



wwPDB X-ray Structure Validation Summary Report ⓘ

May 15, 2020 – 02:17 pm BST

PDB ID : 1DXL
Title : Dihydrolipoamide dehydrogenase of glycine decarboxylase from *Pisum Sativum*
Authors : Faure, M.; Cohen-Addad, C.; Bourguignon, J.; Macherel, D.; Neuburger, M.; Douce, R.
Deposited on : 2000-01-10
Resolution : 3.15 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 ⓘ 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) : **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) : 2.11

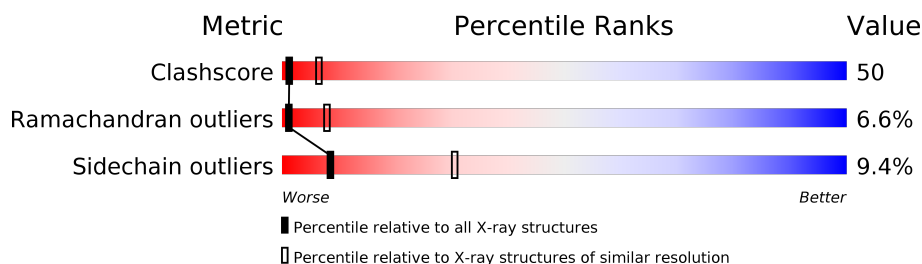
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.15 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	1804 (3.20-3.12)
Ramachandran outliers	138981	1770 (3.20-3.12)
Sidechain outliers	138945	1769 (3.20-3.12)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	470	<div> <div>37%</div> <div>51%</div> <div>10%</div> <div>..</div> </div>
1	B	470	<div> <div>39%</div> <div>50%</div> <div>10%</div> <div>..</div> </div>
1	C	470	<div> <div>36%</div> <div>51%</div> <div>11%</div> <div>.</div> </div>
1	D	470	<div> <div>40%</div> <div>49%</div> <div>9%</div> <div>.</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14240 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 DIHYDROLIPOAMIDE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	467	Total	C	N	O	S	48	1	0
			3487	2203	591	677	16			
1	B	467	Total	C	N	O	S	50	1	0
			3487	2203	591	677	16			
1	C	467	Total	C	N	O	S	77	0	0
			3475	2194	590	675	16			
1	D	467	Total	C	N	O	S	38	0	0
			3475	2194	590	675	16			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	449	HIS	ASN	conflict	UNP P31023
B	449	HIS	ASN	conflict	UNP P31023
C	449	HIS	ASN	conflict	UNP P31023
D	449	HIS	ASN	conflict	UNP P31023

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

- Molecule 3 is water.

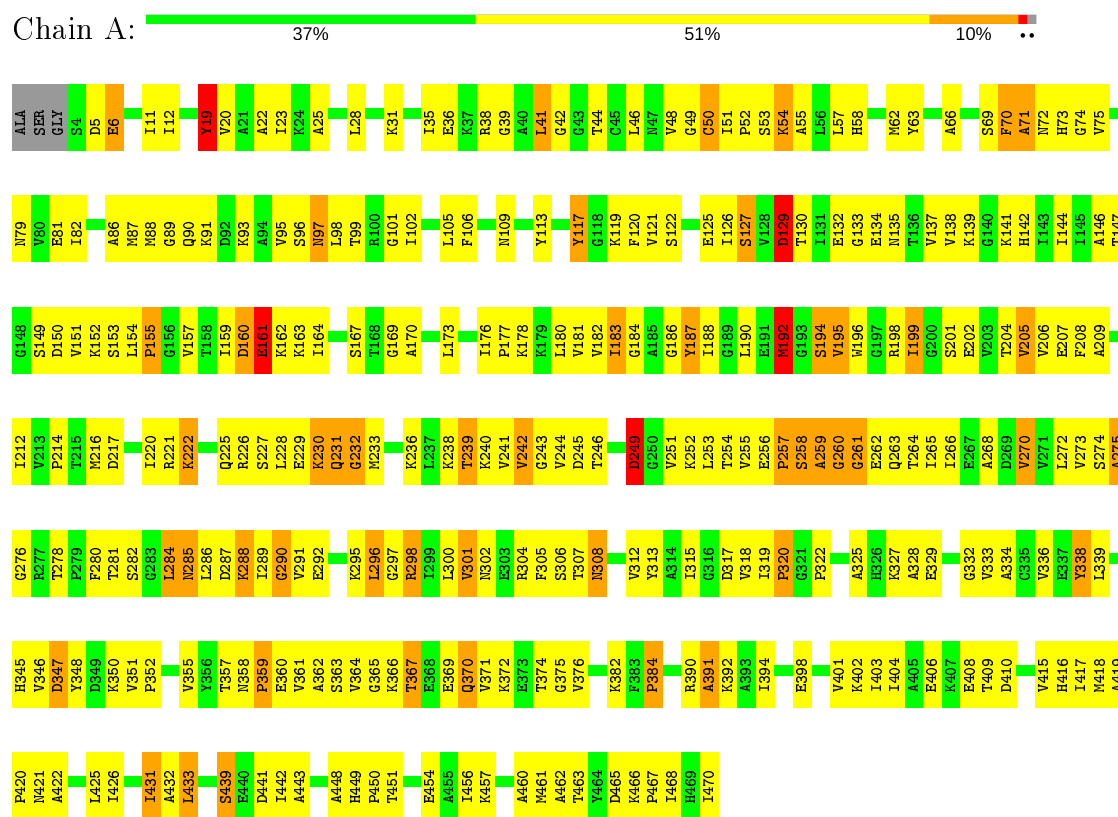
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	33	Total O 33 33	0	0
3	B	23	Total O 23 23	0	0
3	C	25	Total O 25 25	0	0
3	D	23	Total O 23 23	0	0

3 Residue-property plots

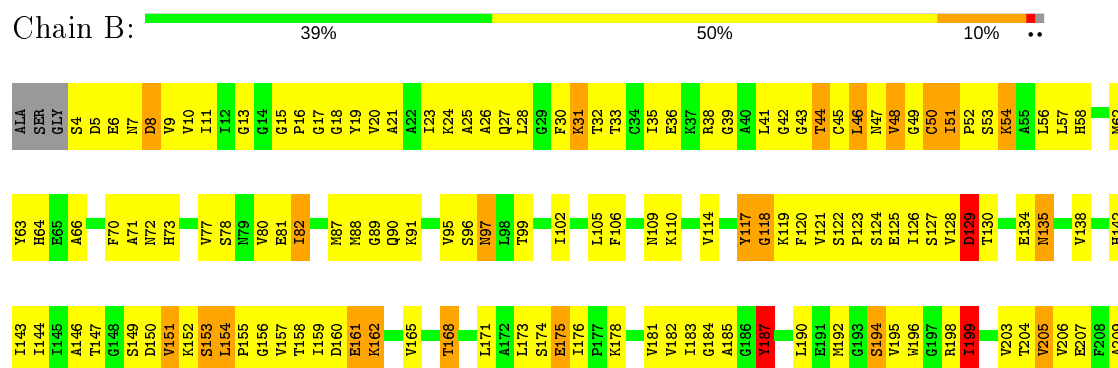
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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.

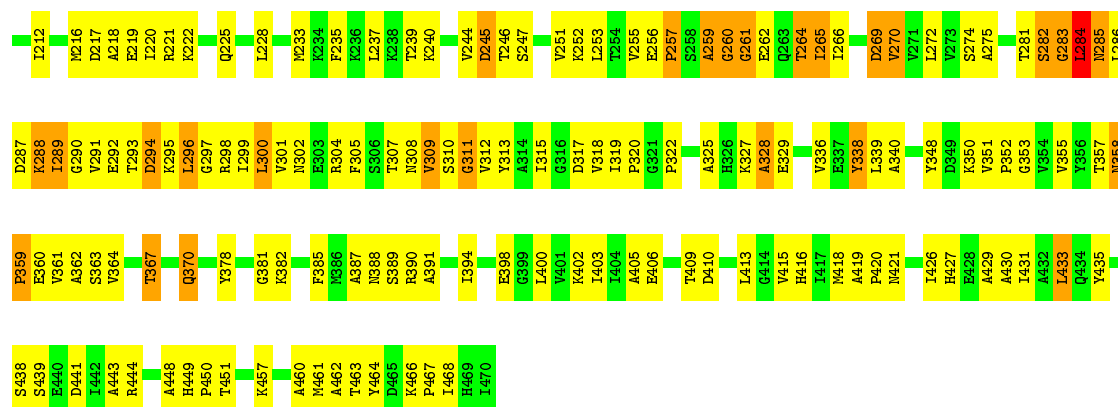
Note EDS was not executed.

• Molecule 1: DIHYDROLIPOAMIDE DEHYDROGENASE



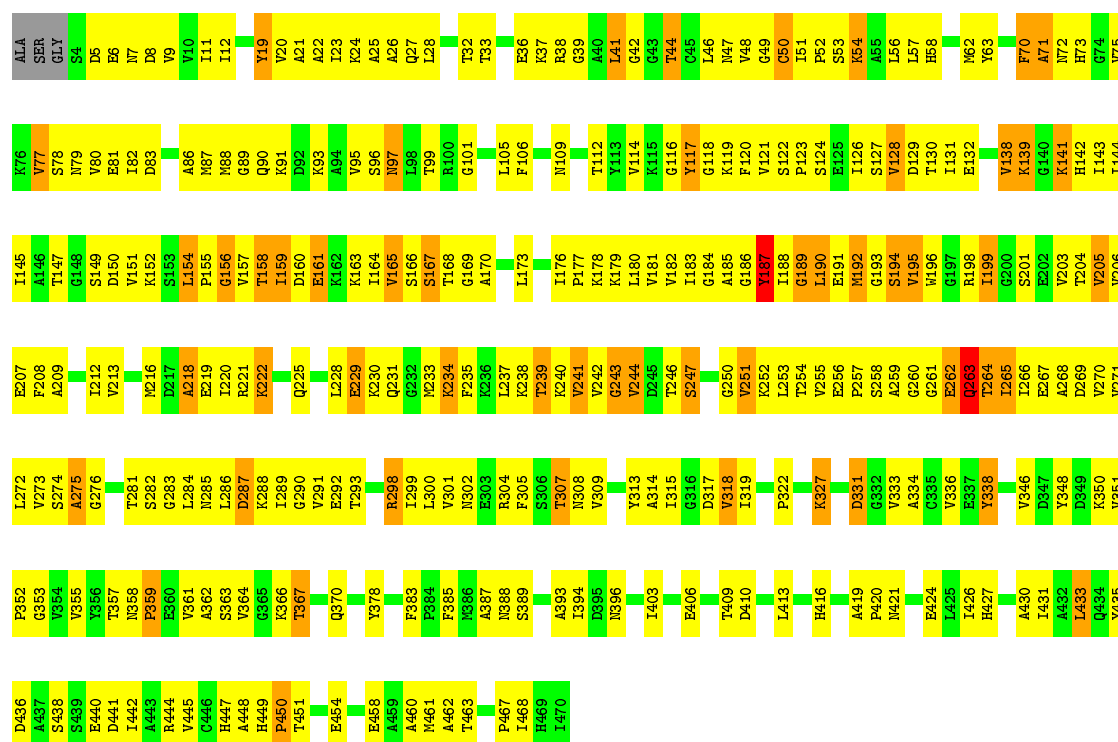
• Molecule 1: DIHYDROLIPOAMIDE DEHYDROGENASE





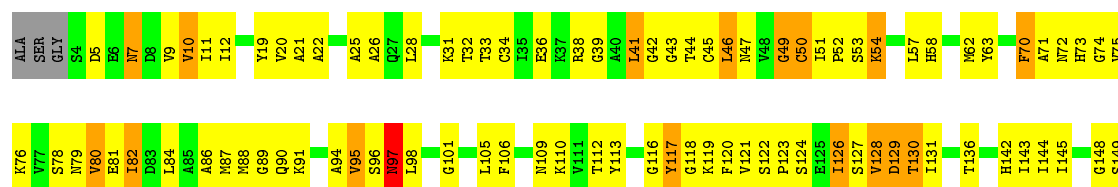
• Molecule 1: DIHYDROLIPOAMIDE DEHYDROGENASE

Chain C: 36% 51% 11%



• Molecule 1: DIHYDROLIPOAMIDE DEHYDROGENASE

Chain D: 40% 49% 9%



D150	V301	I220	D150
V151	N302	R221	V151
K152	E303	K222	K152
S153	R304	Q225	S153
L154	F305	R226	L154
P155	N308	S227	P155
G156	V309	L228	G156
V157	S310	E229	V157
T158	G311	Q230	T158
I159	V312	Q231	I159
D160	Y313	K234	D160
E161	A314	I237	E161
K162	I315	K238	K162
K163	V318	T239	K163
I164	I319	K240	I164
V165	P320	V241	V165
S166	G321	V242	S166
S167	P322	G243	S167
L171	A325	D249	L171
I176	H326	L253	I176
P177	K327	T254	P177
L180	A328	V255	L180
V181	E329	E262	V181
V182	E330	Q263	V182
I183	D331	T264	I183
G184	G332	L265	G184
A185	V333	V270	A185
G186	V338	V273	G186
Y187	I339	S274	Y187
L190	H345	G275	L190
E191	V346	G276	E191
M192	D347	R277	M192
G193	Y348	T278	G193
S194	D349	P279	S194
V195	K350	F280	V195
W196	V351	G283	W196
I199	P352	L284	I199
G200	V354	N285	G200
S201	V355	L286	S201
E202	A356	D287	E202
V203	T357	K288	V203
T204	M358	I289	T204
V205	P359	G290	V205
V206	E360	V291	V206
E207	V361	E292	E207
F208	A362	T293	F208
A209	S363	D294	A209
I212	V364	K295	I212
V213	G365	R298	V213
M216	T367		M216
D217			D217
A218			A218
E219			E219
H449	E368		H449
P450	E369		P450
T451	Q370		T451
N452	V371		N452
S453	F376		S453
I456	E377		I456
K457	F383		K457
B458	P384		B458
A459	F385		A459
A460	M366		A460
N461	S389		N461
A462	R390		A462
T463	I394		T463
Y464	G398		Y464
K466	E399		K466
P467	L400		P467
I468	V401		I468
H469	I403		H469
I470	I404		I470
	A405		
	E406		
	T409		
	D410		
	L413		
	G414		
	V415		
	H416		
	I417		
	N418		
	A419		
	P420		
	N421		
	A422		
	G423		
	E424		
	L425		
	I426		
	H427		
	E428		
	A429		
	A430		
	I431		
	A432		
	L433		
	S438		
	S439		
	E440		
	D441		
	I442		
	A448		

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	100.56Å 108.33Å 202.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 3.15	Depositor
% Data completeness (in resolution range)	86.1 (15.00-3.15)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
Refinement program	CNS 0.4	Depositor
R, R_{free}	0.226 , 0.323	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	14240	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

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: 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	0.84	0/3541	1.02	7/4783 (0.1%)
1	B	0.73	0/3541	0.95	6/4783 (0.1%)
1	C	0.79	1/3527 (0.0%)	0.97	3/4762 (0.1%)
1	D	0.77	0/3528	0.97	3/4765 (0.1%)
All	All	0.78	1/14137 (0.0%)	0.98	19/19093 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	263	GLN	C-N	-6.04	1.20	1.34

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	162	LYS	N-CA-C	6.75	129.24	111.00
1	B	260	GLY	N-CA-C	-5.86	98.44	113.10
1	B	294	ASP	N-CA-C	5.82	126.70	111.00
1	D	31	LYS	N-CA-C	-5.80	95.35	111.00
1	B	44	THR	N-CA-C	-5.78	95.40	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	19	TYR	Sidechain
1	B	187[A]	TYR	Sidechain
1	C	263	GLN	Mainchain

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	3487	0	3552	334	0
1	B	3487	0	3552	362	0
1	C	3475	0	3543	422	0
1	D	3475	0	3544	327	0
2	A	53	0	31	2	0
2	B	53	0	31	2	0
2	C	53	0	31	3	0
2	D	53	0	31	3	0
3	A	33	0	0	2	0
3	B	23	0	0	3	0
3	C	25	0	0	6	0
3	D	23	0	0	6	0
All	All	14240	0	14315	1399	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 50.

The worst 5 of 1399 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:322:PRO:HG2	1:B:327:LYS:HG3	1.25	1.18
1:C:254:THR:HG23	1:C:265:ILE:HD11	1.25	1.18
1:D:243:GLY:HA3	1:D:254:THR:HB	1.25	1.13
1:A:12:ILE:HD11	1:A:126:ILE:CD1	1.81	1.11
1:B:147:THR:HG21	1:B:284:LEU:HD22	1.15	1.11

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	466/470 (99%)	368 (79%)	71 (15%)	27 (6%)	1	11
1	B	466/470 (99%)	357 (77%)	71 (15%)	38 (8%)	1	4
1	C	463/470 (98%)	367 (79%)	62 (13%)	34 (7%)	1	6
1	D	465/470 (99%)	350 (75%)	90 (19%)	25 (5%)	2	12
All	All	1860/1880 (99%)	1442 (78%)	294 (16%)	124 (7%)	1	8

5 of 124 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	50	CYS
1	A	129	ASP
1	A	161	GLU
1	A	201	SER
1	A	232	GLY

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	375/375 (100%)	332 (88%)	43 (12%)	5	22
1	B	375/375 (100%)	346 (92%)	29 (8%)	13	41
1	C	374/375 (100%)	345 (92%)	29 (8%)	12	40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	374/375 (100%)	334 (89%)	40 (11%)	6	25
All	All	1498/1500 (100%)	1357 (91%)	141 (9%)	8	30

5 of 141 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	285	ASN
1	C	90	GLN
1	D	294	ASP
1	B	307	THR
1	B	433	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	421	ASN
1	C	90	GLN
1	D	370	GLN
1	C	61	HIS
1	C	97	ASN

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 carbohydrates 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	C	480	-	51,58,58	2.25	15 (29%)	60,89,89	1.92	15 (25%)
2	FAD	D	480	-	51,58,58	2.28	13 (25%)	60,89,89	1.90	11 (18%)
2	FAD	A	480	-	51,58,58	2.20	10 (19%)	60,89,89	1.86	13 (21%)
2	FAD	B	480	-	51,58,58	2.29	15 (29%)	60,89,89	1.75	12 (20%)

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	C	480	-	-	4/30/50/50	0/6/6/6
2	FAD	D	480	-	-	4/30/50/50	0/6/6/6
2	FAD	A	480	-	-	4/30/50/50	0/6/6/6
2	FAD	B	480	-	-	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	D	480	FAD	C4X-C10	8.57	1.47	1.38
2	B	480	FAD	C4X-C10	8.20	1.47	1.38
2	C	480	FAD	C4X-C10	8.16	1.47	1.38
2	A	480	FAD	C4X-C10	7.62	1.46	1.38
2	B	480	FAD	O4B-C1B	5.79	1.49	1.41

The worst 5 of 51 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	480	FAD	C4-N3-C2	8.17	122.04	115.14
2	D	480	FAD	C4-N3-C2	8.15	122.02	115.14
2	A	480	FAD	C4-N3-C2	7.99	121.89	115.14
2	B	480	FAD	C4-N3-C2	7.12	121.16	115.14
2	C	480	FAD	C4X-C4-N3	-5.64	115.72	123.43

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

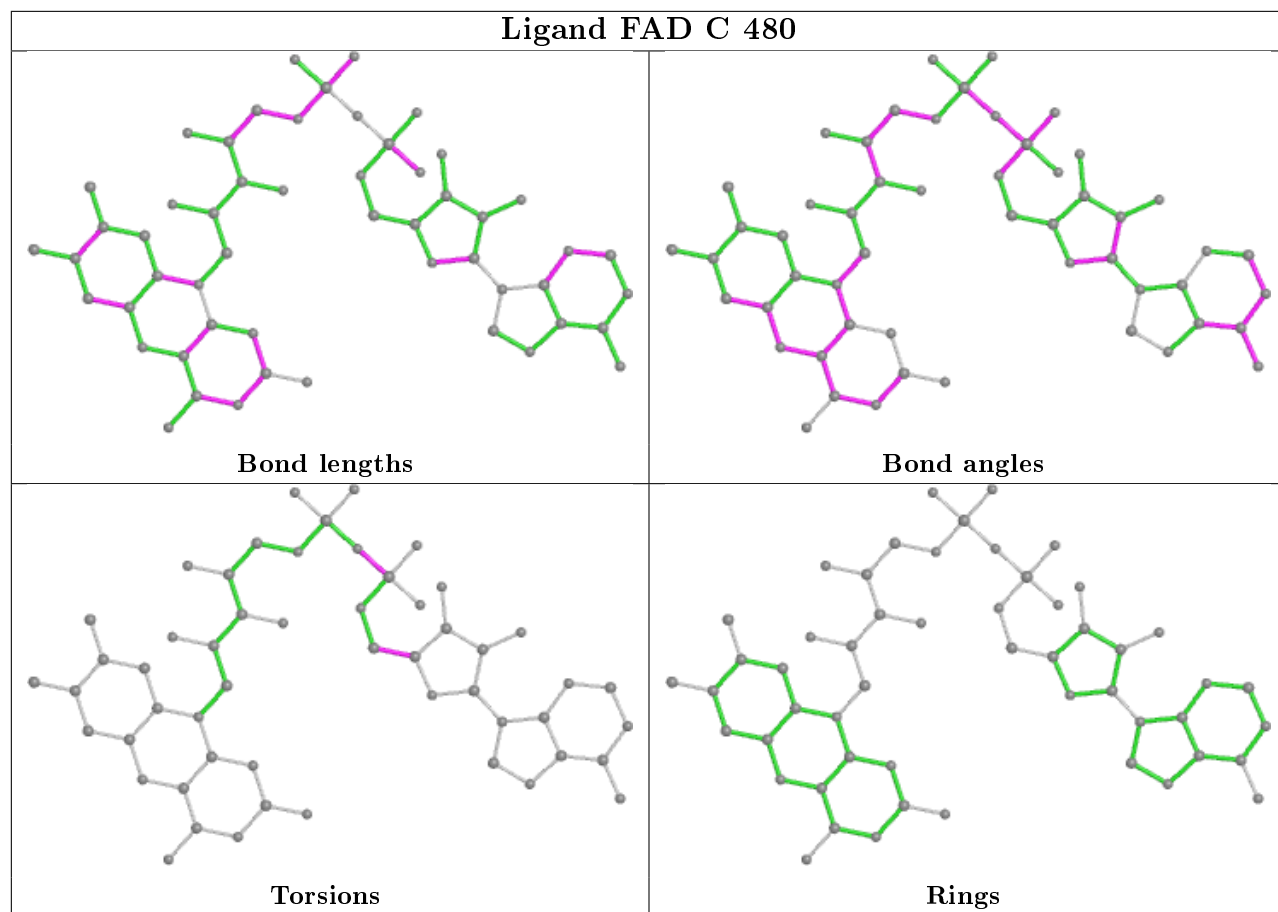
Mol	Chain	Res	Type	Atoms
2	C	480	FAD	O4B-C4B-C5B-O5B
2	A	480	FAD	O4B-C4B-C5B-O5B
2	C	480	FAD	P-O3P-PA-O1A
2	B	480	FAD	O4B-C4B-C5B-O5B
2	D	480	FAD	O4B-C4B-C5B-O5B

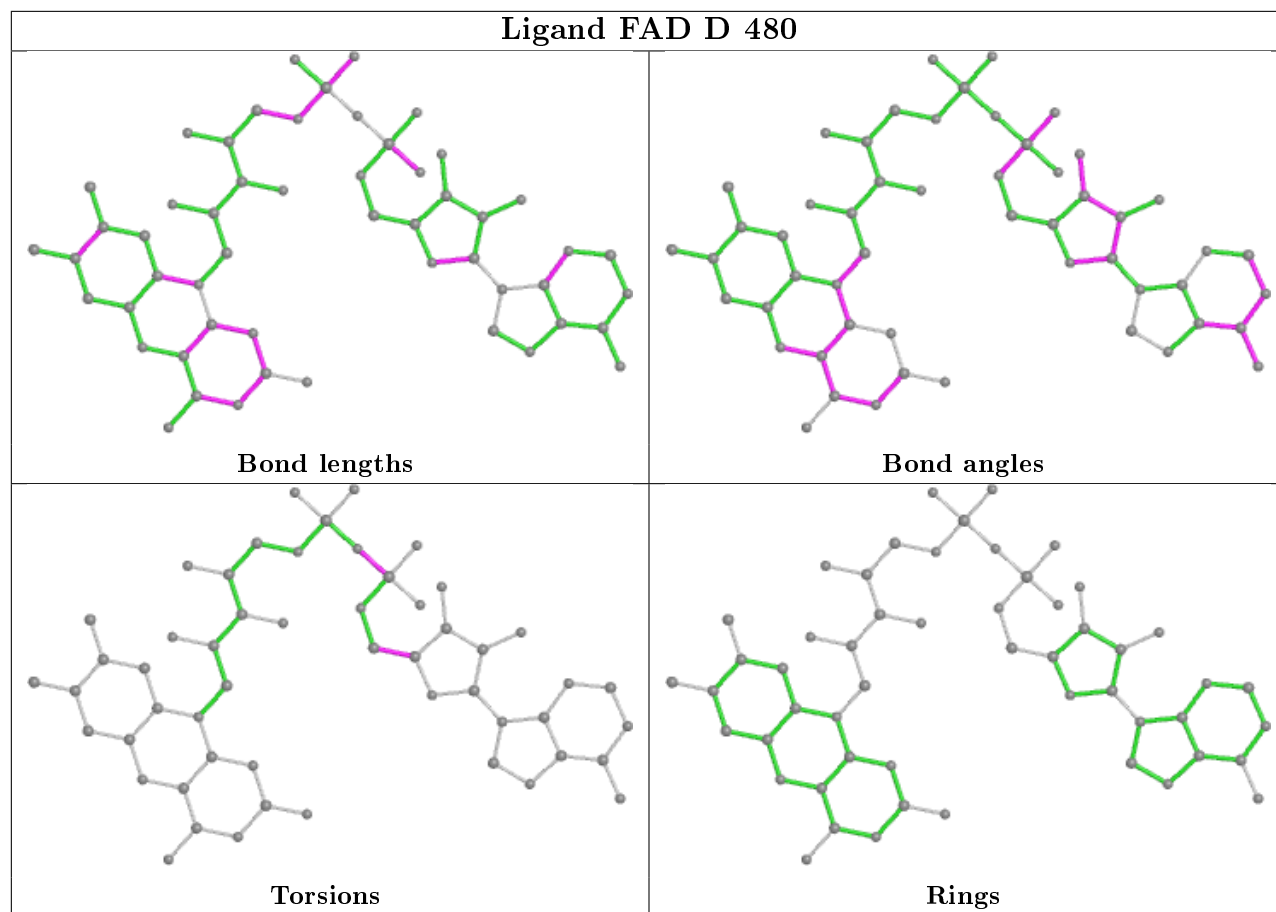
There are no ring outliers.

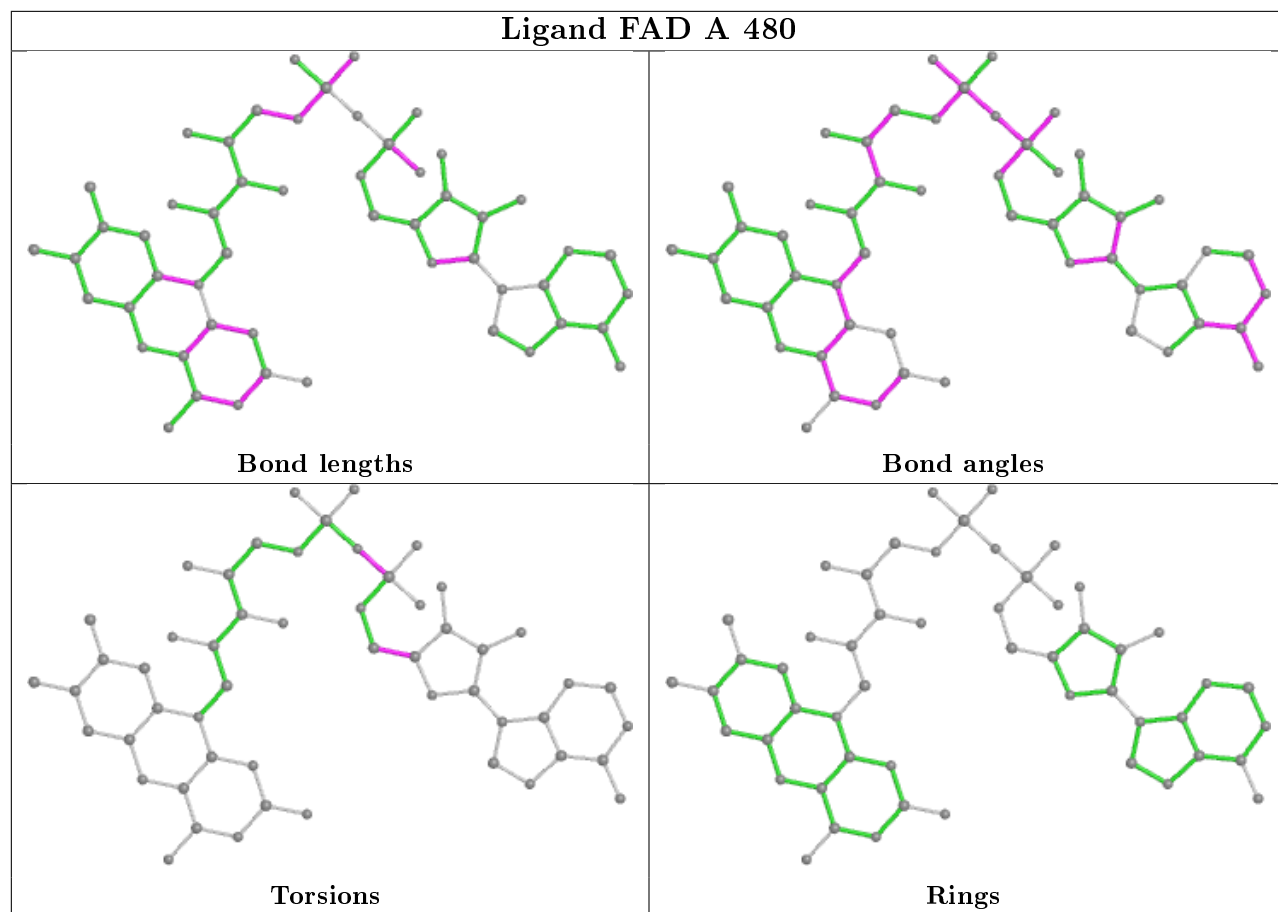
4 monomers are involved in 10 short contacts:

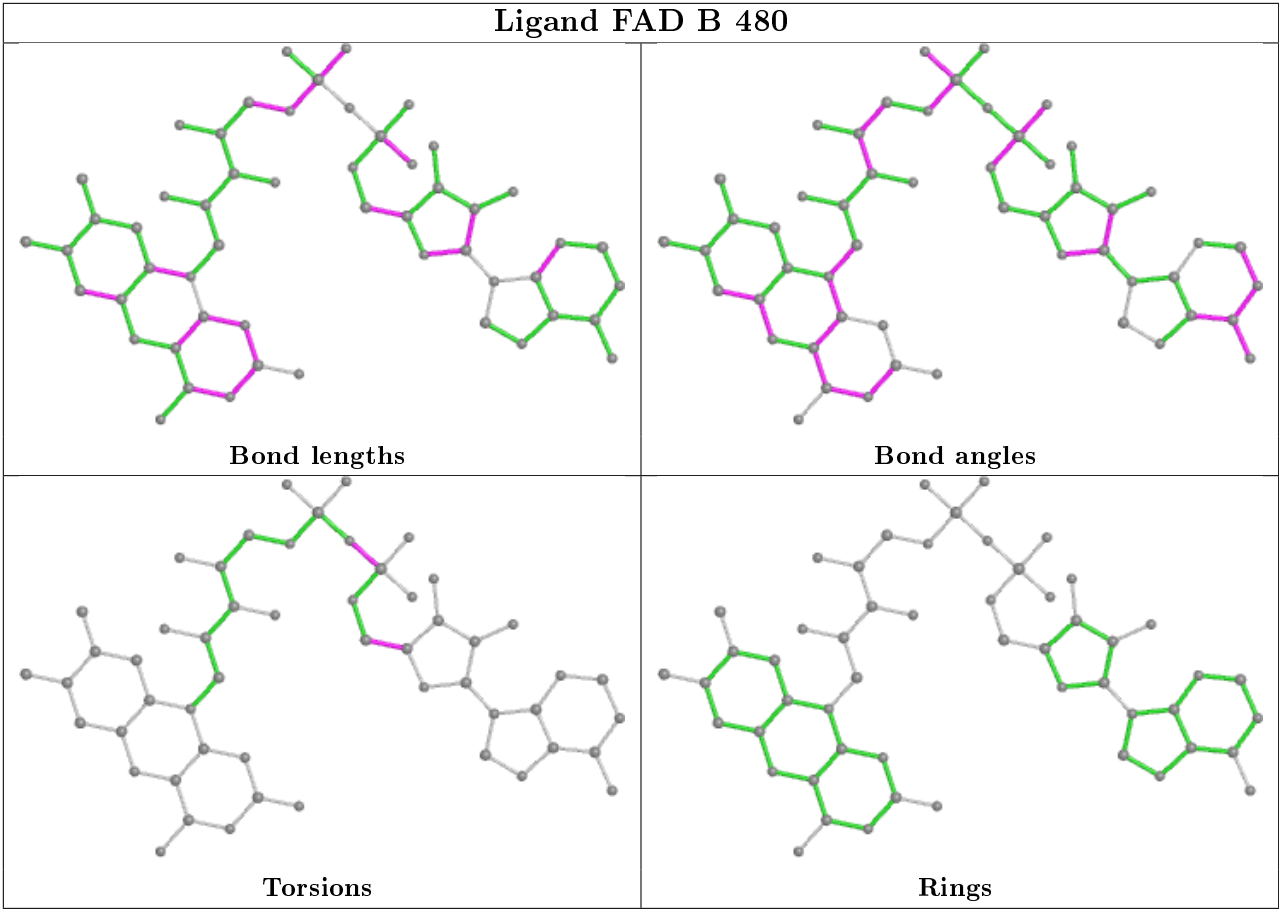
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	480	FAD	3	0
2	D	480	FAD	3	0
2	A	480	FAD	2	0
2	B	480	FAD	2	0

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









5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	258:SER	C	259:ALA	N	2.22
1	C	263:GLN	C	264:THR	N	1.20

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.