wwPDB X-ray Structure Validation Summary Report (i)

Jun 13, 2024 – 07:27 AM EDT

PDB ID	:	1MOK
Title	:	NADPH DEPENDENT 2-KETOPROPYL COENZYME M OXIDOREDUCTASE/CARBOXYLASE
Authors	:	Nocek, B.; Jang, S.B.; Jeong, M.S.; Clark, D.D.; Ensign, S.A.; Peters, J.W.
Deposited on	:	2002-09-09
Resolution	:	2.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (1)) were used in the production of this report:

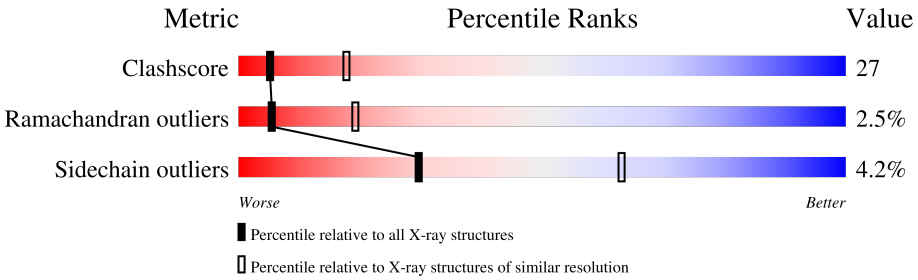
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	523	53% 43% .
1	B	523	56% 40% .
1	C	523	54% 42% . .
1	D	523	50% 45% .

2 Entry composition (i)

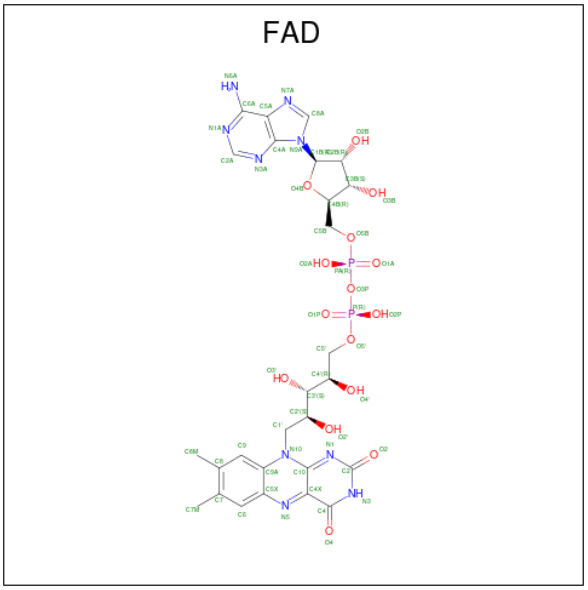
There are 2 unique types of molecules in this entry. The entry contains 16304 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 orf3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	522	Total	C	N	O	S	0	0	0
			4023	2546	699	755	23			
1	B	522	Total	C	N	O	S	0	0	0
			4023	2546	699	755	23			
1	C	522	Total	C	N	O	S	0	0	0
			4023	2546	699	755	23			
1	D	522	Total	C	N	O	S	0	0	0
			4023	2546	699	755	23			

- 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		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

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

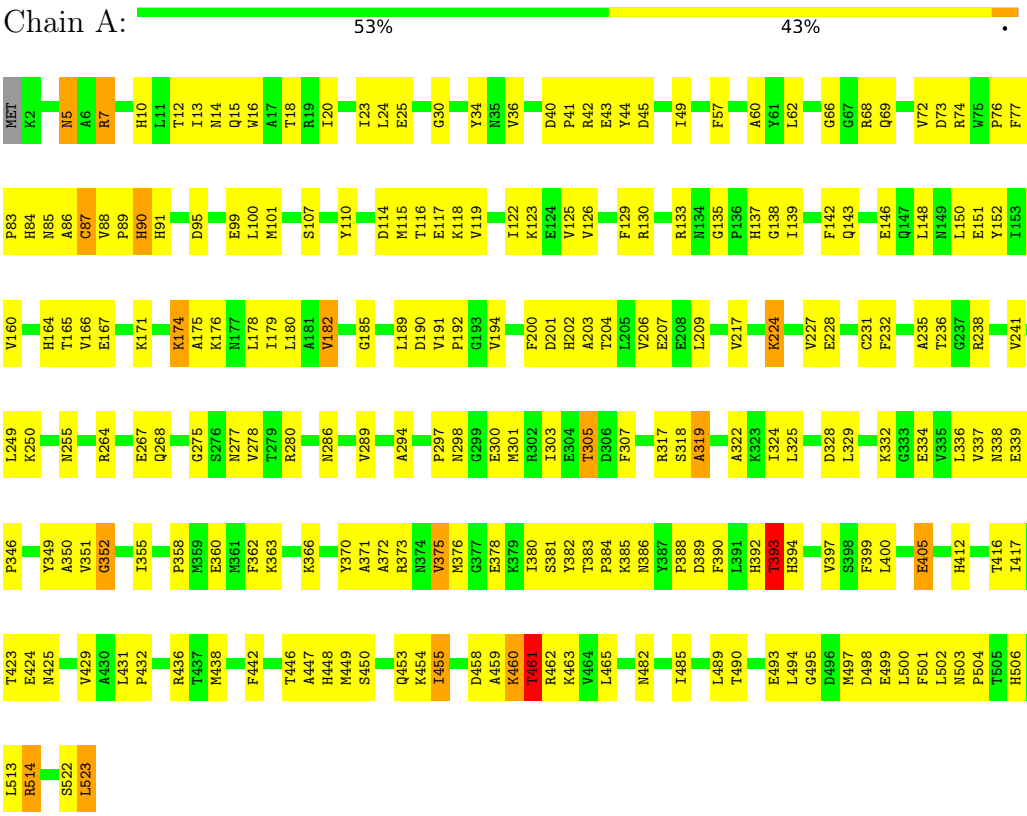
3 Residue-property plots (i)

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. 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. 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.

Note EDS was not executed.

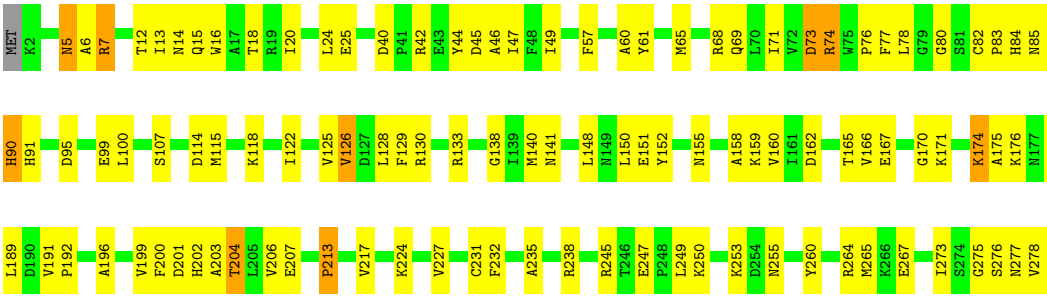
- Molecule 1: orf3

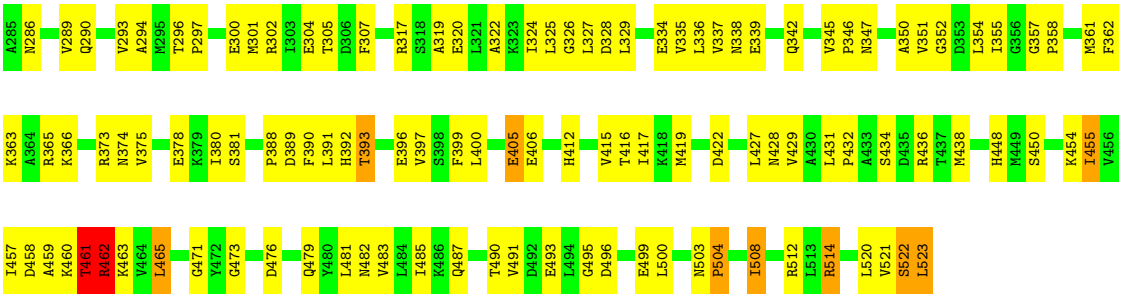
Chain A:



- Molecule 1: orf3

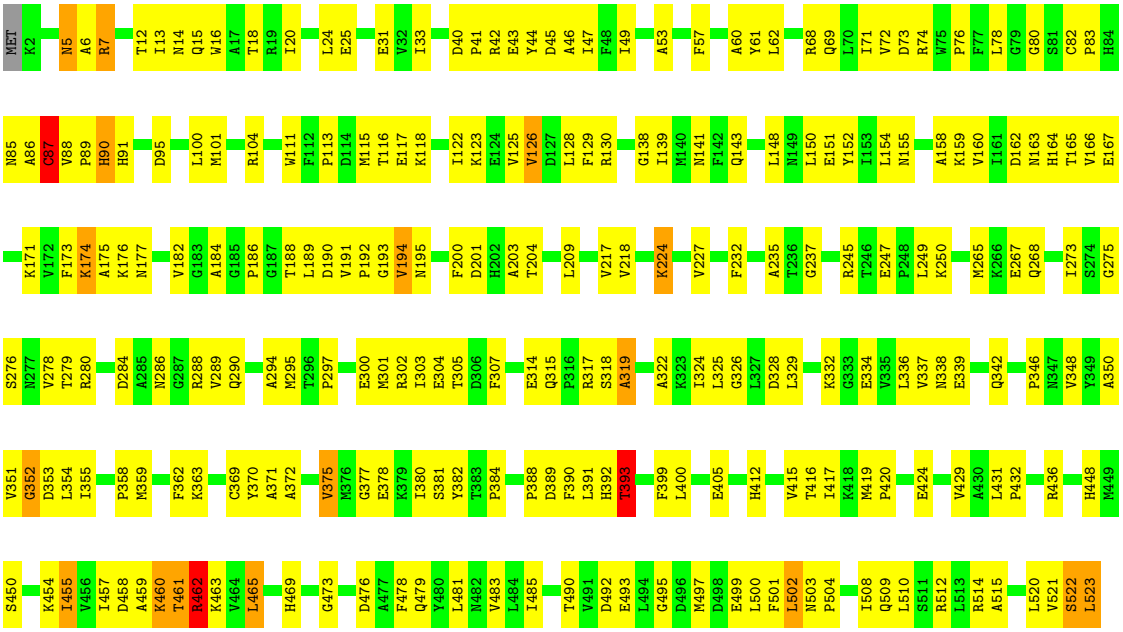
Chain B:





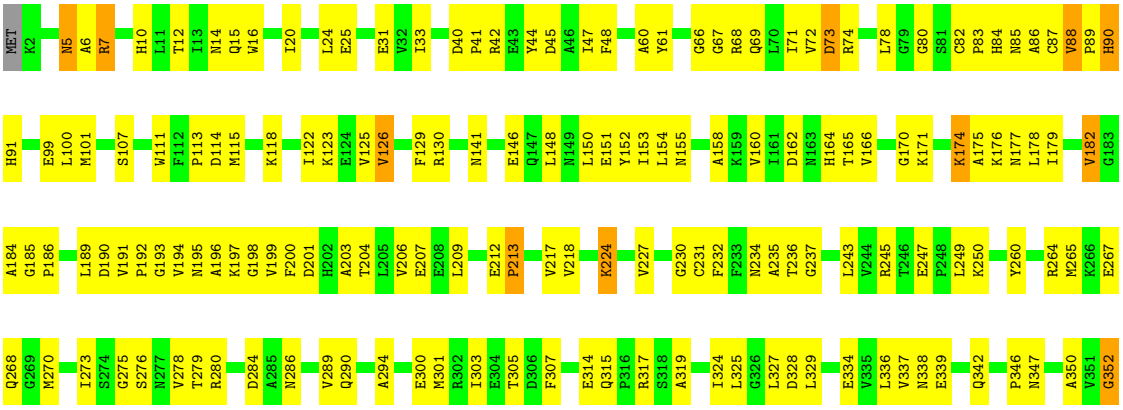
• Molecule 1: orf3

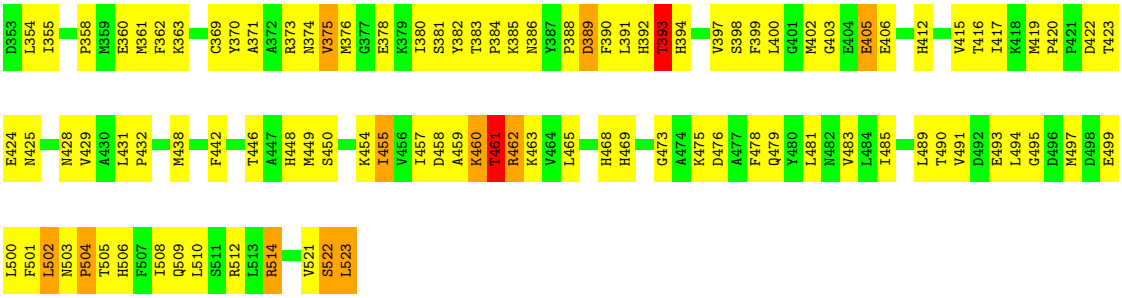
Chain C:



• Molecule 1: orf3

Chain D:




D353 L354 I355 P358 M359 E360 M361 F362 K363 C369 Y370 A371 A372 R373 N374 V375 M376 G377 E378 K379 I380 S381 Y382 T383 P384 K385 N386 Y387 P388 D389 F390 L391 H392 T393 H394 V397 S398 F399 L400 G401 M402 G403 E404 E405 E406 H412 V415 T416 I417 K418 M419 P420 P421 D422 T423
E424 N425 N428 V429 A430 L431 P432 M438 F442 T446 A447 H448 M449 S450 K454 I455 V456 I457 D458 A459 K460 T461 R462 K463 V464 L465 H468 H469 G473 A474 K475 D476 A477 F478 Q479 Y480 L481 N482 V483 L484 I485 L489 T490 V491 D492 E493 L494 G495 D496 M497 D498 E499
L500 F501 L502 N503 P504 T505 H506 F507 I508 Q509 L510 S511 R512 L513 R514 V521 S522 L523

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	65.60Å 87.50Å 100.70Å 72.00° 73.40° 69.81°	Depositor
Resolution (Å)	19.99 – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) (19.99-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.225 , 0.277	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	16304	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.48	1/4106 (0.0%)	0.66	2/5556 (0.0%)
1	B	0.53	2/4106 (0.0%)	0.71	4/5556 (0.1%)
1	C	0.48	1/4106 (0.0%)	0.67	4/5556 (0.1%)
1	D	0.50	1/4106 (0.0%)	0.67	2/5556 (0.0%)
All	All	0.50	5/16424 (0.0%)	0.68	12/22224 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	523	LEU	C-O	-16.04	0.92	1.23
1	D	523	LEU	C-O	-15.27	0.94	1.23
1	C	523	LEU	C-O	-15.03	0.94	1.23
1	A	523	LEU	C-O	-14.81	0.95	1.23
1	B	73	ASP	C-N	-7.01	1.18	1.34

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	523	LEU	CA-C-O	12.25	145.82	120.10
1	D	523	LEU	CA-C-O	11.65	144.57	120.10
1	A	523	LEU	CA-C-O	10.93	143.06	120.10
1	C	523	LEU	CA-C-O	10.14	141.41	120.10
1	B	462	ARG	NE-CZ-NH2	7.37	123.98	120.30

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	4023	0	3980	222	0
1	B	4023	0	3979	217	0
1	C	4023	0	3980	234	0
1	D	4023	0	3980	231	0
2	A	53	0	31	6	0
2	B	53	0	31	6	0
2	C	53	0	31	9	0
2	D	53	0	31	12	0
All	All	16304	0	16043	864	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 27.

The worst 5 of 864 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:C:460:LYS:O	1:C:461:THR:HB	1.39	1.08
1:C:82:CYS:HA	1:C:86:ALA:HB3	1.38	1.05
1:A:82:CYS:HA	1:A:86:ALA:HB3	1.42	1.00
1:D:40:ASP:OD1	1:D:42:ARG:HG2	1.64	0.98
1:C:165:THR:HG22	1:C:174:LYS:HG3	1.46	0.97

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	520/523 (99%)	449 (86%)	60 (12%)	11 (2%)	7	23
1	B	520/523 (99%)	447 (86%)	62 (12%)	11 (2%)	7	23
1	C	520/523 (99%)	456 (88%)	51 (10%)	13 (2%)	5	19
1	D	520/523 (99%)	450 (86%)	54 (10%)	16 (3%)	4	14
All	All	2080/2092 (99%)	1802 (87%)	227 (11%)	51 (2%)	5	19

5 of 51 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	224	LYS
1	A	319	ALA
1	A	462	ARG
1	B	224	LYS
1	B	462	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	423/424 (100%)	407 (96%)	16 (4%)	33	67
1	B	423/424 (100%)	405 (96%)	18 (4%)	29	62
1	C	423/424 (100%)	407 (96%)	16 (4%)	33	67
1	D	423/424 (100%)	402 (95%)	21 (5%)	24	56
All	All	1692/1696 (100%)	1621 (96%)	71 (4%)	30	63

5 of 71 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	182	VAL
1	D	234	ASN
1	D	455	ILE
1	B	305	THR
1	B	204	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 63 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	412	HIS
1	D	255	ASN
1	C	90	HIS
1	D	234	ASN
1	D	412	HIS

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)

4 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	$\#\|Z\| > 2$
2	FAD	A	524	-	53,58,58	2.39	14 (26%)	68,89,89	1.28	10 (14%)
2	FAD	C	524	-	53,58,58	2.34	13 (24%)	68,89,89	1.29	10 (14%)
2	FAD	D	524	-	53,58,58	2.39	13 (24%)	68,89,89	1.26	8 (11%)
2	FAD	B	524	-	53,58,58	2.37	13 (24%)	68,89,89	1.30	10 (14%)

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	A	524	-	-	4/30/50/50	0/6/6/6
2	FAD	C	524	-	-	3/30/50/50	0/6/6/6
2	FAD	D	524	-	-	3/30/50/50	0/6/6/6
2	FAD	B	524	-	-	4/30/50/50	0/6/6/6

The worst 5 of 53 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	524	FAD	C4X-N5	7.56	1.45	1.30
2	D	524	FAD	C4A-N3A	7.28	1.45	1.35
2	D	524	FAD	C4X-N5	7.13	1.44	1.30
2	A	524	FAD	C4X-N5	6.85	1.44	1.30
2	C	524	FAD	C4A-N3A	6.84	1.45	1.35

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	524	FAD	C1'-N10-C9A	-3.06	115.41	120.51
2	B	524	FAD	C1'-N10-C9A	-3.04	115.45	120.51
2	D	524	FAD	C1'-N10-C9A	-3.02	115.48	120.51
2	A	524	FAD	C1'-N10-C9A	-2.89	115.70	120.51
2	D	524	FAD	C5X-C9A-N10	-2.88	114.98	117.95

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	524	FAD	P-O3P-PA-O1A
2	B	524	FAD	P-O3P-PA-O1A
2	D	524	FAD	P-O3P-PA-O1A
2	C	524	FAD	P-O3P-PA-O1A
2	C	524	FAD	O4B-C4B-C5B-O5B

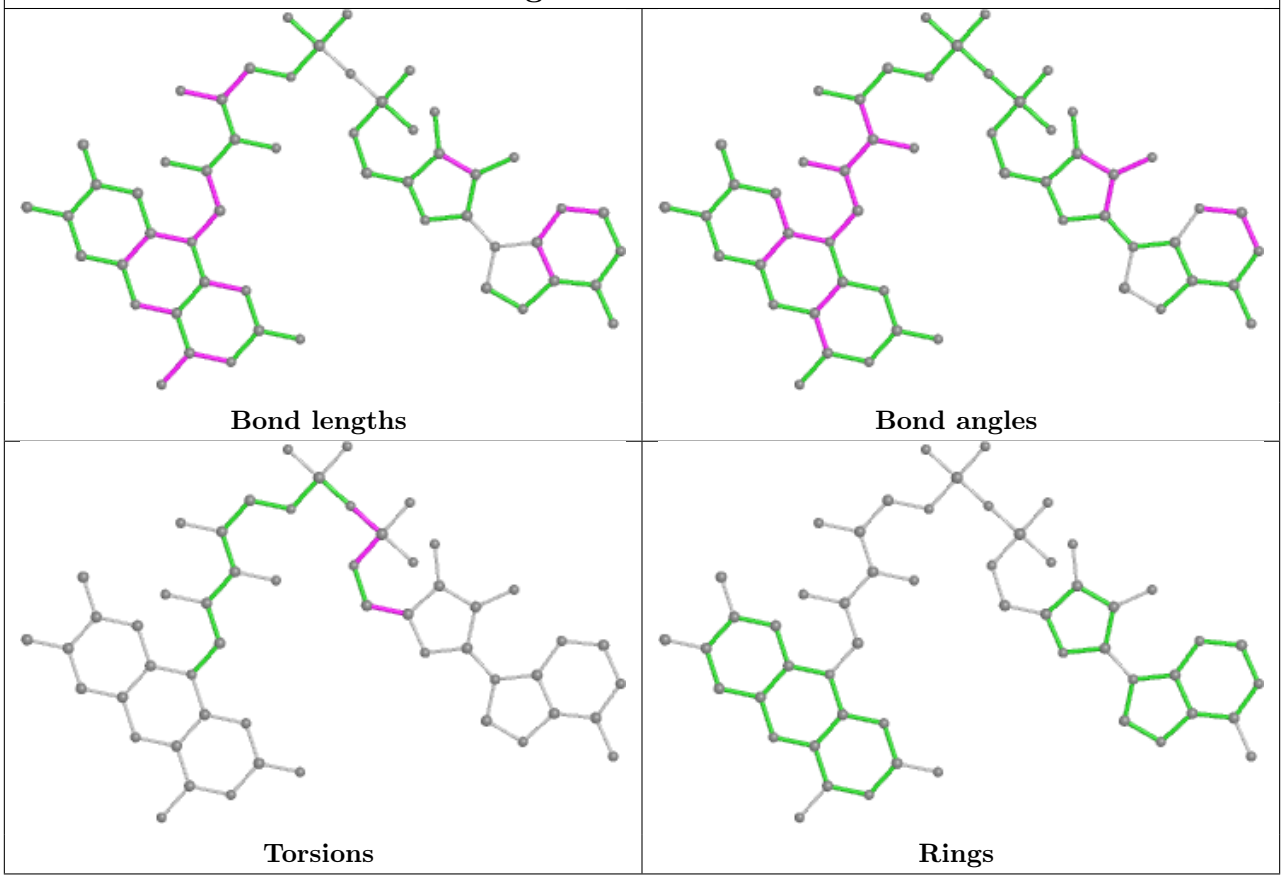
There are no ring outliers.

4 monomers are involved in 33 short contacts:

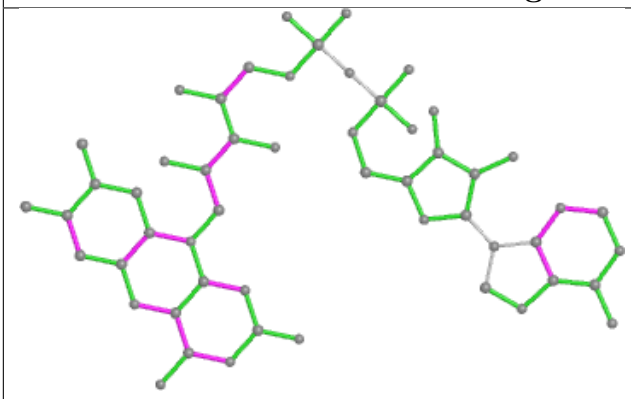
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	524	FAD	6	0
2	C	524	FAD	9	0
2	D	524	FAD	12	0
2	B	524	FAD	6	0

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.

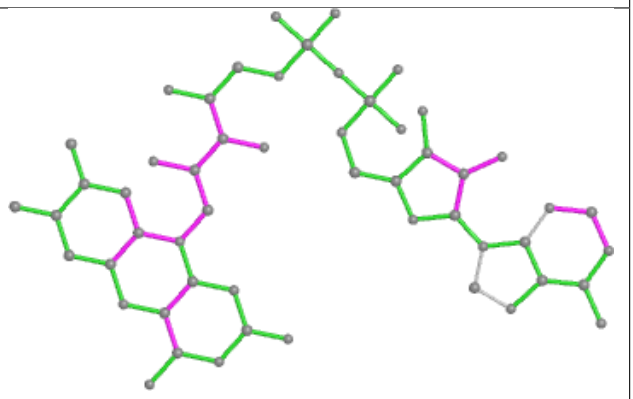
Ligand FAD A 524



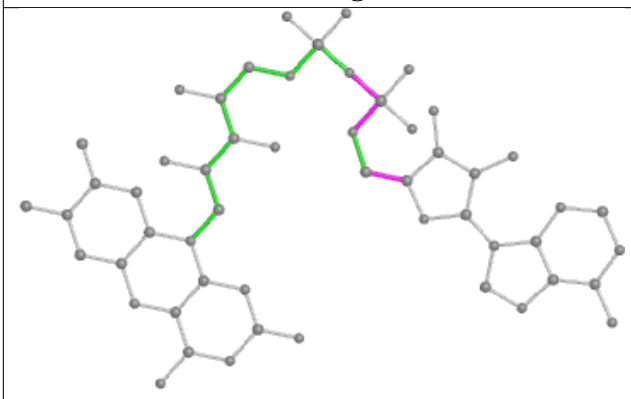
Ligand FAD C 524



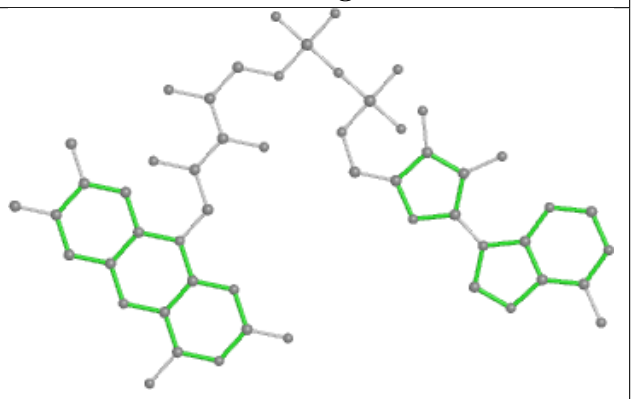
Bond lengths



Bond angles

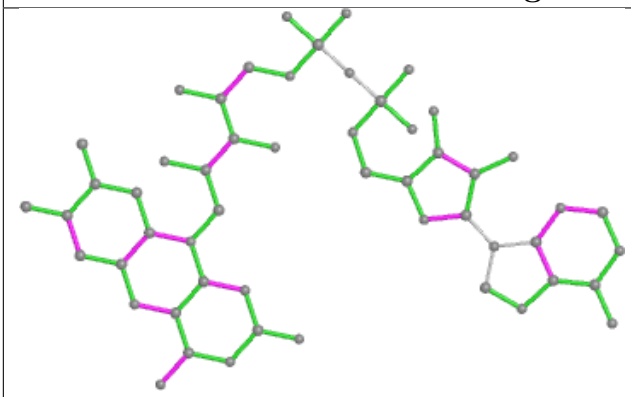


Torsions

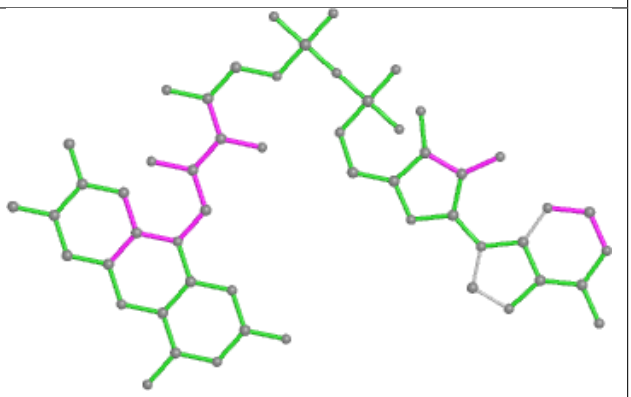


Rings

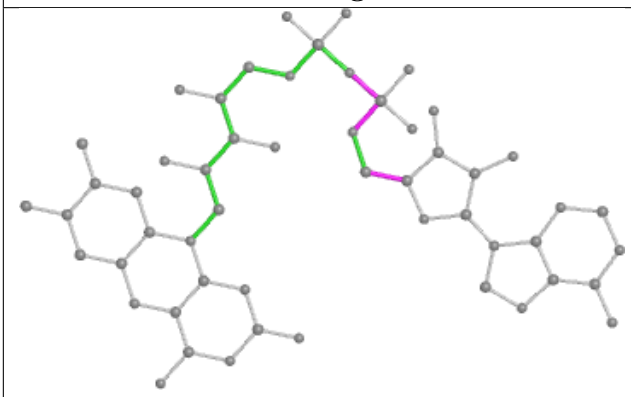
Ligand FAD D 524



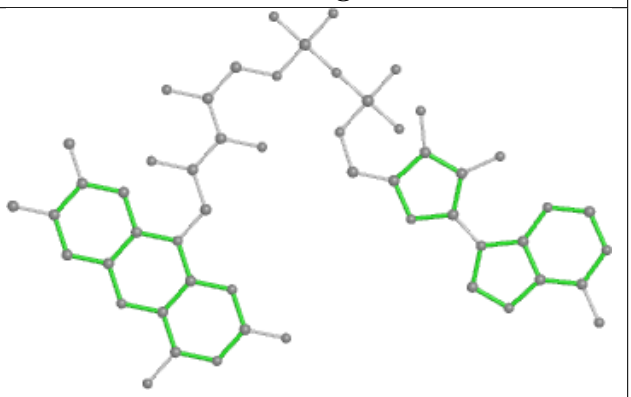
Bond lengths



Bond angles

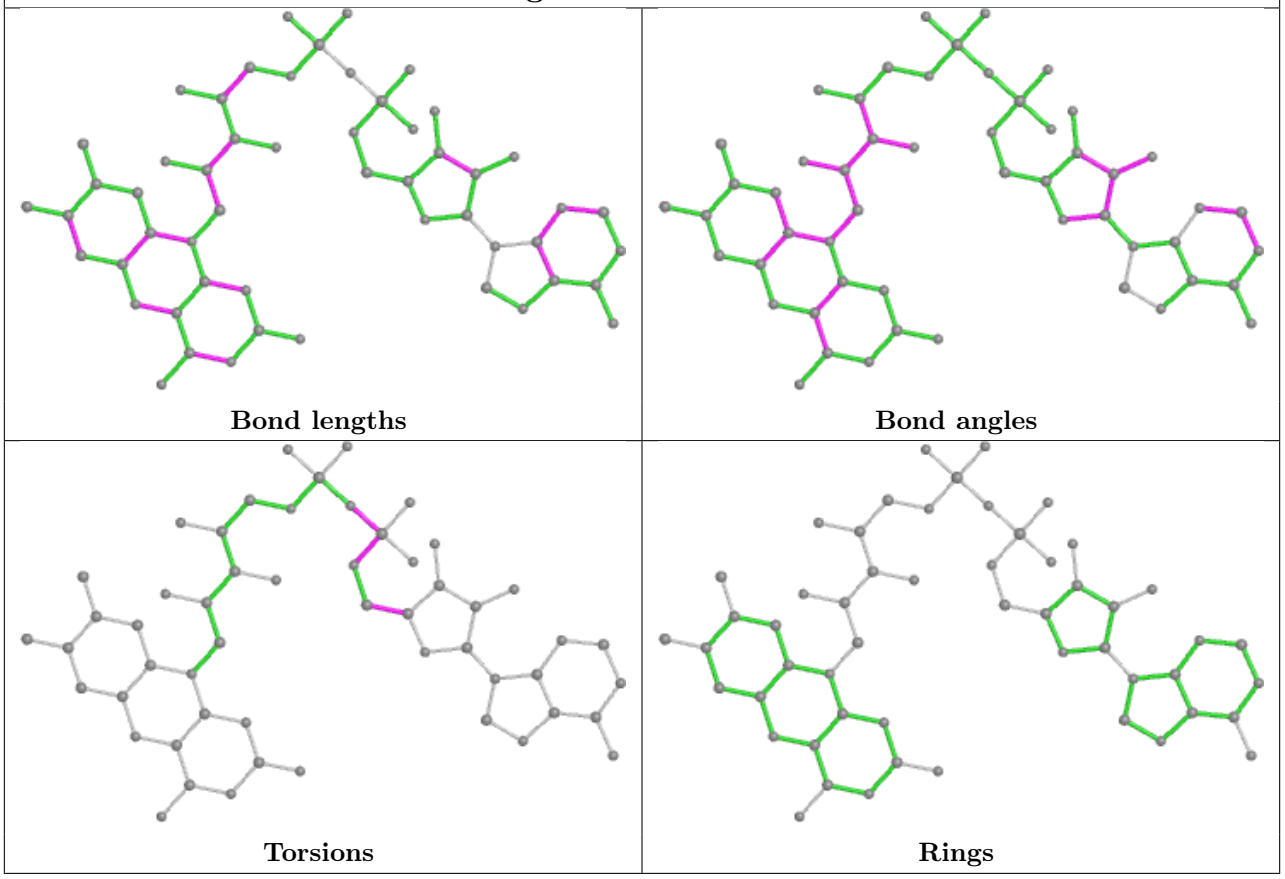


Torsions



Rings

Ligand FAD B 524



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	73:ASP	C	74:ARG	N	1.17

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.