Full wwPDB X-ray Structure Validation Report ⓘ

Nov 23, 2023 – 02:36 AM JST

PDB ID	:	7Y0A
Title	:	Crystal structure of human short-chain acyl-CoA dehydrogenase
Authors	:	Huang, Y.; Xu, Y.; Li, J.
Deposited on	:	2022-06-04
Resolution	:	2.32 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

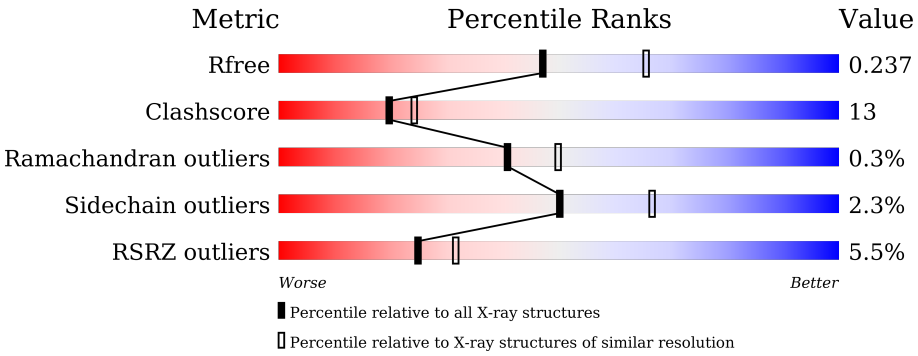
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.32 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	5974 (2.34-2.30)
Clashscore	141614	6604 (2.34-2.30)
Ramachandran outliers	138981	6523 (2.34-2.30)
Sidechain outliers	138945	6523 (2.34-2.30)
RSRZ outliers	127900	5855 (2.34-2.30)

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	398	5% 71% 25%
1	B	398	5% 73% 22%
1	C	398	5% 72% 23%
1	D	398	7% 67% 28%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 12081 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 Short-chain specific acyl-CoA dehydrogenase, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	385	Total	C	N	O	S	0	0	0
			2879	1825	493	542	19			
1	B	383	Total	C	N	O	S	0	0	0
			2861	1812	491	538	20			
1	C	387	Total	C	N	O	S	0	2	0
			2900	1840	499	541	20			
1	D	385	Total	C	N	O	S	0	0	0
			2884	1827	492	545	20			

There are 40 discrepancies between the modelled and reference sequences:

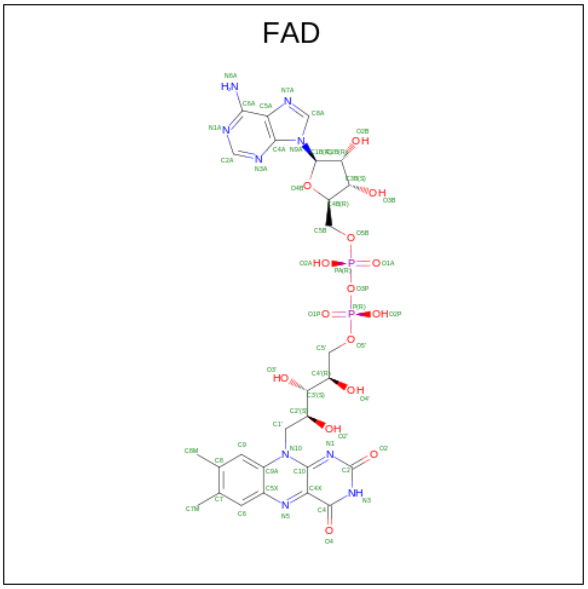
Chain	Residue	Modelled	Actual	Comment	Reference
A	23	MET	-	initiating methionine	UNP P16219
A	24	GLY	-	expression tag	UNP P16219
A	413	LEU	-	expression tag	UNP P16219
A	414	GLU	-	expression tag	UNP P16219
A	415	HIS	-	expression tag	UNP P16219
A	416	HIS	-	expression tag	UNP P16219
A	417	HIS	-	expression tag	UNP P16219
A	418	HIS	-	expression tag	UNP P16219
A	419	HIS	-	expression tag	UNP P16219
A	420	HIS	-	expression tag	UNP P16219
B	23	MET	-	initiating methionine	UNP P16219
B	24	GLY	-	expression tag	UNP P16219
B	413	LEU	-	expression tag	UNP P16219
B	414	GLU	-	expression tag	UNP P16219
B	415	HIS	-	expression tag	UNP P16219
B	416	HIS	-	expression tag	UNP P16219
B	417	HIS	-	expression tag	UNP P16219
B	418	HIS	-	expression tag	UNP P16219
B	419	HIS	-	expression tag	UNP P16219
B	420	HIS	-	expression tag	UNP P16219
C	23	MET	-	initiating methionine	UNP P16219

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	24	GLY	-	expression tag	UNP P16219
C	413	LEU	-	expression tag	UNP P16219
C	414	GLU	-	expression tag	UNP P16219
C	415	HIS	-	expression tag	UNP P16219
C	416	HIS	-	expression tag	UNP P16219
C	417	HIS	-	expression tag	UNP P16219
C	418	HIS	-	expression tag	UNP P16219
C	419	HIS	-	expression tag	UNP P16219
C	420	HIS	-	expression tag	UNP P16219
D	23	MET	-	initiating methionine	UNP P16219
D	24	GLY	-	expression tag	UNP P16219
D	413	LEU	-	expression tag	UNP P16219
D	414	GLU	-	expression tag	UNP P16219
D	415	HIS	-	expression tag	UNP P16219
D	416	HIS	-	expression tag	UNP P16219
D	417	HIS	-	expression tag	UNP P16219
D	418	HIS	-	expression tag	UNP P16219
D	419	HIS	-	expression tag	UNP P16219
D	420	HIS	-	expression tag	UNP P16219

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



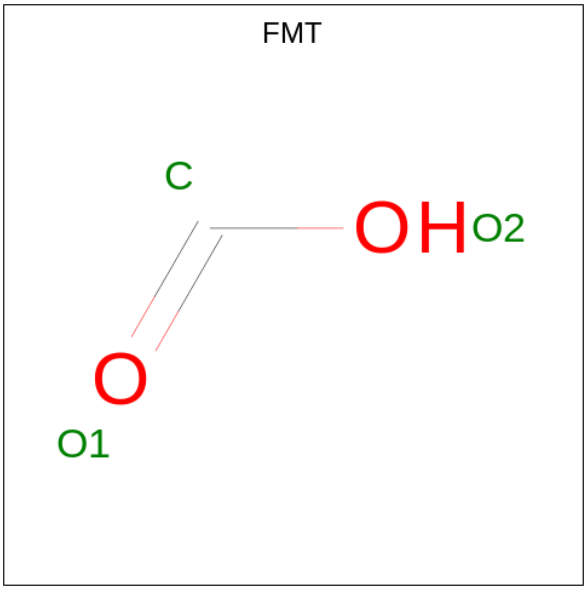
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

Continued on next page...

Continued from previous page...

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

- Molecule 3 is FORMIC ACID (three-letter code: FMT) (formula: CH_2O_2).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 3 1 2	0	0
3	B	1	Total C O 3 1 2	0	0
3	C	1	Total C O 3 1 2	0	0
3	D	1	Total C O 3 1 2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	98	Total O 98 98	0	0
4	B	43	Total O 43 43	0	0

Continued on next page...

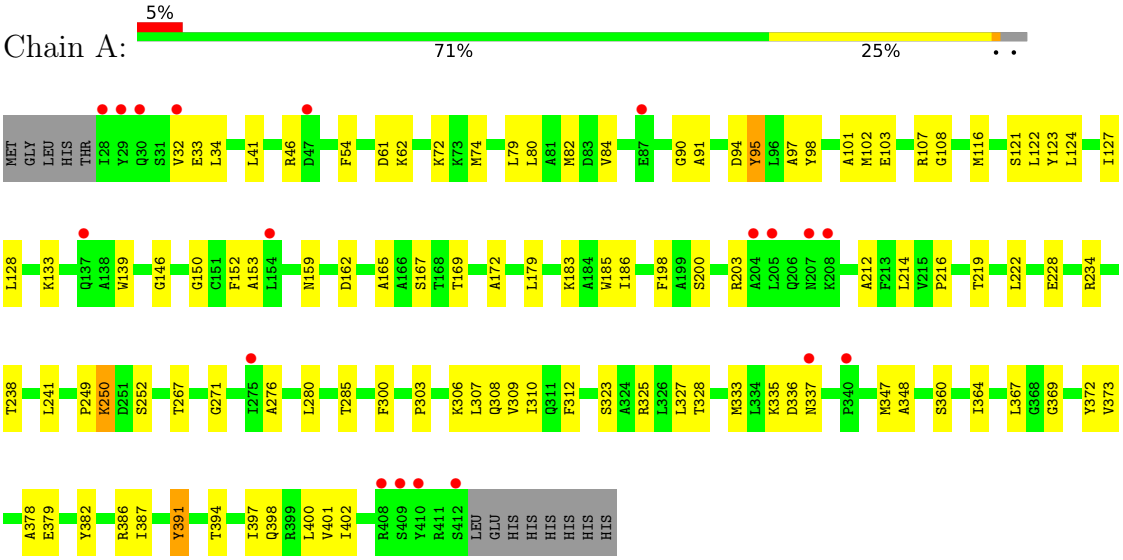
Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	105	Total O 105 105	0	0
4	D	87	Total O 87 87	0	0

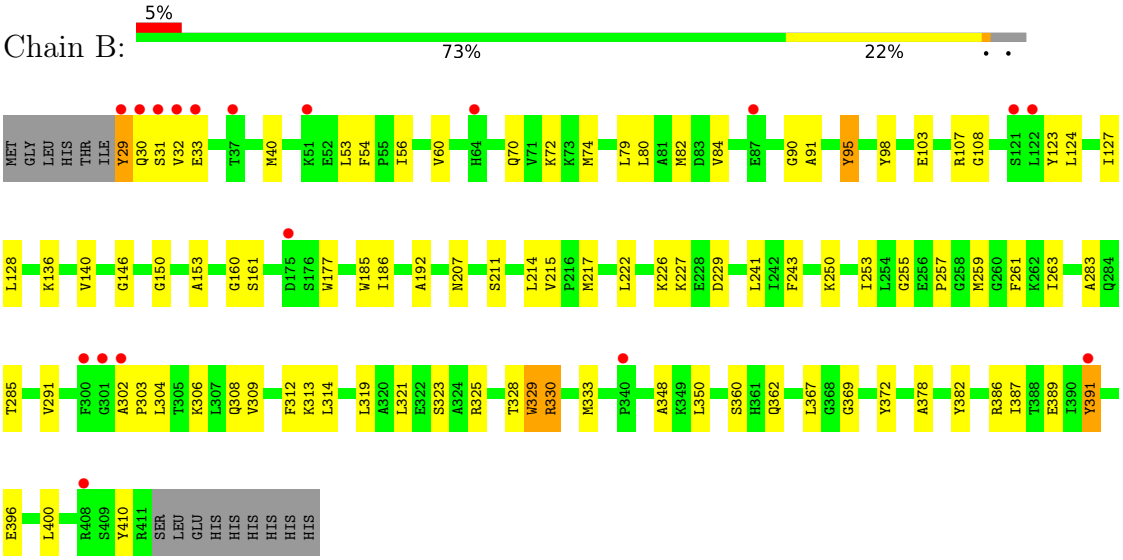
3 Residue-property plots (i)

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: Short-chain specific acyl-CoA dehydrogenase, mitochondrial

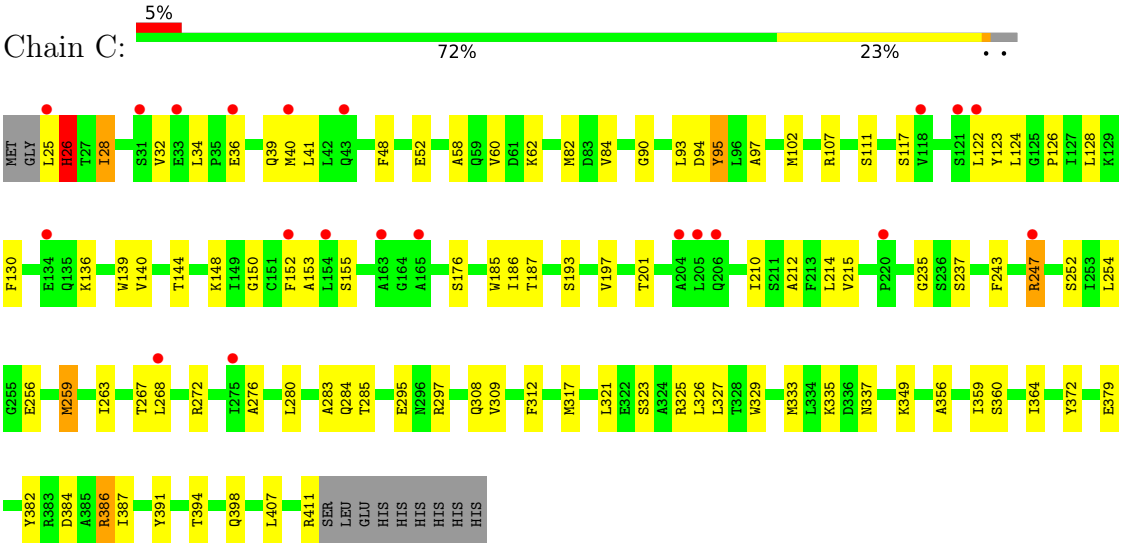


• Molecule 1: Short-chain specific acyl-CoA dehydrogenase, mitochondrial



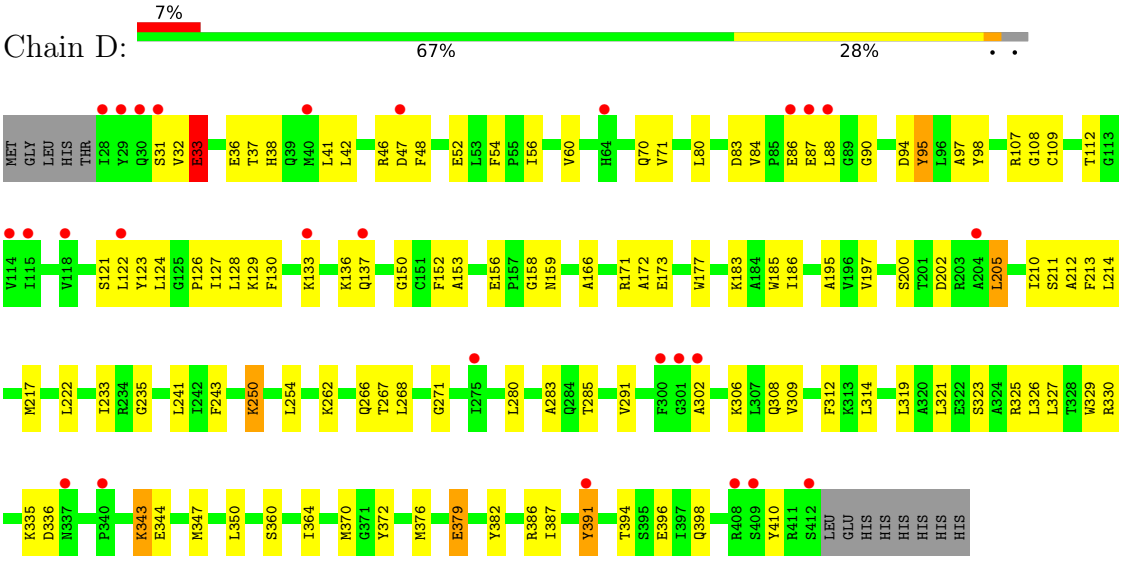
• Molecule 1: Short-chain specific acyl-CoA dehydrogenase, mitochondrial

Chain C:



• Molecule 1: Short-chain specific acyl-CoA dehydrogenase, mitochondrial

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	78.89Å 138.49Å 150.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.49 – 2.32 28.49 – 2.32	Depositor EDS
% Data completeness (in resolution range)	99.7 (28.49-2.32) 99.7 (28.49-2.32)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.22 (at 2.31Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.195 , 0.239 0.195 , 0.237	Depositor DCC
R_{free} test set	2011 reflections (2.79%)	wwPDB-VP
Wilson B-factor (Å^2)	23.0	Xtriage
Anisotropy	0.889	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 33.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	12081	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.95% 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: FMT, 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	0.47	0/2930	0.60	0/3963
1	B	0.74	4/2912 (0.1%)	0.67	1/3938 (0.0%)
1	C	1.03	7/2965 (0.2%)	0.73	3/4011 (0.1%)
1	D	0.91	9/2935 (0.3%)	0.67	1/3968 (0.0%)
All	All	0.82	20/11742 (0.2%)	0.67	5/15880 (0.0%)

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	295	GLU	CD-OE2	-8.56	1.16	1.25
1	D	344	GLU	CD-OE1	-8.52	1.16	1.25
1	D	344	GLU	CD-OE2	-8.31	1.16	1.25
1	C	295	GLU	CD-OE1	-8.06	1.16	1.25
1	D	156	GLU	CD-OE2	-7.62	1.17	1.25
1	C	111	SER	CB-OG	-7.12	1.32	1.42
1	D	329	TRP	CB-CG	-6.52	1.38	1.50
1	D	379	GLU	CD-OE2	-6.20	1.18	1.25
1	C	210	ILE	C-O	-5.64	1.12	1.23
1	C	386	ARG	CZ-NH2	-5.56	1.25	1.33
1	B	330	ARG	CZ-NH2	-5.53	1.25	1.33
1	D	156	GLU	CD-OE1	-5.44	1.19	1.25
1	C	337	ASN	C-O	-5.44	1.13	1.23
1	B	329	TRP	CD2-CE2	-5.30	1.34	1.41
1	D	330	ARG	CZ-NH2	-5.21	1.26	1.33
1	C	297	ARG	CZ-NH1	-5.18	1.26	1.33
1	B	329	TRP	CB-CG	-5.13	1.41	1.50
1	D	158	GLY	C-O	-5.03	1.15	1.23
1	D	330	ARG	CZ-NH1	-5.02	1.26	1.33
1	B	329	TRP	CG-CD1	-5.01	1.29	1.36

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	259	MET	CG-SD-CE	11.30	118.29	100.20
1	B	31	SER	N-CA-CB	5.66	118.99	110.50
1	D	33	GLU	OE1-CD-OE2	-5.23	117.02	123.30
1	C	26	HIS	N-CA-C	5.19	125.01	111.00
1	C	94	ASP	CB-CG-OD1	5.01	122.81	118.30

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	2879	0	2895	86	0
1	B	2861	0	2865	85	0
1	C	2900	0	2917	72	0
1	D	2884	0	2892	89	0
2	A	53	0	31	9	0
2	B	53	0	31	14	0
2	C	53	0	31	7	0
2	D	53	0	31	6	0
3	A	3	0	1	0	0
3	B	3	0	1	0	0
3	C	3	0	1	0	0
3	D	3	0	1	0	0
4	A	98	0	0	4	0
4	B	43	0	0	1	0
4	C	105	0	0	2	0
4	D	87	0	0	0	0
All	All	12081	0	11697	298	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 13.

All (298) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:262:LYS:HE3	1:D:266:GLN:NE2	1.54	1.19
1:D:262:LYS:CE	1:D:266:GLN:HE21	1.73	1.01
1:D:262:LYS:HE3	1:D:266:GLN:HE21	0.84	1.00
1:D:387:ILE:HD11	2:D:601:FAD:HM83	1.51	0.90
1:B:387:ILE:HD11	2:B:501:FAD:HM83	1.58	0.85
1:A:387:ILE:HG13	1:A:391:TYR:CD1	2.16	0.80
1:A:33:GLU:HG2	1:C:28:ILE:HB	1.61	0.80
1:A:387:ILE:HD11	2:A:601:FAD:HM83	1.63	0.79
1:A:84:VAL:HG22	1:A:128:LEU:HD11	1.68	0.75
1:A:347:MET:HG3	1:A:402:ILE:HD12	1.68	0.74
1:A:387:ILE:HG13	1:A:391:TYR:CE1	2.23	0.73
1:C:372:TYR:CZ	1:D:387:ILE:HB	2.24	0.72
1:A:303:PRO:HG2	1:A:306:LYS:HG2	1.70	0.72
1:D:370:MET:CE	1:D:376:MET:HG2	2.21	0.71
1:B:387:ILE:HG13	1:B:391:TYR:CD1	2.25	0.70
1:B:302:ALA:HB1	1:B:303:PRO:HD2	1.71	0.70
1:D:387:ILE:HG13	1:D:391:TYR:CE1	2.27	0.70
1:D:172:ALA:HB1	1:D:250:LYS:HZ1	1.58	0.69
1:D:87:GLU:HG2	1:D:88:LEU:HD12	1.75	0.68
1:B:84:VAL:HG22	1:B:128:LEU:HD11	1.76	0.68
1:C:95:TYR:CD2	1:C:335:LYS:HE3	2.28	0.68
1:A:122:LEU:HB3	1:A:152:PHE:HB2	1.74	0.68
1:A:398:GLN:O	1:A:402:ILE:HG12	1.95	0.67
1:A:387:ILE:HB	1:B:372:TYR:CZ	2.31	0.66
1:D:370:MET:HE2	1:D:376:MET:HG2	1.78	0.65
1:C:153:ALA:HA	1:C:186:ILE:HD12	1.77	0.65
1:D:387:ILE:HG13	1:D:391:TYR:CD1	2.31	0.65
1:B:302:ALA:HB1	1:B:306:LYS:HD3	1.79	0.65
1:B:302:ALA:HB1	1:B:303:PRO:CD	2.28	0.64
1:C:122:LEU:HB3	1:C:152:PHE:HB2	1.79	0.64
1:D:107:ARG:HG3	1:D:285:THR:HB	1.79	0.64
1:A:372:TYR:CZ	1:B:387:ILE:HB	2.33	0.63
1:C:36:GLU:HG2	1:C:40:MET:HE2	1.80	0.63
1:D:84:VAL:HA	1:D:128:LEU:HD11	1.80	0.63
1:D:86:GLU:HG3	1:D:90:GLY:O	1.98	0.63
1:A:308:GLN:HB3	1:D:309:VAL:HG23	1.80	0.63
1:A:327:LEU:HD11	1:C:323:SER:OG	2.00	0.61
1:C:84:VAL:HB	1:C:90:GLY:HA3	1.83	0.61
2:B:501:FAD:H61A	1:D:308:GLN:HE22	1.50	0.60
1:B:153:ALA:HA	1:B:186:ILE:HD12	1.83	0.60
1:D:387:ILE:CD1	2:D:601:FAD:HM83	2.27	0.60
1:C:185:TRP:O	2:C:502:FAD:C4X	2.50	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:364:ILE:HD11	1:D:379:GLU:HA	1.83	0.59
1:C:387:ILE:HD11	2:C:502:FAD:HM83	1.84	0.59
1:B:312:PHE:CE2	1:C:309:VAL:HG21	2.38	0.58
1:D:84:VAL:HG21	1:D:124:LEU:HD13	1.84	0.58
1:C:387:ILE:HB	1:D:372:TYR:CZ	2.39	0.58
1:B:215:VAL:HG11	1:B:243:PHE:HE1	1.69	0.58
1:B:84:VAL:HB	1:B:90:GLY:HA3	1.85	0.57
1:C:107:ARG:HG3	1:C:285:THR:HB	1.86	0.57
1:B:387:ILE:HG13	1:B:391:TYR:CE1	2.40	0.57
1:A:122:LEU:HB3	1:A:152:PHE:CB	2.35	0.56
1:A:153:ALA:HA	1:A:186:ILE:HD12	1.87	0.56
1:C:123:TYR:CG	1:C:150:GLY:HA3	2.39	0.56
1:C:309:VAL:CG1	2:D:601:FAD:H2A	2.35	0.56
1:B:107:ARG:HG3	1:B:285:THR:HB	1.87	0.56
1:B:387:ILE:CD1	2:B:501:FAD:HM83	2.32	0.55
1:A:159:ASN:HD21	1:A:162:ASP:HB3	1.70	0.55
1:B:70:GLN:O	1:B:74:MET:HE2	2.06	0.55
1:B:160:GLY:HA3	2:B:501:FAD:H5'2	1.88	0.55
1:A:309:VAL:HG21	1:D:312:PHE:CE2	2.41	0.55
1:C:82:MET:HE3	1:C:93:LEU:HD12	1.89	0.55
1:B:74:MET:HG2	1:B:79:LEU:HD12	1.88	0.55
1:A:82:MET:HE1	1:A:101:ALA:HB3	1.88	0.55
1:A:203:ARG:NH1	4:A:704:HOH:O	2.39	0.55
1:C:384:ASP:OD1	4:C:601:HOH:O	2.18	0.54
1:A:185:TRP:O	2:A:601:FAD:C4X	2.55	0.54
1:A:84:VAL:HG21	1:A:124:LEU:HD13	1.90	0.54
1:C:256:GLU:HG2	1:C:259:MET:HE2	1.90	0.54
1:C:325:ARG:HD3	1:C:329:TRP:CZ2	2.43	0.54
1:B:80:LEU:HD12	1:B:146:GLY:HA2	1.91	0.53
1:A:387:ILE:CD1	2:A:601:FAD:HM83	2.36	0.53
1:B:400:LEU:HD11	2:B:501:FAD:N6A	2.24	0.53
1:A:107:ARG:HG3	1:A:285:THR:HB	1.90	0.53
1:B:226:LYS:HZ2	1:B:227:LYS:H	1.57	0.53
1:C:185:TRP:HB3	2:C:502:FAD:C9A	2.38	0.53
1:C:407:LEU:O	1:C:411:ARG:HD2	2.09	0.53
1:D:42:LEU:HD21	1:D:46:ARG:HH11	1.73	0.53
1:C:122:LEU:HB3	1:C:152:PHE:CB	2.39	0.52
1:D:42:LEU:HD21	1:D:46:ARG:NH1	2.25	0.52
1:B:84:VAL:HG21	1:B:124:LEU:HD13	1.91	0.52
1:A:159:ASN:ND2	1:A:165:ALA:HB3	2.25	0.52
1:A:360:SER:OG	1:A:382:TYR:HA	2.08	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:34:LEU:HB2	1:C:39:GLN:HG2	1.90	0.52
1:B:226:LYS:NZ	1:B:227:LYS:H	2.07	0.52
1:B:313:LYS:HG2	1:B:362:GLN:OE1	2.10	0.52
1:B:82:MET:HA	1:B:91:ALA:HB3	1.92	0.51
1:B:309:VAL:HG21	1:C:312:PHE:CE2	2.45	0.51
1:A:46:ARG:HH11	1:A:107:ARG:CZ	2.23	0.51
1:A:372:TYR:CG	1:B:387:ILE:HD13	2.45	0.51
1:D:48:PHE:CE1	1:D:52:GLU:HG3	2.45	0.51
1:D:302:ALA:HB1	1:D:306:LYS:HG3	1.93	0.51
1:C:26:HIS:CD2	1:C:333:MET:HG2	2.45	0.51
1:D:177:TRP:CD1	1:D:250:LYS:HA	2.45	0.51
1:A:159:ASN:ND2	1:A:162:ASP:HB3	2.25	0.51
1:C:84:VAL:HG22	1:C:128:LEU:HD11	1.92	0.51
1:B:29:TYR:CE2	1:D:33:GLU:HG3	2.46	0.50
1:B:309:VAL:HG22	1:B:313:LYS:HD2	1.93	0.50
1:D:185:TRP:O	2:D:601:FAD:C4X	2.59	0.50
1:D:283:ALA:HB3	1:D:321:LEU:HD13	1.93	0.50
1:D:122:LEU:HB3	1:D:152:PHE:CG	2.47	0.50
1:D:183:LYS:HB2	1:D:241:LEU:HB2	1.92	0.50
1:B:308:GLN:HB3	1:C:308:GLN:HB2	1.94	0.50
1:C:153:ALA:HB3	1:C:197:VAL:HG22	1.94	0.49
1:A:102:MET:HA	1:A:116:MET:HE1	1.92	0.49
1:A:307:LEU:HD13	2:B:501:FAD:C5A	2.42	0.49
1:B:319:LEU:HD13	1:D:350:LEU:HD23	1.94	0.49
1:B:217:MET:HG2	1:B:222:LEU:CD2	2.41	0.49
1:A:172:ALA:HB1	4:A:703:HOH:O	2.12	0.49
1:A:300:PHE:HE2	2:B:501:FAD:H2A	1.77	0.49
1:C:41:LEU:HD22	1:C:97:ALA:HB1	1.95	0.49
1:B:207:ASN:HB2	1:B:261:PHE:CG	2.48	0.49
1:C:372:TYR:HE1	1:D:386:ARG:HB3	1.77	0.49
1:C:139:TRP:CG	1:C:214:LEU:HD13	2.48	0.49
1:B:177:TRP:CD1	1:B:250:LYS:HA	2.48	0.48
1:C:309:VAL:HG12	2:D:601:FAD:H2A	1.94	0.48
1:A:84:VAL:HB	1:A:90:GLY:HA3	1.96	0.48
1:D:84:VAL:HB	1:D:90:GLY:HA3	1.96	0.48
1:A:250:LYS:NZ	4:A:703:HOH:O	2.36	0.48
1:B:95:TYR:HA	1:B:98:TYR:HB3	1.95	0.48
1:B:192:ALA:C	1:B:217:MET:HE3	2.34	0.48
1:C:386:ARG:HB3	1:D:372:TYR:HE1	1.77	0.48
1:A:386:ARG:HB3	1:B:372:TYR:HE1	1.79	0.48
1:B:396:GLU:HB2	2:B:501:FAD:O2B	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:133:LYS:O	1:D:137:GLN:HG3	2.14	0.47
1:B:103:GLU:OE2	1:B:325:ARG:NH2	2.33	0.47
1:B:185:TRP:O	2:B:501:FAD:C4X	2.61	0.47
1:B:323:SER:HB2	1:D:323:SER:OG	2.14	0.47
1:B:54:PHE:CD2	1:B:108:GLY:HA2	2.49	0.47
1:C:214:LEU:O	1:C:252:SER:HB3	2.15	0.47
2:A:601:FAD:H2A	1:B:309:VAL:CG1	2.44	0.47
1:A:276:ALA:O	1:A:280:LEU:HG	2.15	0.47
1:B:29:TYR:CZ	1:D:33:GLU:HG3	2.49	0.47
1:B:329:TRP:HB3	1:B:333:MET:CE	2.44	0.47
1:C:84:VAL:HG21	1:C:124:LEU:HD13	1.96	0.47
1:A:34:LEU:HD23	1:A:34:LEU:HA	1.61	0.47
1:A:121:SER:HB3	1:A:271:GLY:HA2	1.95	0.47
1:A:82:MET:HE3	1:A:98:TYR:HD1	1.79	0.47
1:A:103:GLU:OE2	1:A:325:ARG:NH1	2.47	0.47
1:A:312:PHE:CZ	1:D:309:VAL:HG21	2.50	0.47
1:D:37:THR:HG23	1:D:38:HIS:ND1	2.28	0.47
1:A:122:LEU:HB3	1:A:152:PHE:CG	2.50	0.46
1:A:328:THR:HA	1:A:348:ALA:HB1	1.96	0.46
2:A:601:FAD:H51A	1:B:304:LEU:HD11	1.97	0.46
1:D:172:ALA:HB1	1:D:250:LYS:NZ	2.27	0.46
1:A:133:LYS:HD2	1:A:133:LYS:HA	1.81	0.46
1:B:217:MET:HG2	1:B:222:LEU:HD21	1.97	0.46
1:A:222:LEU:HD11	1:A:241:LEU:HG	1.97	0.46
1:D:41:LEU:CD2	1:D:97:ALA:HB1	2.45	0.46
1:B:54:PHE:CE2	1:B:108:GLY:HA2	2.49	0.46
1:C:360:SER:OG	1:C:382:TYR:HA	2.15	0.46
1:D:94:ASP:HB2	1:D:336:ASP:CG	2.36	0.46
1:A:153:ALA:O	1:A:183:LYS:HE2	2.16	0.46
1:D:48:PHE:CD1	1:D:52:GLU:HG3	2.51	0.46
1:D:222:LEU:HD13	1:D:243:PHE:CE1	2.51	0.46
1:A:32:VAL:HG22	1:C:333:MET:HB3	1.97	0.46
1:A:41:LEU:HD22	1:A:97:ALA:HB1	1.98	0.46
1:A:387:ILE:CG1	1:A:391:TYR:CE1	2.97	0.46
1:A:123:TYR:CG	1:A:150:GLY:HA3	2.51	0.46
1:C:60:VAL:HG13	1:C:235:GLY:HA3	1.98	0.46
1:A:300:PHE:CE2	2:B:501:FAD:H2A	2.51	0.45
1:C:36:GLU:HG2	1:C:40:MET:CE	2.43	0.45
1:C:394:THR:O	1:C:398:GLN:HG2	2.17	0.45
1:D:212:ALA:HB3	1:D:254:LEU:HB3	1.98	0.45
1:A:94:ASP:HB2	1:A:336:ASP:OD1	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:394:THR:O	1:A:398:GLN:HG2	2.16	0.45
1:C:48:PHE:CE1	1:C:52:GLU:HG3	2.50	0.45
2:C:502:FAD:H2'	2:C:502:FAD:C9	2.46	0.45
1:D:128:LEU:HD23	1:D:128:LEU:HA	1.77	0.45
1:A:328:THR:HA	1:A:348:ALA:CB	2.47	0.45
1:C:256:GLU:H	1:C:259:MET:HE3	1.81	0.45
1:A:169:THR:O	1:A:179:LEU:HA	2.17	0.45
1:A:367:LEU:HD22	1:A:378:ALA:HB2	1.99	0.45
1:B:386:ARG:NH1	1:B:389:GLU:HB2	2.31	0.45
1:C:276:ALA:HB2	1:C:349:LYS:HA	1.99	0.45
1:C:325:ARG:HD2	4:C:665:HOH:O	2.16	0.45
1:A:94:ASP:HB2	1:A:336:ASP:CG	2.37	0.45
1:D:129:LYS:HB3	1:D:130:PHE:CD2	2.52	0.45
1:B:127:ILE:HG12	1:B:214:LEU:HD21	1.99	0.44
1:C:155:SER:OG	2:C:502:FAD:H1'1	2.17	0.44
1:D:122:LEU:HB3	1:D:152:PHE:HB2	1.99	0.44
1:B:29:TYR:CD2	1:D:33:GLU:OE2	2.70	0.44
1:B:330:ARG:HD3	1:D:326:LEU:HD21	1.99	0.44
1:C:364:ILE:HD11	1:C:379:GLU:HA	1.99	0.44
1:D:211:SER:HB2	1:D:213:PHE:CE2	2.53	0.44
1:A:369:GLY:HA2	2:B:501:FAD:HM81	1.98	0.44
1:C:212:ALA:HB3	1:C:254:LEU:HB3	1.98	0.44
2:A:601:FAD:HM81	1:B:369:GLY:HA2	2.00	0.44
1:C:386:ARG:HA	1:C:386:ARG:HD2	1.72	0.44
1:D:71:VAL:HG13	1:D:80:LEU:HD11	1.99	0.44
1:C:95:TYR:CE2	1:C:335:LYS:HE3	2.52	0.44
1:C:140:VAL:O	1:C:144:THR:HG23	2.18	0.44
1:C:272:ARG:NE	1:C:398:GLN:HE22	2.15	0.44
1:D:83:ASP:OD2	1:D:335:LYS:NZ	2.49	0.44
1:A:216:PRO:HG2	1:A:219:THR:HB	1.99	0.44
1:B:323:SER:HB3	1:D:327:LEU:HD11	2.00	0.44
1:D:88:LEU:HD21	1:D:136:LYS:HD2	1.99	0.44
1:D:122:LEU:HB3	1:D:152:PHE:CB	2.48	0.44
1:A:153:ALA:HB1	1:A:183:LYS:HG3	1.98	0.44
1:B:329:TRP:HB3	1:B:333:MET:HE2	1.98	0.44
1:C:326:LEU:HD23	1:C:326:LEU:HA	1.83	0.44
1:C:387:ILE:CD1	2:C:502:FAD:HM83	2.46	0.44
1:C:58:ALA:HB1	1:C:62:LYS:HE3	2.00	0.43
1:D:195:ALA:HB2	1:D:217:MET:SD	2.58	0.43
1:B:29:TYR:CE2	1:D:33:GLU:CD	2.91	0.43
1:A:95:TYR:HA	1:A:98:TYR:HB3	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:130:PHE:CD2	1:C:263:ILE:HG12	2.53	0.43
1:C:187:THR:HA	1:C:237:SER:O	2.19	0.43
1:D:126:PRO:HD3	1:D:267:THR:HG23	2.00	0.43
1:B:29:TYR:CE2	1:D:33:GLU:CG	3.02	0.43
1:A:61:ASP:OD1	1:A:234:ARG:HD3	2.18	0.43
1:B:328:THR:HA	1:B:348:ALA:HB1	2.00	0.43
1:D:396:GLU:H	1:D:396:GLU:CD	2.21	0.43
1:A:400:LEU:HD11	2:A:601:FAD:N1A	2.33	0.43
1:B:30:GLN:CD	1:B:30:GLN:H	2.22	0.43
1:D:123:TYR:CG	1:D:150:GLY:HA3	2.53	0.43
1:D:394:THR:O	1:D:398:GLN:HG2	2.19	0.43
1:B:161:SER:N	2:B:501:FAD:H5'2	2.33	0.43
1:D:183:LYS:HB3	1:D:186:ILE:HD11	2.00	0.43
1:D:314:LEU:HD23	1:D:314:LEU:HA	1.83	0.43
1:A:387:ILE:HD12	1:A:387:ILE:HA	1.78	0.43
1:B:123:TYR:CG	1:B:150:GLY:HA3	2.53	0.43
1:B:410:TYR:CG	1:D:291:VAL:HG11	2.53	0.43
1:C:317:MET:HG2	1:C:359:ILE:HA	2.01	0.43
1:D:109:CYS:HB3	1:D:112:THR:HB	1.99	0.43
1:A:364:ILE:HD11	1:A:379:GLU:HA	2.01	0.43
1:B:291:VAL:HG11	1:D:410:TYR:CG	2.54	0.43
1:D:127:ILE:HG12	1:D:214:LEU:HD21	2.00	0.43
1:C:102:MET:SD	1:C:117:SER:HB2	2.59	0.42
1:D:171:ARG:NH1	1:D:173:GLU:OE2	2.49	0.42
1:C:148:LYS:HB3	1:C:193:SER:HB2	2.01	0.42
1:D:280:LEU:HD11	1:D:325:ARG:HA	2.00	0.42
1:A:310:ILE:HD11	2:B:501:FAD:H1B	2.01	0.42
1:B:283:ALA:HB3	1:B:321:LEU:HD13	2.00	0.42
1:A:333:MET:HB2	1:C:32:VAL:HG21	2.01	0.42
1:B:30:GLN:C	1:B:32:VAL:H	2.22	0.42
1:B:396:GLU:OE1	2:B:501:FAD:O2B	2.36	0.42
1:A:397:ILE:O	1:A:401:VAL:HG23	2.19	0.42
1:A:153:ALA:HA	1:A:186:ILE:CD1	2.50	0.42
1:B:56:ILE:HD12	1:B:60:VAL:HG21	2.01	0.42
1:D:268:LEU:HD23	1:D:268:LEU:HA	1.91	0.42
1:A:228:GLU:HB2	1:A:238:THR:HB	2.00	0.42
1:A:323:SER:HB2	1:C:327:LEU:HD11	2.01	0.42
2:A:601:FAD:H2A	1:B:309:VAL:HG11	2.02	0.42
1:B:386:ARG:HA	1:B:386:ARG:HD2	1.80	0.42
1:D:121:SER:HB3	1:D:271:GLY:HA2	2.02	0.42
1:C:283:ALA:HB2	1:C:356:ALA:HA	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:54:PHE:CD2	1:D:108:GLY:HA2	2.55	0.42
1:A:139:TRP:CG	1:A:214:LEU:HD13	2.55	0.41
1:B:360:SER:OG	1:B:382:TYR:HA	2.20	0.41
1:B:367:LEU:HD22	1:B:378:ALA:HB2	2.01	0.41
1:C:268:LEU:HD23	1:C:268:LEU:HA	1.88	0.41
1:A:82:MET:HA	1:A:91:ALA:HB3	2.02	0.41
1:C:126:PRO:HD3	1:C:267:THR:HG23	2.01	0.41
1:D:166:ALA:HB3	1:D:210:ILE:HD12	2.02	0.41
1:A:74:MET:HB3	1:A:79:LEU:HB2	2.01	0.41
1:A:80:LEU:HD12	1:A:146:GLY:HA2	2.02	0.41
1:A:387:ILE:HD13	1:B:372:TYR:CG	2.55	0.41
1:C:276:ALA:O	1:C:280:LEU:HG	2.20	0.41
1:C:372:TYR:CG	1:D:387:ILE:HD13	2.55	0.41
1:D:54:PHE:CE2	1:D:108:GLY:HA2	2.56	0.41
1:A:249:PRO:O	1:A:252:SER:HB2	2.20	0.41
1:A:337:ASN:ND2	4:A:714:HOH:O	2.50	0.41
1:C:136:LYS:O	1:C:140:VAL:HB	2.20	0.41
1:C:215:VAL:HG11	1:C:243:PHE:HE1	1.85	0.41
1:B:259:MET:O	1:B:263:ILE:HG13	2.20	0.41
1:D:95:TYR:HA	1:D:98:TYR:HB3	2.02	0.41
1:D:343:LYS:HD3	1:D:347:MET:CE	2.50	0.41
1:B:29:TYR:OH	1:D:33:GLU:HG3	2.19	0.41
1:B:350:LEU:HD23	1:D:319:LEU:HD13	2.02	0.41
1:D:360:SER:OG	1:D:382:TYR:HA	2.21	0.41
1:A:152:PHE:CE1	1:A:267:THR:HG21	2.56	0.41
1:A:198:PHE:CE1	1:A:212:ALA:HB2	2.56	0.41
1:B:211:SER:OG	1:B:257:PRO:HA	2.21	0.41
2:C:502:FAD:H2'	2:C:502:FAD:H9	2.01	0.41
1:D:202:ASP:HB3	1:D:205:LEU:HD22	2.02	0.41
1:D:233:ILE:HD11	2:D:601:FAD:HM73	2.02	0.41
1:A:82:MET:HE3	1:A:82:MET:HB2	1.97	0.41
1:B:222:LEU:HD11	1:B:241:LEU:HG	2.03	0.41
1:D:153:ALA:HB3	1:D:197:VAL:HG22	2.02	0.41
1:D:370:MET:HE2	1:D:376:MET:CG	2.48	0.41
1:A:54:PHE:CE1	1:A:108:GLY:HA2	2.56	0.41
1:D:60:VAL:HG13	1:D:235:GLY:HA3	2.03	0.41
1:A:373:VAL:HG11	1:B:185:TRP:HZ3	1.86	0.41
1:B:53:LEU:O	1:B:56:ILE:HG13	2.21	0.41
1:B:314:LEU:HD23	1:B:314:LEU:HA	1.92	0.40
1:C:58:ALA:O	1:C:62:LYS:HG3	2.21	0.40
1:A:62:LYS:HE3	1:B:229:ASP:OD2	2.20	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:303:PRO:HD2	1:B:306:LYS:HD3	2.04	0.40
1:B:72:LYS:HE3	4:B:621:HOH:O	2.21	0.40
1:A:123:TYR:O	1:A:127:ILE:HG13	2.22	0.40
1:B:253:ILE:HG12	1:B:255:GLY:O	2.22	0.40
1:C:124:LEU:HD22	1:C:140:VAL:HG13	2.03	0.40
1:D:56:ILE:HD13	1:D:70:GLN:CD	2.42	0.40
1:A:185:TRP:HB3	2:A:601:FAD:C9A	2.52	0.40
1:B:136:LYS:O	1:B:140:VAL:HB	2.21	0.40
1:C:284:GLN:OE1	1:C:321:LEU:HD21	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	383/398 (96%)	367 (96%)	16 (4%)	0	100	100
1	B	381/398 (96%)	361 (95%)	19 (5%)	1 (0%)	41	50
1	C	387/398 (97%)	376 (97%)	10 (3%)	1 (0%)	41	50
1	D	383/398 (96%)	367 (96%)	13 (3%)	3 (1%)	19	23
All	All	1534/1592 (96%)	1471 (96%)	58 (4%)	5 (0%)	41	50

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	33	GLU
1	C	26	HIS
1	D	33	GLU
1	D	31	SER
1	D	32	VAL

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	291/309 (94%)	284 (98%)	7 (2%)	49	65
1	B	287/309 (93%)	283 (99%)	4 (1%)	67	80
1	C	293/309 (95%)	285 (97%)	8 (3%)	44	60
1	D	291/309 (94%)	282 (97%)	9 (3%)	40	55
All	All	1162/1236 (94%)	1134 (98%)	28 (2%)	50	65

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	72	LYS
1	A	95	TYR
1	A	167	SER
1	A	200	SER
1	A	250	LYS
1	A	335	LYS
1	A	391	TYR
1	B	29	TYR
1	B	40	MET
1	B	95	TYR
1	B	391	TYR
1	C	25	LEU
1	C	28	ILE
1	C	95	TYR
1	C	176	SER
1	C	201	THR
1	C	247[A]	ARG
1	C	247[B]	ARG
1	C	391	TYR
1	D	36	GLU
1	D	47	ASP
1	D	95	TYR
1	D	159	ASN
1	D	200	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	205	LEU
1	D	250	LYS
1	D	343	LYS
1	D	391	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	337	ASN
1	B	39	GLN
1	C	337	ASN
1	D	266	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry

8 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	FMT	C	501	-	2,2,2	0.55	0	1,1,1	0.22	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	FAD	D	601	-	53,58,58	2.61	30 (56%)	68,89,89	1.37	12 (17%)
3	FMT	B	502	-	2,2,2	0.64	0	1,1,1	0.21	0
3	FMT	D	602	-	2,2,2	0.64	0	1,1,1	0.23	0
2	FAD	C	502	-	53,58,58	2.65	31 (58%)	68,89,89	1.50	17 (25%)
2	FAD	B	501	-	53,58,58	0.66	0	68,89,89	0.97	5 (7%)
3	FMT	A	602	-	2,2,2	0.66	0	1,1,1	0.32	0
2	FAD	A	601	-	53,58,58	0.59	1 (1%)	68,89,89	0.69	2 (2%)

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
2	FAD	B	501	-	-	11/30/50/50	0/6/6/6
2	FAD	C	502	-	-	5/30/50/50	0/6/6/6
2	FAD	A	601	-	-	3/30/50/50	0/6/6/6
2	FAD	D	601	-	-	6/30/50/50	0/6/6/6

All (62) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	601	FAD	C5X-N5	-5.87	1.28	1.39
2	D	601	FAD	C4-N3	-5.67	1.28	1.38
2	C	502	FAD	C4-N3	-5.64	1.28	1.38
2	D	601	FAD	P-O1P	-4.93	1.33	1.50
2	C	502	FAD	P-O1P	-4.79	1.33	1.50
2	C	502	FAD	C5X-N5	-4.79	1.30	1.39
2	C	502	FAD	C4A-N3A	-4.75	1.29	1.35
2	D	601	FAD	PA-O2A	-4.43	1.34	1.55
2	D	601	FAD	PA-O1A	-4.20	1.36	1.50
2	D	601	FAD	C6-C7	-4.15	1.33	1.39
2	C	502	FAD	C9-C9A	-3.93	1.33	1.39
2	D	601	FAD	P-O2P	-3.92	1.36	1.55
2	C	502	FAD	P-O2P	-3.91	1.37	1.55
2	C	502	FAD	PA-O1A	-3.90	1.37	1.50
2	C	502	FAD	C6-C7	-3.66	1.34	1.39
2	C	502	FAD	C5A-N7A	-3.65	1.26	1.39
2	D	601	FAD	C5A-N7A	-3.58	1.26	1.39
2	C	502	FAD	C8A-N7A	-3.51	1.28	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	601	FAD	C9-C9A	-3.47	1.34	1.39
2	C	502	FAD	O4-C4	-3.46	1.17	1.23
2	C	502	FAD	C6-C5X	-3.42	1.34	1.40
2	D	601	FAD	C4A-N3A	-3.41	1.30	1.35
2	D	601	FAD	C2-N3	-3.38	1.31	1.39
2	D	601	FAD	O4B-C4B	-3.29	1.37	1.45
2	C	502	FAD	C2B-C1B	-3.28	1.48	1.53
2	C	502	FAD	C2A-N1A	-3.23	1.27	1.33
2	C	502	FAD	C9A-C5X	3.13	1.46	1.41
2	C	502	FAD	C2-N3	-3.12	1.31	1.39
2	C	502	FAD	C9-C8	-3.03	1.35	1.39
2	C	502	FAD	PA-O2A	-3.02	1.41	1.55
2	D	601	FAD	C8A-N7A	-2.98	1.29	1.34
2	D	601	FAD	PA-O5B	-2.98	1.47	1.59
2	D	601	FAD	O2-C2	-2.93	1.18	1.24
2	D	601	FAD	C6-C5X	-2.92	1.35	1.40
2	C	502	FAD	O4B-C4B	-2.85	1.38	1.45
2	C	502	FAD	C2-N1	-2.76	1.30	1.36
2	D	601	FAD	O2B-C2B	-2.58	1.36	1.43
2	C	502	FAD	O4B-C1B	-2.56	1.37	1.41
2	C	502	FAD	P-O5'	-2.52	1.49	1.59
2	D	601	FAD	O4-C4	-2.50	1.18	1.23
2	D	601	FAD	O4B-C1B	-2.49	1.37	1.41
2	D	601	FAD	P-O5'	-2.49	1.49	1.59
2	D	601	FAD	O4'-C4'	-2.48	1.38	1.43
2	D	601	FAD	O3'-C3'	-2.47	1.37	1.43
2	D	601	FAD	C2-N1	-2.42	1.31	1.36
2	C	502	FAD	C8M-C8	-2.38	1.46	1.51
2	C	502	FAD	C2B-C3B	-2.35	1.46	1.53
2	C	502	FAD	C10-N1	-2.34	1.28	1.33
2	C	502	FAD	PA-O5B	-2.31	1.49	1.59
2	D	601	FAD	C9-C8	-2.30	1.36	1.39
2	C	502	FAD	O2B-C2B	-2.30	1.37	1.43
2	D	601	FAD	C1'-N10	-2.29	1.42	1.48
2	D	601	FAD	C7M-C7	-2.27	1.46	1.51
2	D	601	FAD	C2B-C3B	-2.22	1.47	1.53
2	D	601	FAD	C9A-N10	-2.18	1.37	1.41
2	C	502	FAD	O5'-C5'	-2.18	1.36	1.44
2	C	502	FAD	C1'-N10	-2.15	1.42	1.48
2	D	601	FAD	C2B-C1B	-2.14	1.50	1.53
2	C	502	FAD	O2-C2	-2.07	1.20	1.24
2	C	502	FAD	O3'-C3'	-2.01	1.38	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	FAD	PA-O5B	-2.01	1.51	1.59
2	D	601	FAD	C2A-N3A	-2.01	1.28	1.32

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	501	FAD	O2P-P-O5'	3.93	126.02	107.75
2	C	502	FAD	N3A-C2A-N1A	-3.35	123.44	128.68
2	C	502	FAD	C1B-N9A-C4A	-3.30	120.84	126.64
2	A	601	FAD	P-O3P-PA	-3.15	122.01	132.83
2	C	502	FAD	C1'-N10-C9A	2.88	125.32	120.51
2	C	502	FAD	O4'-C4'-C3'	2.80	115.91	109.10
2	C	502	FAD	C5X-C9A-N10	2.79	120.83	117.95
2	B	501	FAD	C3B-C2B-C1B	-2.76	96.83	100.98
2	B	501	FAD	O4B-C1B-C2B	-2.74	102.93	106.93
2	D	601	FAD	C4X-C10-N1	-2.69	118.48	124.73
2	D	601	FAD	C1B-N9A-C4A	-2.67	121.96	126.64
2	C	502	FAD	C9A-N10-C10	-2.60	116.72	120.77
2	D	601	FAD	C4'-C3'-C2'	2.59	118.75	113.36
2	C	502	FAD	C4-C4X-N5	2.58	121.90	118.23
2	C	502	FAD	N3-C2-N1	2.56	124.40	119.38
2	C	502	FAD	C2A-N1A-C6A	2.48	123.00	118.75
2	C	502	FAD	O2-C2-N1	-2.45	117.77	121.83
2	D	601	FAD	C2A-N1A-C6A	2.44	122.92	118.75
2	C	502	FAD	C4-N3-C2	-2.36	121.28	125.64
2	D	601	FAD	N3-C2-N1	2.35	123.99	119.38
2	C	502	FAD	O3B-C3B-C4B	-2.34	104.28	111.05
2	D	601	FAD	C4A-C5A-N7A	-2.31	106.99	109.40
2	C	502	FAD	C4X-C4-N3	2.26	118.93	113.19
2	A	601	FAD	C5A-C6A-N6A	2.24	123.76	120.35
2	C	502	FAD	O4'-C4'-C5'	-2.23	104.90	109.92
2	D	601	FAD	O4B-C4B-C3B	2.21	109.49	105.11
2	C	502	FAD	C4X-C10-N1	-2.20	119.64	124.73
2	D	601	FAD	O2'-C2'-C1'	2.13	114.96	109.80
2	D	601	FAD	N10-C10-N1	2.13	124.48	118.35
2	B	501	FAD	P-O3P-PA	-2.07	125.71	132.83
2	D	601	FAD	O2P-P-O5'	2.05	117.27	107.75
2	C	502	FAD	C4X-C10-N10	2.04	119.47	116.48
2	B	501	FAD	C5A-C6A-N6A	2.04	123.45	120.35
2	D	601	FAD	C6-C5X-C9A	2.03	121.81	118.94
2	D	601	FAD	N3A-C2A-N1A	-2.01	125.53	128.68
2	C	502	FAD	C6-C5X-C9A	2.01	121.77	118.94

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	FAD	C5B-O5B-PA-O2A
2	B	501	FAD	C5B-O5B-PA-O1A
2	B	501	FAD	C1'-C2'-C3'-O3'
2	B	501	FAD	C1'-C2'-C3'-C4'
2	B	501	FAD	C5'-O5'-P-O1P
2	B	501	FAD	C5'-O5'-P-O2P
2	C	502	FAD	C5B-O5B-PA-O1A
2	D	601	FAD	C5B-O5B-PA-O1A
2	B	501	FAD	O2'-C2'-C3'-O3'
2	D	601	FAD	O2'-C2'-C3'-O3'
2	B	501	FAD	O2'-C2'-C3'-C4'
2	D	601	FAD	O2'-C2'-C3'-C4'
2	B	501	FAD	C5B-O5B-PA-O3P
2	C	502	FAD	C5B-O5B-PA-O3P
2	D	601	FAD	C5B-O5B-PA-O3P
2	C	502	FAD	C5B-O5B-PA-O2A
2	D	601	FAD	C5B-O5B-PA-O2A
2	D	601	FAD	C1'-C2'-C3'-O3'
2	C	502	FAD	O2'-C2'-C3'-C4'
2	C	502	FAD	O2'-C2'-C3'-O3'
2	A	601	FAD	C5B-O5B-PA-O3P
2	B	501	FAD	C5'-O5'-P-O3P
2	B	501	FAD	P-O3P-PA-O1A
2	B	501	FAD	P-O3P-PA-O2A
2	A	601	FAD	C5B-O5B-PA-O1A

There are no ring outliers.

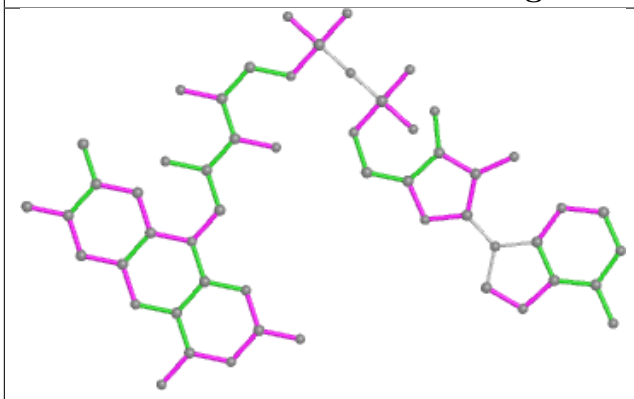
4 monomers are involved in 36 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	601	FAD	6	0
2	C	502	FAD	7	0
2	B	501	FAD	14	0
2	A	601	FAD	9	0

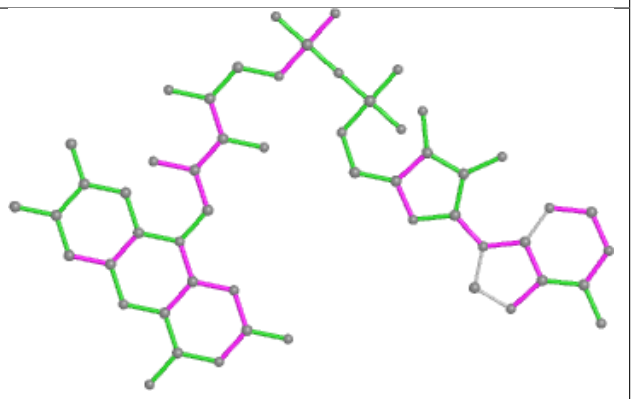
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

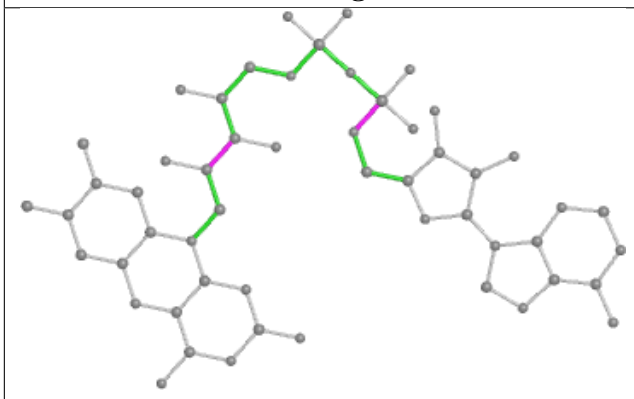
Ligand FAD D 601



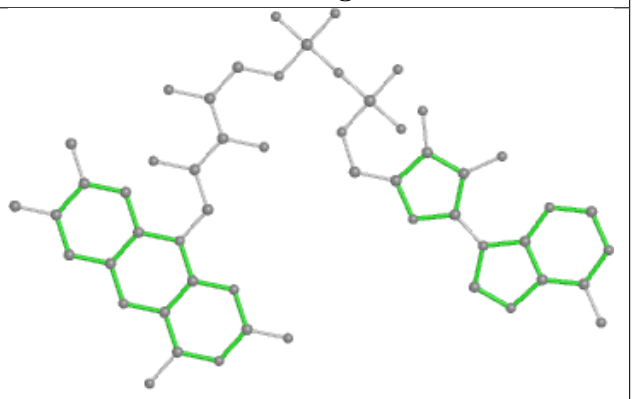
Bond lengths



Bond angles

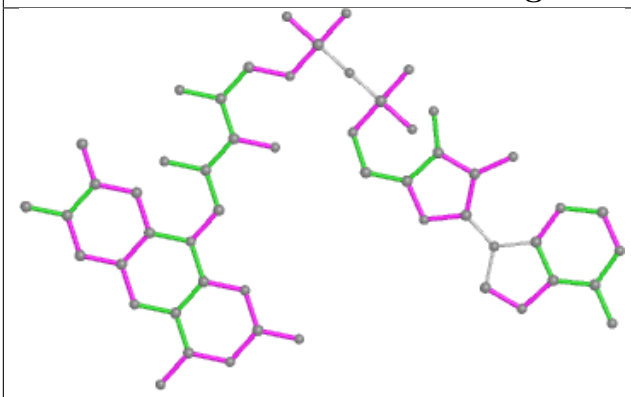


Torsions

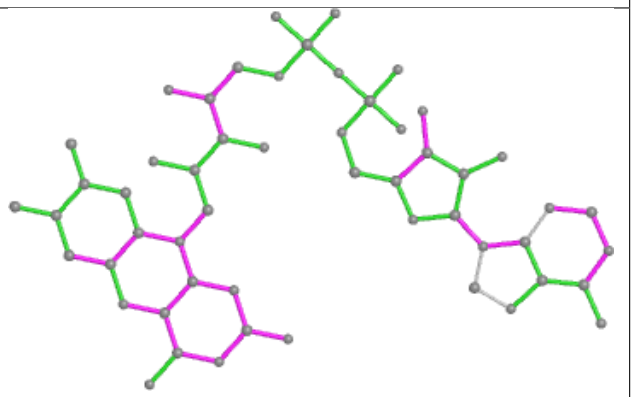


Rings

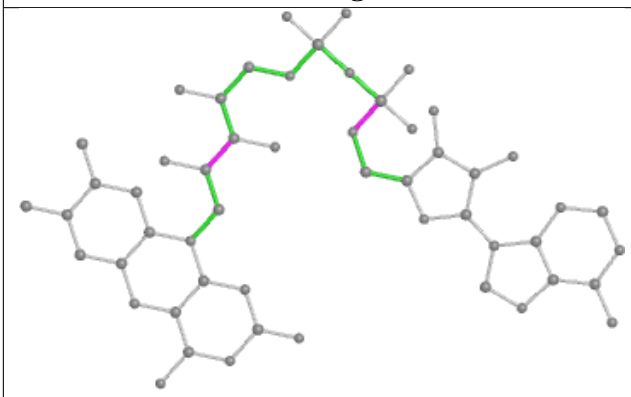
Ligand FAD C 502



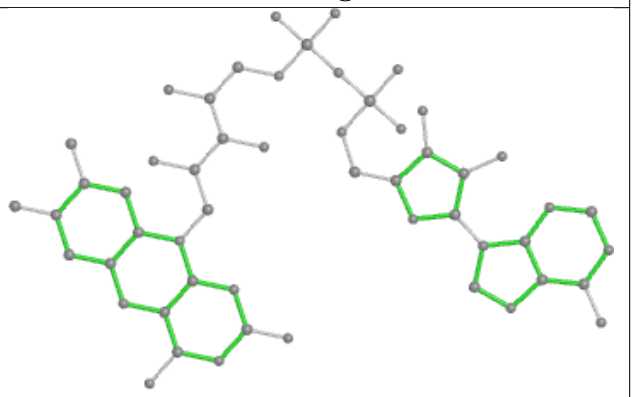
Bond lengths



Bond angles

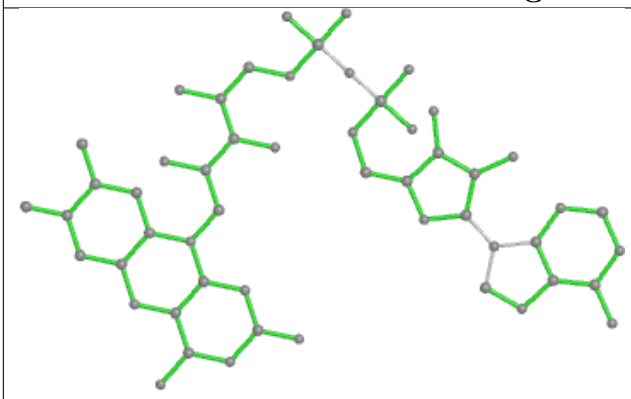


Torsions

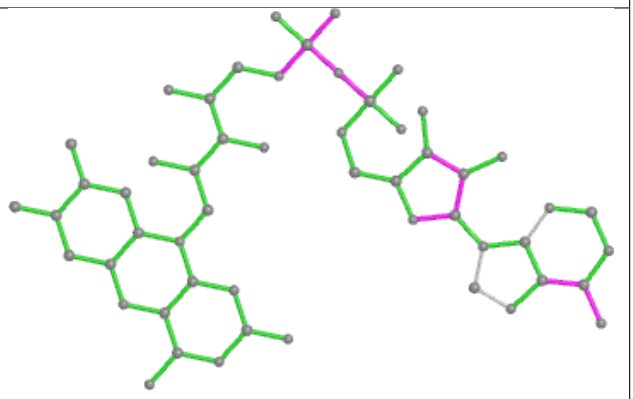


Rings

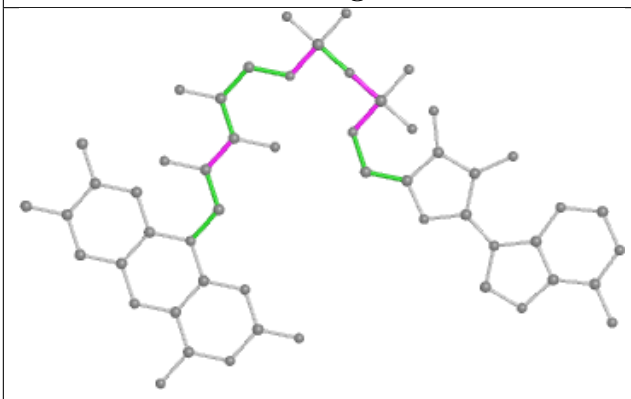
Ligand FAD B 501



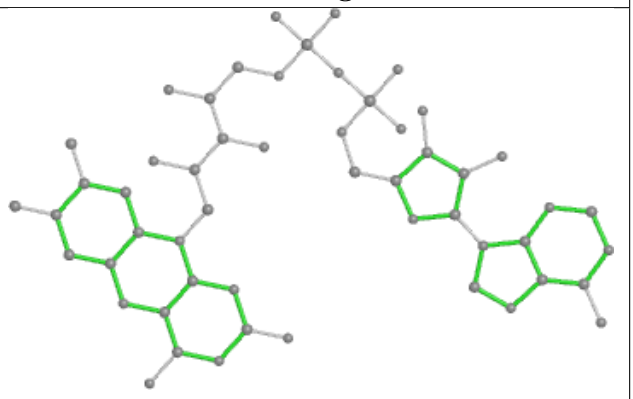
Bond lengths



Bond angles

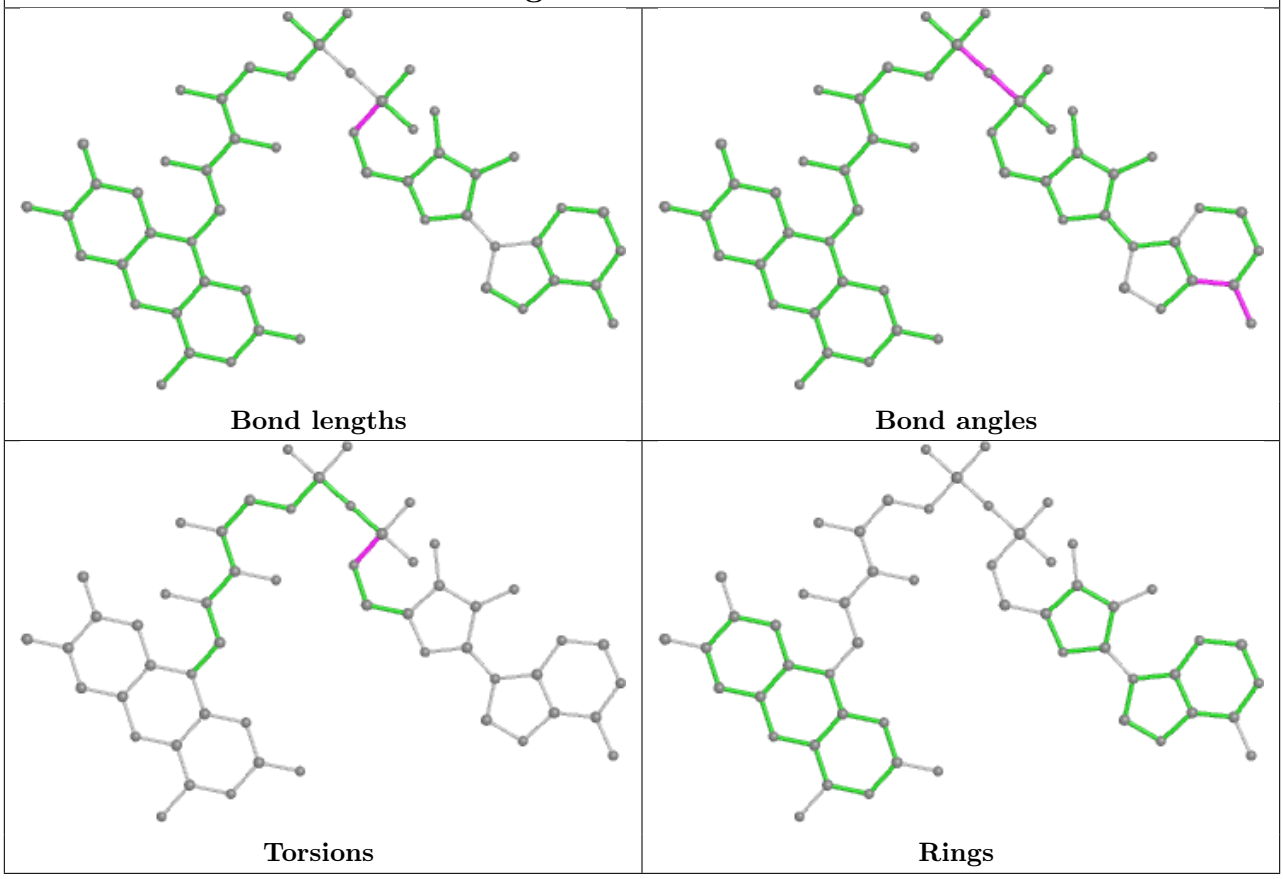


Torsions



Rings

Ligand FAD A 601



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

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	385/398 (96%)	0.34	19 (4%)	29	37	13, 21, 36, 54	0
1	B	383/398 (96%)	0.27	18 (4%)	31	38	13, 20, 34, 56	0
1	C	387/398 (97%)	0.28	21 (5%)	25	32	14, 22, 36, 50	0
1	D	385/398 (96%)	0.37	27 (7%)	16	22	15, 22, 37, 58	0
All	All	1540/1592 (96%)	0.32	85 (5%)	25	31	13, 21, 36, 58	0

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	32	VAL	7.8
1	B	30	GLN	5.2
1	B	302	ALA	5.2
1	D	300	PHE	4.6
1	B	300	PHE	4.6
1	D	31	SER	4.2
1	A	29	TYR	4.0
1	D	29	TYR	3.8
1	C	25	LEU	3.8
1	D	118	VAL	3.8
1	C	220	PRO	3.8
1	D	412	SER	3.7
1	A	32	VAL	3.7
1	C	204	ALA	3.7
1	A	409	SER	3.6
1	A	28	ILE	3.6
1	D	30	GLN	3.6
1	D	408	ARG	3.5
1	D	28	ILE	3.5
1	A	412	SER	3.5
1	A	408	ARG	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	204	ALA	3.3
1	C	40	MET	3.3
1	C	31	SER	3.3
1	D	301	GLY	3.1
1	D	86	GLU	3.1
1	A	410	TYR	3.1
1	D	133	LYS	3.0
1	B	175	ASP	2.9
1	D	122	LEU	2.9
1	B	31	SER	2.9
1	A	30	GLN	2.8
1	A	154	LEU	2.8
1	D	40	MET	2.8
1	D	115	ILE	2.8
1	C	205	LEU	2.8
1	A	207	ASN	2.7
1	C	165	ALA	2.7
1	C	36	GLU	2.6
1	D	409	SER	2.6
1	A	205	LEU	2.6
1	A	87	GLU	2.6
1	D	88	LEU	2.5
1	B	33	GLU	2.5
1	C	206	GLN	2.5
1	D	47	ASP	2.5
1	C	122	LEU	2.5
1	B	87	GLU	2.5
1	C	163	ALA	2.5
1	A	208	LYS	2.5
1	B	122	LEU	2.4
1	D	337	ASN	2.4
1	B	408	ARG	2.4
1	D	391	TYR	2.4
1	C	33	GLU	2.4
1	D	275	ILE	2.4
1	C	152	PHE	2.4
1	D	87	GLU	2.3
1	B	340	PRO	2.3
1	C	268	LEU	2.3
1	B	391	TYR	2.3
1	C	154	LEU	2.2
1	A	275	ILE	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	301	GLY	2.2
1	C	275	ILE	2.2
1	D	340	PRO	2.2
1	C	134	GLU	2.2
1	C	118	VAL	2.2
1	C	121	SER	2.2
1	B	51	LYS	2.1
1	D	64	HIS	2.1
1	A	340	PRO	2.1
1	D	114	VAL	2.1
1	C	43	GLN	2.1
1	B	121	SER	2.1
1	B	64	HIS	2.1
1	A	47	ASP	2.1
1	A	137	GLN	2.1
1	D	302	ALA	2.1
1	A	337	ASN	2.0
1	B	37	THR	2.0
1	D	204	ALA	2.0
1	D	137	GLN	2.0
1	C	247[A]	ARG	2.0
1	B	29	TYR	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, 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
2	FAD	B	501	53/53	0.91	0.17	15,19,28,32	0

Continued on next page...

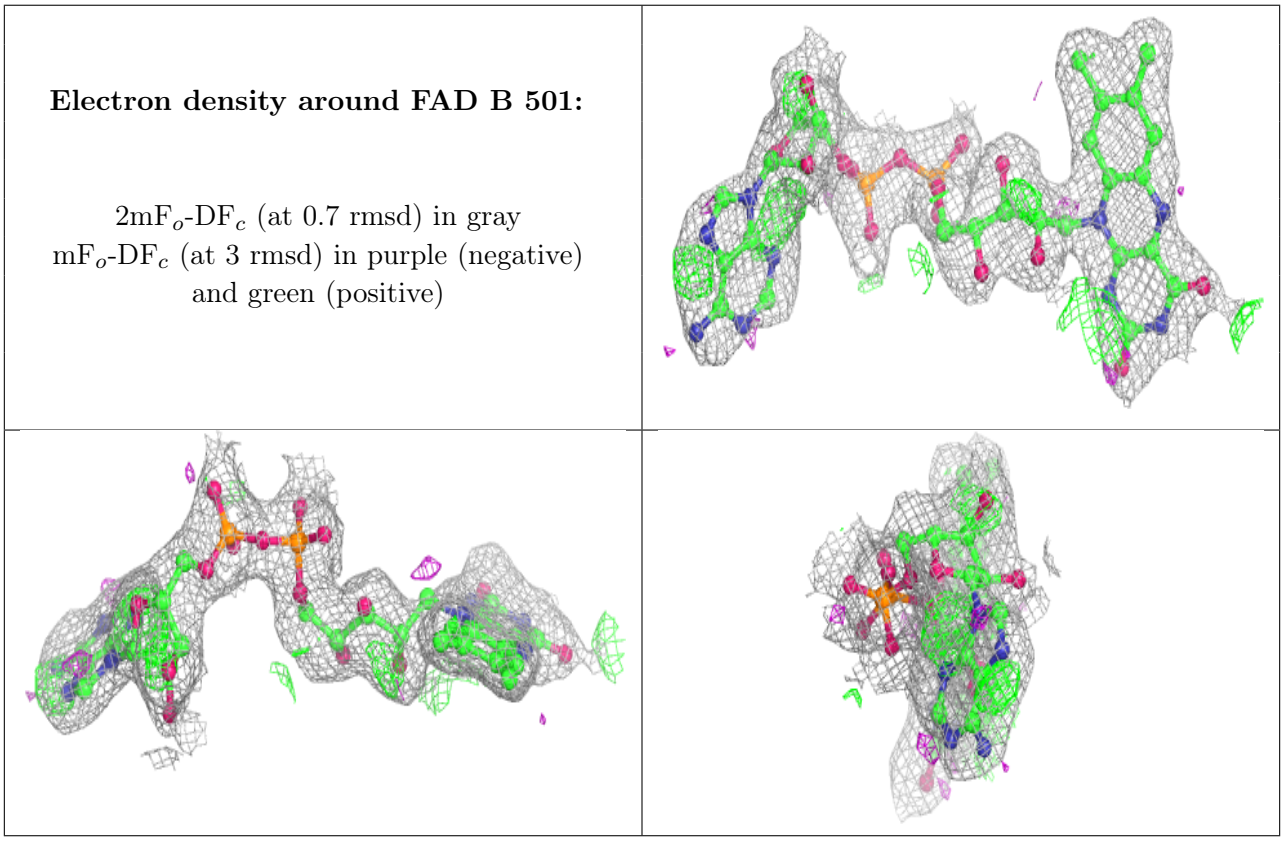
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	FMT	D	602	3/3	0.91	0.12	23,23,25,31	0
2	FAD	C	502	53/53	0.93	0.13	15,19,24,24	0
2	FAD	A	601	53/53	0.94	0.14	14,18,21,23	0
3	FMT	C	501	3/3	0.95	0.11	24,24,27,31	0
2	FAD	D	601	53/53	0.95	0.11	15,18,21,23	0
3	FMT	B	502	3/3	0.96	0.09	21,21,24,25	0
3	FMT	A	602	3/3	0.97	0.08	22,22,27,29	0

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

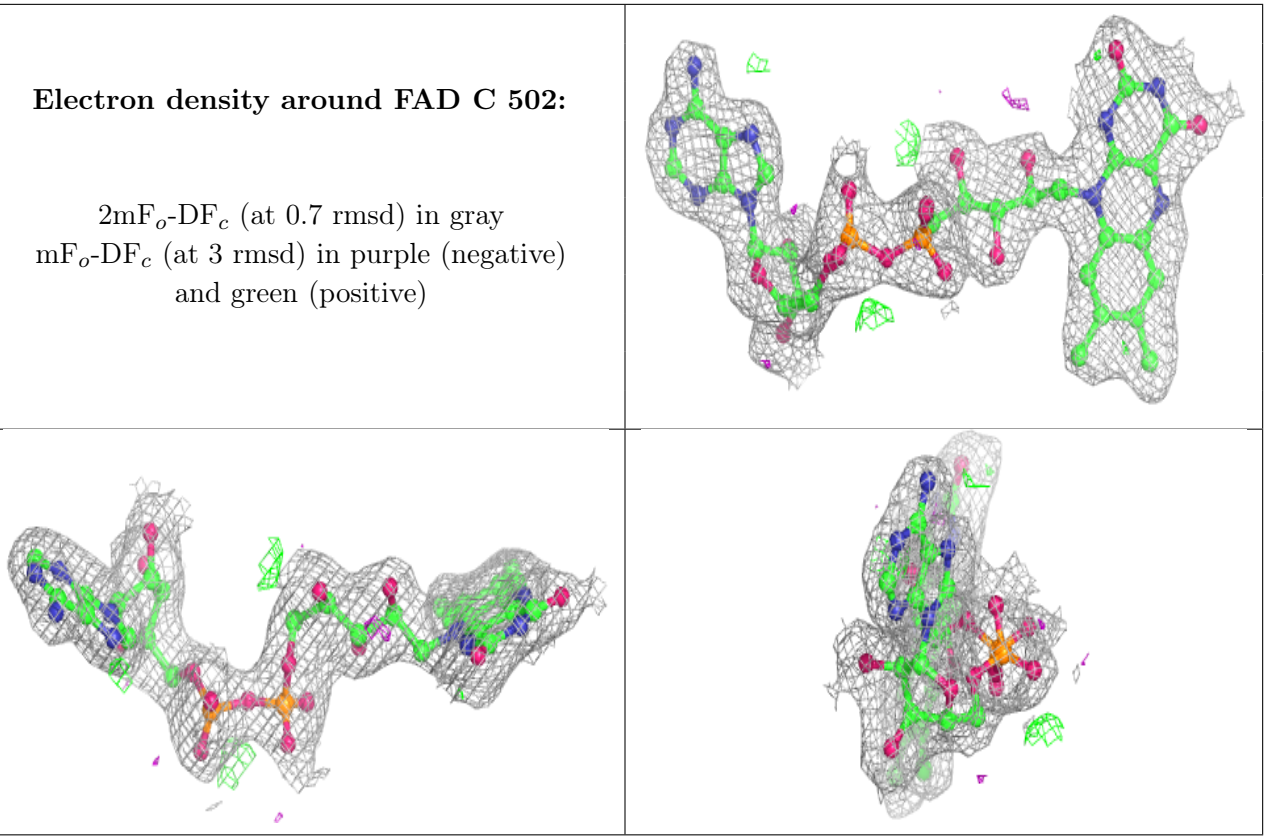
Electron density around FAD B 501:

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



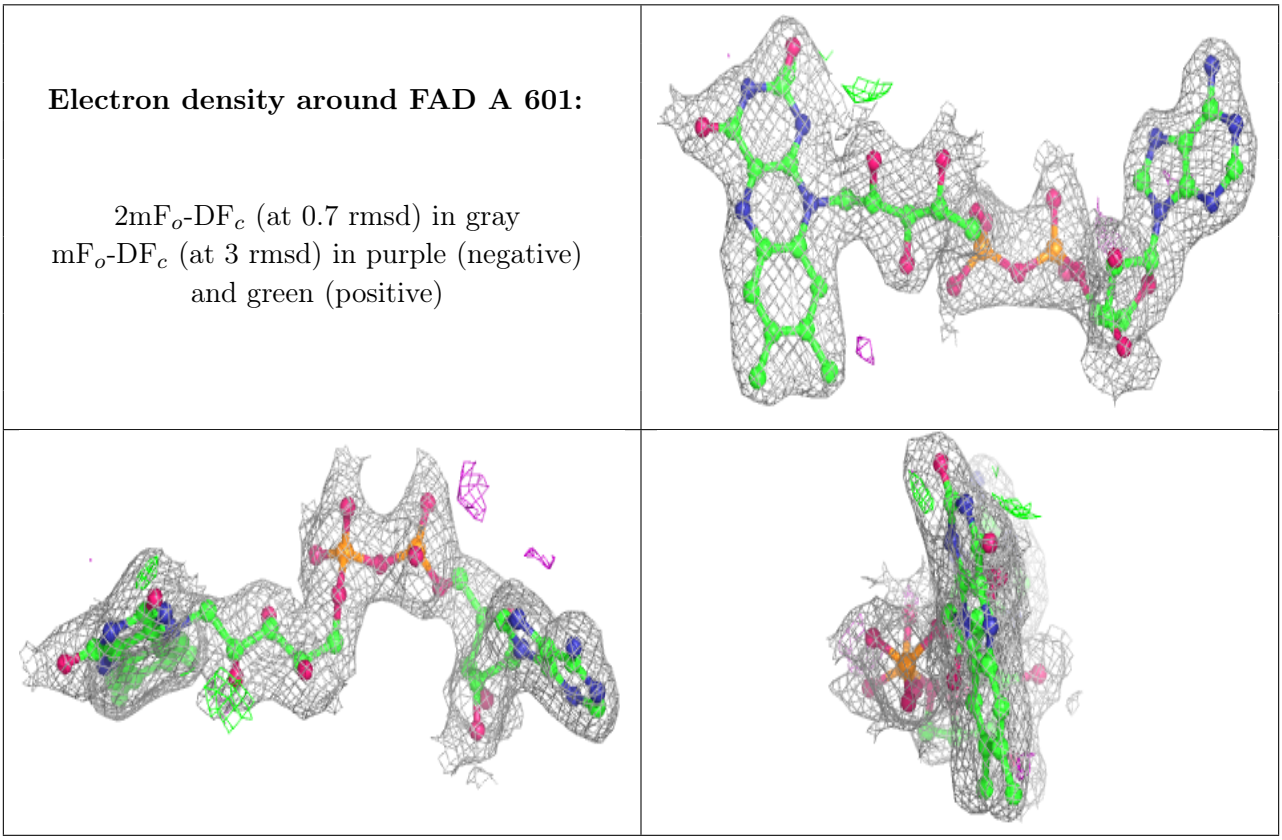
Electron density around FAD C 502:

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



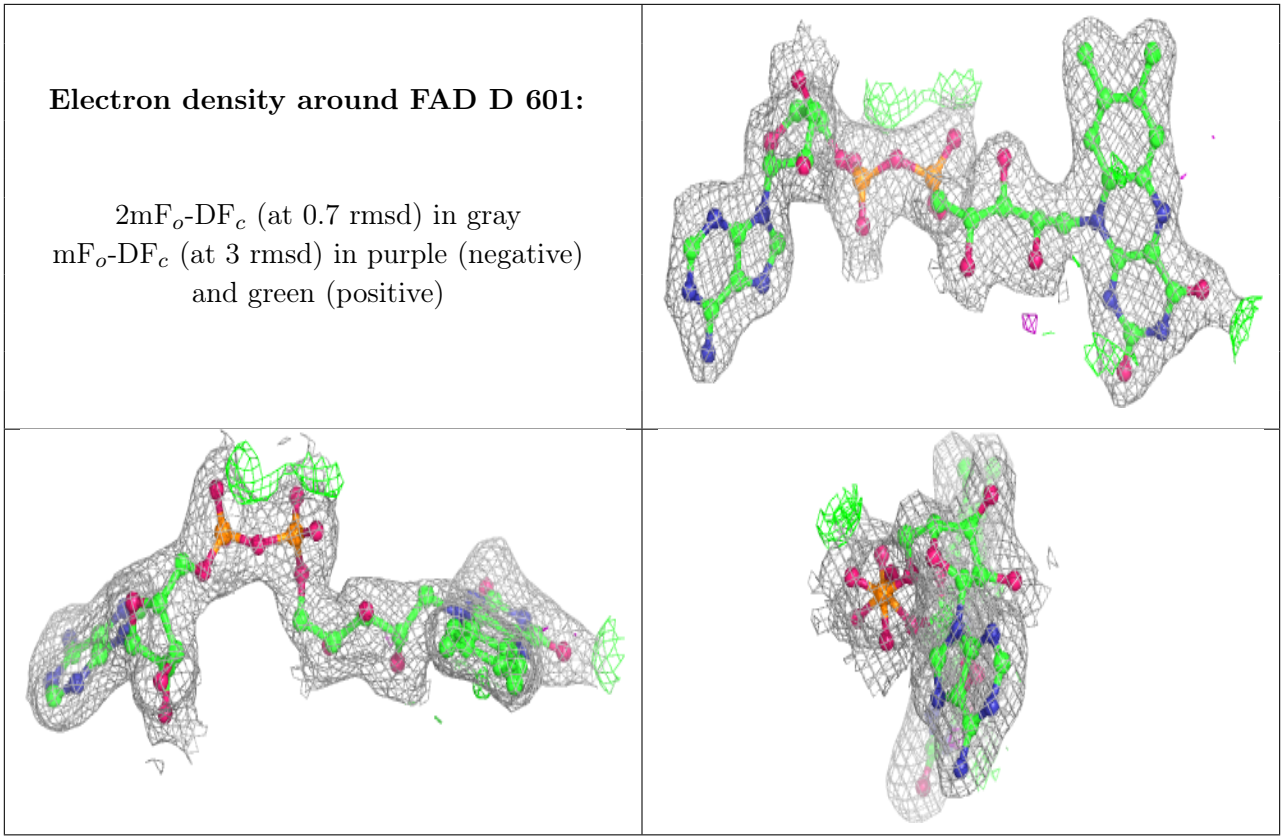
Electron density around FAD A 601:

$2mF_o$-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 601:

$2mF_o$-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.