Full wwPDB X-ray Structure Validation Report ⓘ

Jun 7, 2020 – 03:35 am BST

PDB ID	:	6I4T
Title	:	Crystal structure of the disease-causing I445M mutant of the human dihydrolipoamide dehydrogenase
Authors	:	Szabo, E.; Wilk, P.; Zambo, Z.; Torocsik, B.; Weiss, M.S.; Adam-Vizi, V.; Ambrus, A.
Deposited on	:	2018-11-10
Resolution	:	1.82 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 following versions of software and data (see references ⓘ) were used in the production of this report:

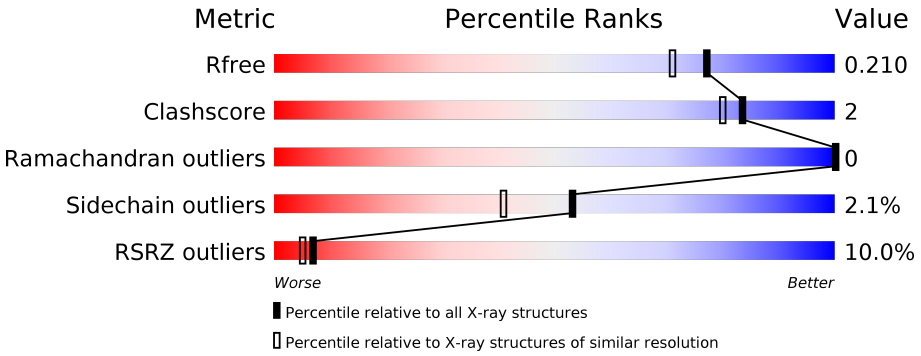
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 1.82 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	7484 (1.84-1.80)
Clashscore	141614	8401 (1.84-1.80)
Ramachandran outliers	138981	8290 (1.84-1.80)
Sidechain outliers	138945	8290 (1.84-1.80)
RSRZ outliers	127900	7371 (1.84-1.80)

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 on 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	496	8% 89% 6% 5%
1	B	496	11% 91% 6% .

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 15098 atoms, of which 7366 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 Dihydrolipoyl dehydrogenase, mitochondrial.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	472	Total	C	H	N	O	S	0	10	0
			7173	2243	3618	611	677	24			
1	B	481	Total	C	H	N	O	S	0	7	0
			7268	2275	3664	620	686	23			

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	initiating methionine	UNP P09622
A	-20	ALA	-	expression tag	UNP P09622
A	-19	SER	-	expression tag	UNP P09622
A	-18	TRP	-	expression tag	UNP P09622
A	-17	SER	-	expression tag	UNP P09622
A	-16	HIS	-	expression tag	UNP P09622
A	-15	PRO	-	expression tag	UNP P09622
A	-14	GLN	-	expression tag	UNP P09622
A	-13	PHE	-	expression tag	UNP P09622
A	-12	GLU	-	expression tag	UNP P09622
A	-11	LYS	-	expression tag	UNP P09622
A	-10	GLY	-	expression tag	UNP P09622
A	-9	ALA	-	expression tag	UNP P09622
A	-8	LEU	-	expression tag	UNP P09622
A	-7	GLU	-	expression tag	UNP P09622
A	-6	VAL	-	expression tag	UNP P09622
A	-5	LEU	-	expression tag	UNP P09622
A	-4	PHE	-	expression tag	UNP P09622
A	-3	GLN	-	expression tag	UNP P09622
A	-2	GLY	-	expression tag	UNP P09622
A	-1	PRO	-	expression tag	UNP P09622
A	0	GLY	-	expression tag	UNP P09622
A	445	MET	ILE	engineered mutation	UNP P09622
B	-21	MET	-	initiating methionine	UNP P09622
B	-20	ALA	-	expression tag	UNP P09622

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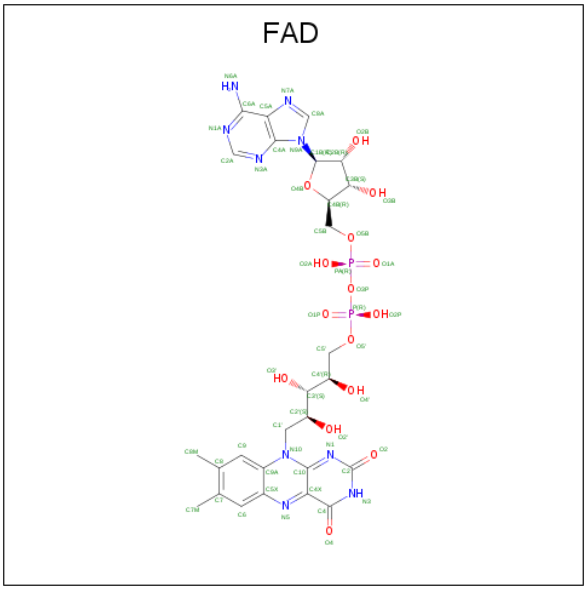
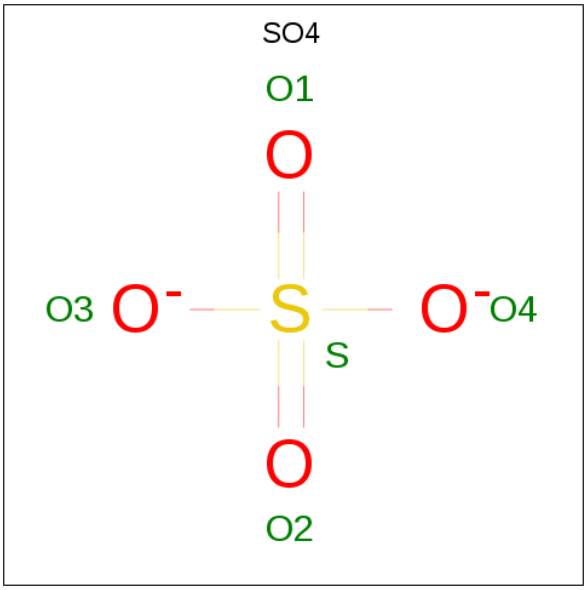
Chain	Residue	Modelled	Actual	Comment	Reference
B	-19	SER	-	expression tag	UNP P09622
B	-18	TRP	-	expression tag	UNP P09622
B	-17	SER	-	expression tag	UNP P09622
B	-16	HIS	-	expression tag	UNP P09622
B	-15	PRO	-	expression tag	UNP P09622
B	-14	GLN	-	expression tag	UNP P09622
B	-13	PHE	-	expression tag	UNP P09622
B	-12	GLU	-	expression tag	UNP P09622
B	-11	LYS	-	expression tag	UNP P09622
B	-10	GLY	-	expression tag	UNP P09622
B	-9	ALA	-	expression tag	UNP P09622
B	-8	LEU	-	expression tag	UNP P09622
B	-7	GLU	-	expression tag	UNP P09622
B	-6	VAL	-	expression tag	UNP P09622
B	-5	LEU	-	expression tag	UNP P09622
B	-4	PHE	-	expression tag	UNP P09622
B	-3	GLN	-	expression tag	UNP P09622
B	-2	GLY	-	expression tag	UNP P09622
B	-1	PRO	-	expression tag	UNP P09622
B	0	GLY	-	expression tag	UNP P09622
B	445	MET	ILE	engineered mutation	UNP P09622

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



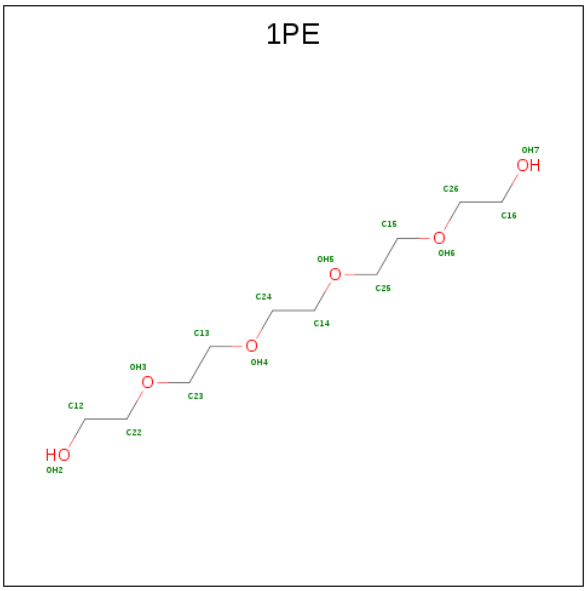
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	P	0	0
			84	27	31	9	15	2		
2	B	1	Total	C	H	N	O	P	0	0
			84	27	31	9	15	2		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	O	S		0	0
			5	4	1			
3	A	1	Total	O	S		0	0
			5	4	1			
3	A	1	Total	O	S		0	0
			5	4	1			
3	A	1	Total	O	S		0	0
			5	4	1			
3	B	1	Total	O	S		0	0
			5	4	1			
3	B	1	Total	O	S		0	0
			5	4	1			
3	B	1	Total	O	S		0	0
			5	4	1			
3	B	1	Total	O	S		0	0
			5	4	1			

- Molecule 4 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			38	10	22	6		

- Molecule 5 is water.

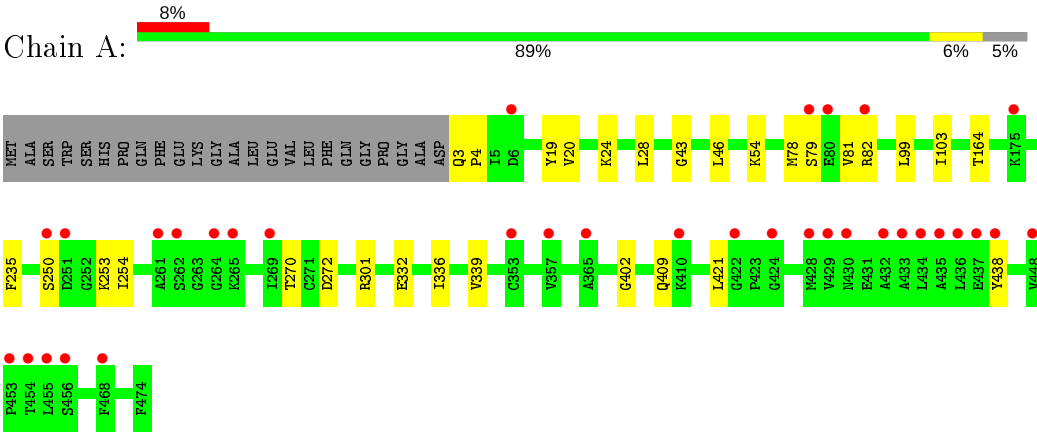
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	226	Total	O	0	0
			226	226		
5	B	185	Total	O	0	0
			185	185		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

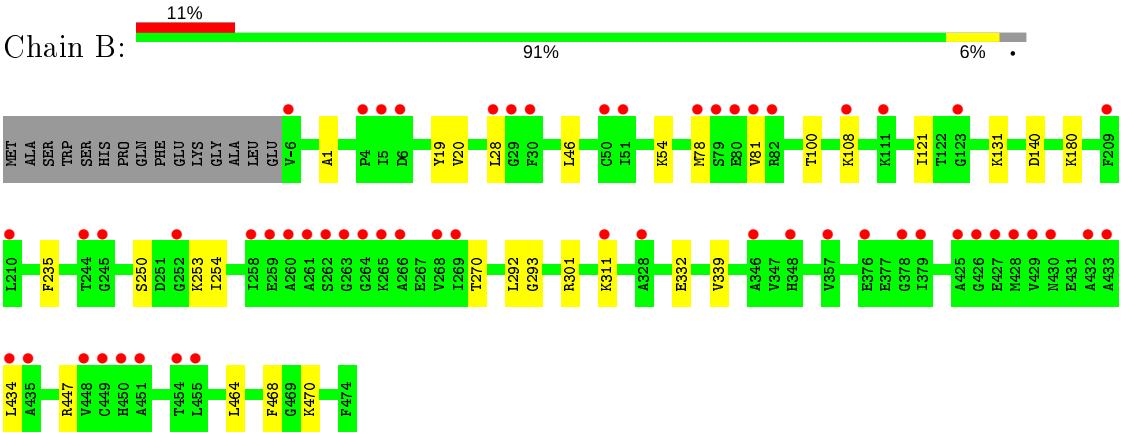
- Molecule 1: Dihydrolipoyl dehydrogenase, mitochondrial

Chain A:



- Molecule 1: Dihydrolipoyl dehydrogenase, mitochondrial

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	118.92Å 169.00Å 60.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.60 – 1.82 48.63 – 1.82	Depositor EDS
% Data completeness (in resolution range)	98.2 (45.60-1.82) 98.4 (48.63-1.82)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.04 (at 1.82Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.191 , 0.210 0.191 , 0.210	Depositor DCC
R_{free} test set	2097 reflections (1.94%)	wwPDB-VP
Wilson B-factor (Å^2)	28.5	Xtriage
Anisotropy	0.736	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 41.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	15098	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.02% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, FAD, 1PE

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	0.33	0/3644	0.55	0/4918
1	B	0.32	0/3683	0.54	0/4973
All	All	0.32	0/7327	0.54	0/9891

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

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	3555	3618	3614	17	0
1	B	3604	3664	3671	20	0
2	A	53	31	31	1	0
2	B	53	31	31	0	0
3	A	20	0	0	0	0
3	B	20	0	0	0	0
4	A	16	22	22	6	0
5	A	226	0	0	1	0
5	B	185	0	0	1	0
All	All	7732	7366	7369	35	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 (35) 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:A:81:VAL:HG22	1:B:78:MET:HG2	1.80	0.64
1:B:180:LYS:HE3	1:B:270:THR:O	1.99	0.61
1:B:464:LEU:HD12	1:B:468:PHE:HD2	1.66	0.60
1:A:164:THR:HB	1:A:254:ILE:HD11	1.84	0.59
1:A:180:LYS:HE3	1:A:270:THR:O	2.04	0.57
1:B:1:ALA:O	1:B:131:LYS:NZ	2.35	0.56
1:B:293:GLY:O	1:B:311:LYS:NZ	2.26	0.54
1:B:464:LEU:HD12	1:B:468:PHE:CD2	2.44	0.53
1:A:78:MET:HG2	1:B:81:VAL:HG22	1.91	0.52
1:B:254:ILE:N	1:B:254:ILE:HD12	2.25	0.52
1:B:253:LYS:C	1:B:254:ILE:HD12	2.30	0.52
1:A:28:LEU:HD12	1:A:339:VAL:HG12	1.93	0.51
4:A:506:1PE:H142	1:B:464:LEU:HD11	1.92	0.51
4:A:506:1PE:H262	1:B:447:ARG:HA	1.93	0.50
1:A:46[A]:LEU:HD11	1:A:99:LEU:HB2	1.94	0.49
1:A:253:LYS:NZ	1:A:272:ASP:OD1	2.46	0.49
1:A:20:VAL:HG11	1:A:332:GLU:HG3	1.96	0.48
1:A:24:LYS:HZ3	4:A:506:1PE:H142	1.81	0.46
1:B:434:LEU:O	1:B:434:LEU:HD23	2.16	0.46
1:A:3:GLN:N	1:A:4:PRO:HD2	2.31	0.46
1:B:46[A]:LEU:HD21	1:B:100:THR:HA	1.98	0.45
1:B:20:VAL:HG11	1:B:332:GLU:HG3	1.99	0.45
1:A:24:LYS:NZ	4:A:506:1PE:OH4	2.46	0.45
1:B:28:LEU:HD12	1:B:339:VAL:HG12	1.99	0.44
1:A:402:GLY:HA3	1:A:421:LEU:O	2.17	0.44
1:B:46[A]:LEU:CD2	1:B:100:THR:HG22	2.47	0.44
1:A:43:GLY:HA2	2:A:501:FAD:O3B	2.19	0.43
1:B:46[A]:LEU:HD21	1:B:100:THR:CA	2.50	0.42
1:A:24:LYS:NZ	4:A:506:1PE:OH3	2.52	0.42
1:B:108:LYS:NZ	5:B:608:HOH:O	2.52	0.42
1:A:336:ILE:HG21	4:A:506:1PE:H252	2.01	0.42
1:A:164:THR:CB	1:A:254:ILE:HD11	2.51	0.40
5:A:607:HOH:O	1:B:46[B]:LEU:HD11	2.20	0.40
1:A:46[B]:LEU:HD22	1:A:103:ILE:HD12	2.03	0.40
1:B:121:ILE:HG21	1:B:292:LEU:HD11	2.01	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	480/496 (97%)	471 (98%)	9 (2%)	0	100	100
1	B	486/496 (98%)	477 (98%)	9 (2%)	0	100	100
All	All	966/992 (97%)	948 (98%)	18 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	382/390 (98%)	373 (98%)	9 (2%)	49	35
1	B	385/390 (99%)	378 (98%)	7 (2%)	59	48
All	All	767/780 (98%)	751 (98%)	16 (2%)	53	41

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	TYR
1	A	54	LYS
1	A	79	SER
1	A	82	ARG
1	A	235	PHE
1	A	250	SER
1	A	301	ARG
1	A	409	GLN

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Mol	Chain	Res	Type
1	A	438	TYR
1	B	19	TYR
1	B	54	LYS
1	B	140	ASP
1	B	235	PHE
1	B	250	SER
1	B	301	ARG
1	B	470	LYS

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

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

11 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	SO4	A	502	-	4,4,4	0.14	0	6,6,6	0.06	0
3	SO4	B	503	-	4,4,4	0.15	0	6,6,6	0.24	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	FAD	A	501	-	51,58,58	1.22	4 (7%)	60,89,89	2.19	7 (11%)
2	FAD	B	501	-	51,58,58	1.30	5 (9%)	60,89,89	2.17	7 (11%)
4	1PE	A	506	-	15,15,15	0.56	0	14,14,14	0.40	0
3	SO4	B	502	-	4,4,4	0.12	0	6,6,6	0.07	0
3	SO4	A	504	-	4,4,4	0.13	0	6,6,6	0.13	0
3	SO4	A	503	-	4,4,4	0.23	0	6,6,6	0.10	0
3	SO4	B	505	-	4,4,4	0.16	0	6,6,6	0.17	0
3	SO4	A	505	-	4,4,4	0.12	0	6,6,6	0.10	0
3	SO4	B	504	-	4,4,4	0.14	0	6,6,6	0.10	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
4	1PE	A	506	-	-	8/13/13/13	-
2	FAD	A	501	-	-	2/30/50/50	0/6/6/6
2	FAD	B	501	-	-	2/30/50/50	0/6/6/6

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	FAD	C4X-C10	5.61	1.44	1.38
2	A	501	FAD	C4X-C10	5.29	1.44	1.38
2	B	501	FAD	C4-N3	3.89	1.39	1.33
2	A	501	FAD	C4-N3	3.14	1.38	1.33
2	B	501	FAD	C4-C4X	2.54	1.45	1.41
2	A	501	FAD	C9A-N10	2.50	1.41	1.38
2	B	501	FAD	C9A-N10	2.38	1.41	1.38
2	A	501	FAD	C4-C4X	2.23	1.45	1.41
2	B	501	FAD	C5X-N5	2.06	1.38	1.35

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	501	FAD	C4-N3-C2	12.59	125.77	115.14
2	B	501	FAD	C4-N3-C2	12.30	125.52	115.14
2	B	501	FAD	C4X-C4-N3	-7.01	113.85	123.43
2	A	501	FAD	C4X-C4-N3	-6.67	114.31	123.43
2	A	501	FAD	C10-C4X-N5	4.92	124.66	121.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	501	FAD	C10-C4X-N5	4.48	124.36	121.26
2	A	501	FAD	C4-C4X-C10	-3.96	117.33	119.95
2	B	501	FAD	C4-C4X-C10	-3.74	117.48	119.95
2	A	501	FAD	C4X-C10-N10	-3.60	116.61	120.30
2	B	501	FAD	C1'-N10-C9A	3.56	121.09	118.29
2	B	501	FAD	C4X-C10-N10	-3.45	116.76	120.30
2	A	501	FAD	C1'-N10-C9A	3.30	120.89	118.29
2	B	501	FAD	C5A-C6A-N6A	2.30	123.85	120.35
2	A	501	FAD	C5A-C6A-N6A	2.30	123.84	120.35

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	FAD	PA-O3P-P-O5'
2	B	501	FAD	PA-O3P-P-O5'
4	A	506	1PE	OH6-C15-C25-OH5
4	A	506	1PE	OH7-C16-C26-OH6
4	A	506	1PE	OH4-C13-C23-OH3
2	B	501	FAD	O4B-C4B-C5B-O5B
4	A	506	1PE	C15-C25-OH5-C14
4	A	506	1PE	C16-C26-OH6-C15
4	A	506	1PE	OH2-C12-C22-OH3
2	A	501	FAD	O4B-C4B-C5B-O5B
4	A	506	1PE	OH5-C14-C24-OH4
4	A	506	1PE	C24-C14-OH5-C25

There are no ring outliers.

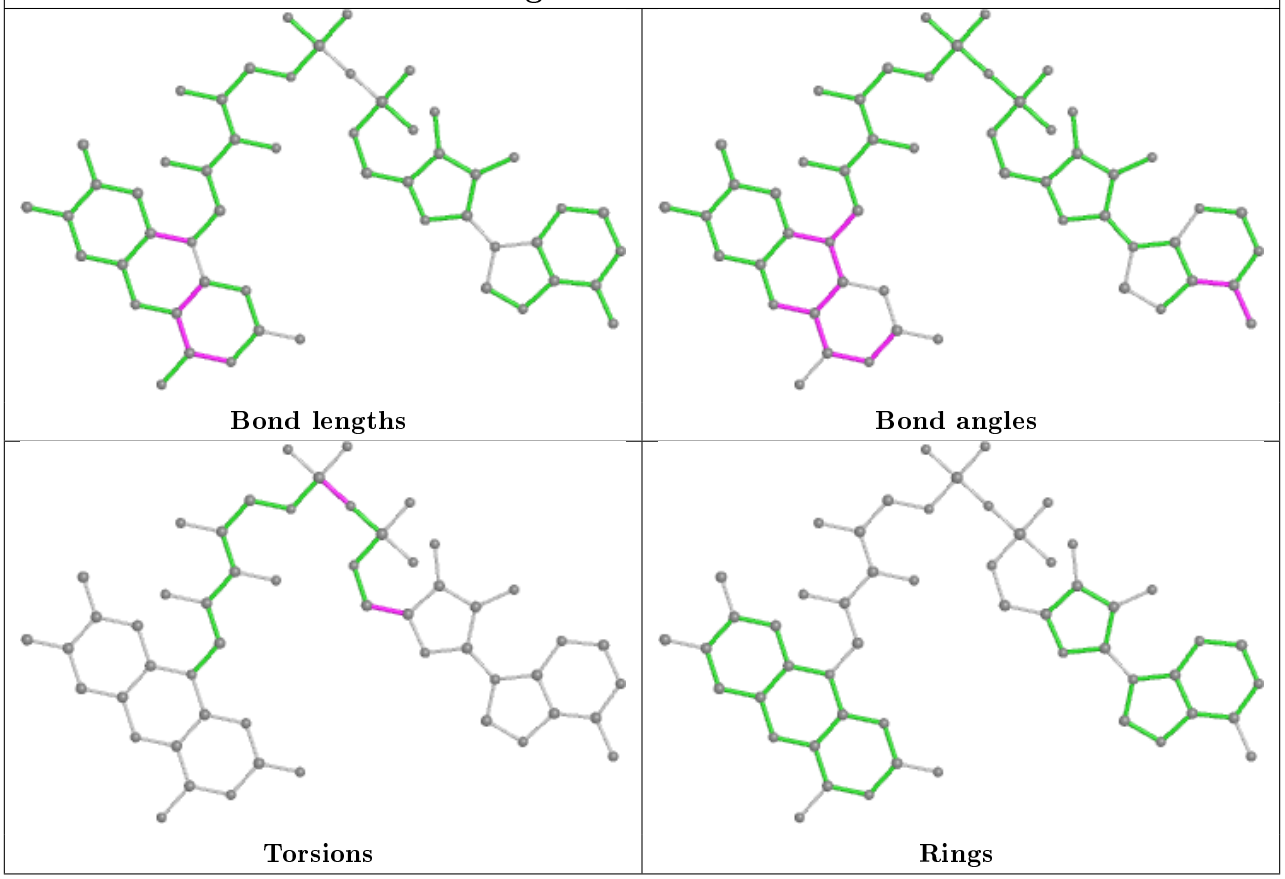
2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	FAD	1	0
4	A	506	1PE	6	0

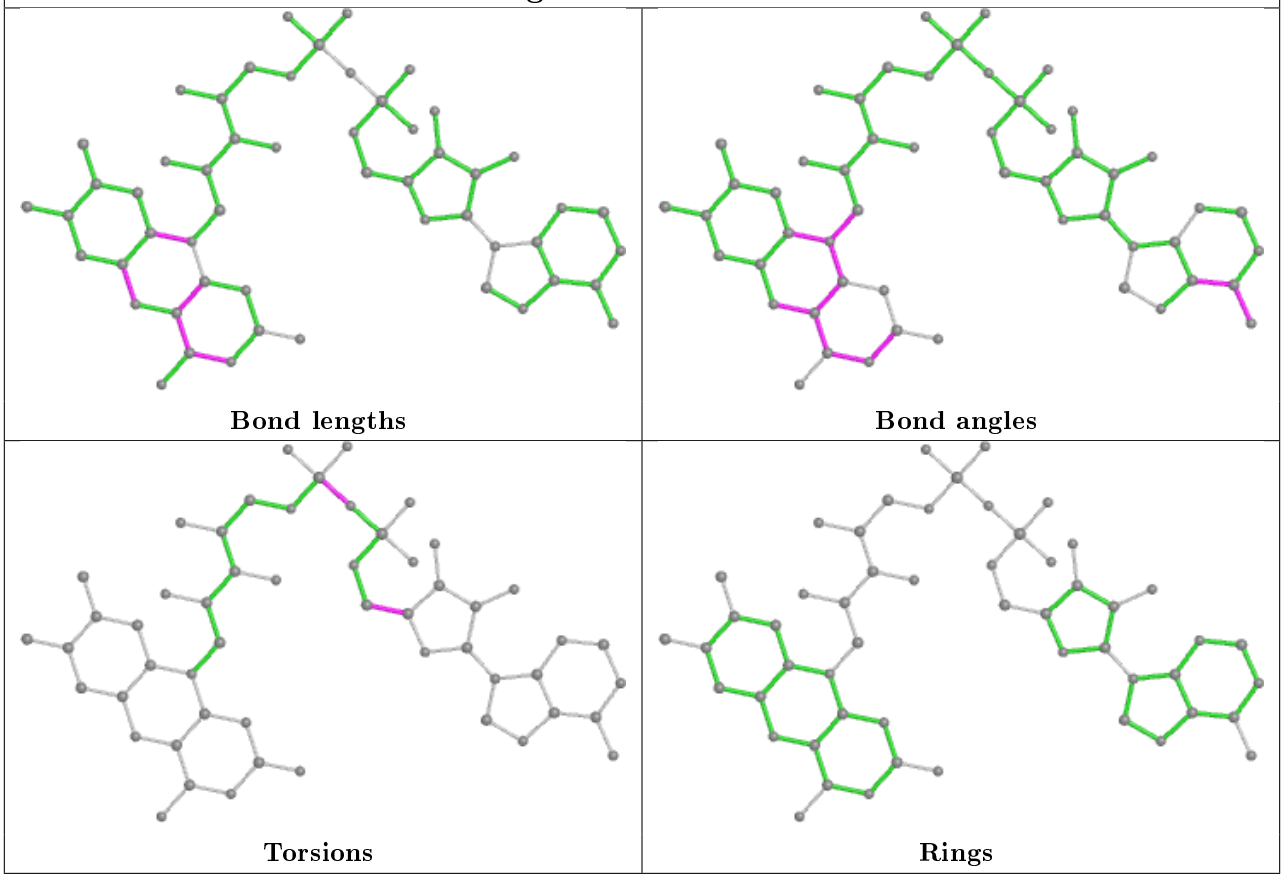
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 FAD A 501



Ligand FAD B 501



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	472/496 (95%)	0.38	38 (8%) 12 9	24, 38, 62, 110	0
1	B	481/496 (96%)	0.49	57 (11%) 4 3	27, 44, 68, 99	0
All	All	953/992 (96%)	0.44	95 (9%) 7 5	24, 41, 66, 110	0

All (95) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	261	ALA	5.2
1	B	264	GLY	5.1
1	A	265	LYS	4.8
1	A	262	SER	4.7
1	B	266	ALA	4.7
1	B	79	SER	4.6
1	A	79	SER	4.6
1	B	449	CYS	4.0
1	A	250	SER	3.9
1	A	261	ALA	3.6
1	B	265	LYS	3.6
1	B	262	SER	3.5
1	B	252	GLY	3.5
1	A	468	PHE	3.3
1	A	454	THR	3.3
1	A	428	MET	3.3
1	B	6	ASP	3.3
1	B	434	LEU	3.2
1	B	80	GLU	3.2
1	A	455	LEU	3.2
1	B	451	ALA	3.2
1	A	451	ALA	3.2
1	A	251	ASP	3.1
1	B	-6	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	379	ILE	3.0
1	A	80	GLU	3.0
1	A	433	ALA	3.0
1	B	268	VAL	2.9
1	B	81	VAL	2.9
1	B	269	ILE	2.8
1	B	448	VAL	2.8
1	B	263	GLY	2.8
1	B	28	LEU	2.7
1	A	82	ARG	2.7
1	B	82	ARG	2.7
1	B	435	ALA	2.6
1	B	346	ALA	2.6
1	A	353	CYS	2.6
1	B	428	MET	2.6
1	A	434	LEU	2.6
1	A	432	ALA	2.5
1	A	449	CYS	2.5
1	B	328	ALA	2.5
1	B	29	GLY	2.5
1	A	410	LYS	2.5
1	B	433	ALA	2.5
1	A	365	ALA	2.5
1	A	264	GLY	2.5
1	B	5	ILE	2.4
1	B	348[A]	HIS	2.4
1	B	210	LEU	2.4
1	A	456	SER	2.4
1	B	429	VAL	2.4
1	B	108	LYS	2.4
1	A	437[A]	GLU	2.4
1	B	454	THR	2.4
1	A	422	GLY	2.4
1	A	429	VAL	2.4
1	A	209	PHE	2.3
1	B	259	GLU	2.3
1	A	436	LEU	2.3
1	B	450	HIS	2.3
1	B	209	PHE	2.3
1	B	260	ALA	2.3
1	B	357	VAL	2.3
1	A	453	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	4	PRO	2.2
1	B	426	GLY	2.2
1	A	435	ALA	2.2
1	B	78	MET	2.2
1	A	357	VAL	2.2
1	B	378	GLY	2.2
1	A	430	ASN	2.2
1	A	6	ASP	2.2
1	B	245	GLY	2.2
1	B	432	ALA	2.2
1	A	448	VAL	2.2
1	B	376	GLU	2.1
1	B	30	PHE	2.1
1	B	123	GLY	2.1
1	A	269	ILE	2.1
1	B	311	LYS	2.1
1	A	438	TYR	2.1
1	B	51	ILE	2.1
1	A	450	HIS	2.1
1	B	455	LEU	2.1
1	A	424	GLY	2.1
1	B	244	THR	2.1
1	B	427	GLU	2.0
1	A	175	LYS	2.0
1	B	425	ALA	2.0
1	B	258	ILE	2.0
1	B	430	ASN	2.0
1	B	111	LYS	2.0
1	B	50[A]	CYS	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 carbohydrates in this entry.

6.4 Ligands

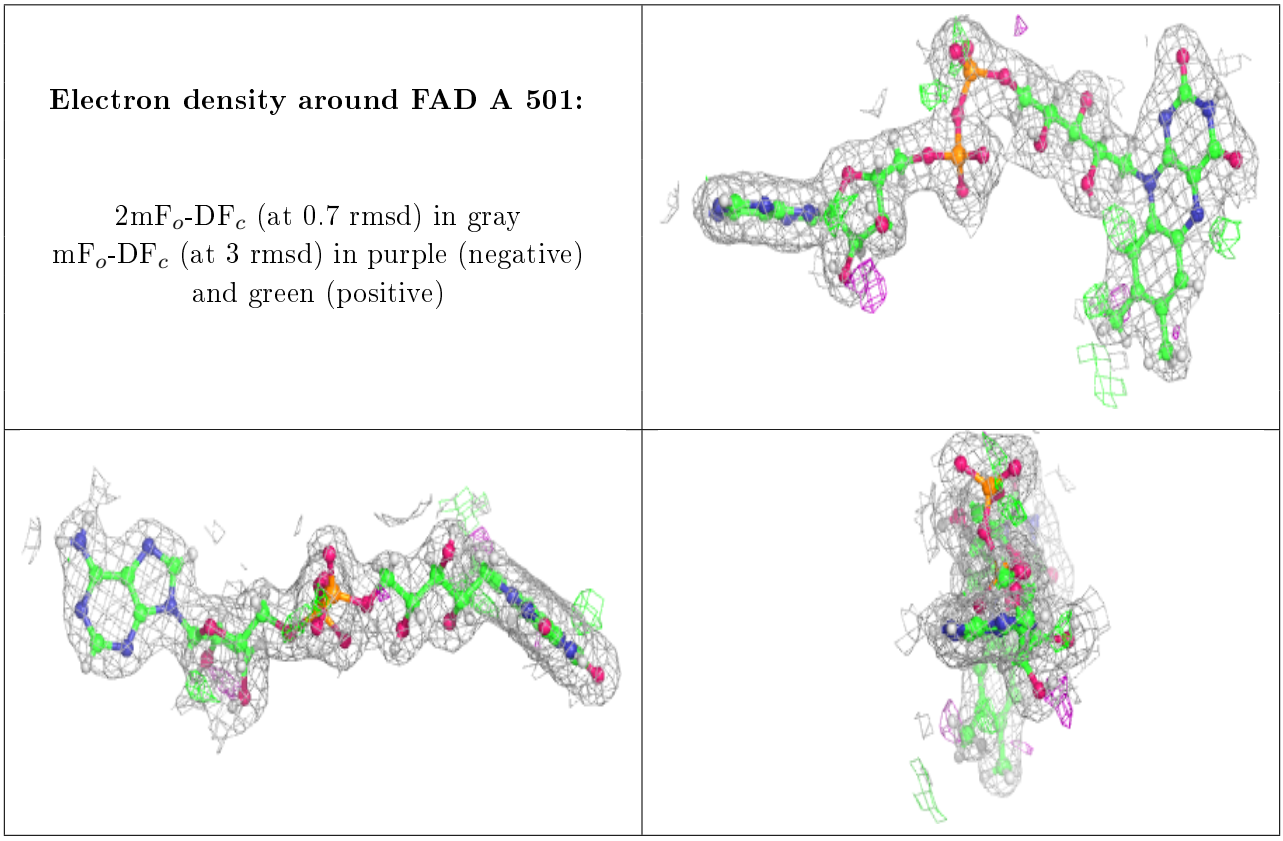
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	1PE	A	506	16/16	0.81	0.17	53,66,80,80	0
3	SO4	B	504	5/5	0.87	0.21	100,100,100,100	0
3	SO4	B	505	5/5	0.92	0.24	72,72,72,72	0
3	SO4	B	503	5/5	0.93	0.14	70,70,70,70	0
3	SO4	A	504	5/5	0.94	0.17	96,96,96,96	0
3	SO4	A	505	5/5	0.95	0.10	73,73,73,73	0
3	SO4	A	503	5/5	0.95	0.07	57,57,57,58	0
2	FAD	A	501	53/53	0.96	0.12	24,28,35,36	0
3	SO4	B	502	5/5	0.97	0.07	66,66,67,67	0
2	FAD	B	501	53/53	0.97	0.11	24,30,36,37	0
3	SO4	A	502	5/5	0.97	0.08	58,58,59,59	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.

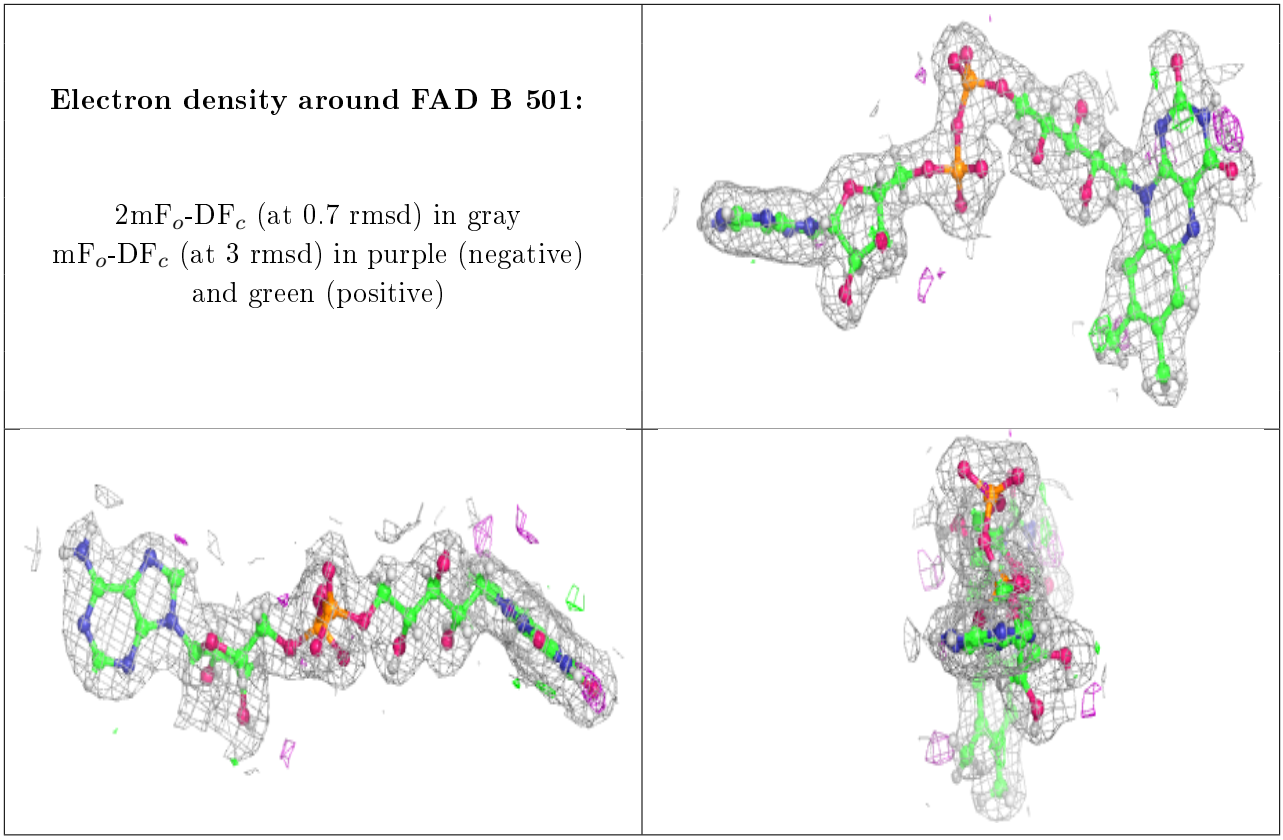
Electron density around FAD A 501:

$2mF_o$-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 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

There are no such residues in this entry.