



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 06:36 AM UTC

PDB ID : 1DXL / pdb_00001dxl
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 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

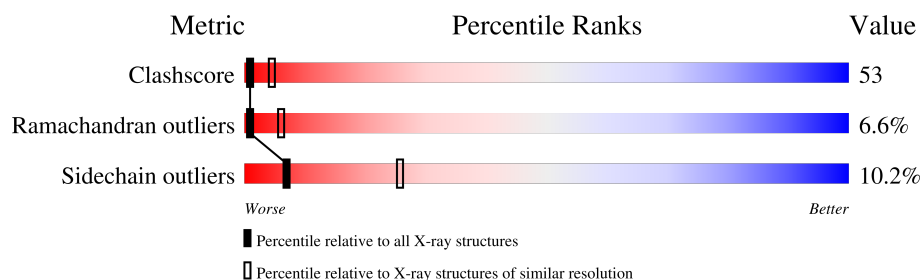
1 Overall quality at a glance

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	190562	2486 (3.20-3.12)
Ramachandran outliers	187476	2405 (3.20-3.12)
Sidechain outliers	187428	2404 (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 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	470	30% 50% 18% ..
1	B	470	34% 47% 17% ..
1	C	470	30% 52% 15% ..
1	D	470	34% 50% 13% ..

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 (CCD ID: 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.

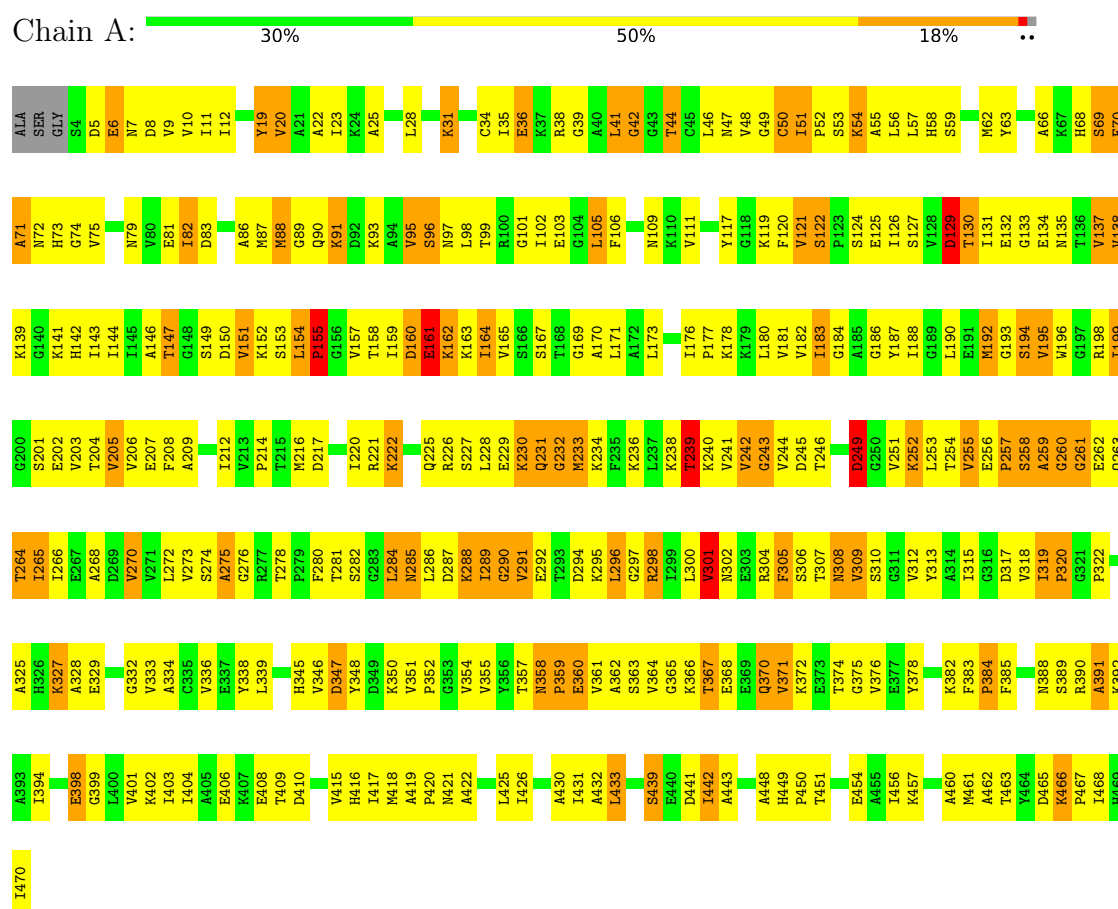
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	33	Total O 33 33	0	0
3	B	23	Total O 23 23	0	0
3	C	25	Total O 25 25	0	0
3	D	23	Total O 23 23	0	0

3 Residue-property plots

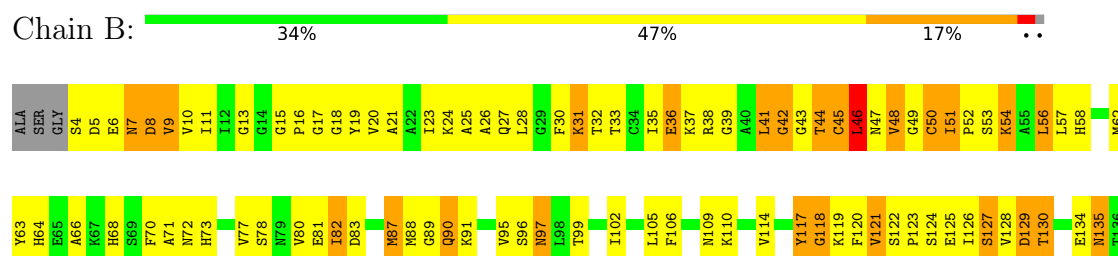
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

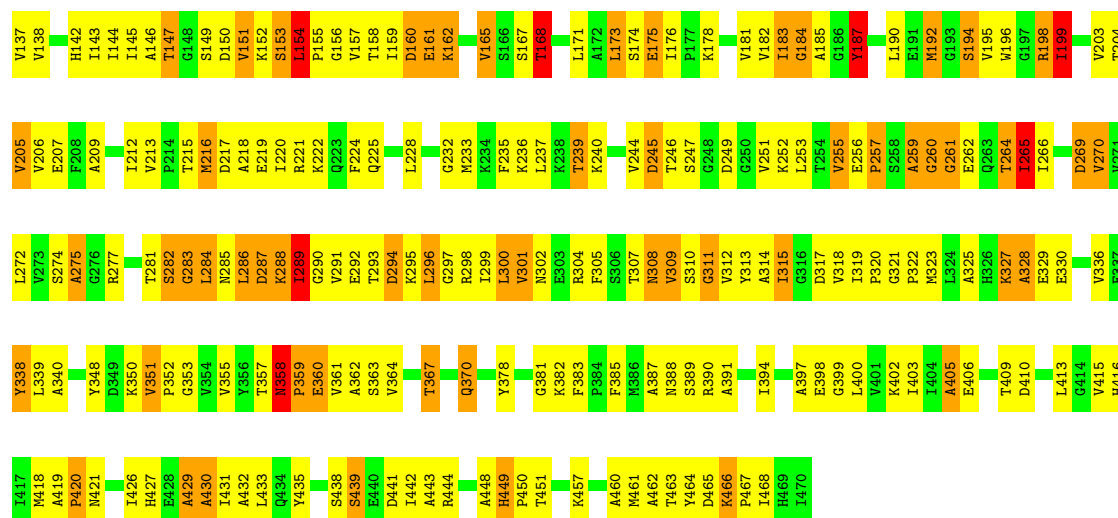
Note EDS was not executed.

• Molecule 1: DIHYDROLIPOAMIDE DEHYDROGENASE



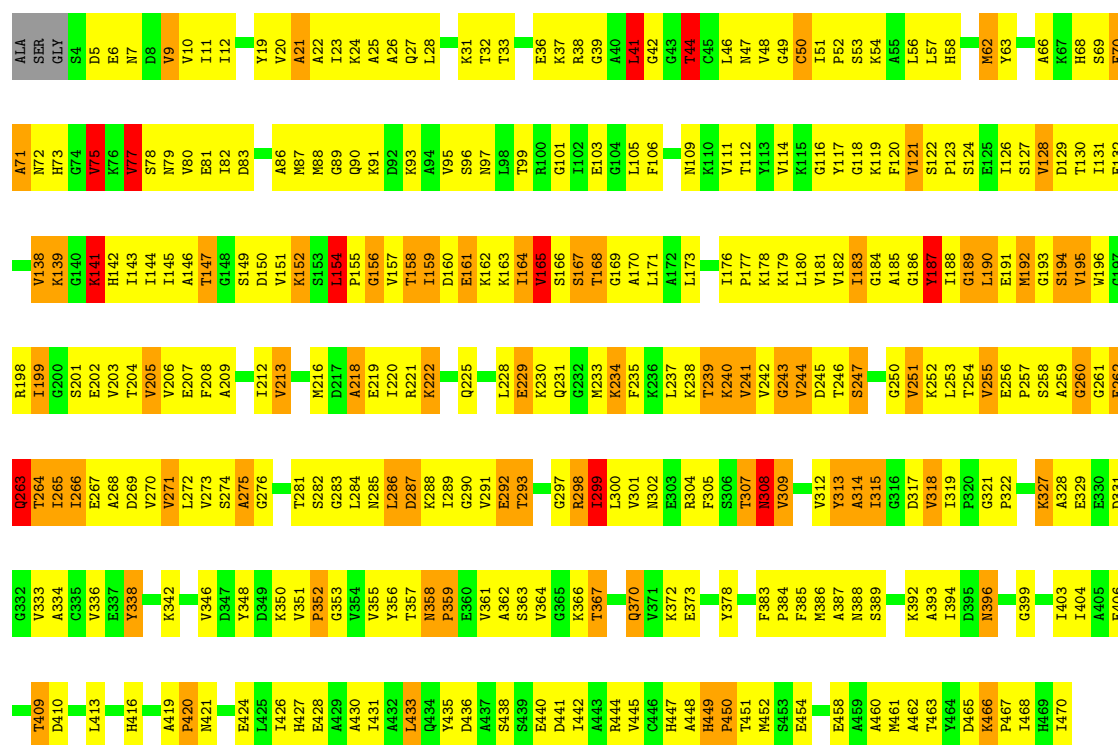
• Molecule 1: DIHYDROLIPOAMIDE DEHYDROGENASE





● Molecule 1: DIHYDROLIPOAMIDE DEHYDROGENASE

Chain C: 30% 52% 15% ..



● Molecule 1: DIHYDROLIPOAMIDE DEHYDROGENASE

Chain D: 34% 50% 13% ..



A422	P352	G283	V205	V138	N72
G423	G353	L284	V206	H142	H73
E424	V354	N285	E207	I143	G74
L425	V355	L286	F208	I144	V75
I426	Y356	D287	A209	I145	K76
H427	T357	K288	I212	A146	V77
E428	H358	I289	V213	T147	S78
A429	F359	G290	V213	G148	N79
A430	V360	V291	N216	S149	V80
I431	V361	E292	D217	D150	E81
A432	A362	T293	A218	D150	I82
L433	S363	D294	E219	V151	D83
S438	V364	K295	I220	K152	L84
S439	G365	R298	R221	S153	A85
E440	K366	F301	K222	L154	A86
D441	T367	N302	Q225	P155	M87
E442	E368	F303	R226	G156	M88
A448	V376	R304	L228	V157	G89
P450	E377	F305	E229	T158	Q90
T451	V380	N308	Q231	I159	K91
S453	V382	V309	G232	D160	A94
E454	F383	G311	M233	E161	V95
A455	V312	V313	K234	K162	S96
I456	F385	A314	L237	I164	N97
K457	M386	I315	K238	V165	L98
E458	S389	V318	T239	S167	G101
A459	R390	I319	V241	L171	I102
A460	A391	P320	V242	A172	E103
M461	K392	G321	G243	L173	G104
A462	A393	P322	V244	I176	F106
T463	I394	M323	D249	P177	N109
Y464	E398	L324	L253	L180	K110
D465	G399	A325	T254	V181	V111
K466	L400	H326	V255	V182	T112
P467	V401	K327	E262	I183	Y113
I468	K402	E329	Q263	G184	G116
H469	I403	F330	T264	A185	Y117
V470	I404	D331	I265	G186	G118
A470	A405	G332	V270	Y187	K119
	E406	V333	V273	L190	F120
	T409	A334	S274	E191	V121
	D410	G335	A275	M192	S122
	L413	V336	G276	G193	P123
	G414	L339	R277	S194	S124
	V415	H345	T278	V195	E125
	H416	V346	E279	W196	I126
	I417	D347	G276	G197	S127
	M418	Y348	R277	R198	V128
	A419	D349	T278	I199	D129
	P420	K350	F280	G200	T130
	N421	V351	T281	S201	I131
			S282	E202	E132
				V203	T136
				T204	V137

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	1.11	14/3541 (0.4%)	1.49	55/4783 (1.1%)
1	B	1.00	4/3541 (0.1%)	1.46	61/4783 (1.3%)
1	C	1.05	9/3527 (0.3%)	1.46	53/4762 (1.1%)
1	D	1.04	8/3528 (0.2%)	1.43	47/4765 (1.0%)
All	All	1.05	35/14137 (0.2%)	1.46	216/19093 (1.1%)

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

The worst 5 of 35 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	263	GLN	C-N	-9.67	1.20	1.33
1	D	301	VAL	CA-CB	-7.79	1.47	1.55
1	A	301	VAL	CA-CB	-6.95	1.45	1.55
1	A	289	ILE	CA-CB	-6.62	1.47	1.54
1	C	315	ILE	CA-CB	-6.50	1.43	1.55

The worst 5 of 216 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	358	ASN	CA-C-N	-15.87	103.32	120.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	358	ASN	C-N-CA	-15.87	103.32	120.14
1	B	44	THR	N-CA-C	-15.03	95.40	114.04
1	B	162	LYS	N-CA-C	12.91	129.24	113.23
1	D	399	GLY	N-CA-C	12.28	124.57	112.04

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	356	0
1	B	3487	0	3552	388	0
1	C	3475	0	3543	441	0
1	D	3475	0	3544	359	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	1495	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 53.

The worst 5 of 1495 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	8
1	B	466/470 (99%)	357 (77%)	71 (15%)	38 (8%)	0	3
1	C	463/470 (98%)	367 (79%)	62 (13%)	34 (7%)	1	5
1	D	465/470 (99%)	350 (75%)	90 (19%)	25 (5%)	1	9
All	All	1860/1880 (99%)	1442 (78%)	294 (16%)	124 (7%)	1	6

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%)	333 (89%)	42 (11%)	6	22
1	B	375/375 (100%)	340 (91%)	35 (9%)	8	29
1	C	374/375 (100%)	338 (90%)	36 (10%)	8	28
1	D	374/375 (100%)	335 (90%)	39 (10%)	7	24
All	All	1498/1500 (100%)	1346 (90%)	152 (10%)	7	26

5 of 152 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	34	CYS
1	D	298	ARG
1	D	76	LYS
1	D	194	SER
1	D	384	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 45 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	109	ASN
1	D	7	ASN
1	C	225	GLN
1	C	396	ASN
1	D	68	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry

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	480	-	58,58,58	2.58	17 (29%)	85,89,89	1.31	8 (9%)
2	FAD	B	480	-	58,58,58	2.34	16 (27%)	85,89,89	1.29	8 (9%)
2	FAD	D	480	-	58,58,58	2.31	16 (27%)	85,89,89	1.33	9 (10%)
2	FAD	C	480	-	58,58,58	2.30	19 (32%)	85,89,89	1.27	10 (11%)

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	480	-	-	4/34/50/50	0/6/6/6
2	FAD	B	480	-	-	4/34/50/50	0/6/6/6
2	FAD	D	480	-	-	4/34/50/50	0/6/6/6
2	FAD	C	480	-	-	4/34/50/50	0/6/6/6

The worst 5 of 68 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	480	FAD	P-O3P	-14.34	1.44	1.59
2	D	480	FAD	P-O3P	-11.96	1.46	1.59
2	B	480	FAD	P-O3P	-11.05	1.47	1.59
2	C	480	FAD	P-O3P	-10.52	1.48	1.59
2	C	480	FAD	PA-O2A	-5.26	1.31	1.55

The worst 5 of 35 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	480	FAD	O2A-PA-O3P	4.37	119.08	107.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	480	FAD	O4B-C1B-N9A	-4.25	99.92	108.09
2	B	480	FAD	O2A-PA-O3P	4.05	118.23	107.27
2	A	480	FAD	C4B-O4B-C1B	-3.99	100.65	109.47
2	D	480	FAD	C4B-O4B-C1B	-3.57	101.59	109.47

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

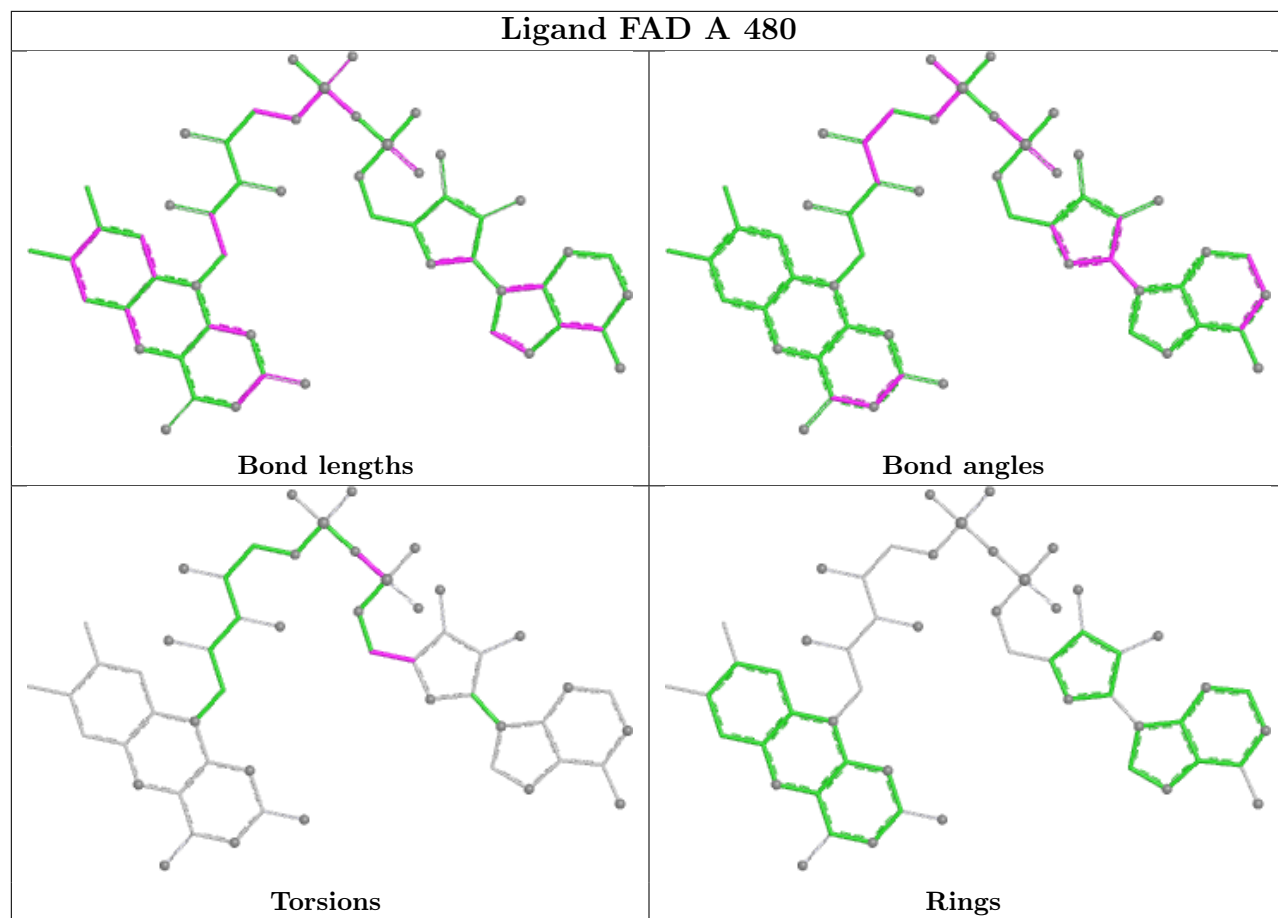
Mol	Chain	Res	Type	Atoms
2	A	480	FAD	O4B-C4B-C5B-O5B
2	C	480	FAD	O4B-C4B-C5B-O5B
2	C	480	FAD	P-O3P-PA-O1A
2	B	480	FAD	O4B-C4B-C5B-O5B
2	A	480	FAD	C3B-C4B-C5B-O5B

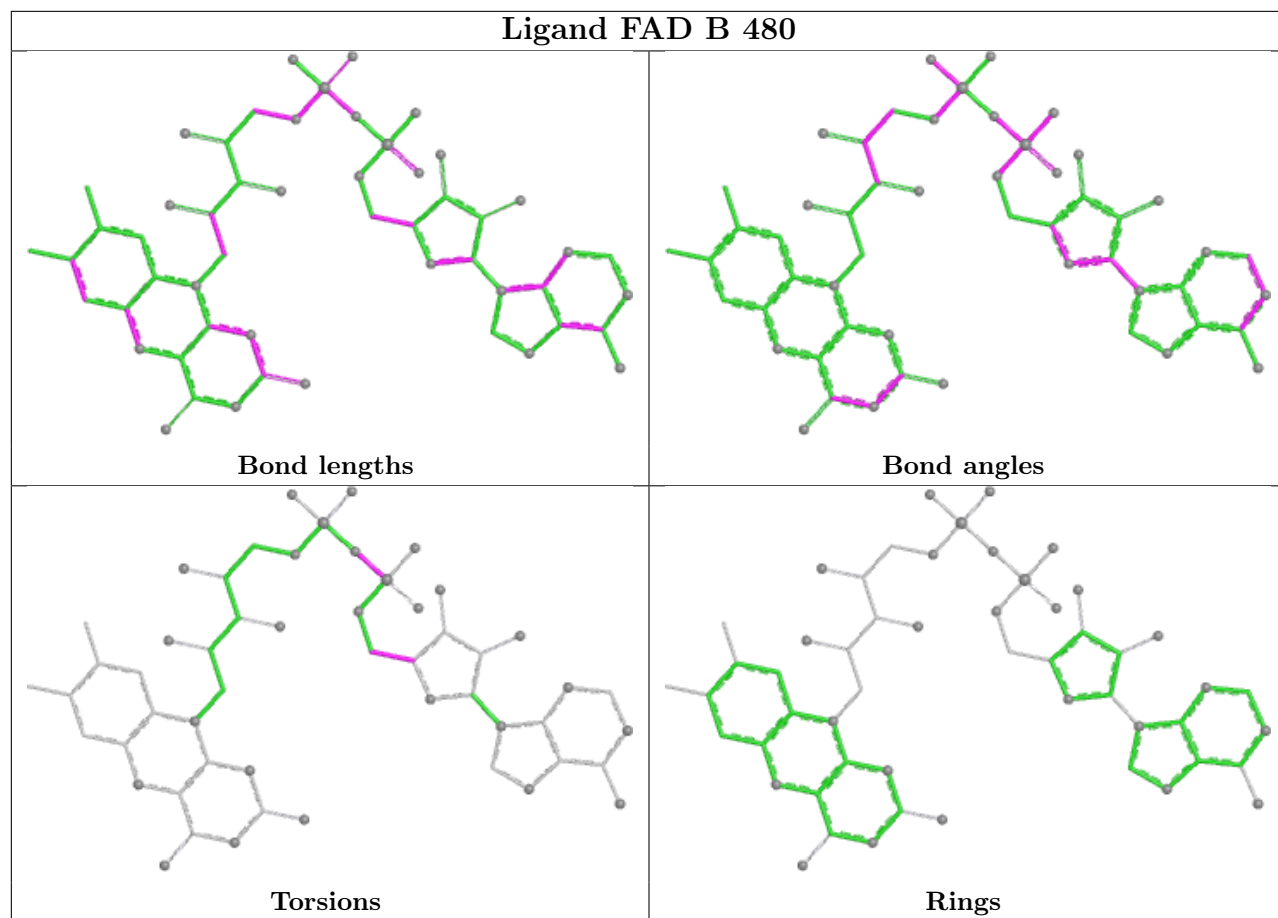
There are no ring outliers.

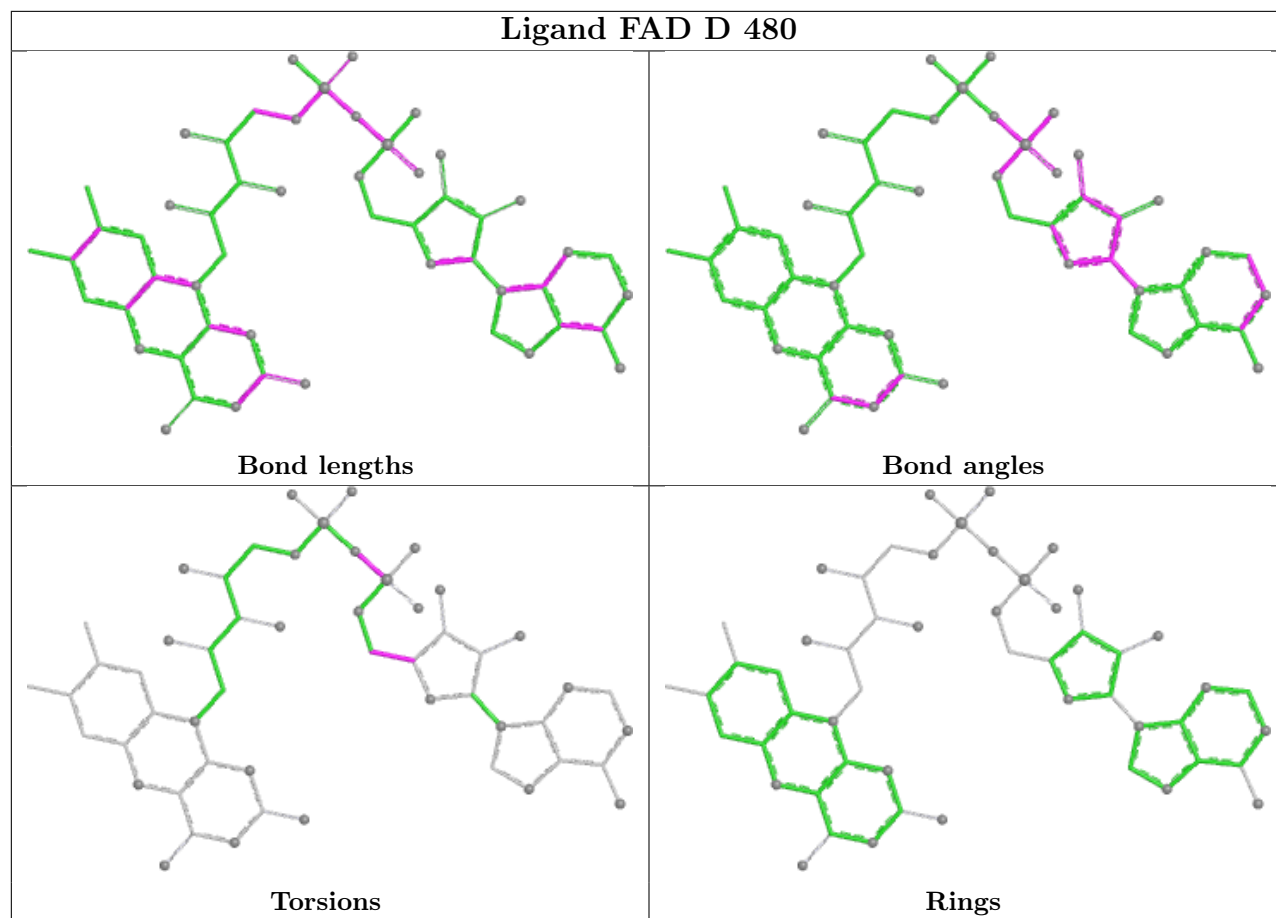
4 monomers are involved in 10 short contacts:

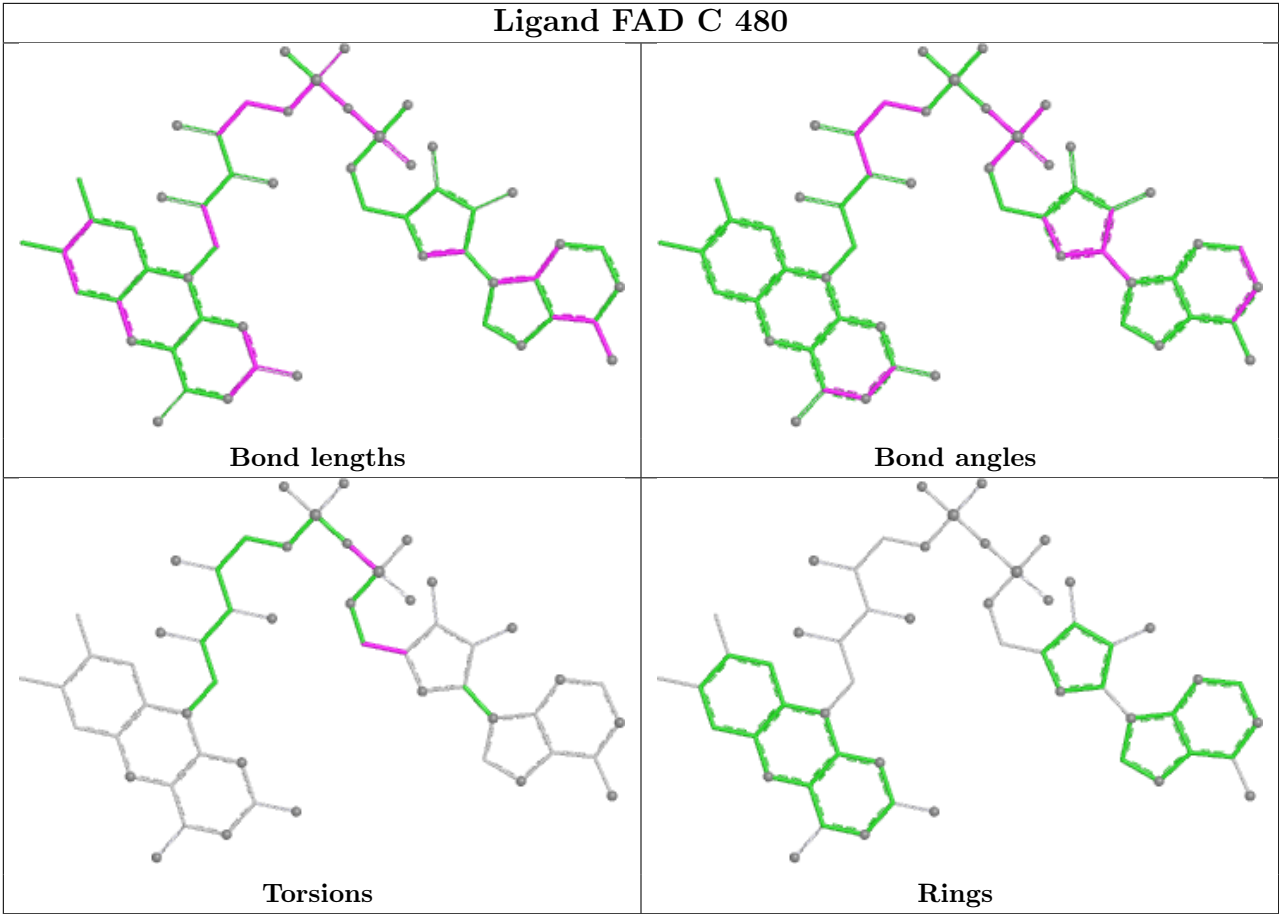
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	480	FAD	2	0
2	B	480	FAD	2	0
2	D	480	FAD	3	0
2	C	480	FAD	3	0

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