Full wwPDB X-ray Structure Validation Report (i)

Nov 1, 2023 – 01:38 PM JST

PDB ID	:	5HXW
Title	:	L-amino acid deaminase from Proteus vulgaris
Authors	:	Zhou, H.; Ju, Y.; Niu, L.; Teng, M.
Deposited on	:	2016-01-31
Resolution	:	2.63 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 (i) 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 (i)) were used in the production of this report:

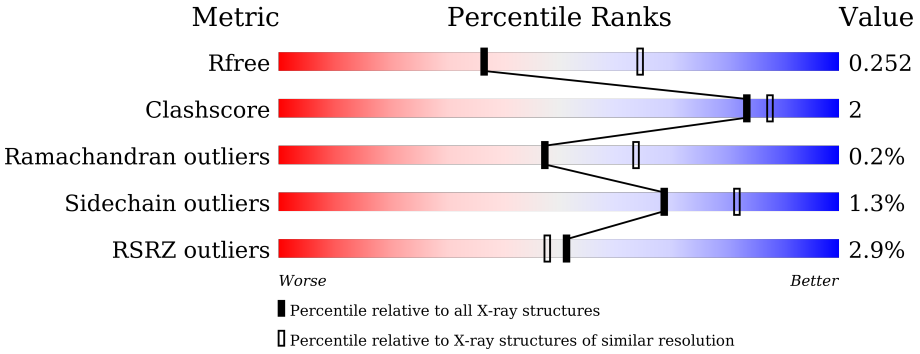
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.63 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}	130704	1426 (2.66-2.62)
Clashscore	141614	1472 (2.66-2.62)
Ramachandran outliers	138981	1446 (2.66-2.62)
Sidechain outliers	138945	1446 (2.66-2.62)
RSRZ outliers	127900	1408 (2.66-2.62)

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	454	88% 8% 5%
1	B	454	.% 89% 6% 5%
1	C	454	3% 89% 5% 5%
1	D	454	3% 89% 5% 5%
1	E	454	3% 86% 9% 5%
1	F	454	6% 90% • 5%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 20385 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 L-amino acid deaminase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	433	3342	2134	561	636	11	0	0	0
1	B	432	3324	2120	560	633	11	0	1	0
1	C	430	3252	2080	540	620	12	0	2	0
1	D	430	3254	2072	542	629	11	0	0	0
1	E	430	3284	2097	546	630	11	0	2	0
1	F	430	3205	2038	535	622	10	0	1	0

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	18	MET	-	expression tag	UNP Q9LCB2
A	19	ARG	-	expression tag	UNP Q9LCB2
A	20	GLY	-	expression tag	UNP Q9LCB2
A	21	SER	-	expression tag	UNP Q9LCB2
A	22	HIS	-	expression tag	UNP Q9LCB2
A	23	HIS	-	expression tag	UNP Q9LCB2
A	24	HIS	-	expression tag	UNP Q9LCB2
A	25	HIS	-	expression tag	UNP Q9LCB2
A	26	HIS	-	expression tag	UNP Q9LCB2
A	27	HIS	-	expression tag	UNP Q9LCB2
A	28	GLY	-	expression tag	UNP Q9LCB2
A	29	SER	-	expression tag	UNP Q9LCB2
B	18	MET	-	expression tag	UNP Q9LCB2
B	19	ARG	-	expression tag	UNP Q9LCB2
B	20	GLY	-	expression tag	UNP Q9LCB2
B	21	SER	-	expression tag	UNP Q9LCB2
B	22	HIS	-	expression tag	UNP Q9LCB2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	23	HIS	-	expression tag	UNP Q9LCB2
B	24	HIS	-	expression tag	UNP Q9LCB2
B	25	HIS	-	expression tag	UNP Q9LCB2
B	26	HIS	-	expression tag	UNP Q9LCB2
B	27	HIS	-	expression tag	UNP Q9LCB2
B	28	GLY	-	expression tag	UNP Q9LCB2
B	29	SER	-	expression tag	UNP Q9LCB2
C	18	MET	-	expression tag	UNP Q9LCB2
C	19	ARG	-	expression tag	UNP Q9LCB2
C	20	GLY	-	expression tag	UNP Q9LCB2
C	21	SER	-	expression tag	UNP Q9LCB2
C	22	HIS	-	expression tag	UNP Q9LCB2
C	23	HIS	-	expression tag	UNP Q9LCB2
C	24	HIS	-	expression tag	UNP Q9LCB2
C	25	HIS	-	expression tag	UNP Q9LCB2
C	26	HIS	-	expression tag	UNP Q9LCB2
C	27	HIS	-	expression tag	UNP Q9LCB2
C	28	GLY	-	expression tag	UNP Q9LCB2
C	29	SER	-	expression tag	UNP Q9LCB2
D	18	MET	-	expression tag	UNP Q9LCB2
D	19	ARG	-	expression tag	UNP Q9LCB2
D	20	GLY	-	expression tag	UNP Q9LCB2
D	21	SER	-	expression tag	UNP Q9LCB2
D	22	HIS	-	expression tag	UNP Q9LCB2
D	23	HIS	-	expression tag	UNP Q9LCB2
D	24	HIS	-	expression tag	UNP Q9LCB2
D	25	HIS	-	expression tag	UNP Q9LCB2
D	26	HIS	-	expression tag	UNP Q9LCB2
D	27	HIS	-	expression tag	UNP Q9LCB2
D	28	GLY	-	expression tag	UNP Q9LCB2
D	29	SER	-	expression tag	UNP Q9LCB2
E	18	MET	-	expression tag	UNP Q9LCB2
E	19	ARG	-	expression tag	UNP Q9LCB2
E	20	GLY	-	expression tag	UNP Q9LCB2
E	21	SER	-	expression tag	UNP Q9LCB2
E	22	HIS	-	expression tag	UNP Q9LCB2
E	23	HIS	-	expression tag	UNP Q9LCB2
E	24	HIS	-	expression tag	UNP Q9LCB2
E	25	HIS	-	expression tag	UNP Q9LCB2
E	26	HIS	-	expression tag	UNP Q9LCB2
E	27	HIS	-	expression tag	UNP Q9LCB2
E	28	GLY	-	expression tag	UNP Q9LCB2

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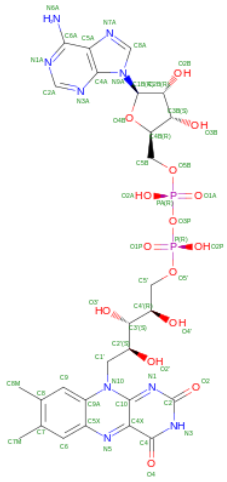
Chain	Residue	Modelled	Actual	Comment	Reference
E	29	SER	-	expression tag	UNP Q9LCB2
F	18	MET	-	expression tag	UNP Q9LCB2
F	19	ARG	-	expression tag	UNP Q9LCB2
F	20	GLY	-	expression tag	UNP Q9LCB2
F	21	SER	-	expression tag	UNP Q9LCB2
F	22	HIS	-	expression tag	UNP Q9LCB2
F	23	HIS	-	expression tag	UNP Q9LCB2
F	24	HIS	-	expression tag	UNP Q9LCB2
F	25	HIS	-	expression tag	UNP Q9LCB2
F	26	HIS	-	expression tag	UNP Q9LCB2
F	27	HIS	-	expression tag	UNP Q9LCB2
F	28	GLY	-	expression tag	UNP Q9LCB2
F	29	SER	-	expression tag	UNP Q9LCB2

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

FAD



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

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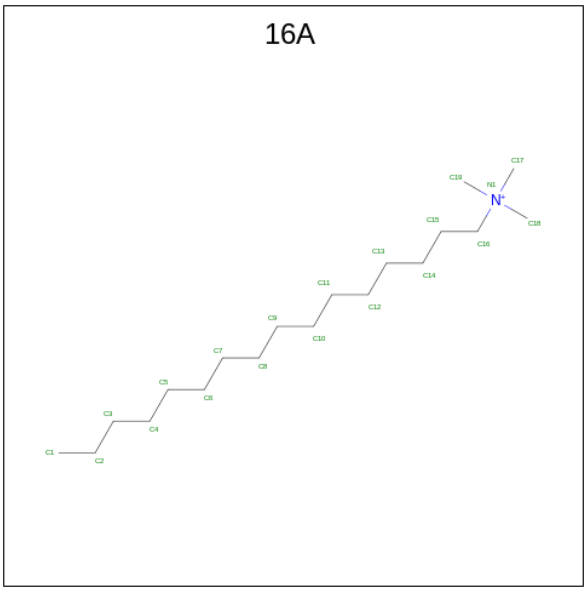
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	E	1	53	27	9	15	2	0	0
			Total	C	N	O	P		
2	F	1	53	27	9	15	2	0	0

- Molecule 3 is CETYL-TRIMETHYL-AMMONIUM (three-letter code: 16A) (formula: $C_{19}H_{42}N$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	N		
3	A	1	20	19	1	0	0
			Total	C	N		
3	A	1	20	19	1	0	0
			Total	C	N		
3	A	1	20	19	1	0	0
			Total	C	N		
3	B	1	20	19	1	0	0
			Total	C	N		
3	B	1	20	19	1	0	0
			Total	C	N		
3	B	1	20	19	1	0	0
			Total	C	N		
3	B	1	20	19	1	0	0
			Total	C	N		
3	B	1	20	19	1	0	0
			Total	C	N		
3	C	1	20	19	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	N		
3	D	1	20	19	1	0	0
			Total	C	N		
3	D	1	20	19	1	0	0
			Total	C	N		
3	D	1	20	19	1	0	0
			Total	C	N		
3	E	1	20	19	1	0	0
			Total	C	N		
3	F	1	20	19	1	0	0
			Total	C	N		
3	F	1	20	19	1	0	0

- Molecule 4 is water.

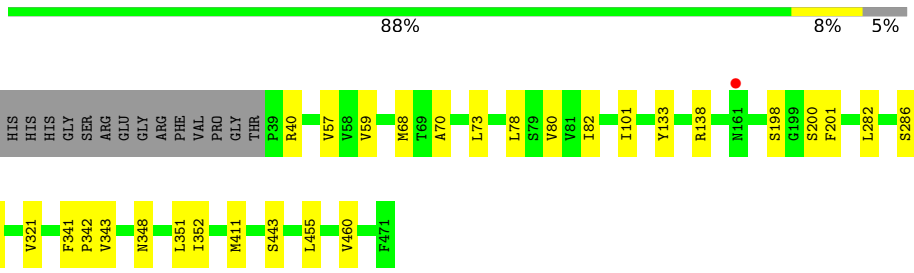
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	28	28	28	0	0
			Total	O		
4	B	18	18	18	0	0
			Total	O		
4	C	19	19	19	0	0
			Total	O		
4	D	16	16	16	0	0
			Total	O		
4	E	15	15	15	0	0
			Total	O		
4	F	10	10	10	0	0

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.

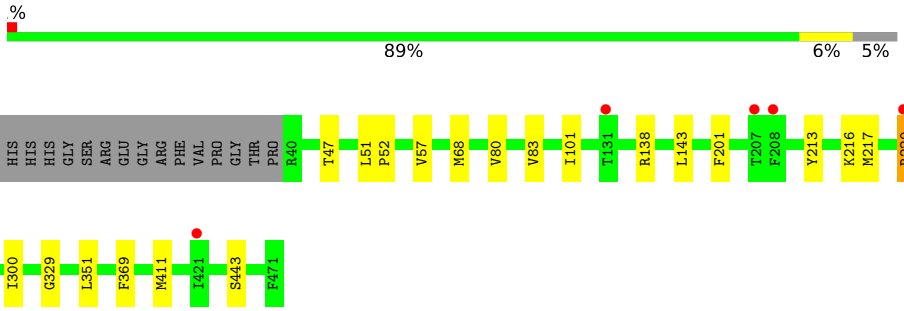
• Molecule 1: L-amino acid deaminase

Chain A:



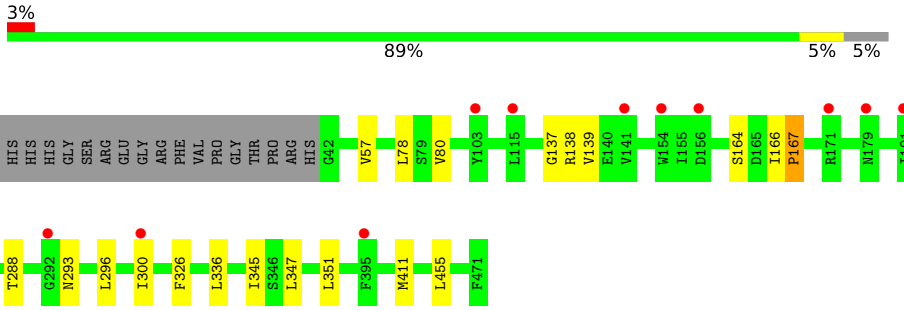
• Molecule 1: L-amino acid deaminase

Chain B:



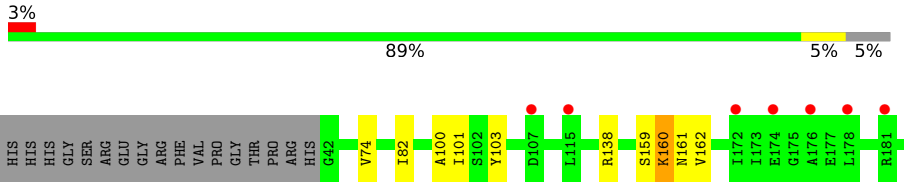
• Molecule 1: L-amino acid deaminase

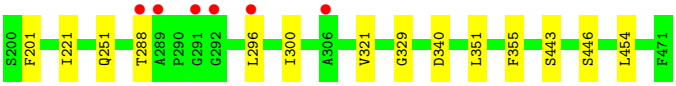
Chain C:



• Molecule 1: L-amino acid deaminase

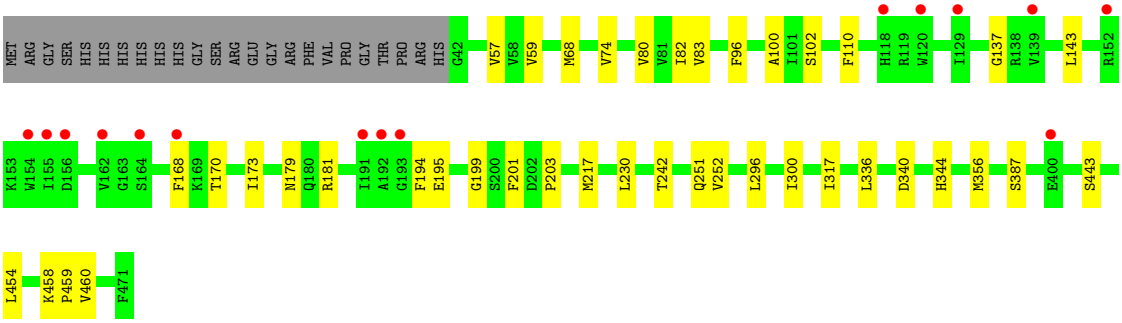
Chain D:





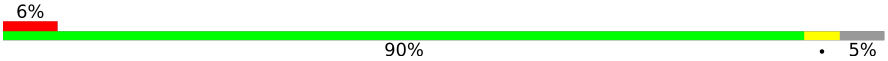
• Molecule 1: L-amino acid deaminase

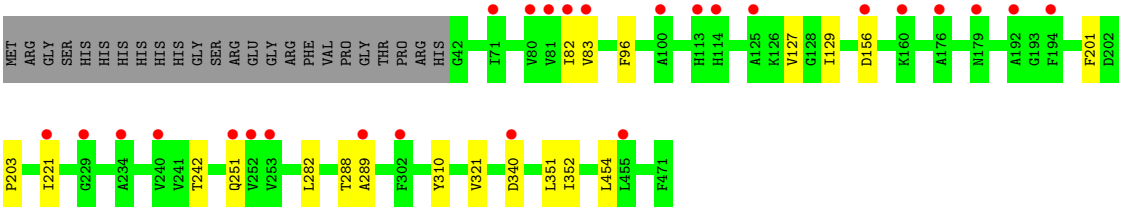
Chain E:



• Molecule 1: L-amino acid deaminase

Chain F:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	100.31Å 104.58Å 105.42Å 64.52° 73.06° 61.17°	Depositor
Resolution (Å)	94.63 – 2.63 49.26 – 2.63	Depositor EDS
% Data completeness (in resolution range)	97.1 (94.63-2.63) 97.1 (49.26-2.63)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.19 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.221 , 0.252 0.221 , 0.252	Depositor DCC
R_{free} test set	4861 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	68.3	Xtriage
Anisotropy	0.451	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 52.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	20385	wwPDB-VP
Average B, all atoms (Å^2)	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.75% of the height of the origin peak. No significant pseudotranslation is detected.*

[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 16A, FAD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.40	0/3419	0.60	0/4648
1	B	0.40	0/3403	0.60	0/4626
1	C	0.40	0/3329	0.59	0/4534
1	D	0.40	0/3327	0.59	0/4531
1	E	0.40	0/3362	0.59	0/4576
1	F	0.40	0/3277	0.58	0/4469
All	All	0.40	0/20117	0.59	0/27384

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	3342	0	3304	18	0
1	B	3324	0	3268	17	0
1	C	3252	0	3155	15	0
1	D	3254	0	3153	11	0
1	E	3284	0	3194	21	0
1	F	3205	0	3033	7	0
2	A	53	0	31	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	53	0	31	2	0
2	C	53	0	31	2	0
2	D	53	0	31	0	0
2	E	53	0	31	0	0
2	F	53	0	31	0	0
3	A	60	0	126	5	0
3	B	100	0	210	7	0
3	C	20	0	42	1	0
3	D	60	0	126	4	0
3	E	20	0	42	2	0
3	F	40	0	84	0	0
4	A	28	0	0	0	0
4	B	18	0	0	0	0
4	C	19	0	0	0	0
4	D	16	0	0	0	0
4	E	15	0	0	0	0
4	F	10	0	0	0	0
All	All	20385	0	19923	96	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 2.

All (96) 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:B:213:TYR:CE1	1:B:217:MET:HG2	2.08	0.87
1:E:181:ARG:HD2	1:E:194:PHE:CE1	2.16	0.80
1:E:181:ARG:HD2	1:E:194:PHE:HE1	1.51	0.74
1:B:47:THR:HG21	1:B:220:ARG:HG3	1.71	0.73
1:B:213:TYR:O	1:B:216:LYS:N	2.24	0.70
1:A:348:ASN:HA	3:A:503:16A:H182	1.76	0.66
1:E:181:ARG:CD	1:E:194:PHE:HE1	2.09	0.66
1:B:213:TYR:CE1	1:B:217:MET:CG	2.82	0.62
1:C:195:GLU:HG2	1:C:198:SER:HB3	1.81	0.61
1:C:137:GLY:HA2	1:C:195:GLU:O	2.00	0.61
1:E:296:LEU:HB2	1:E:300:ILE:HB	1.84	0.59
1:C:57:VAL:HB	1:C:80:VAL:HG12	1.83	0.59
1:E:173:ILE:HG12	1:E:194:PHE:HB2	1.84	0.59
3:B:504:16A:H101	3:B:506:16A:H91	1.83	0.58
1:E:57:VAL:HG13	1:E:80:VAL:HG12	1.84	0.58
1:D:296:LEU:HB2	1:D:300:ILE:HB	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:ALA:HB1	1:A:80:VAL:HG21	1.87	0.57
1:B:296:LEU:HB2	1:B:300:ILE:HB	1.87	0.56
3:B:502:16A:H151	3:B:503:16A:H161	1.89	0.55
1:B:57:VAL:HB	1:B:80:VAL:HG12	1.90	0.54
1:C:336:LEU:HD11	1:C:345:ILE:HD11	1.90	0.53
1:A:101:ILE:HG22	1:A:198:SER:HB2	1.91	0.53
1:C:296:LEU:HB2	1:C:300:ILE:HB	1.89	0.53
1:F:289:ALA:HB1	1:F:310:TYR:OH	2.10	0.52
1:A:133:TYR:HA	1:A:200:SER:O	2.10	0.52
1:A:316:VAL:HA	1:A:342:PRO:HB2	1.92	0.51
1:C:139:VAL:HA	1:C:193:GLY:O	2.09	0.51
1:E:168:PHE:CZ	1:E:170:THR:HB	2.45	0.51
1:E:74:VAL:HG23	1:E:80:VAL:HG22	1.93	0.51
1:A:296:LEU:HB2	1:A:300:ILE:HB	1.92	0.50
1:C:166:ILE:O	1:C:167:PRO:O	2.30	0.50
1:E:100:ALA:HB3	1:E:199:GLY:HA3	1.94	0.50
1:E:317:ILE:HG21	3:E:502:16A:H82	1.93	0.50
1:A:101:ILE:HG21	1:A:138:ARG:HD2	1.93	0.49
3:A:503:16A:H173	3:D:502:16A:H141	1.94	0.49
1:F:321:VAL:HG12	1:F:351:LEU:HD13	1.95	0.49
1:A:286:SER:HB3	1:A:289:ALA:HB2	1.95	0.48
1:C:347:LEU:HD11	1:C:351:LEU:HD22	1.95	0.47
1:E:96:PHE:CZ	1:E:203:PRO:HA	2.49	0.47
1:E:102:SER:HB2	1:E:110:PHE:CE1	2.49	0.47
1:B:213:TYR:HE1	1:B:217:MET:CG	2.25	0.47
1:F:251:GLN:HB3	1:F:454:LEU:HD11	1.96	0.47
1:D:355:PHE:O	3:D:502:16A:H152	2.15	0.47
3:B:502:16A:H142	3:B:503:16A:H141	1.96	0.47
3:B:502:16A:H172	3:B:506:16A:H41	1.97	0.47
1:C:78:LEU:HD11	1:C:455:LEU:HD21	1.97	0.47
1:B:83:VAL:HG11	1:B:242:THR:HG21	1.97	0.46
1:E:336:LEU:HD11	3:E:502:16A:H193	1.98	0.46
1:C:256:GLY:O	2:C:501:FAD:H8A	2.16	0.46
1:A:68:MET:HG3	1:A:443:SER:HB2	1.98	0.46
1:B:351:LEU:HD23	3:B:502:16A:H131	1.97	0.46
1:D:101:ILE:HG21	1:D:138:ARG:HD2	1.98	0.46
1:D:329:GLY:O	3:D:504:16A:H162	2.16	0.45
1:D:82:ILE:HD12	1:D:221:ILE:HG12	1.98	0.45
1:B:286:SER:HB3	1:B:289:ALA:HB2	1.97	0.45
1:D:251:GLN:HB3	1:D:454:LEU:HD11	1.99	0.45
1:E:74:VAL:HG11	1:E:217:MET:HB3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:VAL:HB	1:A:82:ILE:HG12	2.00	0.44
1:E:59:VAL:HB	1:E:82:ILE:HG12	1.99	0.44
1:B:101:ILE:HG21	1:B:138:ARG:HD2	1.99	0.44
1:D:101:ILE:HD12	1:D:103:TYR:HB3	2.00	0.44
1:D:160:LYS:O	1:D:162:VAL:N	2.50	0.44
3:B:504:16A:H72	3:B:506:16A:H141	1.99	0.44
1:C:164:SER:C	1:C:166:ILE:H	2.20	0.44
1:B:68:MET:HG3	1:B:443:SER:HB2	1.98	0.43
1:C:411:MET:HG3	2:C:501:FAD:C8M	2.48	0.43
1:F:127:VAL:HG12	1:F:129:ILE:H	1.83	0.43
1:B:411:MET:HG3	2:B:501:FAD:C8M	2.49	0.43
3:A:503:16A:C17	3:D:502:16A:H141	2.47	0.43
1:E:83:VAL:HG11	1:E:242:THR:HG21	2.00	0.43
1:A:341:PHE:HA	1:A:342:PRO:HD3	1.85	0.43
1:B:259:TRP:HB3	1:B:369:PHE:HE1	1.83	0.43
1:D:321:VAL:HG12	1:D:351:LEU:HD13	2.00	0.42
1:E:230:LEU:HD22	1:E:252:VAL:HG21	2.00	0.42
1:A:321:VAL:HG12	1:A:351:LEU:HD13	2.00	0.42
1:E:68:MET:HG3	1:E:443:SER:HB2	2.00	0.42
1:A:301:PHE:HE2	1:A:315:ARG:HB3	1.84	0.42
1:F:96:PHE:CZ	1:F:203:PRO:HA	2.54	0.42
1:A:411:MET:SD	3:A:504:16A:H182	2.60	0.42
1:E:137:GLY:HA2	1:E:195:GLU:O	2.20	0.42
1:E:251:GLN:HB3	1:E:454:LEU:HD11	2.02	0.41
1:B:51:LEU:HA	1:B:52:PRO:HD3	1.93	0.41
1:B:411:MET:HG3	2:B:501:FAD:HM81	2.02	0.41
1:E:458:LYS:HA	1:E:459:PRO:HD3	1.85	0.41
1:A:57:VAL:HG11	1:A:73:LEU:HD13	2.01	0.41
1:C:326:PHE:HA	3:C:502:16A:H111	2.01	0.41
1:D:443:SER:HA	1:D:446:SER:HB2	2.03	0.41
1:A:352:ILE:HD11	3:A:503:16A:H142	2.01	0.41
1:B:329:GLY:HA3	3:B:505:16A:H192	2.03	0.41
1:C:138:ARG:HA	1:C:293:ASN:O	2.20	0.41
1:C:138:ARG:HB2	1:C:293:ASN:HB3	2.03	0.41
1:F:83:VAL:HG11	1:F:242:THR:HG21	2.03	0.41
1:A:317:ILE:O	1:A:343:VAL:HA	2.21	0.40
1:D:100:ALA:HB3	1:D:199:GLY:HA3	2.03	0.40
1:F:82:ILE:HD12	1:F:221:ILE:HG12	2.04	0.40
1:A:78:LEU:HD11	1:A:455:LEU:HD21	2.02	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	431/454 (95%)	418 (97%)	12 (3%)	1 (0%)	47	64
1	B	431/454 (95%)	416 (96%)	15 (4%)	0	100	100
1	C	430/454 (95%)	413 (96%)	16 (4%)	1 (0%)	47	64
1	D	428/454 (94%)	412 (96%)	14 (3%)	2 (0%)	29	43
1	E	430/454 (95%)	418 (97%)	12 (3%)	0	100	100
1	F	429/454 (94%)	412 (96%)	17 (4%)	0	100	100
All	All	2579/2724 (95%)	2489 (96%)	86 (3%)	4 (0%)	47	64

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	167	PRO
1	D	160	LYS
1	D	161	ASN
1	A	40	ARG

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	357/379 (94%)	354 (99%)	3 (1%)	81	89
1	B	352/379 (93%)	349 (99%)	3 (1%)	78	88
1	C	335/379 (88%)	333 (99%)	2 (1%)	86	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	339/379 (89%)	334 (98%)	5 (2%)	65	79
1	E	344/379 (91%)	336 (98%)	8 (2%)	50	68
1	F	322/379 (85%)	316 (98%)	6 (2%)	57	74
All	All	2049/2274 (90%)	2022 (99%)	27 (1%)	69	82

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	201	PHE
1	A	282	LEU
1	A	460	VAL
1	B	143	LEU
1	B	201	PHE
1	B	220	ARG
1	C	201	PHE
1	C	288	THR
1	D	74	VAL
1	D	159	SER
1	D	201	PHE
1	D	288	THR
1	D	340	ASP
1	E	143	LEU
1	E	179	ASN
1	E	201	PHE
1	E	340	ASP
1	E	344	HIS
1	E	356	MET
1	E	387	SER
1	E	460	VAL
1	F	156	ASP
1	F	201	PHE
1	F	282	LEU
1	F	288	THR
1	F	340	ASP
1	F	352	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

21 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	16A	B	503	-	19,19,19	0.44	0	21,21,21	0.70	0
2	FAD	E	501	-	53,58,58	1.41	7 (13%)	68,89,89	1.33	11 (16%)
3	16A	C	502	-	19,19,19	0.44	0	21,21,21	0.58	0
2	FAD	C	501	-	53,58,58	1.40	7 (13%)	68,89,89	1.32	10 (14%)
3	16A	A	503	-	19,19,19	0.49	0	21,21,21	0.56	0
2	FAD	B	501	-	53,58,58	1.40	7 (13%)	68,89,89	1.33	13 (19%)
3	16A	F	503	-	19,19,19	0.45	0	21,21,21	0.62	0
3	16A	E	502	-	19,19,19	0.43	0	21,21,21	0.61	0
2	FAD	D	501	-	53,58,58	1.38	6 (11%)	68,89,89	1.33	10 (14%)
2	FAD	F	501	-	53,58,58	1.41	7 (13%)	68,89,89	1.34	11 (16%)
3	16A	B	506	-	19,19,19	0.41	0	21,21,21	0.57	0
3	16A	A	504	-	19,19,19	0.45	0	21,21,21	0.62	0
2	FAD	A	501	-	53,58,58	1.36	6 (11%)	68,89,89	1.38	11 (16%)
3	16A	B	504	-	19,19,19	0.45	0	21,21,21	0.66	0
3	16A	D	504	-	19,19,19	0.44	0	21,21,21	0.66	0
3	16A	B	505	-	19,19,19	0.44	0	21,21,21	0.61	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	16A	D	503	-	19,19,19	0.43	0	21,21,21	0.59	0
3	16A	F	502	-	19,19,19	0.41	0	21,21,21	0.54	0
3	16A	B	502	-	19,19,19	0.38	0	21,21,21	0.63	0
3	16A	D	502	-	19,19,19	0.43	0	21,21,21	0.58	0
3	16A	A	502	-	19,19,19	0.39	0	21,21,21	0.62	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
3	16A	B	503	-	-	10/17/17/17	-
2	FAD	E	501	-	-	1/30/50/50	0/6/6/6
3	16A	C	502	-	-	10/17/17/17	-
2	FAD	C	501	-	-	2/30/50/50	0/6/6/6
3	16A	A	503	-	-	7/17/17/17	-
2	FAD	B	501	-	-	3/30/50/50	0/6/6/6
3	16A	F	503	-	-	8/17/17/17	-
3	16A	E	502	-	-	9/17/17/17	-
2	FAD	D	501	-	-	2/30/50/50	0/6/6/6
2	FAD	F	501	-	-	2/30/50/50	0/6/6/6
3	16A	B	506	-	-	9/17/17/17	-
3	16A	A	504	-	-	10/17/17/17	-
2	FAD	A	501	-	-	2/30/50/50	0/6/6/6
3	16A	B	504	-	-	10/17/17/17	-
3	16A	D	504	-	-	6/17/17/17	-
3	16A	B	505	-	-	9/17/17/17	-
3	16A	D	503	-	-	7/17/17/17	-
3	16A	F	502	-	-	6/17/17/17	-
3	16A	B	502	-	-	12/17/17/17	-
3	16A	D	502	-	-	9/17/17/17	-
3	16A	A	502	-	-	12/17/17/17	-

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	501	FAD	C9A-C5X	5.80	1.50	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	FAD	C9A-C5X	5.76	1.50	1.41
2	F	501	FAD	C9A-C5X	5.76	1.50	1.41
2	D	501	FAD	C9A-C5X	5.74	1.50	1.41
2	B	501	FAD	C9A-C5X	5.71	1.50	1.41
2	A	501	FAD	C9A-C5X	5.29	1.50	1.41
2	F	501	FAD	C8-C7	3.86	1.50	1.40
2	E	501	FAD	C8-C7	3.84	1.50	1.40
2	C	501	FAD	C8-C7	3.78	1.50	1.40
2	D	501	FAD	C8-C7	3.75	1.50	1.40
2	A	501	FAD	C8-C7	3.67	1.50	1.40
2	B	501	FAD	C8-C7	3.60	1.49	1.40
2	E	501	FAD	C5A-C4A	2.81	1.48	1.40
2	C	501	FAD	C4X-N5	2.77	1.36	1.30
2	B	501	FAD	C4X-N5	2.77	1.36	1.30
2	F	501	FAD	C4X-N5	2.74	1.36	1.30
2	A	501	FAD	C4X-N5	2.72	1.36	1.30
2	D	501	FAD	C4X-N5	2.71	1.36	1.30
2	E	501	FAD	C4X-N5	2.70	1.36	1.30
2	D	501	FAD	C5A-C4A	2.69	1.48	1.40
2	B	501	FAD	C5A-C4A	2.67	1.48	1.40
2	C	501	FAD	C5A-C4A	2.66	1.48	1.40
2	F	501	FAD	C5A-C4A	2.64	1.47	1.40
2	A	501	FAD	C5A-C4A	2.58	1.47	1.40
2	E	501	FAD	C10-N10	2.34	1.42	1.37
2	F	501	FAD	C2A-N3A	2.26	1.35	1.32
2	C	501	FAD	C2A-N3A	2.23	1.35	1.32
2	F	501	FAD	C10-N10	2.22	1.42	1.37
2	B	501	FAD	C10-N10	2.22	1.42	1.37
2	A	501	FAD	C2A-N3A	2.20	1.35	1.32
2	E	501	FAD	C2A-N3A	2.17	1.35	1.32
2	B	501	FAD	C4-N3	-2.15	1.34	1.38
2	C	501	FAD	C10-N10	2.14	1.42	1.37
2	F	501	FAD	C4-N3	-2.10	1.34	1.38
2	E	501	FAD	C4-N3	-2.10	1.34	1.38
2	A	501	FAD	C10-N10	2.08	1.41	1.37
2	B	501	FAD	C2A-N3A	2.07	1.35	1.32
2	C	501	FAD	C4-N3	-2.06	1.35	1.38
2	D	501	FAD	C2A-N3A	2.05	1.35	1.32
2	D	501	FAD	C10-N10	2.01	1.41	1.37

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	FAD	N3A-C2A-N1A	-3.82	122.71	128.68
2	F	501	FAD	N3A-C2A-N1A	-3.66	122.95	128.68
2	A	501	FAD	N3A-C2A-N1A	-3.60	123.05	128.68
2	B	501	FAD	N3A-C2A-N1A	-3.50	123.21	128.68
2	C	501	FAD	N3A-C2A-N1A	-3.48	123.23	128.68
2	E	501	FAD	N3A-C2A-N1A	-3.47	123.25	128.68
2	A	501	FAD	C4-C4X-N5	3.27	122.88	118.23
2	B	501	FAD	C4-C4X-N5	3.17	122.75	118.23
2	C	501	FAD	C4-C4X-N5	3.16	122.73	118.23
2	D	501	FAD	C4-C4X-N5	3.10	122.65	118.23
2	B	501	FAD	C4X-C10-N1	-2.97	117.83	124.73
2	E	501	FAD	C4X-C10-N1	-2.97	117.83	124.73
2	F	501	FAD	C4X-C10-N1	-2.95	117.88	124.73
2	E	501	FAD	C4-C4X-N5	2.93	122.40	118.23
2	F	501	FAD	C4-C4X-N5	2.89	122.34	118.23
2	C	501	FAD	C4X-C10-N1	-2.74	118.36	124.73
2	A	501	FAD	C4X-C10-N1	-2.73	118.40	124.73
2	C	501	FAD	P-O3P-PA	-2.72	123.48	132.83
2	A	501	FAD	P-O3P-PA	-2.70	123.56	132.83
2	B	501	FAD	C10-N1-C2	2.68	122.26	116.90
2	E	501	FAD	C10-N1-C2	2.65	122.20	116.90
2	A	501	FAD	C10-N1-C2	2.64	122.17	116.90
2	F	501	FAD	C10-N1-C2	2.64	122.17	116.90
2	D	501	FAD	C4X-C10-N1	-2.63	118.62	124.73
2	C	501	FAD	C10-N1-C2	2.60	122.09	116.90
2	D	501	FAD	P-O3P-PA	-2.54	124.12	132.83
2	D	501	FAD	O2-C2-N1	-2.53	117.63	121.83
2	B	501	FAD	C4A-C5A-N7A	-2.51	106.78	109.40
2	E	501	FAD	O2-C2-N1	-2.49	117.71	121.83
2	D	501	FAD	C10-N1-C2	2.48	121.86	116.90
2	E	501	FAD	C4A-C5A-N7A	-2.47	106.83	109.40
2	C	501	FAD	C4A-C5A-N7A	-2.46	106.83	109.40
2	F	501	FAD	C4A-C5A-N7A	-2.45	106.85	109.40
2	B	501	FAD	P-O3P-PA	-2.38	124.66	132.83
2	A	501	FAD	O2-C2-N1	-2.36	117.92	121.83
2	C	501	FAD	O2-C2-N1	-2.35	117.93	121.83
2	D	501	FAD	C4A-C5A-N7A	-2.34	106.96	109.40
2	E	501	FAD	C4X-C10-N10	2.32	119.87	116.48
2	A	501	FAD	C9A-C5X-N5	-2.31	119.92	122.43
2	F	501	FAD	P-O3P-PA	-2.30	124.93	132.83
2	E	501	FAD	P-O3P-PA	-2.28	124.99	132.83
2	D	501	FAD	O4-C4-C4X	-2.22	120.70	126.60
2	B	501	FAD	C4X-C4-N3	2.21	118.81	113.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	501	FAD	O4-C4-C4X	-2.21	120.73	126.60
2	C	501	FAD	O4-C4-C4X	-2.18	120.81	126.60
2	F	501	FAD	C4X-C4-N3	2.17	118.71	113.19
2	A	501	FAD	O4-C4-C4X	-2.17	120.84	126.60
2	F	501	FAD	C4X-C10-N10	2.16	119.64	116.48
2	B	501	FAD	O2-C2-N1	-2.16	118.24	121.83
2	F	501	FAD	O2-C2-N1	-2.15	118.26	121.83
2	A	501	FAD	C5X-N5-C4X	2.14	121.63	118.07
2	C	501	FAD	C4X-C4-N3	2.14	118.61	113.19
2	B	501	FAD	C5X-N5-C4X	2.12	121.60	118.07
2	E	501	FAD	C4X-C4-N3	2.11	118.56	113.19
2	B	501	FAD	C4X-C10-N10	2.10	119.55	116.48
2	D	501	FAD	C4X-C4-N3	2.10	118.52	113.19
2	A	501	FAD	C4X-C4-N3	2.10	118.51	113.19
2	D	501	FAD	C2A-N1A-C6A	2.06	122.28	118.75
2	B	501	FAD	C9A-C5X-N5	-2.04	120.22	122.43
2	E	501	FAD	O4-C4-C4X	-2.04	121.19	126.60
2	C	501	FAD	C4X-C10-N10	2.04	119.46	116.48
2	A	501	FAD	C4A-C5A-N7A	-2.04	107.28	109.40
2	B	501	FAD	O4-C4-C4X	-2.03	121.21	126.60
2	B	501	FAD	C2A-N1A-C6A	2.02	122.21	118.75
2	F	501	FAD	C3B-C2B-C1B	2.02	104.02	100.98
2	E	501	FAD	C4-N3-C2	-2.01	121.93	125.64

There are no chirality outliers.

All (146) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	501	FAD	O4B-C4B-C5B-O5B
3	B	504	16A	C14-C15-C16-N1
2	A	501	FAD	O4B-C4B-C5B-O5B
2	C	501	FAD	O4B-C4B-C5B-O5B
2	D	501	FAD	C3B-C4B-C5B-O5B
3	A	503	16A	C14-C15-C16-N1
3	A	502	16A	C14-C15-C16-N1
3	A	503	16A	C3-C4-C5-C6
3	A	504	16A	C7-C8-C9-C10
3	B	504	16A	C10-C11-C12-C13
3	D	503	16A	C5-C6-C7-C8
3	F	502	16A	C3-C4-C5-C6
3	A	502	16A	C11-C12-C13-C14
3	B	504	16A	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
3	C	502	16A	C3-C4-C5-C6
3	B	502	16A	C7-C8-C9-C10
3	B	503	16A	C10-C11-C12-C13
3	A	503	16A	C6-C7-C8-C9
3	B	502	16A	C6-C7-C8-C9
3	B	504	16A	C12-C13-C14-C15
3	B	506	16A	C9-C10-C11-C12
3	F	503	16A	C5-C6-C7-C8
3	D	503	16A	C4-C5-C6-C7
3	B	506	16A	C7-C8-C9-C10
3	C	502	16A	C5-C6-C7-C8
3	A	504	16A	C10-C11-C12-C13
3	A	503	16A	C10-C11-C12-C13
3	B	502	16A	C5-C6-C7-C8
3	B	506	16A	C5-C6-C7-C8
3	D	504	16A	C9-C10-C11-C12
3	B	504	16A	C4-C5-C6-C7
3	D	504	16A	C2-C3-C4-C5
3	A	504	16A	C9-C10-C11-C12
3	E	502	16A	C11-C12-C13-C14
3	F	503	16A	C12-C13-C14-C15
3	B	503	16A	C11-C12-C13-C14
3	F	502	16A	C11-C10-C9-C8
3	F	502	16A	C10-C11-C12-C13
3	A	502	16A	C10-C11-C12-C13
3	A	502	16A	C11-C10-C9-C8
3	B	502	16A	C11-C10-C9-C8
3	C	502	16A	C10-C11-C12-C13
3	E	502	16A	C3-C4-C5-C6
3	B	502	16A	C9-C10-C11-C12
3	D	502	16A	C4-C5-C6-C7
3	B	506	16A	C2-C3-C4-C5
3	A	502	16A	C12-C13-C14-C15
3	B	505	16A	C9-C10-C11-C12
3	F	502	16A	C6-C7-C8-C9
3	F	503	16A	C4-C5-C6-C7
3	E	502	16A	C2-C3-C4-C5
2	B	501	FAD	O4B-C4B-C5B-O5B
3	B	502	16A	C11-C12-C13-C14
3	B	503	16A	C11-C10-C9-C8
3	D	502	16A	C12-C13-C14-C15
3	F	503	16A	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
3	B	506	16A	C6-C7-C8-C9
3	D	502	16A	C2-C3-C4-C5
3	F	503	16A	C7-C8-C9-C10
3	B	505	16A	C7-C8-C9-C10
3	E	502	16A	C6-C7-C8-C9
3	F	503	16A	C9-C10-C11-C12
3	A	502	16A	C13-C14-C15-C16
3	C	502	16A	C4-C5-C6-C7
3	B	502	16A	C3-C4-C5-C6
3	B	503	16A	C4-C5-C6-C7
3	C	502	16A	C11-C10-C9-C8
3	D	503	16A	C3-C4-C5-C6
3	D	504	16A	C4-C5-C6-C7
3	B	505	16A	C11-C12-C13-C14
3	B	502	16A	C2-C3-C4-C5
3	D	502	16A	C13-C14-C15-C16
3	D	502	16A	C10-C11-C12-C13
3	C	502	16A	C12-C13-C14-C15
3	B	505	16A	C5-C6-C7-C8
3	B	505	16A	C11-C10-C9-C8
3	B	503	16A	C2-C3-C4-C5
3	B	503	16A	C6-C7-C8-C9
3	B	506	16A	C4-C5-C6-C7
3	F	503	16A	C10-C11-C12-C13
3	C	502	16A	C7-C8-C9-C10
3	E	502	16A	C5-C6-C7-C8
3	A	502	16A	C4-C5-C6-C7
3	A	504	16A	C12-C13-C14-C15
3	D	503	16A	C6-C7-C8-C9
3	B	502	16A	C1-C2-C3-C4
3	E	502	16A	C1-C2-C3-C4
3	D	502	16A	C1-C2-C3-C4
2	A	501	FAD	C3B-C4B-C5B-O5B
3	B	503	16A	C1-C2-C3-C4
3	B	504	16A	C1-C2-C3-C4
3	D	504	16A	C10-C11-C12-C13
3	B	505	16A	C12-C13-C14-C15
2	C	501	FAD	C3B-C4B-C5B-O5B
2	F	501	FAD	O4B-C4B-C5B-O5B
3	A	504	16A	C11-C10-C9-C8
3	A	502	16A	C9-C10-C11-C12
3	F	502	16A	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
3	D	504	16A	C1-C2-C3-C4
3	E	502	16A	C11-C10-C9-C8
3	A	502	16A	C7-C8-C9-C10
3	A	502	16A	C3-C4-C5-C6
3	D	502	16A	C7-C8-C9-C10
3	E	502	16A	C12-C13-C14-C15
3	B	505	16A	C1-C2-C3-C4
3	C	502	16A	C1-C2-C3-C4
3	A	503	16A	C2-C3-C4-C5
3	A	504	16A	C6-C7-C8-C9
3	D	502	16A	C5-C6-C7-C8
3	A	503	16A	C11-C10-C9-C8
3	B	505	16A	C2-C3-C4-C5
3	A	504	16A	C3-C4-C5-C6
3	A	502	16A	C5-C6-C7-C8
3	B	502	16A	C13-C14-C15-C16
3	B	502	16A	C4-C5-C6-C7
3	B	506	16A	C11-C12-C13-C14
3	A	504	16A	C5-C6-C7-C8
3	B	505	16A	C14-C15-C16-N1
3	B	506	16A	C11-C10-C9-C8
3	A	504	16A	C13-C14-C15-C16
3	A	503	16A	C5-C6-C7-C8
3	B	506	16A	C3-C4-C5-C6
3	B	504	16A	C13-C14-C15-C16
3	B	502	16A	C10-C11-C12-C13
3	B	504	16A	C2-C3-C4-C5
3	D	504	16A	C13-C14-C15-C16
3	B	504	16A	C7-C8-C9-C10
3	A	502	16A	C6-C7-C8-C9
2	B	501	FAD	C3B-C4B-C5B-O5B
2	E	501	FAD	O4B-C4B-C5B-O5B
3	C	502	16A	C13-C14-C15-C16
3	B	504	16A	C11-C12-C13-C14
3	D	503	16A	C13-C14-C15-C16
3	D	503	16A	C2-C3-C4-C5
3	F	503	16A	C6-C7-C8-C9
3	D	503	16A	C11-C10-C9-C8
3	D	502	16A	C9-C10-C11-C12
3	B	503	16A	C12-C13-C14-C15
3	C	502	16A	C9-C10-C11-C12
2	F	501	FAD	C3B-C4B-C5B-O5B

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Mol	Chain	Res	Type	Atoms
3	A	504	16A	C14-C15-C16-N1
3	F	502	16A	C11-C12-C13-C14
3	E	502	16A	C7-C8-C9-C10
2	B	501	FAD	O4'-C4'-C5'-O5'
3	B	503	16A	C14-C15-C16-N1
3	B	503	16A	C5-C6-C7-C8

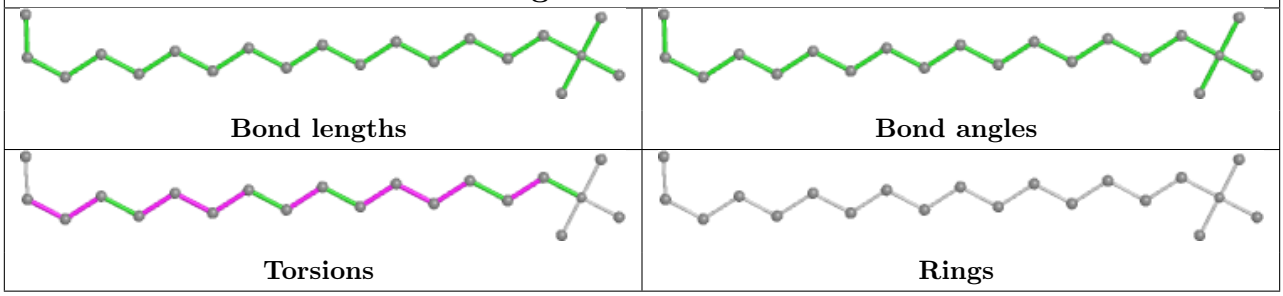
There are no ring outliers.

13 monomers are involved in 21 short contacts:

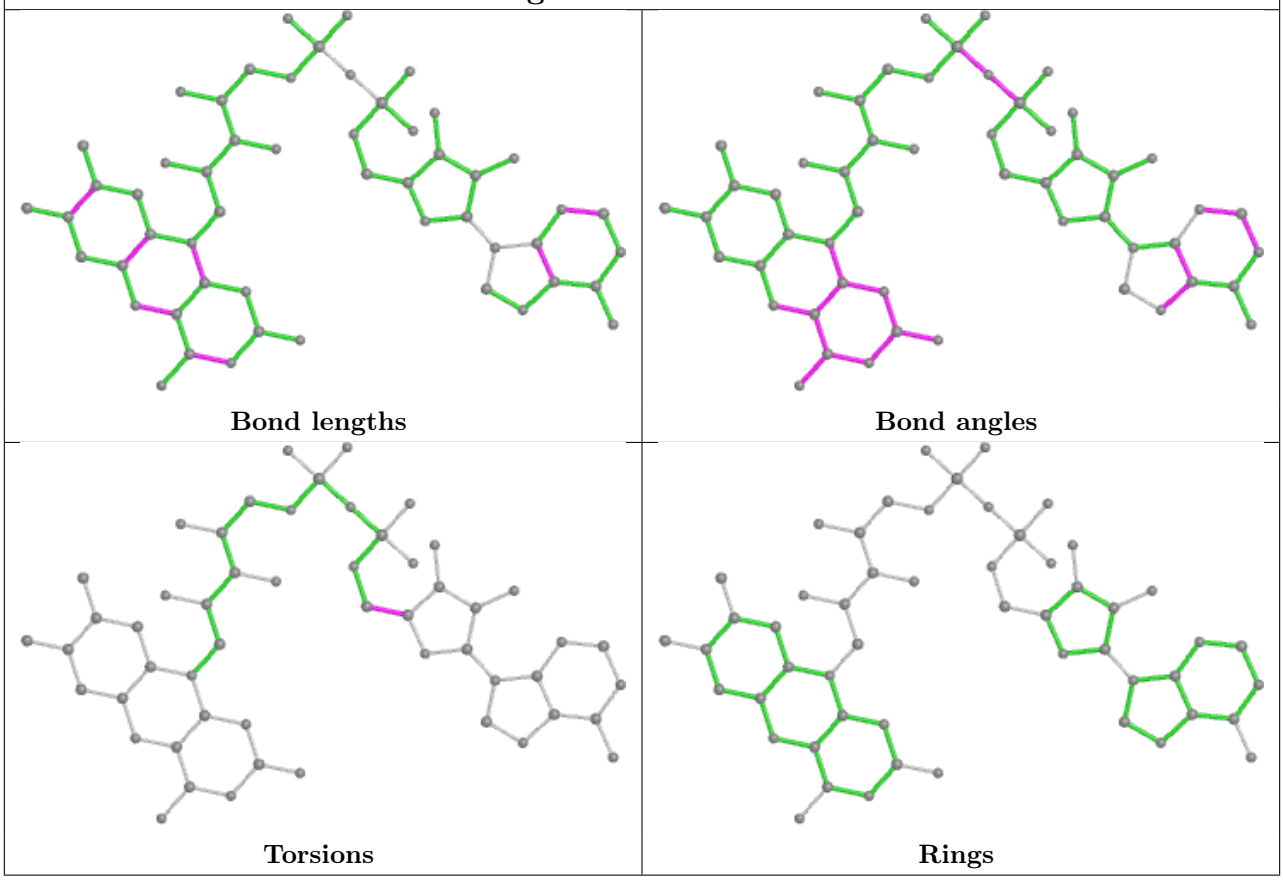
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	503	16A	2	0
3	C	502	16A	1	0
2	C	501	FAD	2	0
3	A	503	16A	4	0
2	B	501	FAD	2	0
3	E	502	16A	2	0
3	B	506	16A	3	0
3	A	504	16A	1	0
3	B	504	16A	2	0
3	D	504	16A	1	0
3	B	505	16A	1	0
3	B	502	16A	4	0
3	D	502	16A	3	0

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 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.

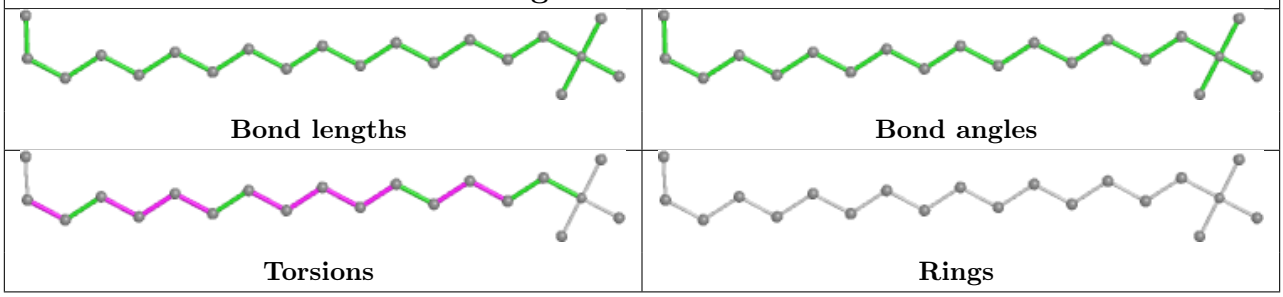
Ligand 16A B 503



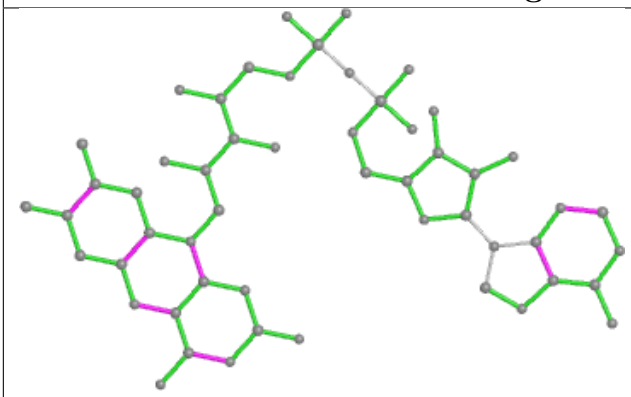
Ligand FAD E 501



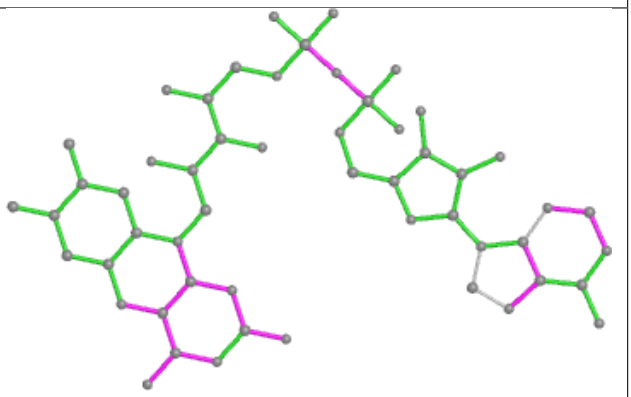
Ligand 16A C 502



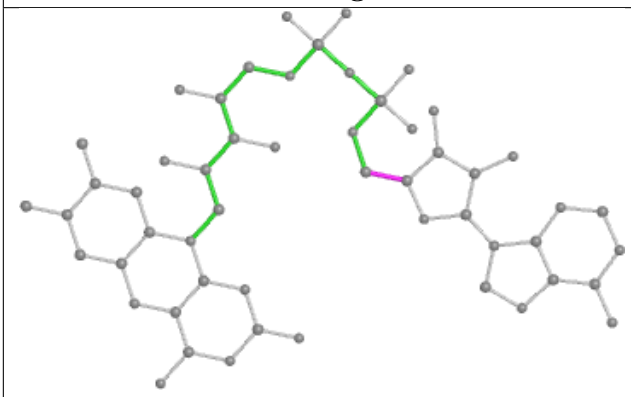
Ligand FAD C 501



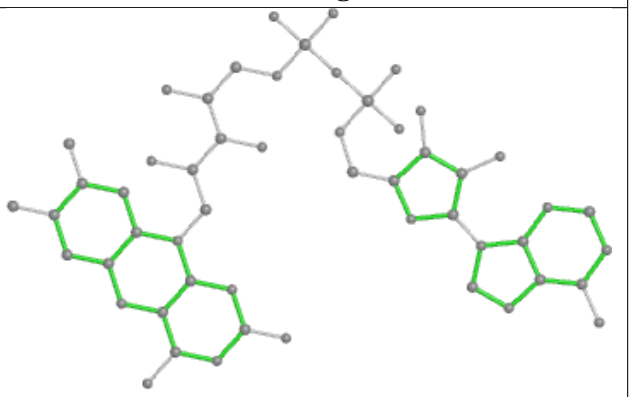
Bond lengths



Bond angles

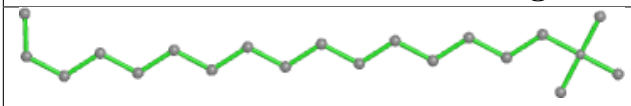


Torsions

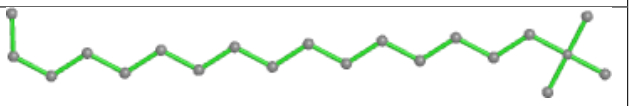


Rings

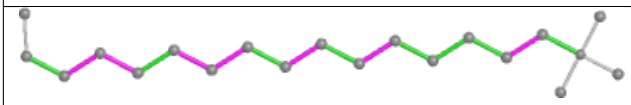
Ligand 16A A 503



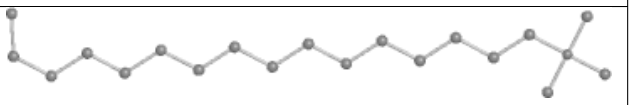
Bond lengths



Bond angles

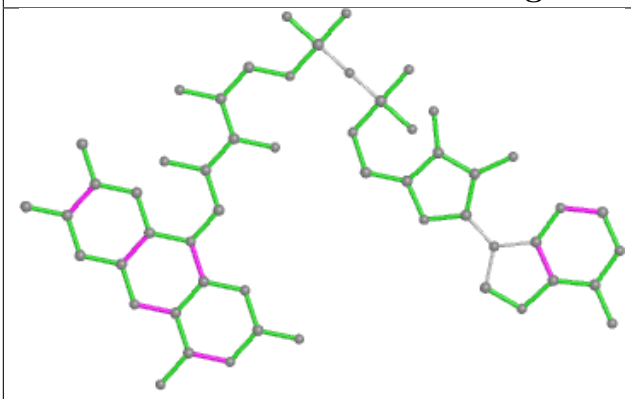


Torsions



Rings

Ligand FAD B 501



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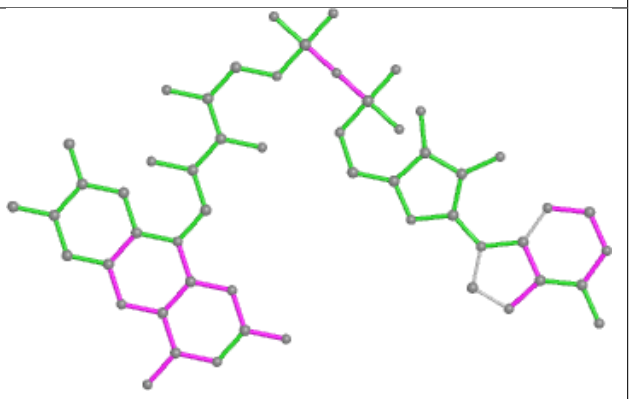
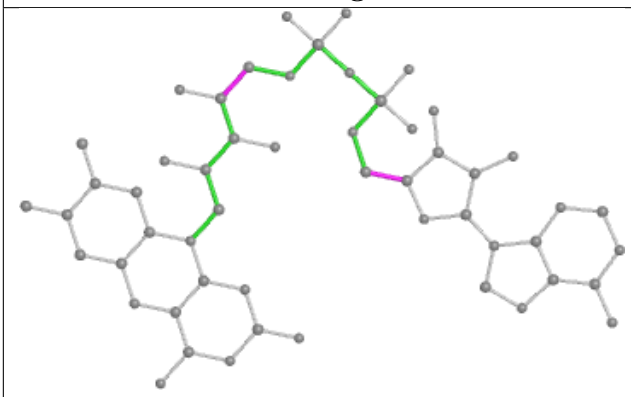
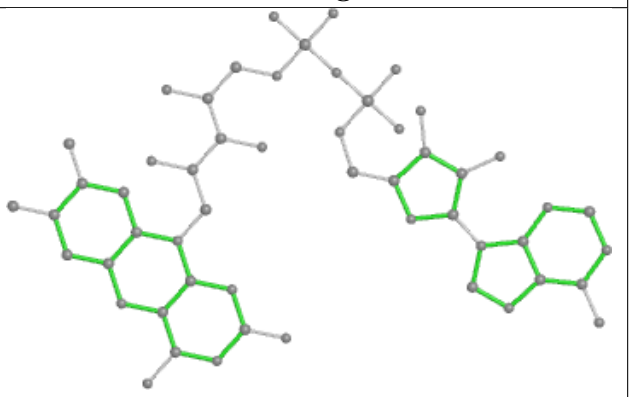


Bond angles

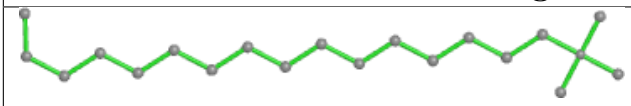


Torsions

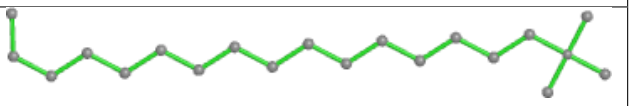


Rings

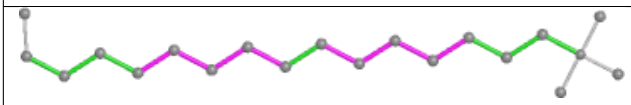
Ligand 16A F 503



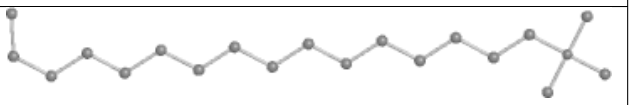
Bond lengths



Bond angles

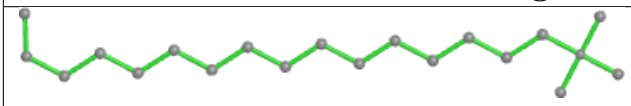


Torsions



Rings

Ligand 16A E 502



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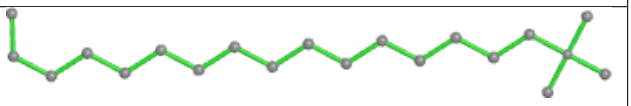
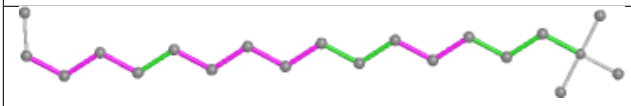


Bond angles



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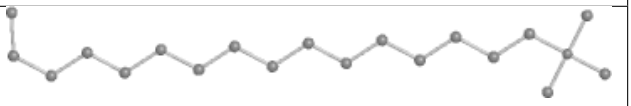
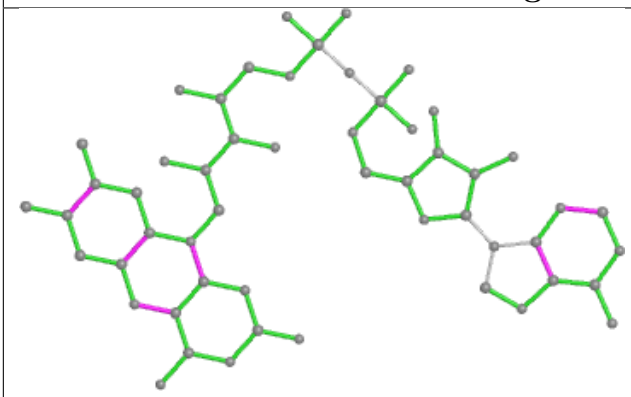
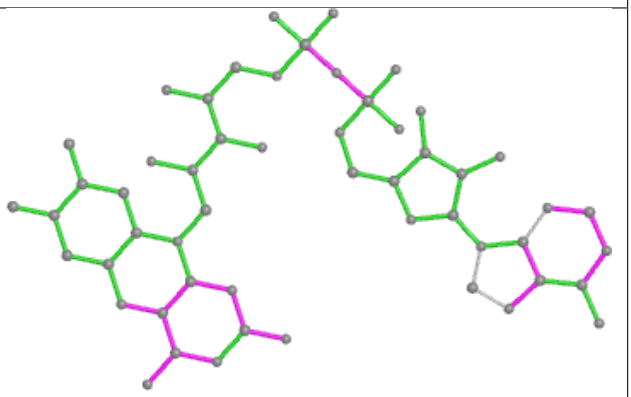


Rings

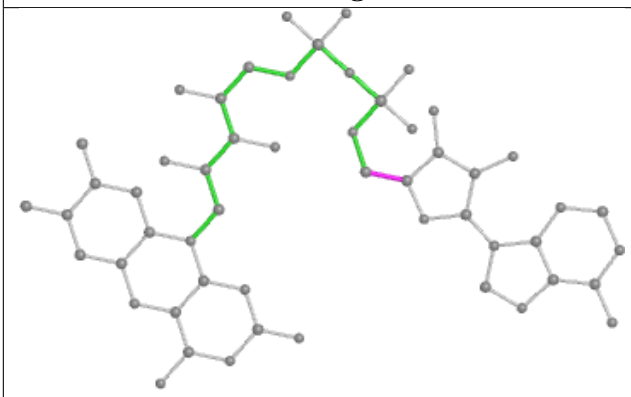
Ligand FAD D 501



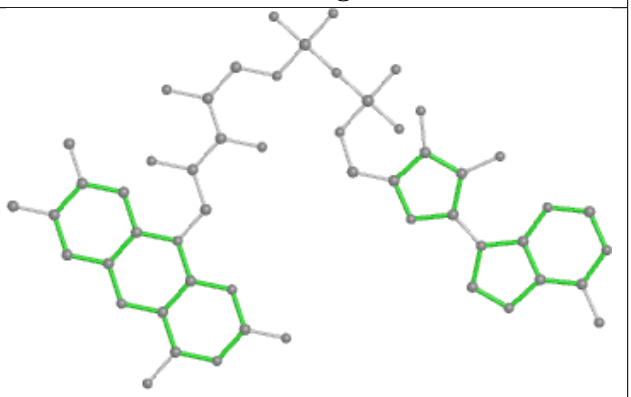
Bond lengths



Bond angles

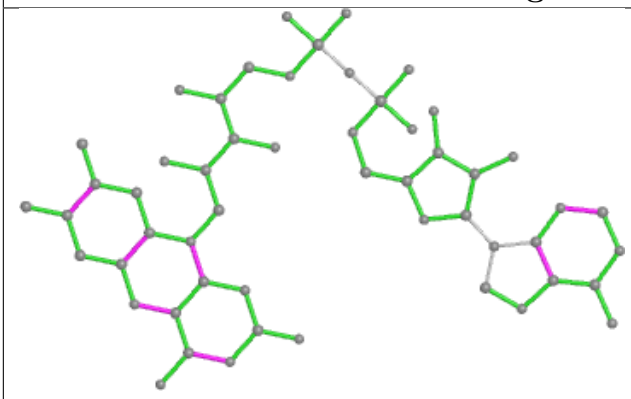


Torsions

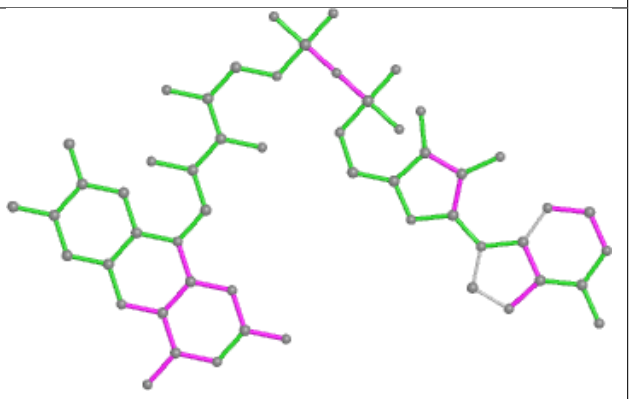


Rings

Ligand FAD F 501



Bond lengths



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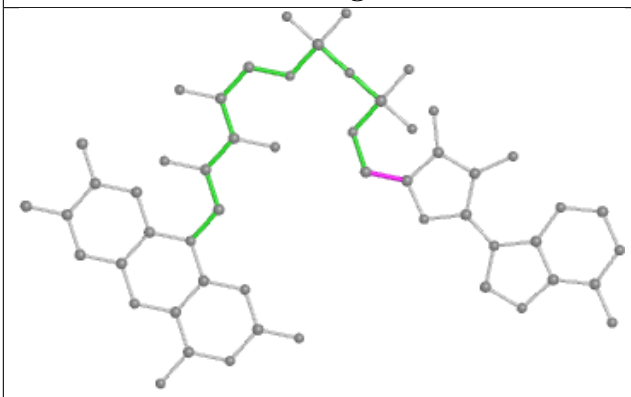
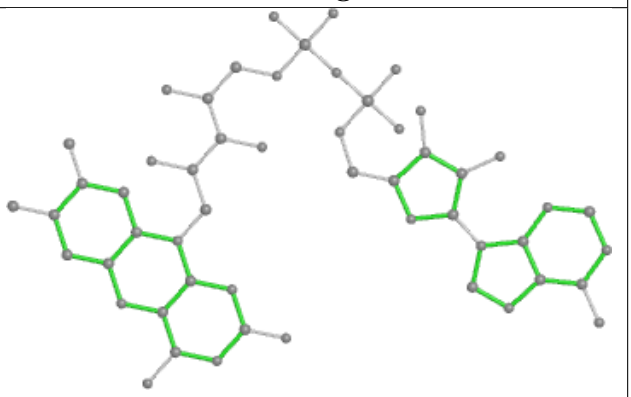
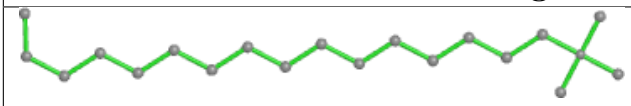


Torsions

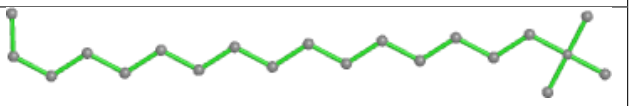


Rings

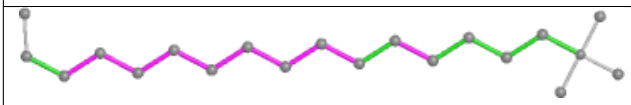
Ligand 16A B 506



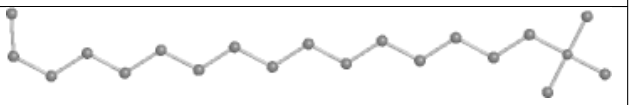
Bond lengths



Bond angles

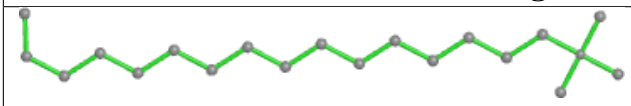


Torsions

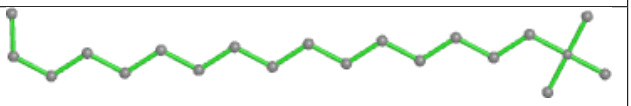


Rings

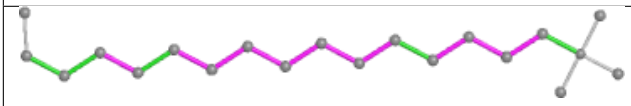
Ligand 16A A 504



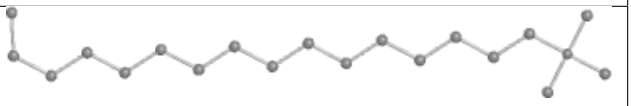
Bond lengths



Bond angles

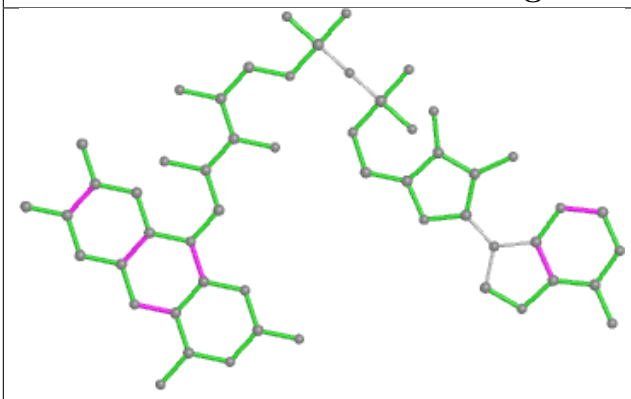


Torsions

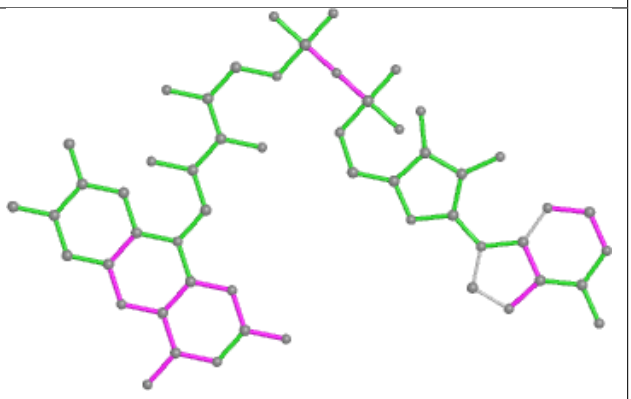


Rings

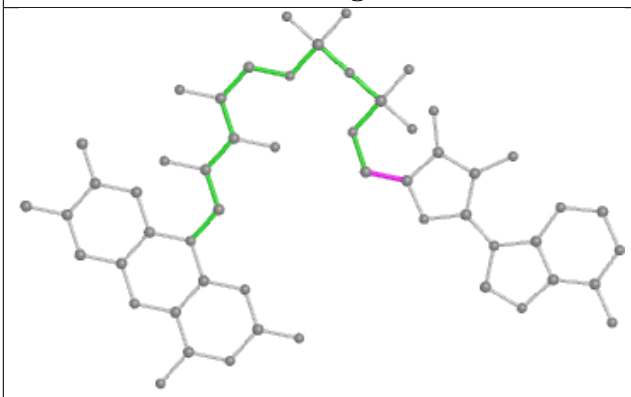
Ligand FAD A 501



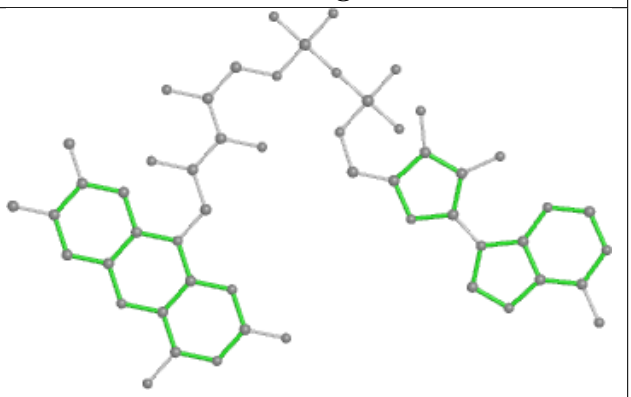
Bond lengths



Bond angles

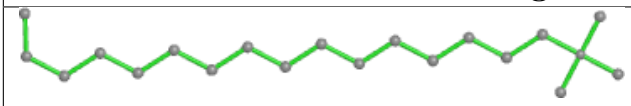


Torsions



Rings

Ligand 16A B 504



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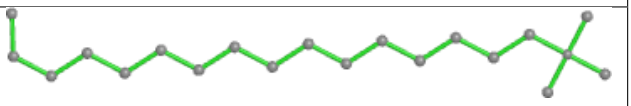
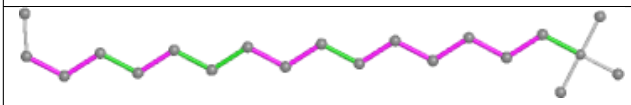


Bond angles



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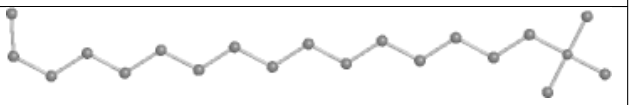
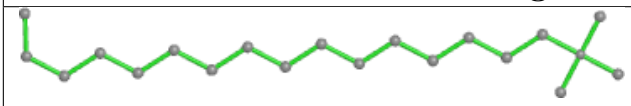
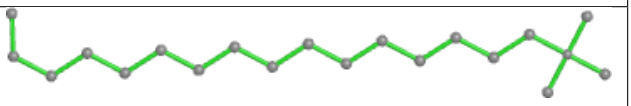


Rings

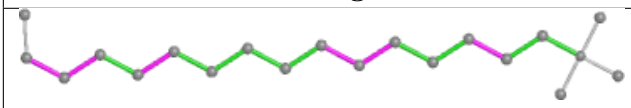
Ligand 16A D 504



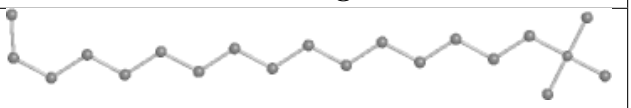
Bond lengths



Bond angles



Torsions



Rings

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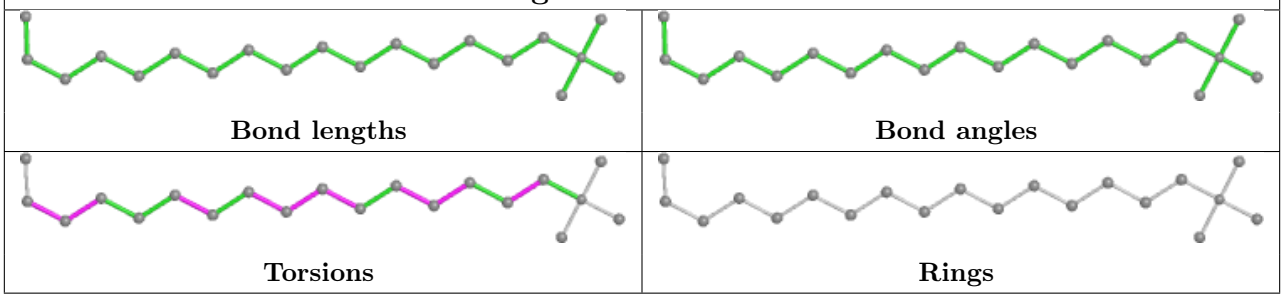

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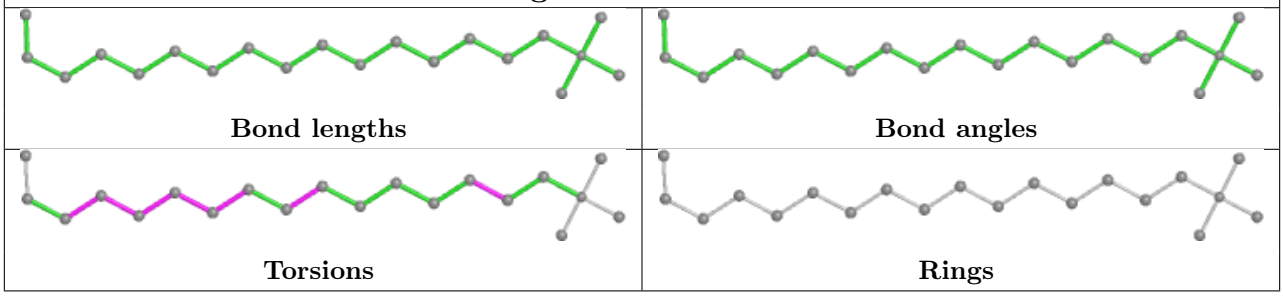
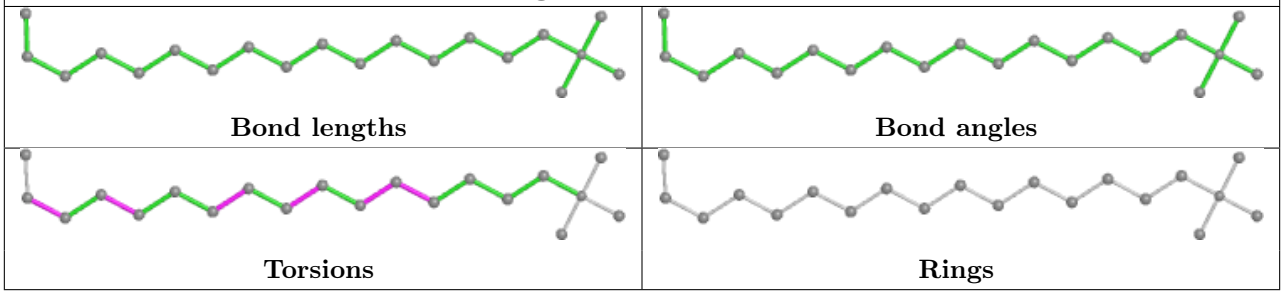
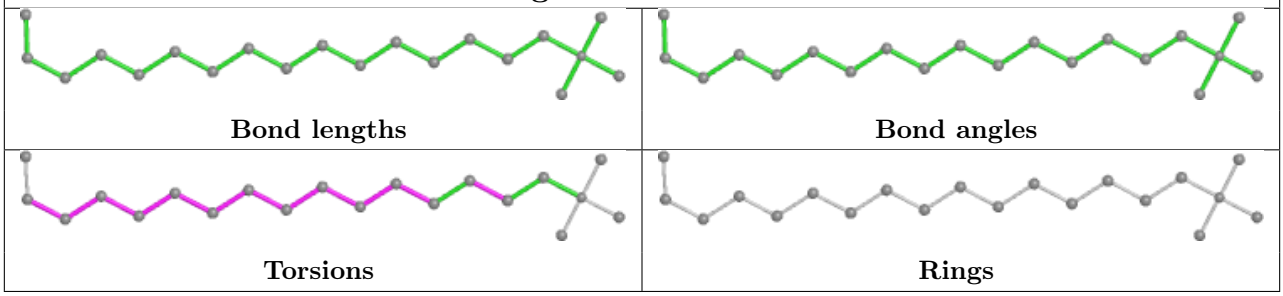


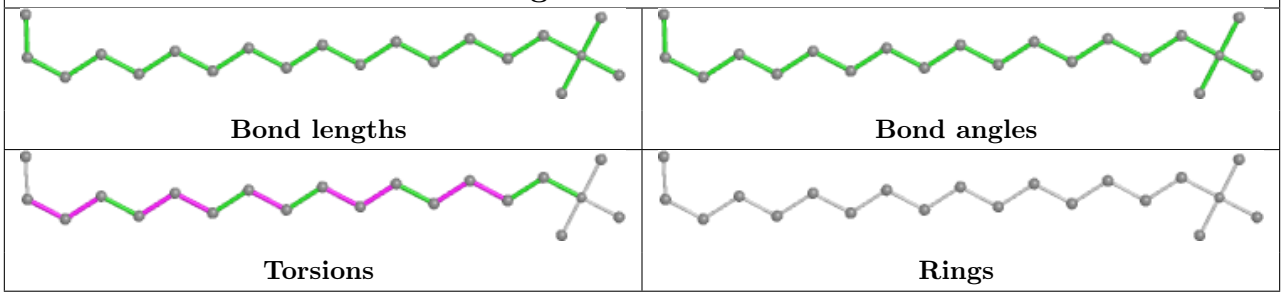
Ligand 16A F 502

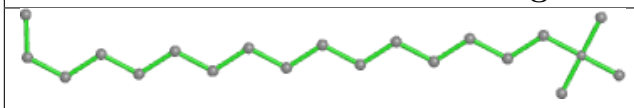
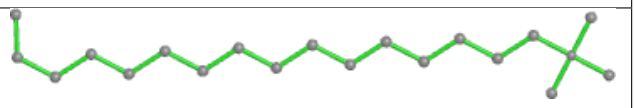
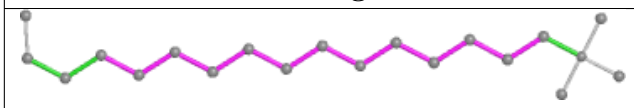
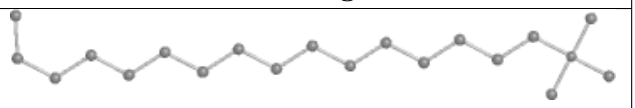


Ligand 16A B 502



Ligand 16A D 502



Ligand 16A A 502	
 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	A	433/454 (95%)	-0.16	1 (0%)	95	96	58, 74, 103, 127	0
1	B	432/454 (95%)	-0.12	5 (1%)	79	77	51, 88, 123, 138	0
1	C	430/454 (94%)	0.15	14 (3%)	46	43	54, 83, 148, 180	0
1	D	430/454 (94%)	0.17	15 (3%)	44	40	56, 93, 155, 192	0
1	E	430/454 (94%)	0.08	15 (3%)	44	40	54, 96, 139, 165	0
1	F	430/454 (94%)	0.29	26 (6%)	21	19	55, 117, 165, 190	0
All	All	2585/2724 (94%)	0.07	76 (2%)	51	48	51, 89, 149, 192	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	192	ALA	7.3
1	C	191	ILE	5.0
1	F	81	VAL	4.9
1	D	176	ALA	4.5
1	F	252	VAL	4.4
1	F	192	ALA	4.2
1	F	194	PHE	4.2
1	D	292	GLY	3.9
1	D	193	GLY	3.9
1	D	192	ALA	3.8
1	C	193	GLY	3.8
1	F	289	ALA	3.7
1	E	139	VAL	3.6
1	E	155	ILE	3.5
1	F	113	HIS	3.4
1	E	191	ILE	3.4
1	A	161	ASN	3.4
1	C	115	LEU	3.2
1	F	156	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
1	F	302	PHE	3.2
1	C	194	PHE	3.2
1	C	179	ASN	3.2
1	E	152	ARG	3.1
1	F	125	ALA	3.1
1	F	176	ALA	3.0
1	F	80	VAL	3.0
1	E	120	TRP	3.0
1	F	455	LEU	2.9
1	C	292	GLY	2.9
1	F	240	VAL	2.9
1	E	156	ASP	2.9
1	E	118	HIS	2.9
1	E	154	TRP	2.8
1	B	131	THR	2.8
1	D	288	THR	2.8
1	F	229	GLY	2.8
1	D	289	ALA	2.8
1	C	103	TYR	2.7
1	F	340	ASP	2.7
1	D	178	LEU	2.6
1	F	100	ALA	2.6
1	F	221	ILE	2.6
1	E	192	ALA	2.6
1	C	171	ARG	2.6
1	D	181	ARG	2.5
1	F	179	ASN	2.5
1	C	154	TRP	2.5
1	D	172	ILE	2.4
1	C	156	ASP	2.4
1	F	83	VAL	2.4
1	F	82	ILE	2.4
1	F	160	LYS	2.3
1	E	164	SER	2.3
1	E	129	ILE	2.3
1	C	141	VAL	2.3
1	E	193	GLY	2.3
1	B	421	ILE	2.2
1	D	296	LEU	2.2
1	B	208	PHE	2.2
1	D	115	LEU	2.2
1	D	174	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	300	ILE	2.2
1	B	207	THR	2.2
1	E	168	PHE	2.2
1	F	234	ALA	2.2
1	D	291	GLY	2.1
1	C	395	PHE	2.1
1	F	71	ILE	2.1
1	D	306	ALA	2.1
1	E	162	VAL	2.1
1	D	107	ASP	2.1
1	F	114	HIS	2.1
1	B	220	ARG	2.1
1	F	253	VAL	2.0
1	E	400	GLU	2.0
1	F	251	GLN	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	16A	A	503	20/20	0.72	0.35	80,89,95,96	0
3	16A	C	502	20/20	0.77	0.29	91,97,100,101	0
3	16A	D	503	20/20	0.79	0.33	71,80,84,84	0
3	16A	B	502	20/20	0.85	0.27	73,79,88,88	0
3	16A	B	503	20/20	0.85	0.33	82,85,88,89	0
3	16A	D	504	20/20	0.85	0.27	72,77,80,81	0
3	16A	E	502	20/20	0.85	0.34	76,80,88,89	0
3	16A	B	504	20/20	0.87	0.31	68,73,86,87	0

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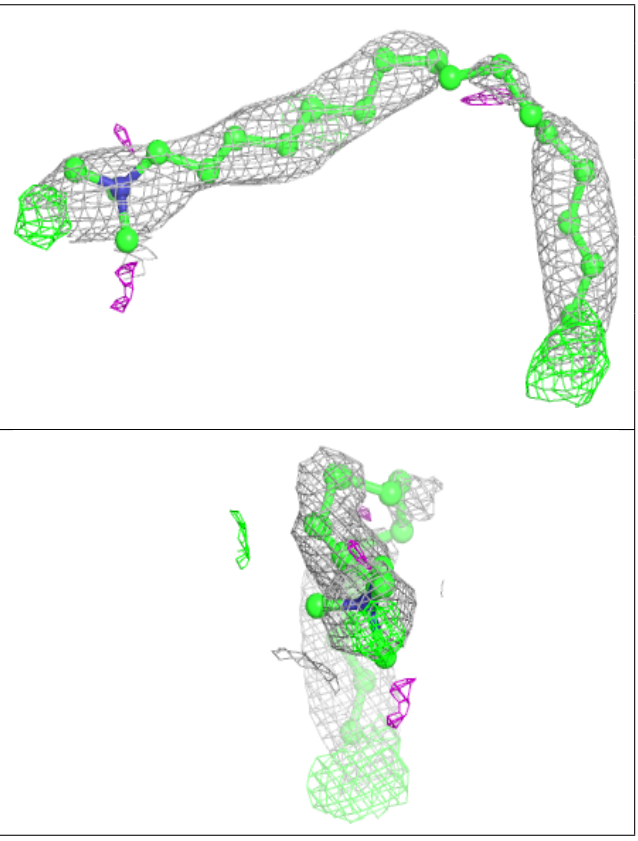
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	16A	D	502	20/20	0.88	0.20	68,71,79,79	0
3	16A	B	505	20/20	0.89	0.22	67,68,73,74	0
3	16A	A	502	20/20	0.89	0.23	64,71,88,88	0
3	16A	B	506	20/20	0.92	0.22	67,69,72,72	0
3	16A	A	504	20/20	0.92	0.27	70,79,89,90	0
3	16A	F	502	20/20	0.92	0.25	67,71,75,76	0
3	16A	F	503	20/20	0.94	0.21	62,75,92,92	0
2	FAD	F	501	53/53	0.96	0.17	77,90,97,102	0
2	FAD	A	501	53/53	0.97	0.16	54,57,62,62	0
2	FAD	C	501	53/53	0.97	0.16	57,60,79,83	0
2	FAD	D	501	53/53	0.97	0.17	62,66,77,79	0
2	FAD	E	501	53/53	0.97	0.15	67,75,85,87	0
2	FAD	B	501	53/53	0.98	0.13	61,69,76,79	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.

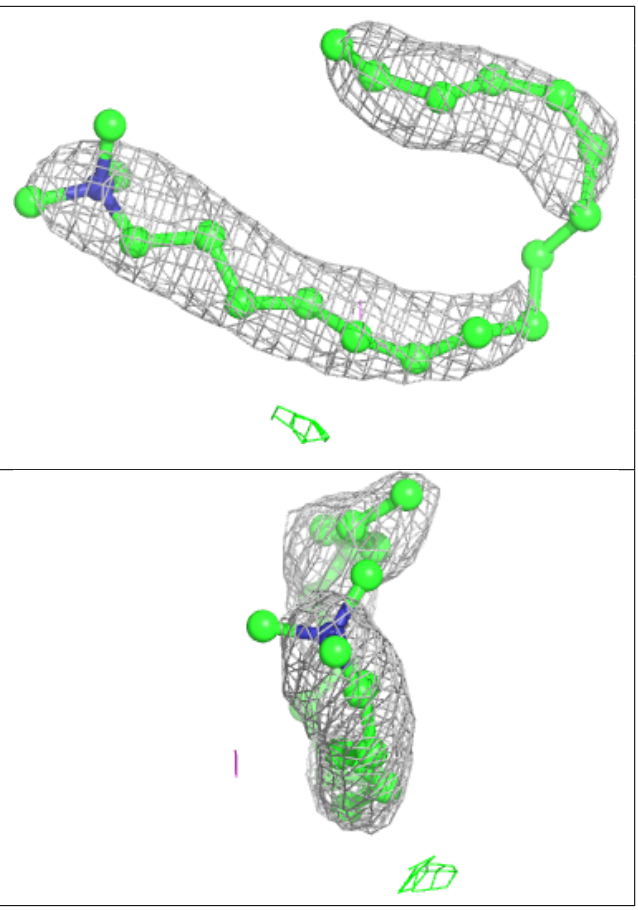
Electron density around 16A A 503:

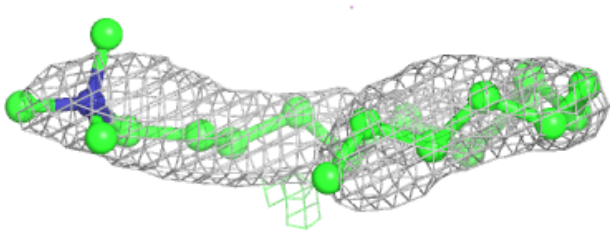
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around 16A C 502:

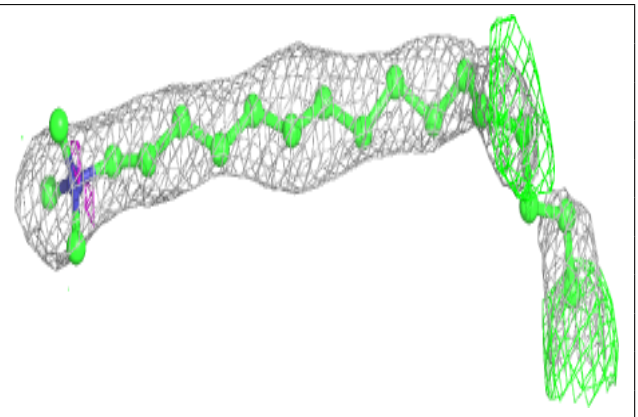
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

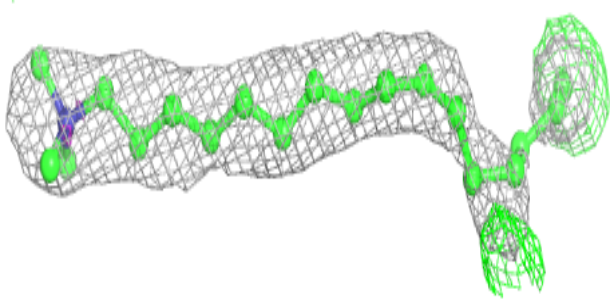


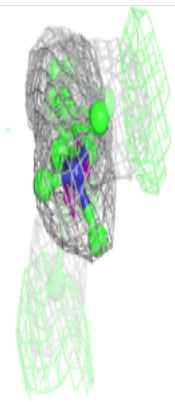


Electron density around 16A D 503:

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

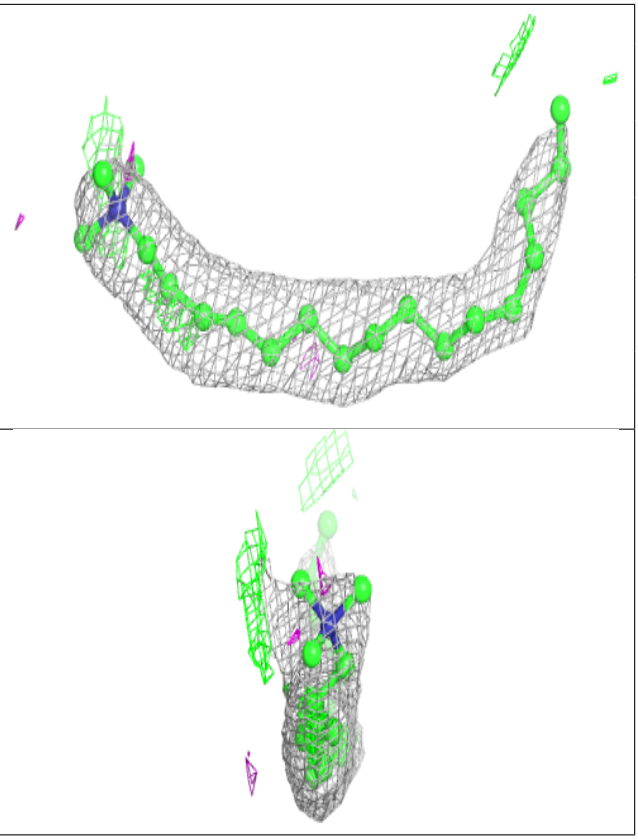






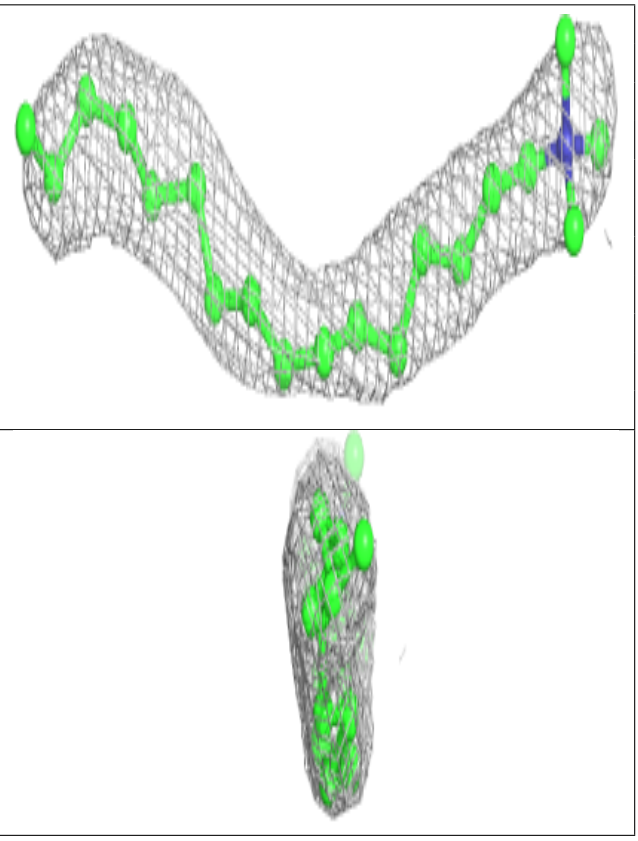
Electron density around 16A B 502:

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



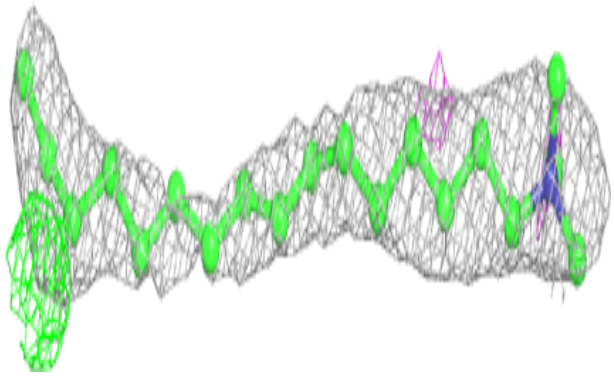
Electron density around 16A B 503:

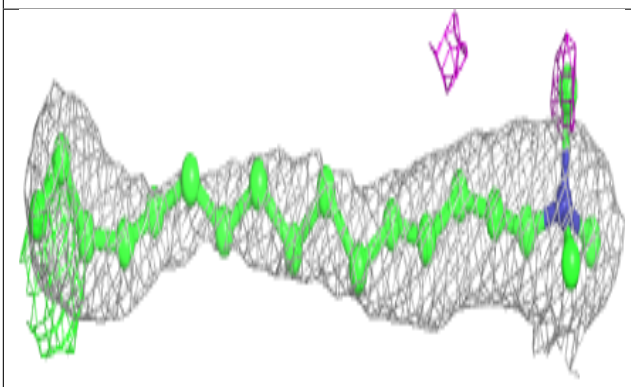
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

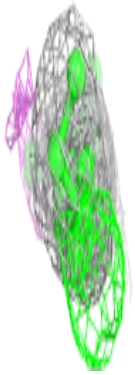


Electron density around 16A D 504:

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

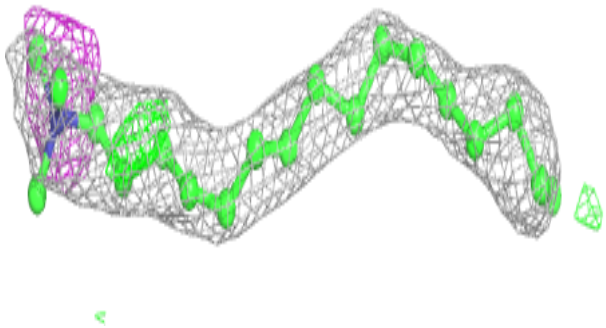


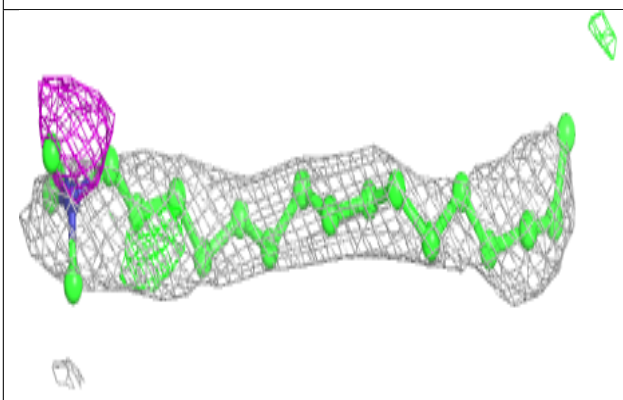


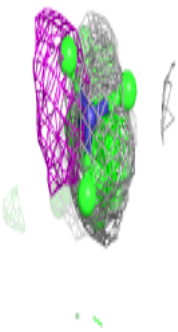


Electron density around 16A E 502:

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

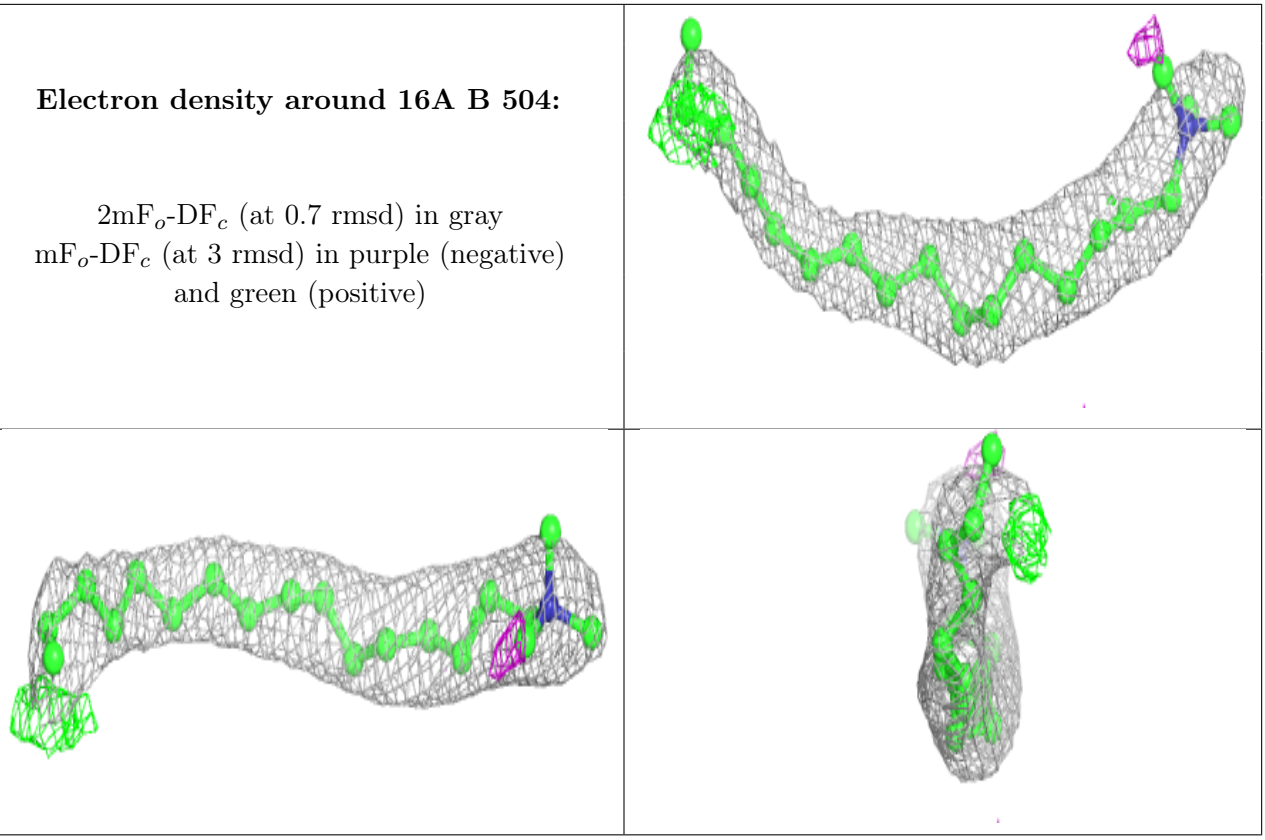






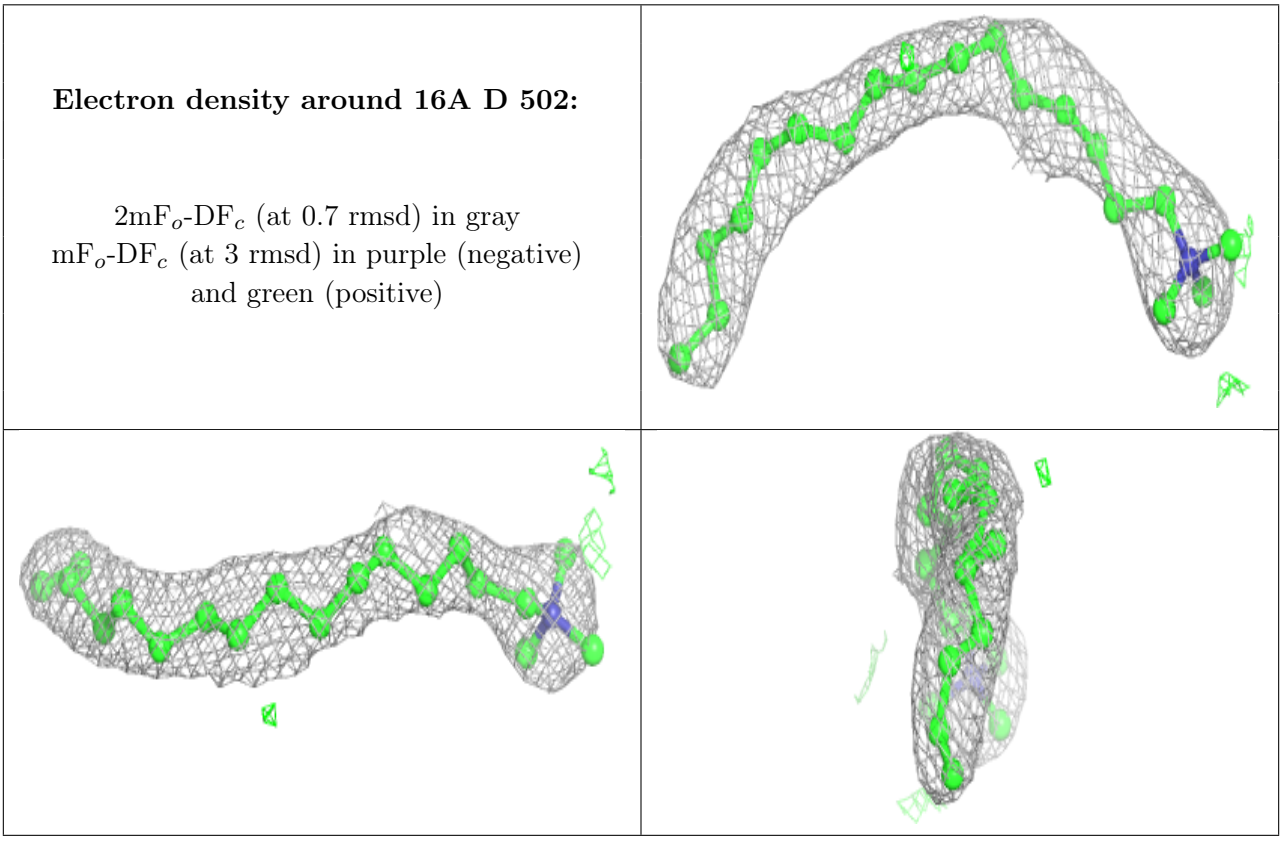
Electron density around 16A B 504:

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



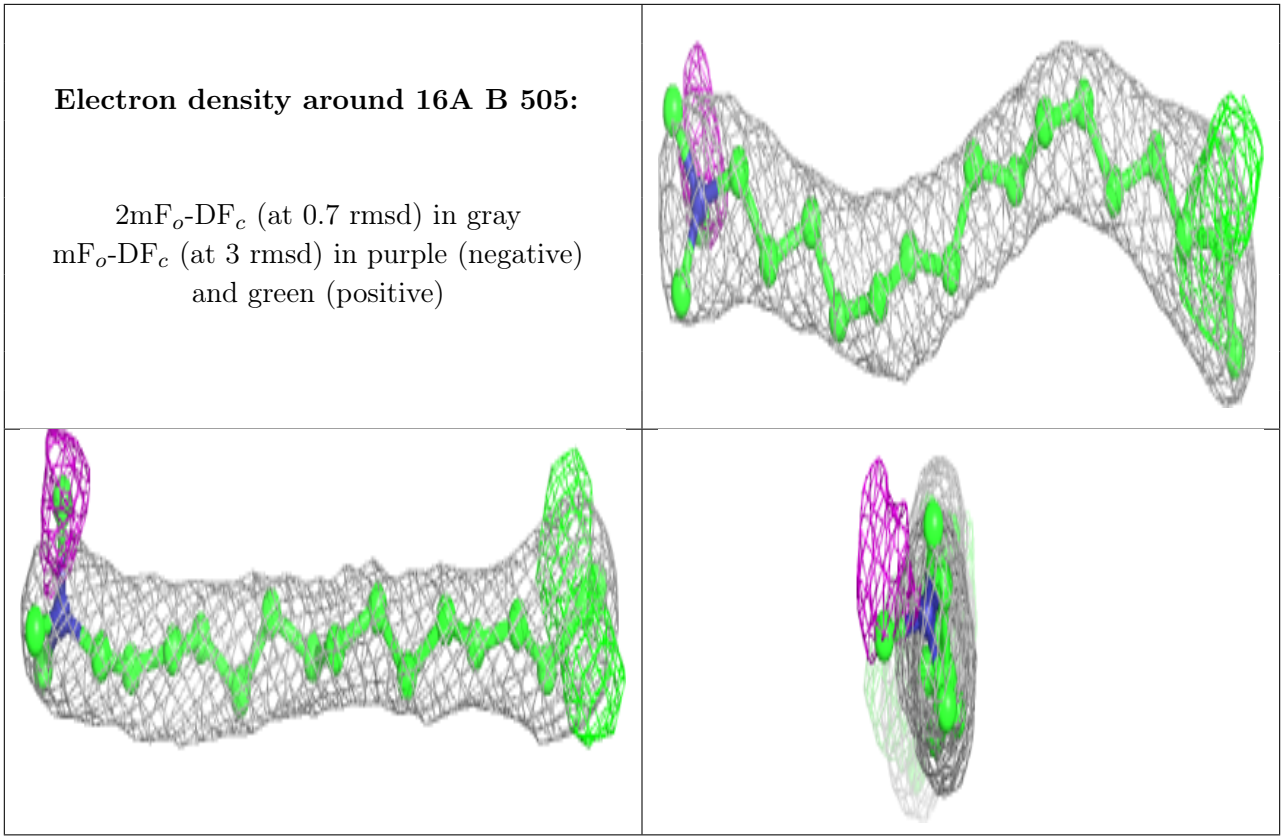
Electron density around 16A D 502:

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



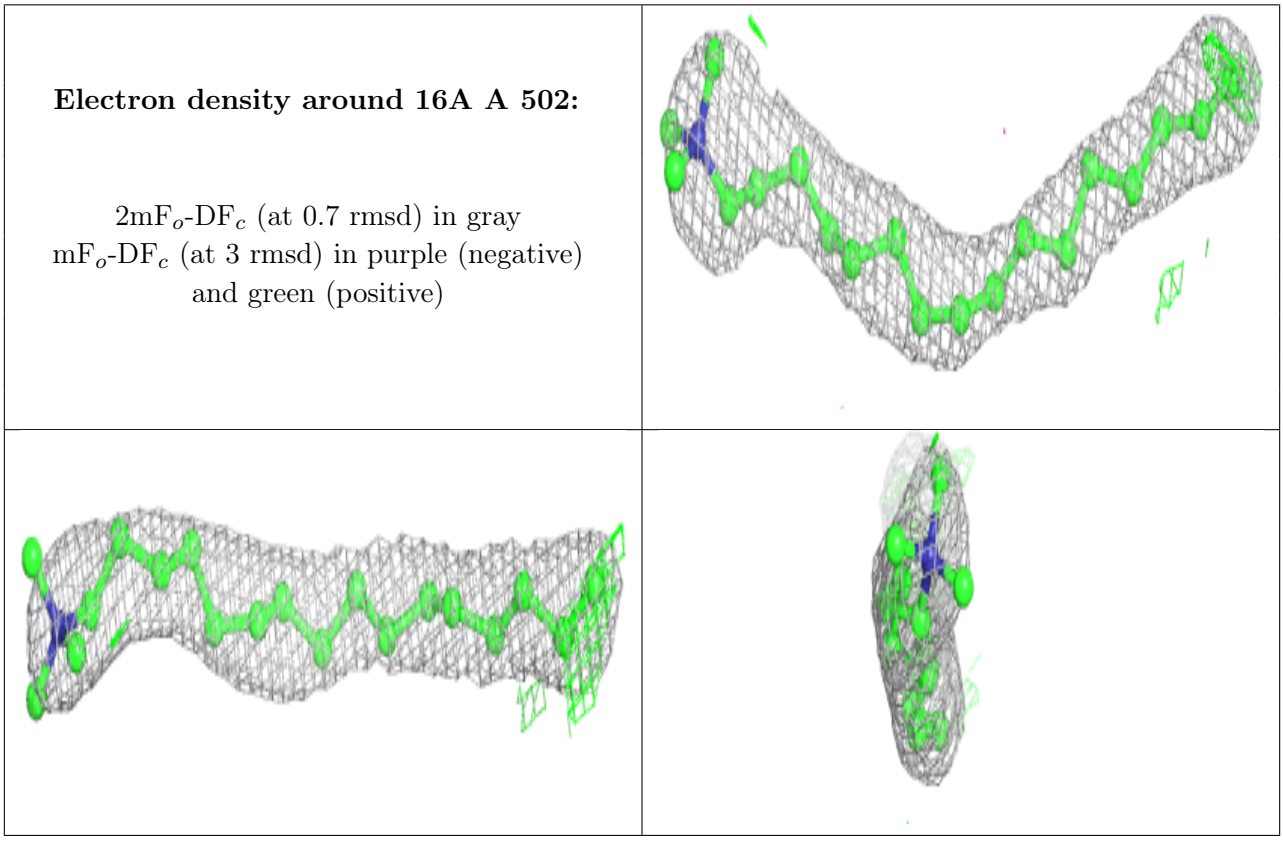
Electron density around 16A B 505:

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



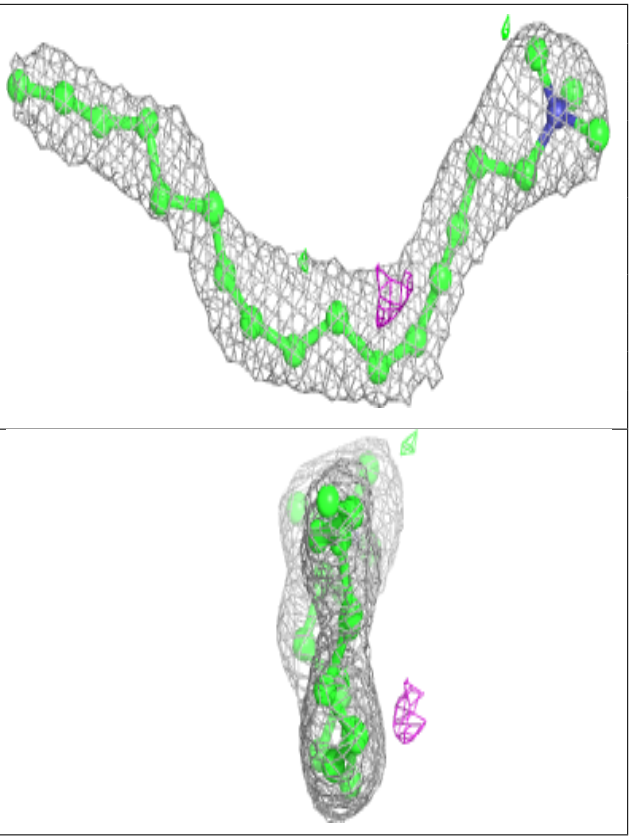
Electron density around 16A A 502:

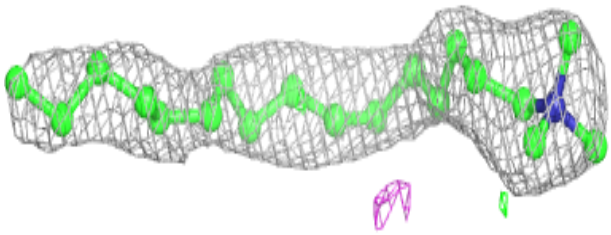
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 16A B 506:

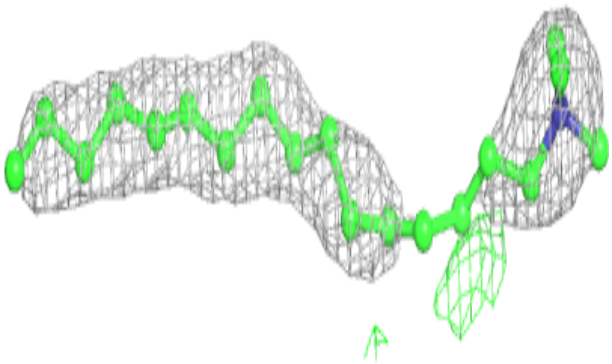
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

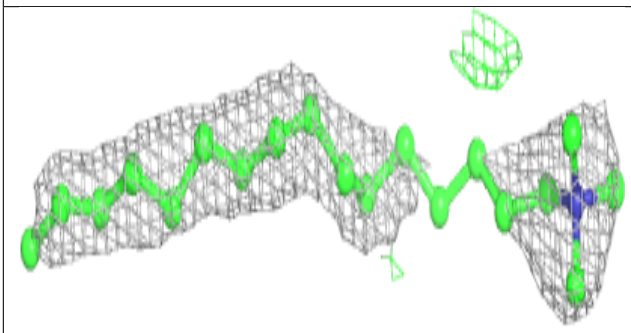


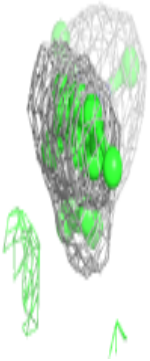


Electron density around 16A A 504:

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

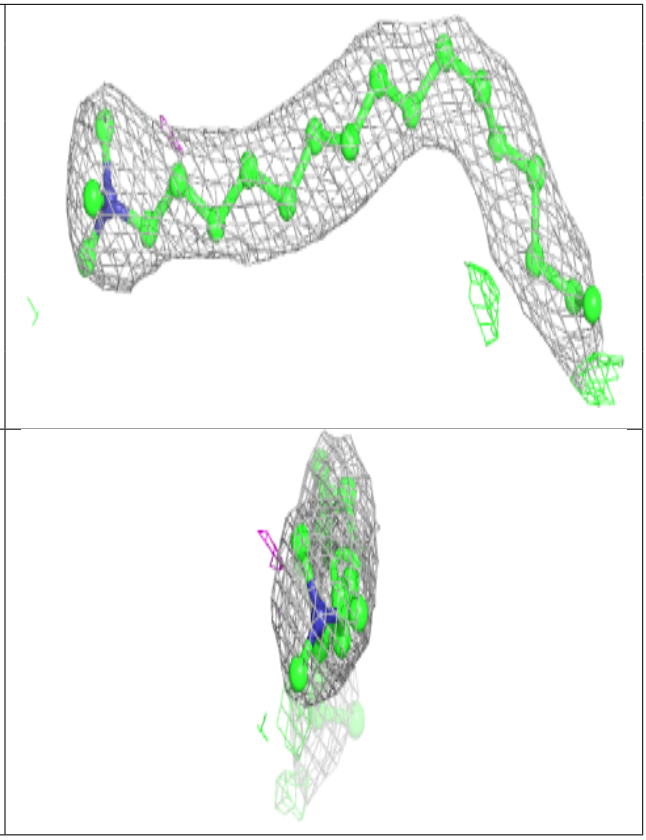






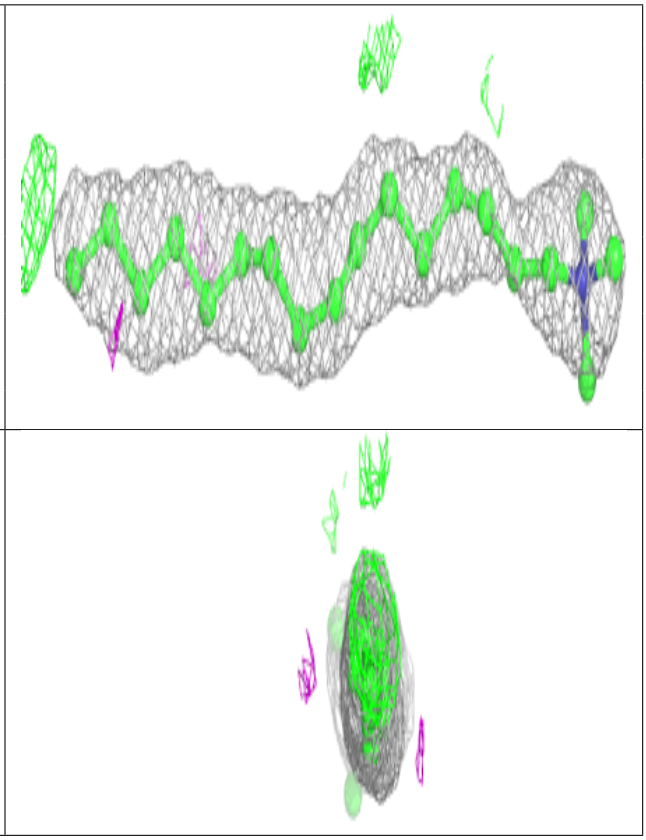
Electron density around 16A F 502:

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



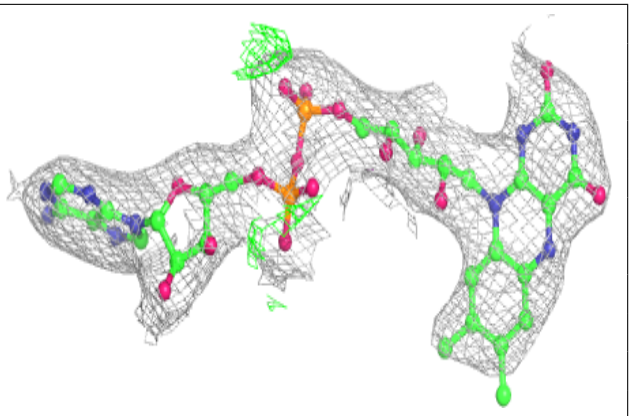
Electron density around 16A F 503:

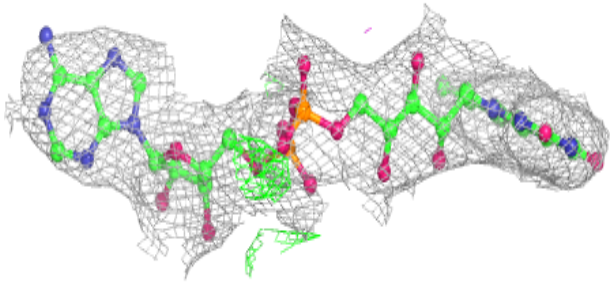
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

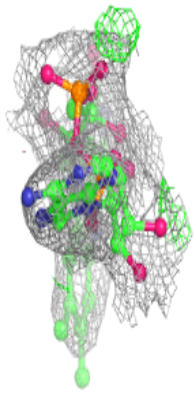


Electron density around FAD F 501:

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

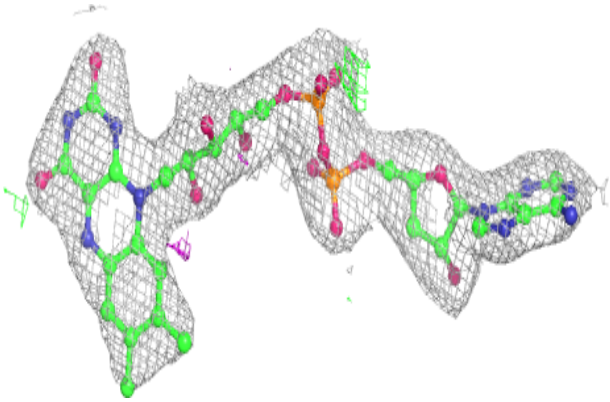


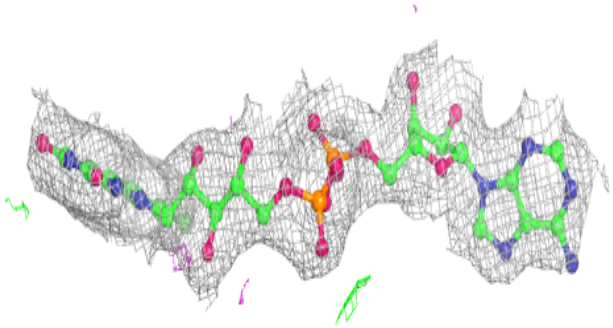


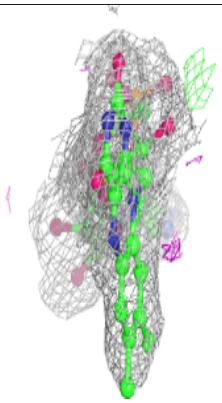


Electron density around FAD A 501:

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

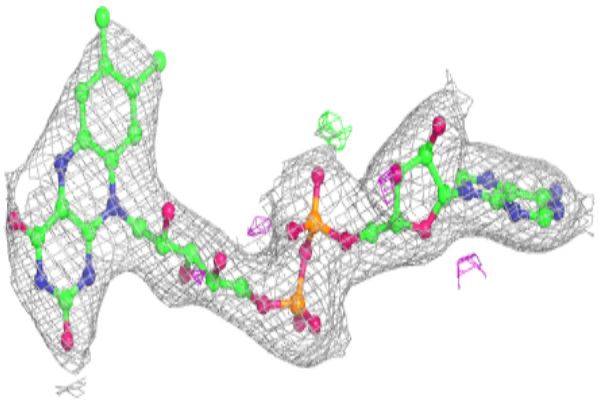


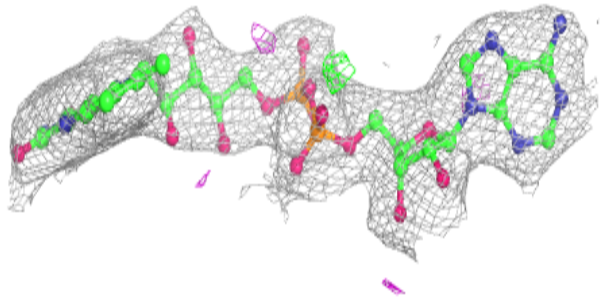


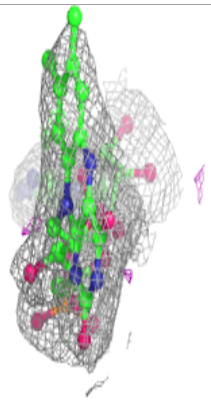


Electron density around FAD C 501:

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

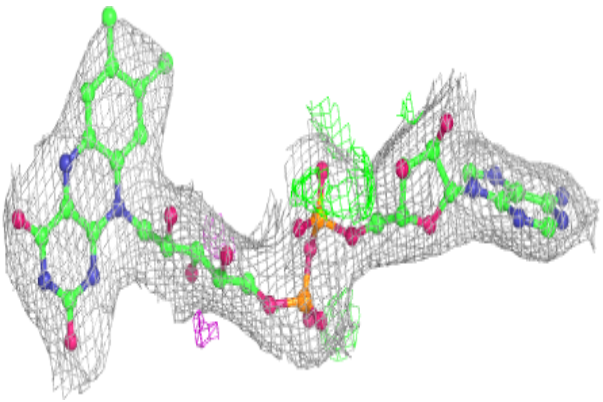


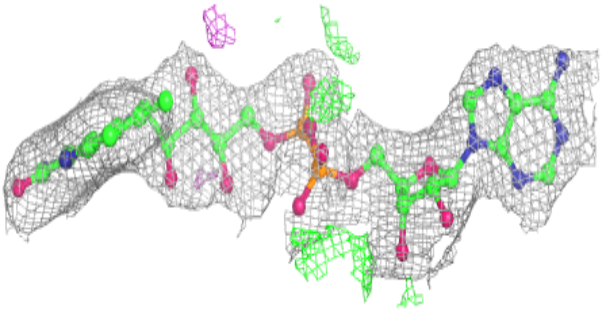


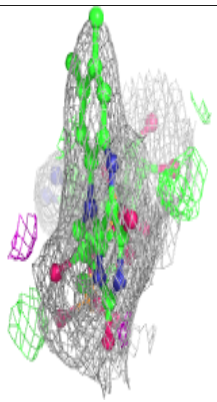


Electron density around FAD D 501:

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

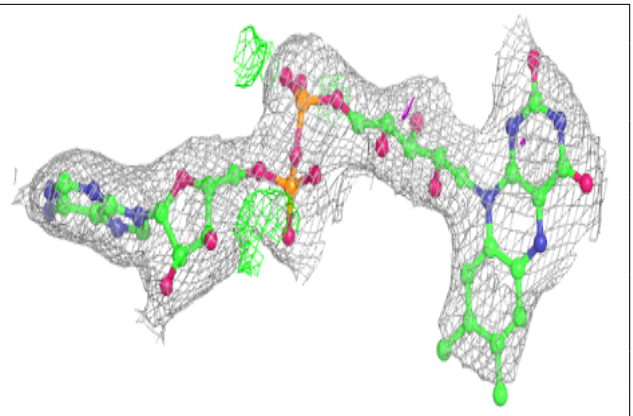


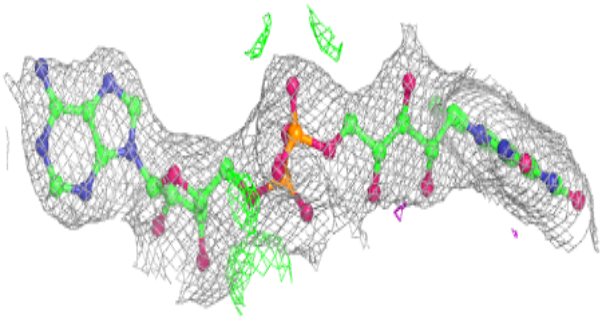


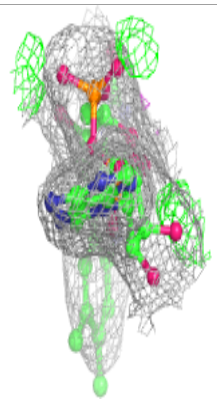


Electron density around FAD E 501:

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

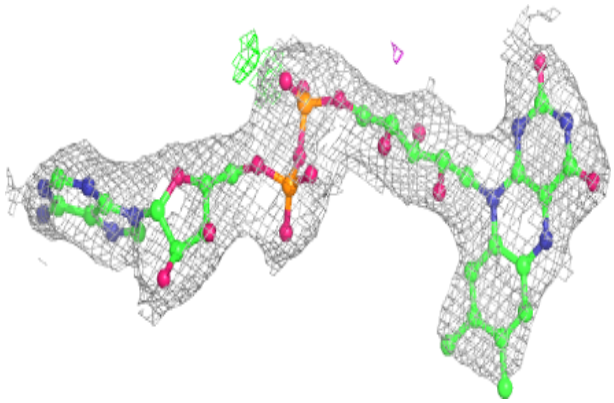


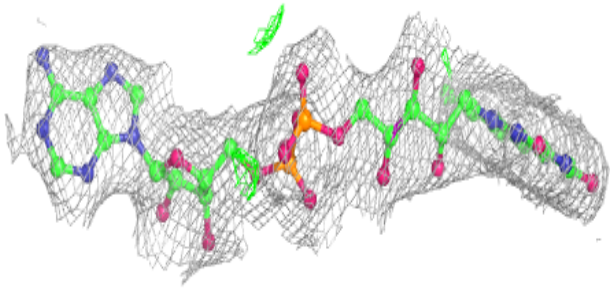




Electron density around FAD B 501:

$2mF_o$-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.