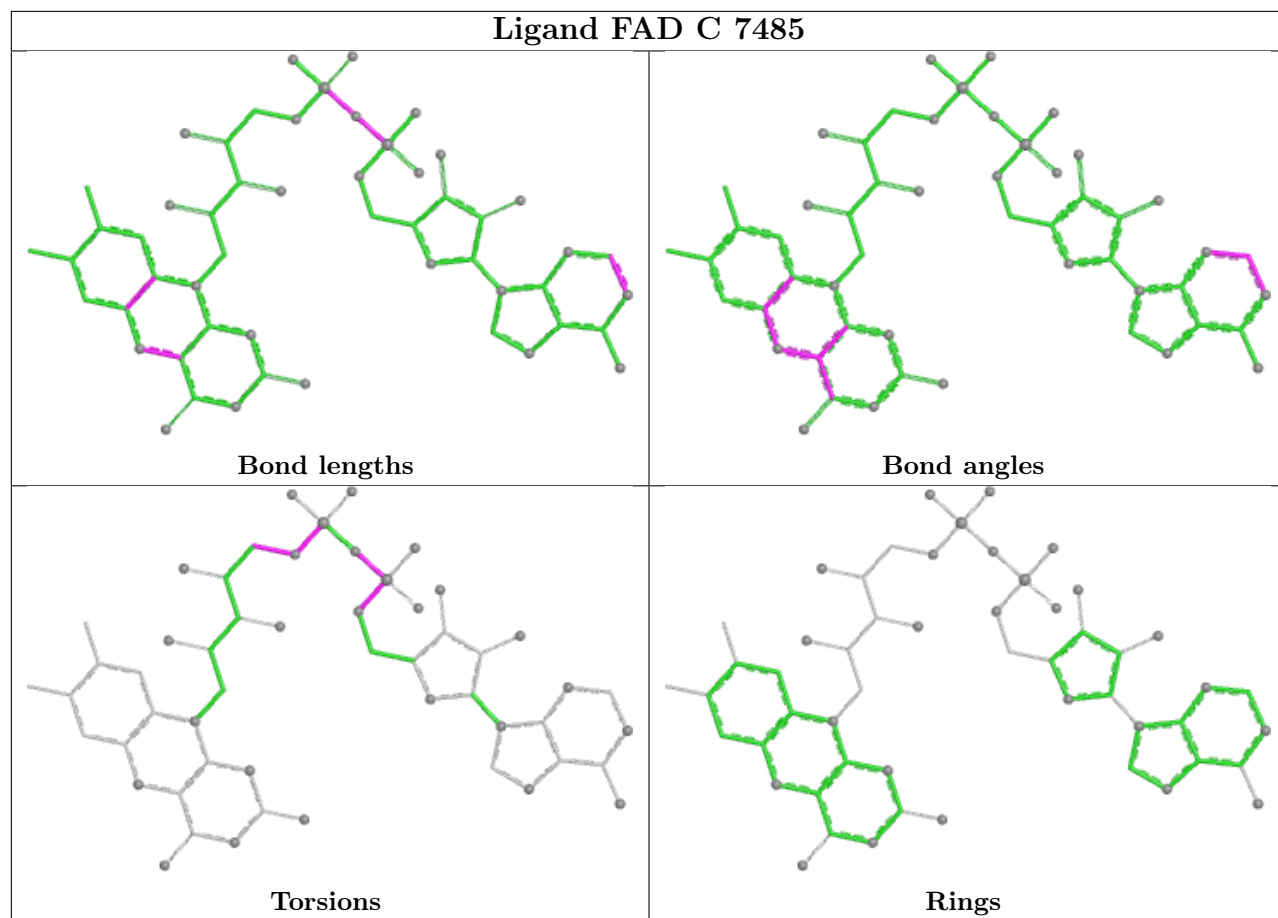
There are no ring outliers.

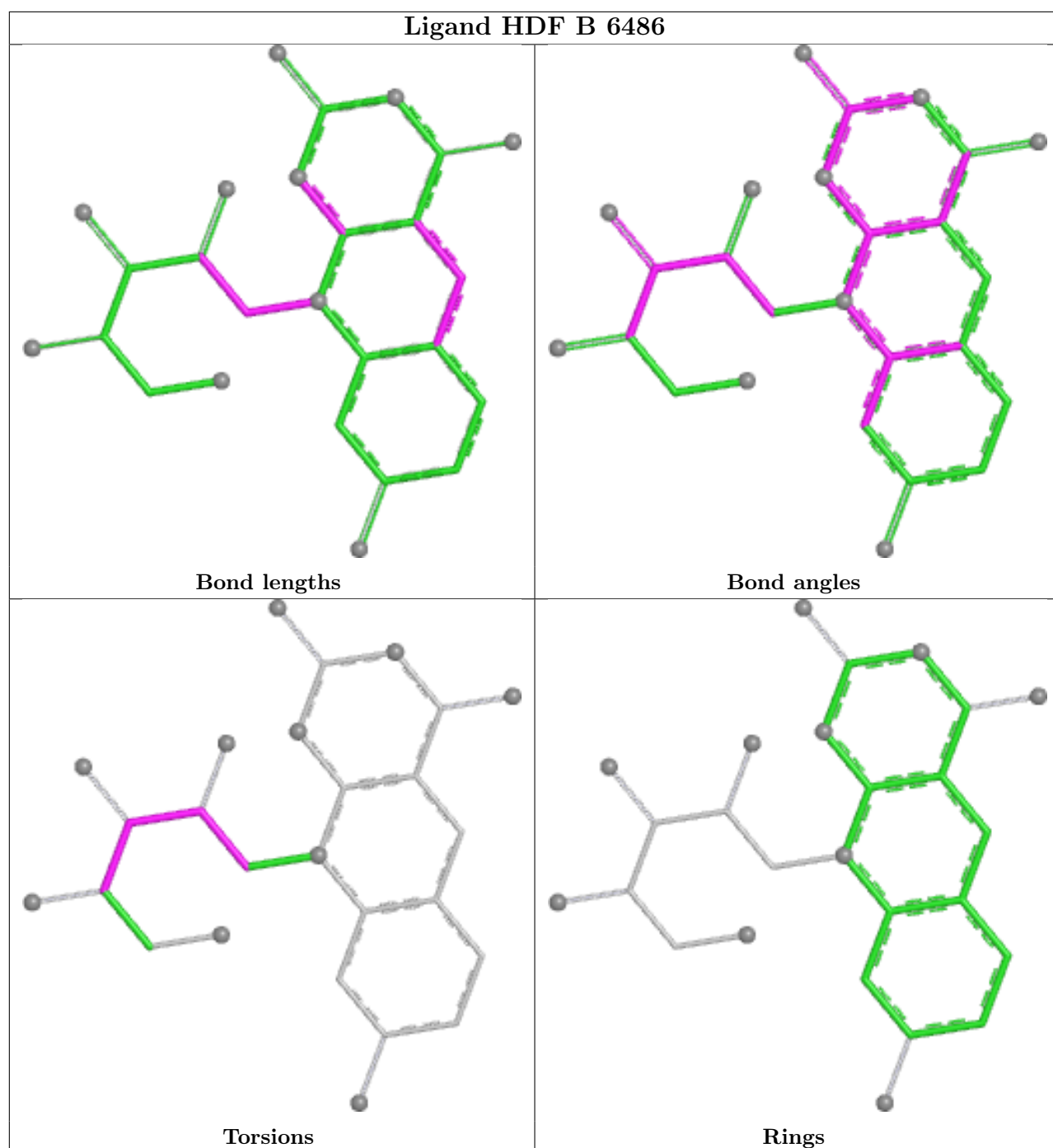
3 monomers are involved in 3 short contacts:

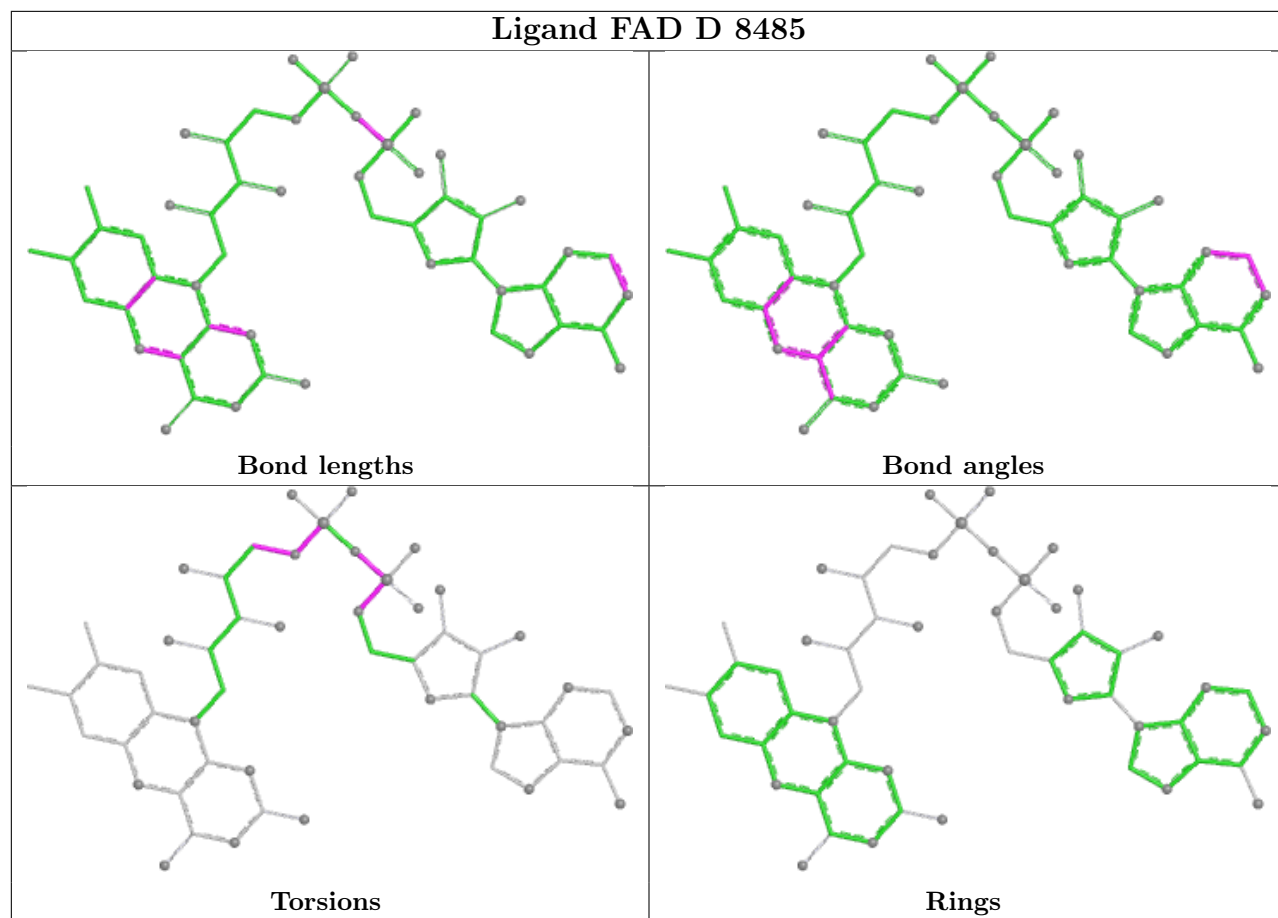
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	7485	FAD	1	0
7	D	8485	FAD	1	0
7	B	6485	FAD	1	0

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

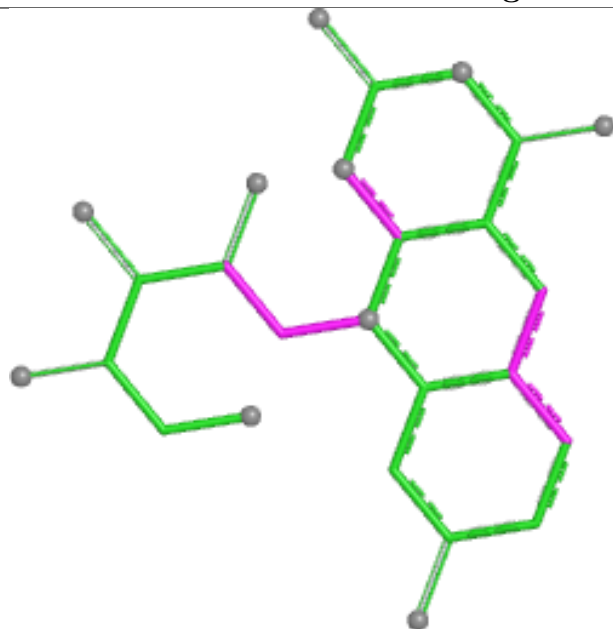




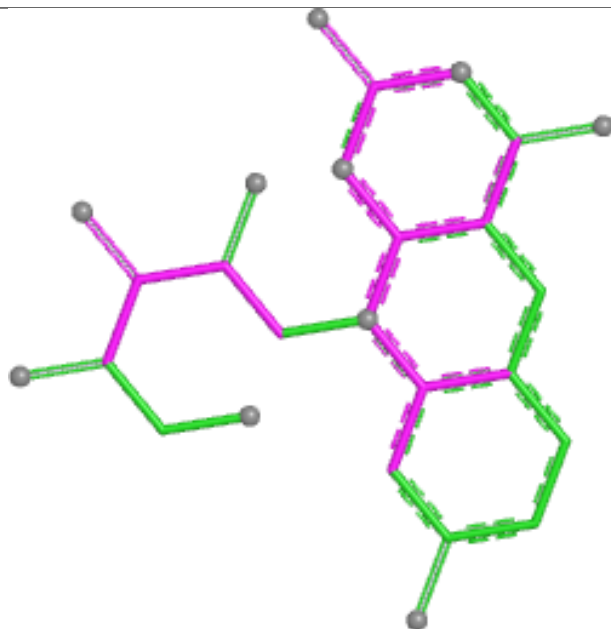




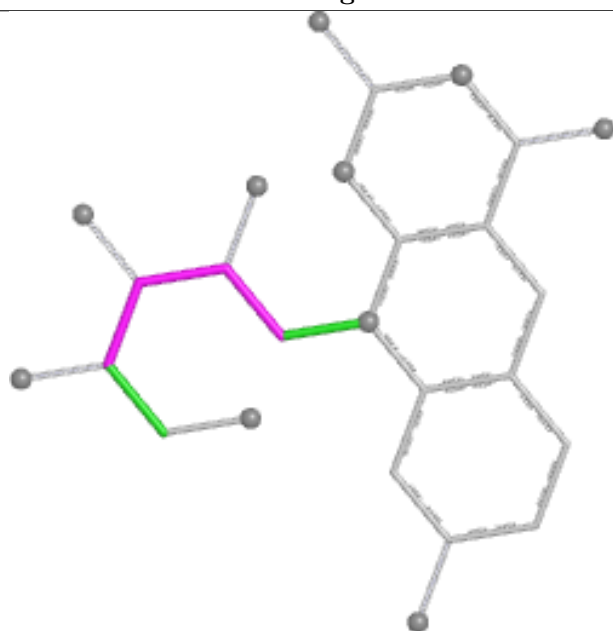
Ligand HDF D 8486



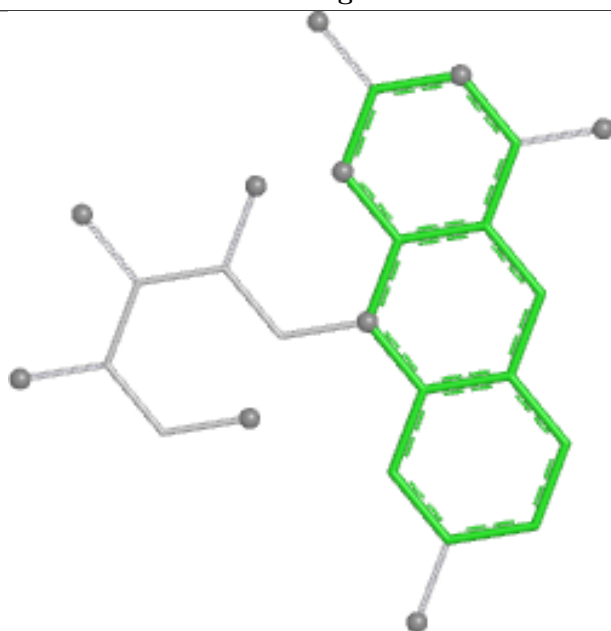
Bond lengths



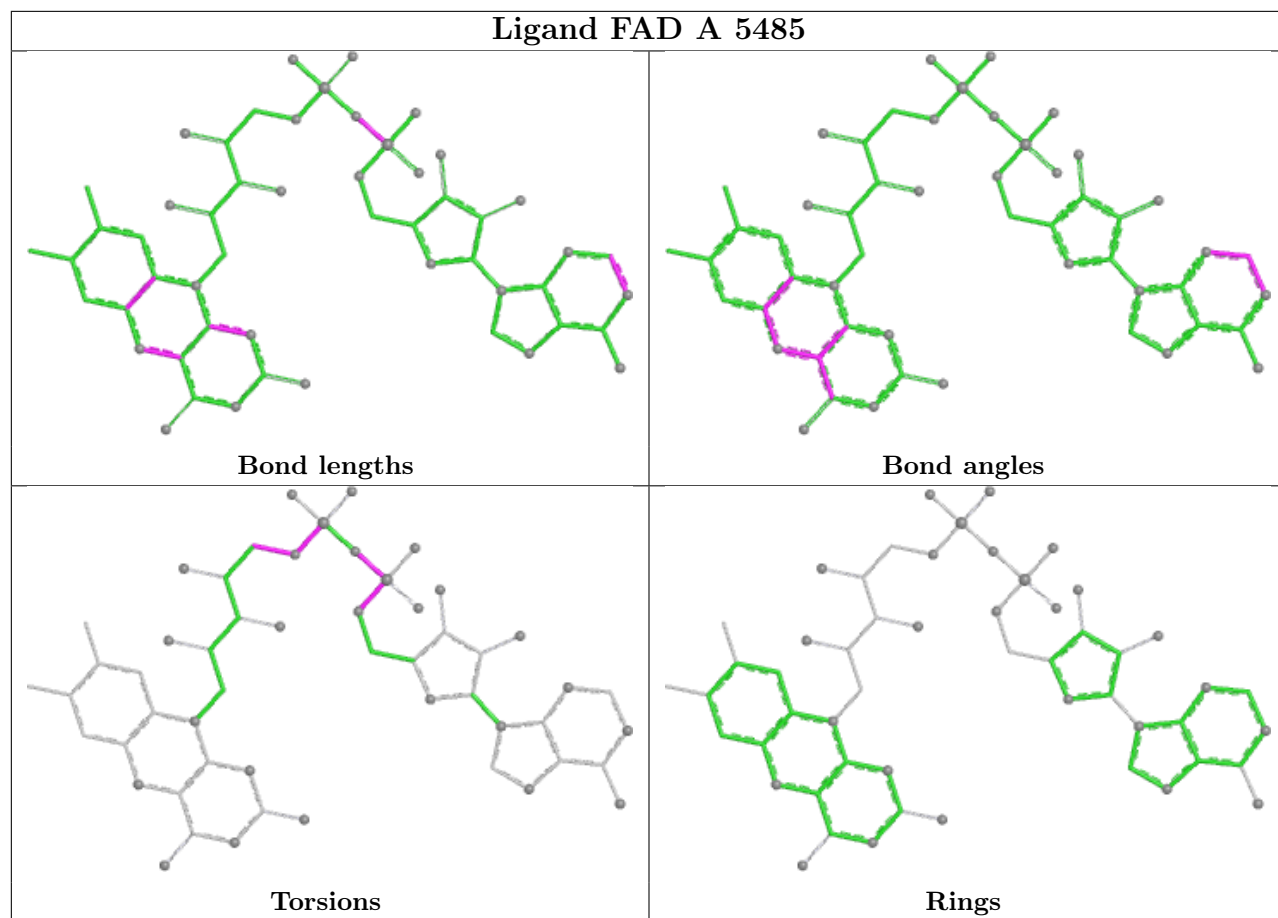
Bond angles

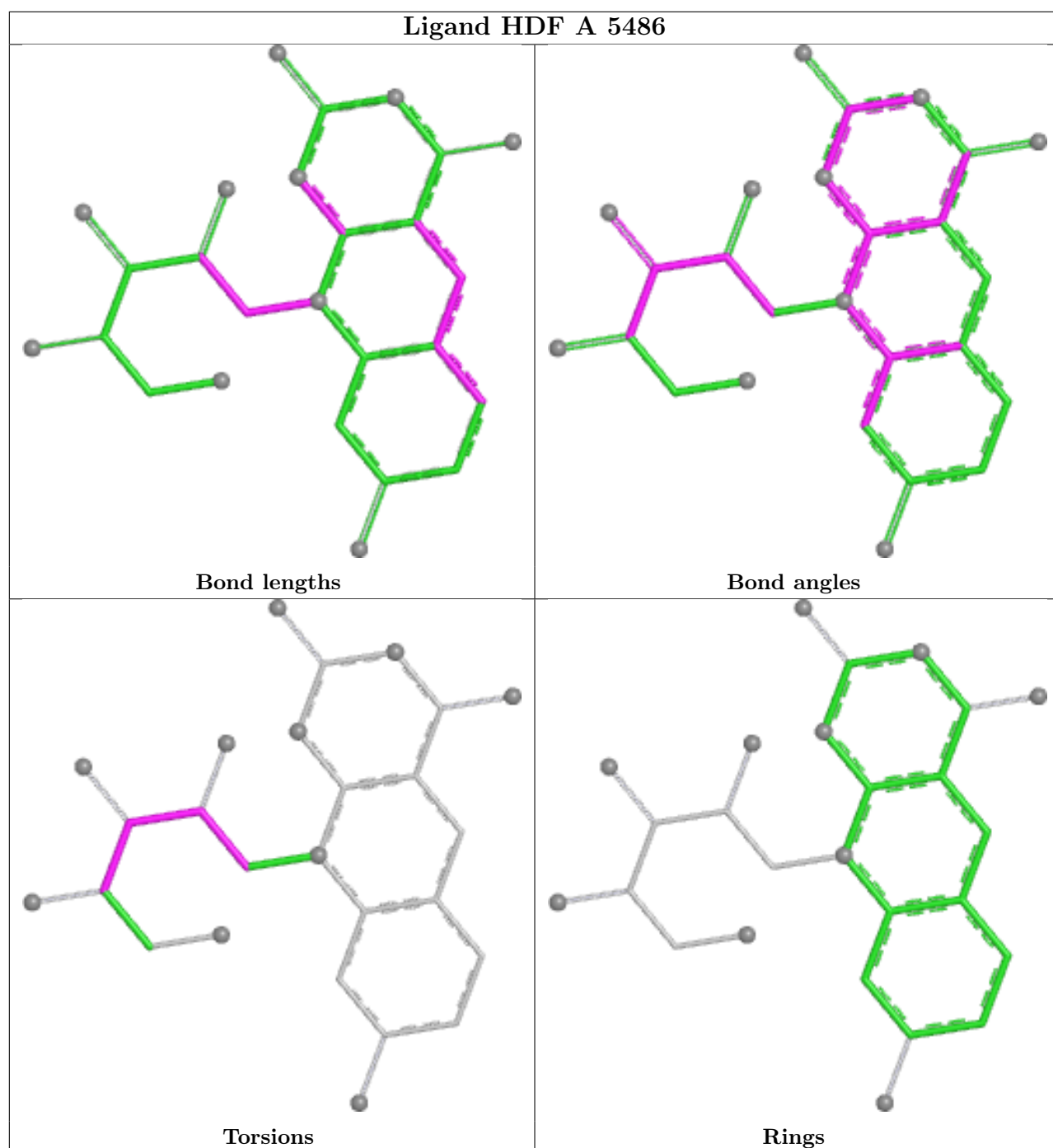


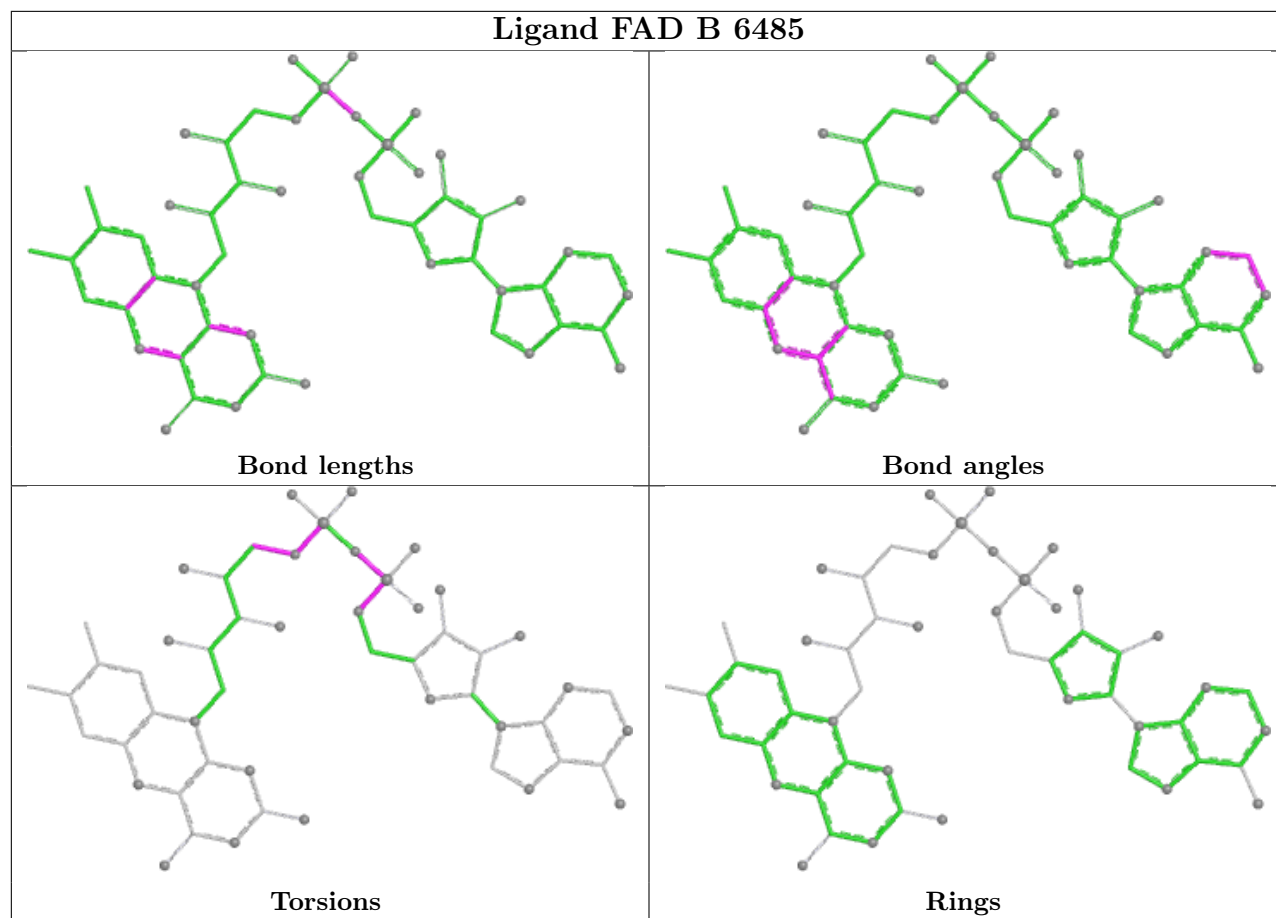
Torsions



Rings







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	I	10/11 (90%)	-0.76	0 100 100	33, 39, 46, 48	10 (100%)
1	K	10/11 (90%)	-0.65	0 100 100	33, 38, 48, 48	10 (100%)
2	J	9/9 (100%)	-0.86	0 100 100	29, 38, 50, 51	9 (100%)
2	L	9/9 (100%)	-0.82	0 100 100	34, 40, 50, 51	9 (100%)
3	M	4/4 (100%)	-0.75	0 100 100	32, 37, 38, 39	4 (100%)
3	O	4/4 (100%)	-0.78	0 100 100	38, 41, 44, 45	4 (100%)
4	N	5/5 (100%)	-0.55	0 100 100	41, 42, 45, 47	5 (100%)
4	P	5/5 (100%)	-0.60	0 100 100	35, 37, 44, 48	5 (100%)
5	A	474/474 (100%)	-1.07	0 100 100	15, 26, 48, 63	1 (0%)
5	B	474/474 (100%)	-1.12	0 100 100	14, 26, 47, 65	2 (0%)
5	C	474/474 (100%)	-1.10	0 100 100	14, 25, 48, 65	0
5	D	474/474 (100%)	-1.07	0 100 100	15, 27, 48, 63	2 (0%)
All	All	1952/1954 (99%)	-1.08	0 100 100	14, 27, 48, 65	61 (3%)

There are no RSRZ outliers to report.

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
1	TCP	I	8	18/18	0.99	0.04	32,34,37,40	18
1	TCP	K	8	18/18	0.99	0.05	33,35,39,42	18

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands

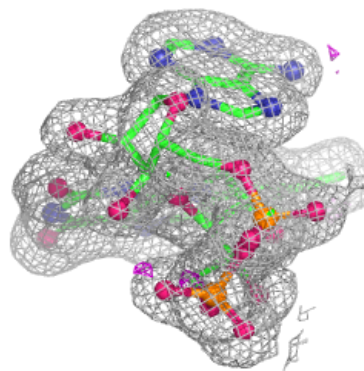
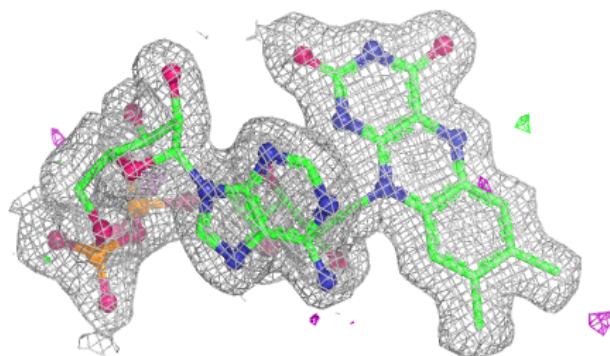
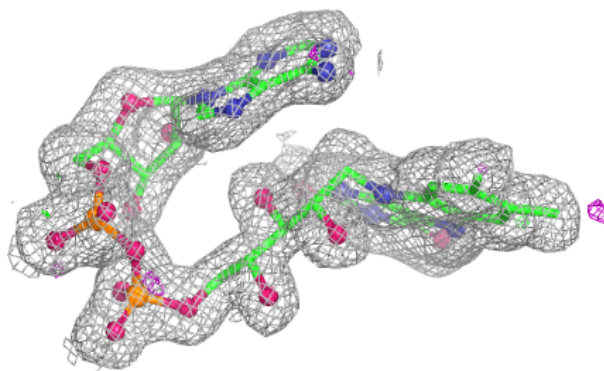
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	MG	A	9002	1/1	0.99	0.03	50,50,50,50	0
6	MG	B	9001	1/1	0.99	0.03	51,51,51,51	0
7	FAD	B	6485	53/53	0.99	0.03	11,16,19,20	0
8	HDF	A	5486	26/26	0.99	0.03	13,18,25,29	0
8	HDF	B	6486	26/26	0.99	0.03	12,16,19,25	0
8	HDF	C	7486	26/26	0.99	0.03	12,16,19,23	0
8	HDF	D	8486	26/26	0.99	0.03	14,18,24,30	0
7	FAD	C	7485	53/53	1.00	0.02	12,16,19,19	0
7	FAD	D	8485	53/53	1.00	0.02	12,16,19,21	0
7	FAD	A	5485	53/53	1.00	0.02	13,16,18,19	0

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

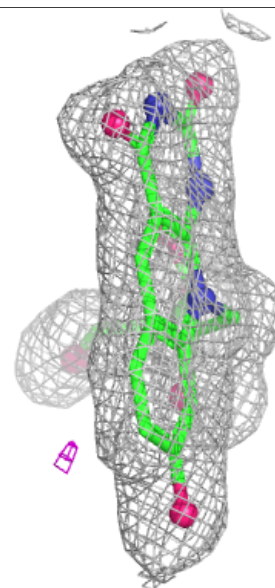
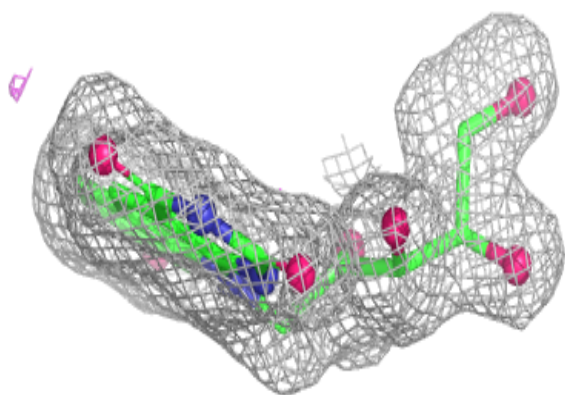
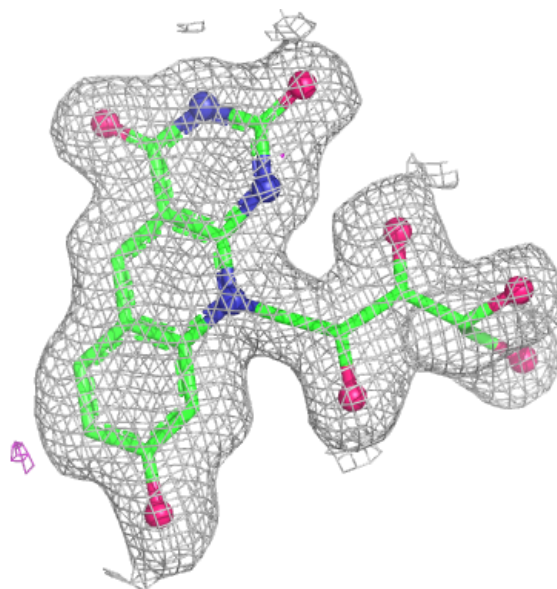
Electron density around FAD B 6485:

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



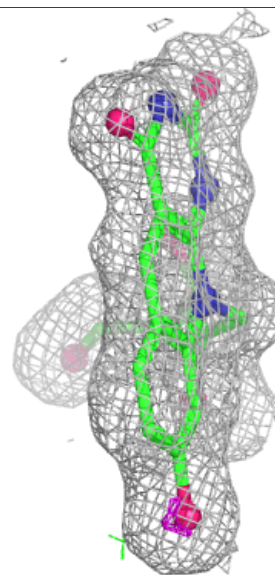
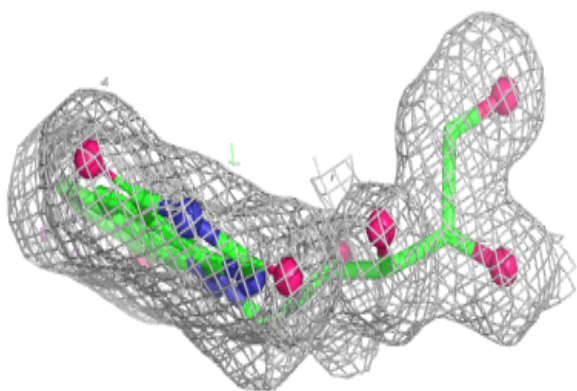
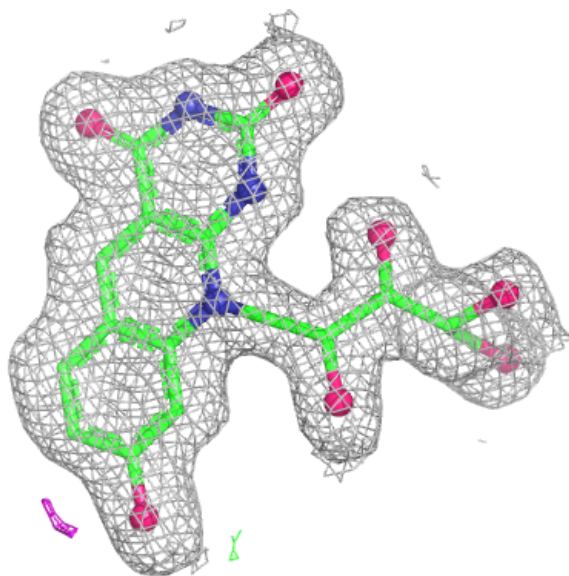
Electron density around HDF A 5486:

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



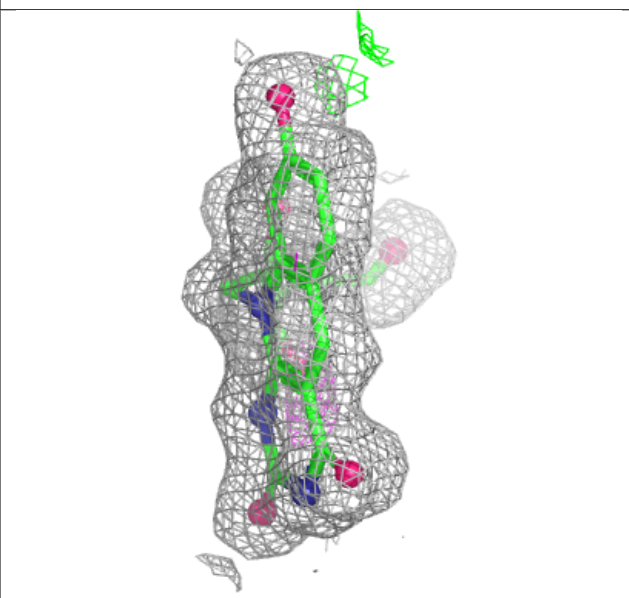
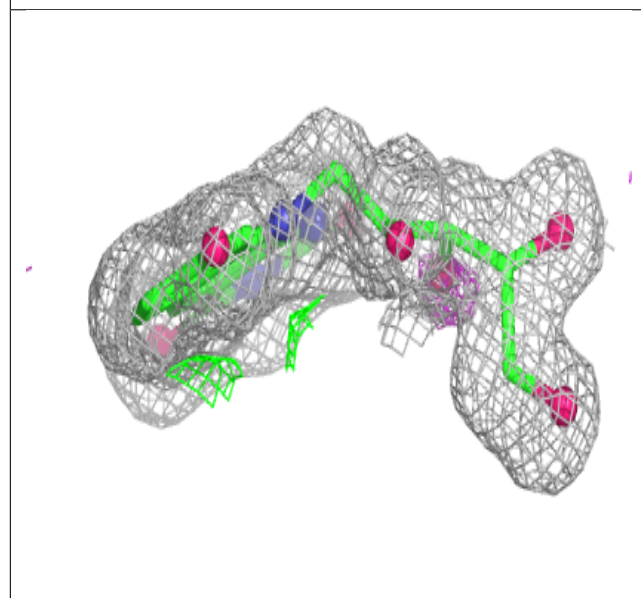
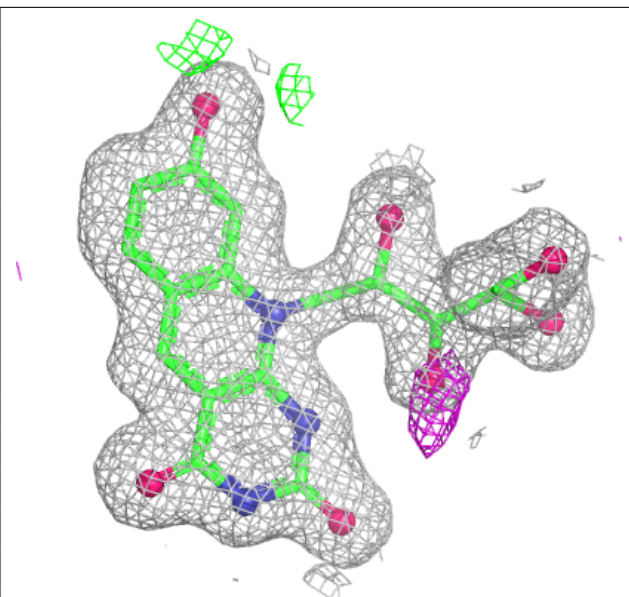
Electron density around HDF B 6486:

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



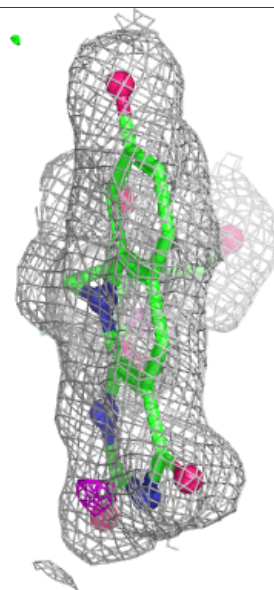
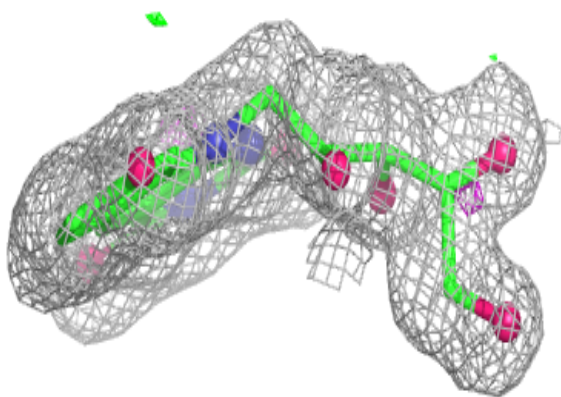
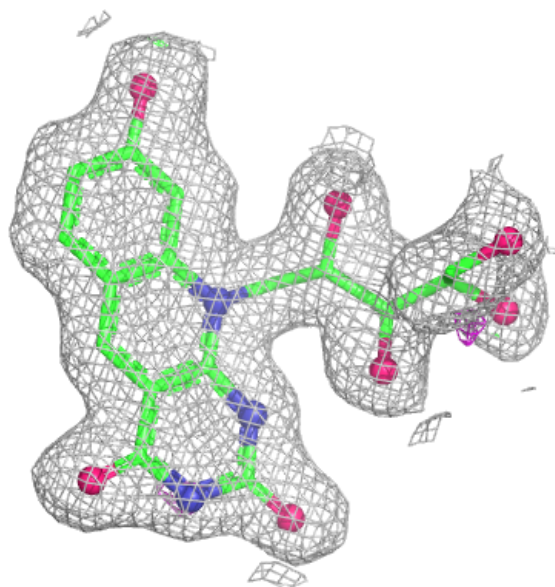
Electron density around HDF C 7486:

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



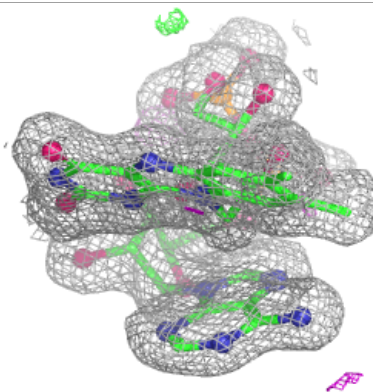
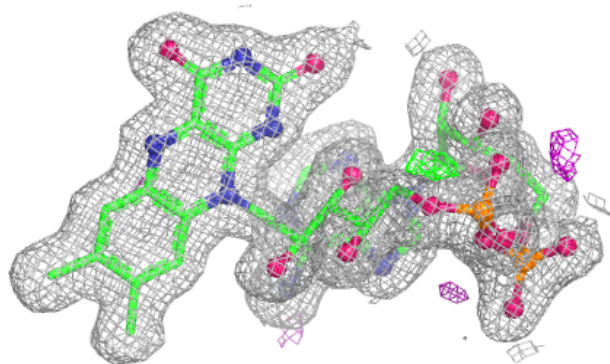
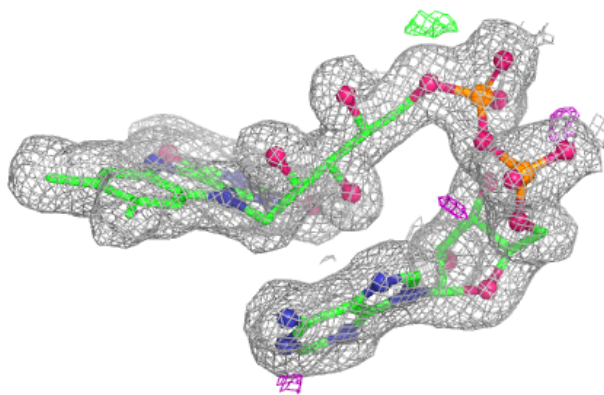
Electron density around HDF D 8486:

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

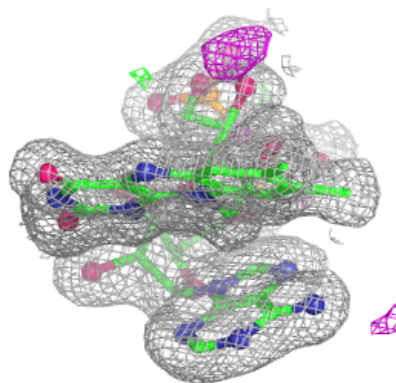
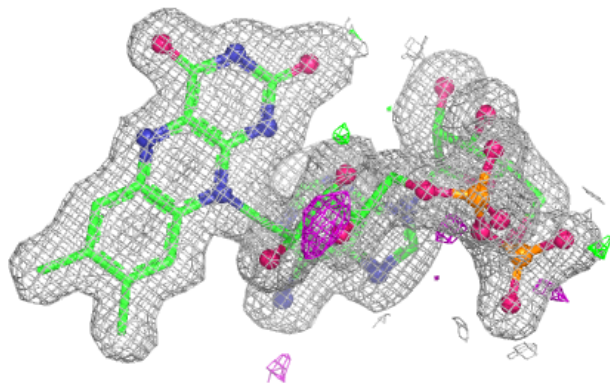
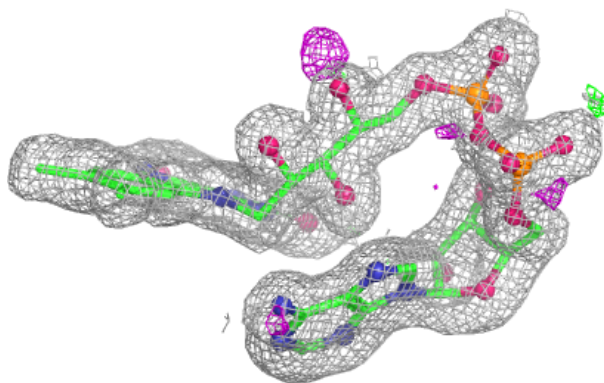


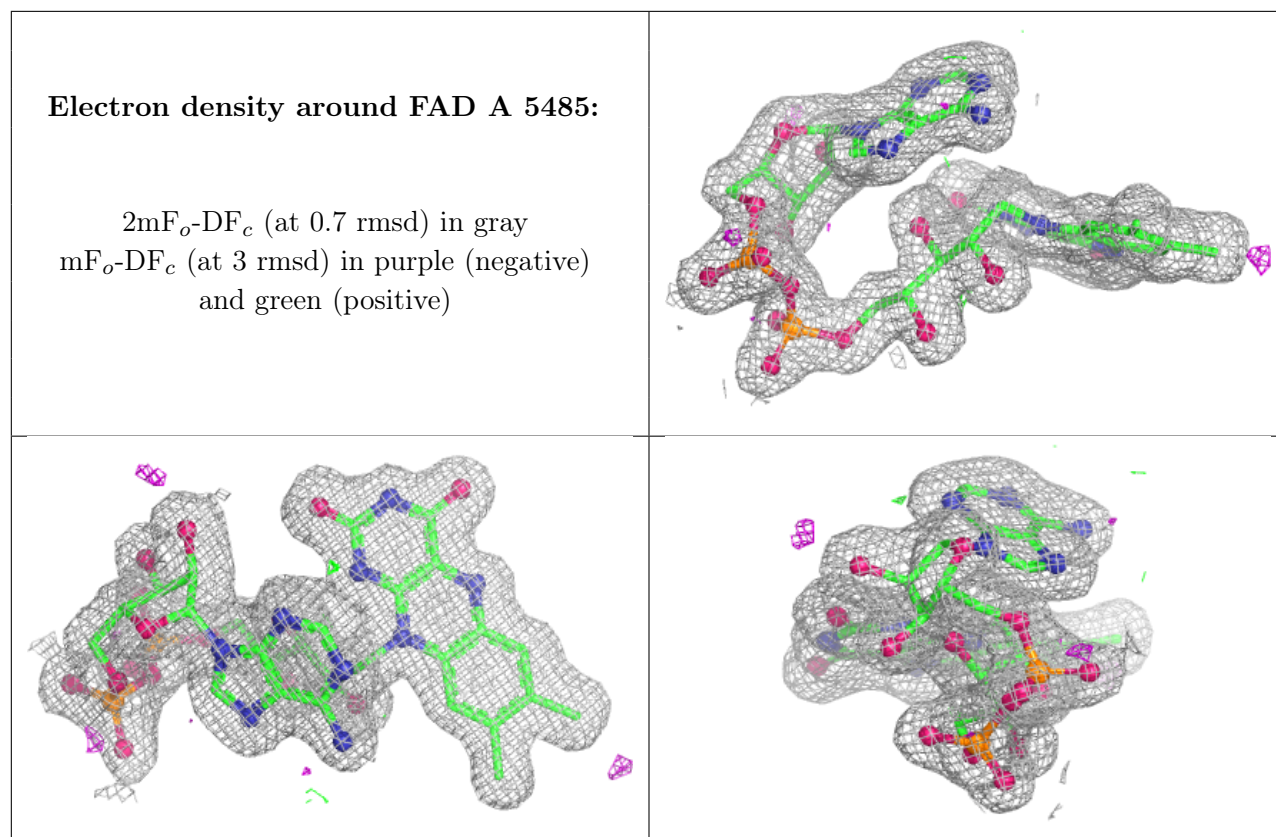
Electron density around FAD C 7485:

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

**Electron density around FAD D 8485:**

$2mF_o-DF_c$ (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.