



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 7, 2019 – 05:20 PM EDT

PDB ID : 1PYD
Title : CATALYTIC CENTERS IN THE THIAMIN DIPHOSPHATE DEPENDENT
ENZYME PYRUVATE DECARBOXYLASE AT 2.4 ANGSTROMS RESO-
LUTION
Authors : Furey, W.; Dyda, F.
Deposited on : 1993-03-23
Resolution : 2.40 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	:	1.8.0 (224370), CSD as540be (2019)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.4

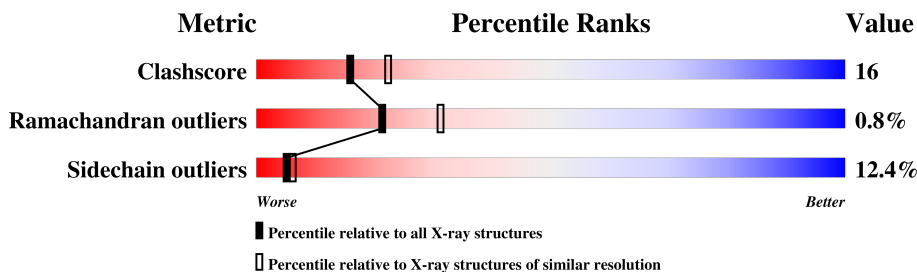
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	122126	3956 (2.40-2.40)
Ramachandran outliers	120053	3897 (2.40-2.40)
Sidechain outliers	120020	3898 (2.40-2.40)

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. 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	556	
1	B	556	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8316 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 PYRUVATE DECARBOXYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	537	Total	C	N	O	S	0	0	0
			4130	2638	694	782	16			
1	B	537	Total	C	N	O	S	0	0	0
			4130	2638	694	782	16			

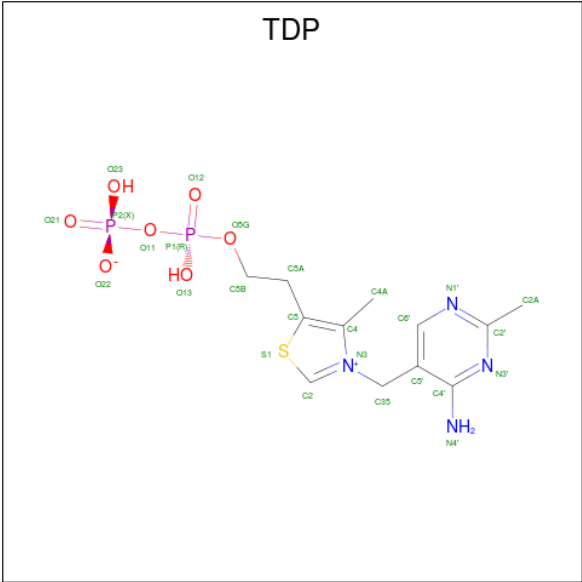
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	55	ALA	ARG	CONFLICT	UNP P06169
A	143	ALA	CYS	CONFLICT	UNP P06169
A	206	ALA	VAL	CONFLICT	UNP P06169
A	208	VAL	ALA	CONFLICT	UNP P06169
A	538	ILE	VAL	CONFLICT	UNP P06169
A	551	LYS	GLU	CONFLICT	UNP P06169
B	55	ALA	ARG	CONFLICT	UNP P06169
B	143	ALA	CYS	CONFLICT	UNP P06169
B	206	ALA	VAL	CONFLICT	UNP P06169
B	208	VAL	ALA	CONFLICT	UNP P06169
B	538	ILE	VAL	CONFLICT	UNP P06169
B	551	LYS	GLU	CONFLICT	UNP P06169

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is THIAMIN DIPHOSPHATE (three-letter code: TDP) (formula: C₁₂H₁₈N₄O₇P₂S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
3	A	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
3	B	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		

- Molecule 4 is water.

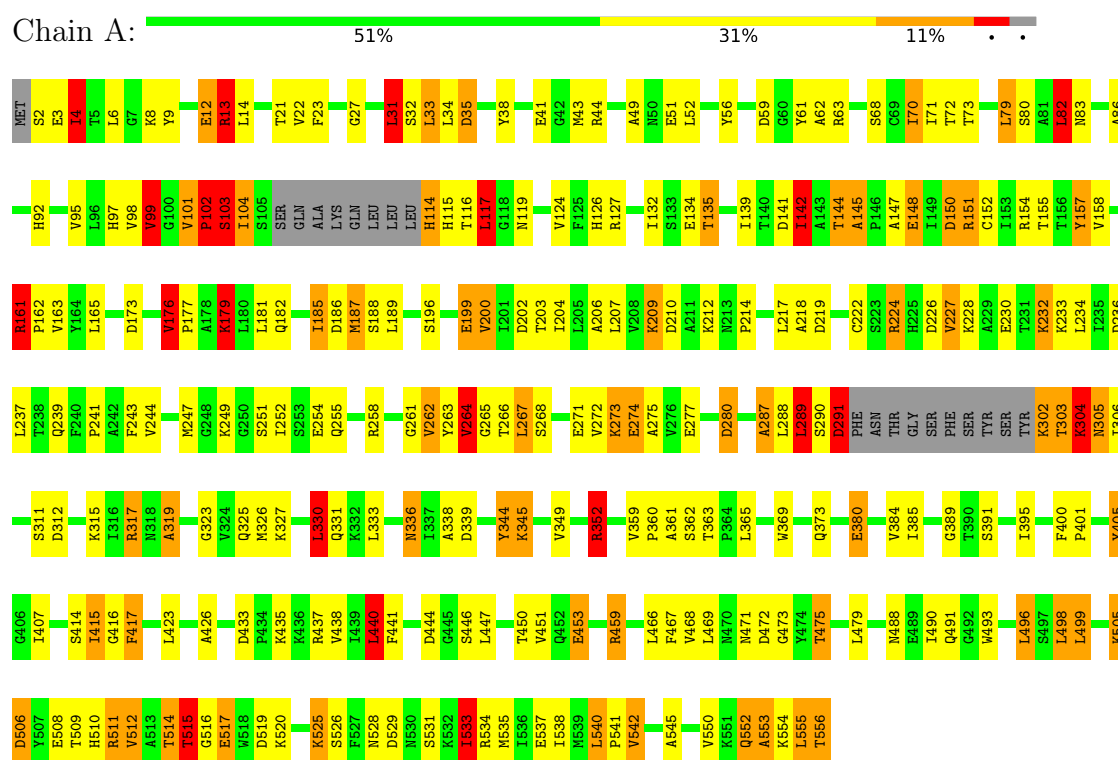
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	O	0	0
			1	1		
4	B	1	Total	O	0	0
			1	1		

3 Residue-property plots

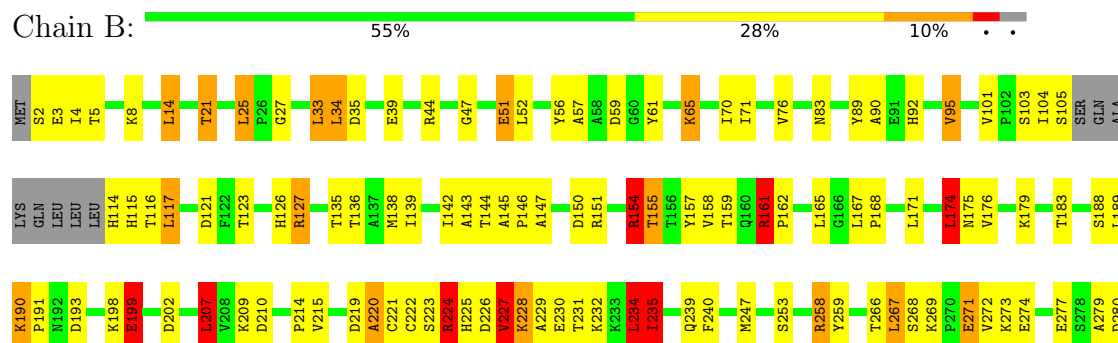
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according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



• Molecule 1: PYRUVATE DECARBOXYLASE



L281	L282	L283	S284	V285	G286	A287	L288	L289	S290	D291	PHE	ASN	THR	GLY	SER	PHE	SER	SER	TYR	SER	TYR	K302	T303	K304	N305	E308	F309	H310	K315	T316	K317	K327	F328	K332	T337	A338	D339	K342	G343	Y344	V349	P350	A351	K352	N356	P364	M370	Q373	
E380	G381	D382	I385	T388	T399	F400	P401	N402	M403	T404	Q409	V410	L411	T418	T422	L423	A426	F427	E431	I432	D433	P434	K435	K436	L440	F441	D444	G445	S446	L447	V451	T456	M457	I458	R459	Y465	L466	N470	N471	D472	G473	Y474	T475	I476	E477				
K478	L479	I480	H481	G482	P483	K484	A485	Q486	Q491	L496	S497	L498	L499	P500	T501	A504	K505	D506	Y507	E508	T509	V512	E517	N518	D519	D524	K525	N528	D529	R534	N535	E536	E537	I538	N539	L540	P541	V542	P546	Q547	N548	L549	V550	K551	Q552	A553	K554	L555	T556

4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	141.95Å 74.67Å 119.95Å 90.00° 116.39° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.40	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.40)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	GPRLSA, X-PLOR	Depositor
R, R_{free}	0.197 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8316	wwPDB-VP
Average B, all atoms (Å ²)	10.0	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: MG, TDP

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	1.06	0/4215	2.24	190/5728 (3.3%)
1	B	1.04	2/4215 (0.0%)	2.27	165/5728 (2.9%)
All	All	1.05	2/8430 (0.0%)	2.26	355/11456 (3.1%)

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
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	39	GLU	CD-OE1	-5.29	1.19	1.25
1	B	517	GLU	CD-OE1	-5.01	1.20	1.25

The worst 5 of 355 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	161	ARG	CD-NE-CZ	23.23	156.13	123.60
1	B	459	ARG	NE-CZ-NH1	22.85	131.73	120.30
1	B	459	ARG	NE-CZ-NH2	-21.18	109.71	120.30
1	B	524	ASP	CB-CG-OD2	19.94	136.25	118.30
1	A	161	ARG	NE-CZ-NH1	19.36	129.98	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	352	ARG	Sidechain
1	B	154	ARG	Sidechain

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	4130	0	4150	139	1
1	B	4130	0	4151	126	1
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	26	0	16	3	0
3	B	26	0	16	3	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
All	All	8316	0	8333	260	1

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 16.

The worst 5 of 260 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)
3:B:557:TDP:H2	3:B:557:TDP:C2	0.97	1.49
3:A:557:TDP:C2	3:A:557:TDP:H2	0.97	1.46
1:B:267:LEU:HD11	1:B:552:GLN:HB2	1.47	0.93
1:B:4:ILE:HD11	1:B:8:LYS:HG2	1.56	0.86
1:B:505:LYS:H	1:B:505:LYS:HD2	1.45	0.81

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:ARG:NH1	1:B:199:GLU:OE2[2_555]	2.08	0.12

5.3 Torsion angles

5.3.1 Protein backbone

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	531/556 (96%)	490 (92%)	37 (7%)	4 (1%)	21	31
1	B	531/556 (96%)	492 (93%)	34 (6%)	5 (1%)	19	27
All	All	1062/1112 (96%)	982 (92%)	71 (7%)	9 (1%)	21	31

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	103	SER
1	A	227	VAL
1	A	304	LYS
1	B	288	LEU
1	B	289	LEU

5.3.2 Protein sidechains

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	447/464 (96%)	389 (87%)	58 (13%)	4	5
1	B	447/464 (96%)	394 (88%)	53 (12%)	6	7
All	All	894/928 (96%)	783 (88%)	111 (12%)	5	6

5 of 111 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	498	LEU

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Mol	Chain	Res	Type
1	B	33	LEU
1	B	466	LEU
1	A	505	LYS
1	A	533	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	20	ASN
1	B	83	ASN
1	B	225	HIS
1	A	552	GLN
1	B	213	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](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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	TDP	A	557	2	22,27,27	1.22	3 (13%)	26,40,40	1.61	6 (23%)
3	TDP	B	557	2	22,27,27	1.41	3 (13%)	26,40,40	1.83	10 (38%)

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
3	TDP	A	557	2	-	6/16/17/17	0/2/2/2
3	TDP	B	557	2	-	4/16/17/17	0/2/2/2

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	557	TDP	P2-O11	3.19	1.64	1.60
3	B	557	TDP	C2'-N3'	-2.51	1.29	1.34
3	A	557	TDP	C35-N3	2.45	1.53	1.48
3	A	557	TDP	P2-O22	-2.39	1.45	1.54
3	A	557	TDP	C4'-N3'	2.05	1.38	1.35

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	557	TDP	C5A-C5-C4	4.36	130.93	127.43
3	A	557	TDP	C5A-C5-C4	3.84	130.52	127.43
3	A	557	TDP	C2A-C2'-N1'	3.20	120.66	117.14
3	A	557	TDP	O22-P2-O21	3.04	122.53	110.53
3	B	557	TDP	C4A-C4-C5	-3.00	121.05	127.60

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

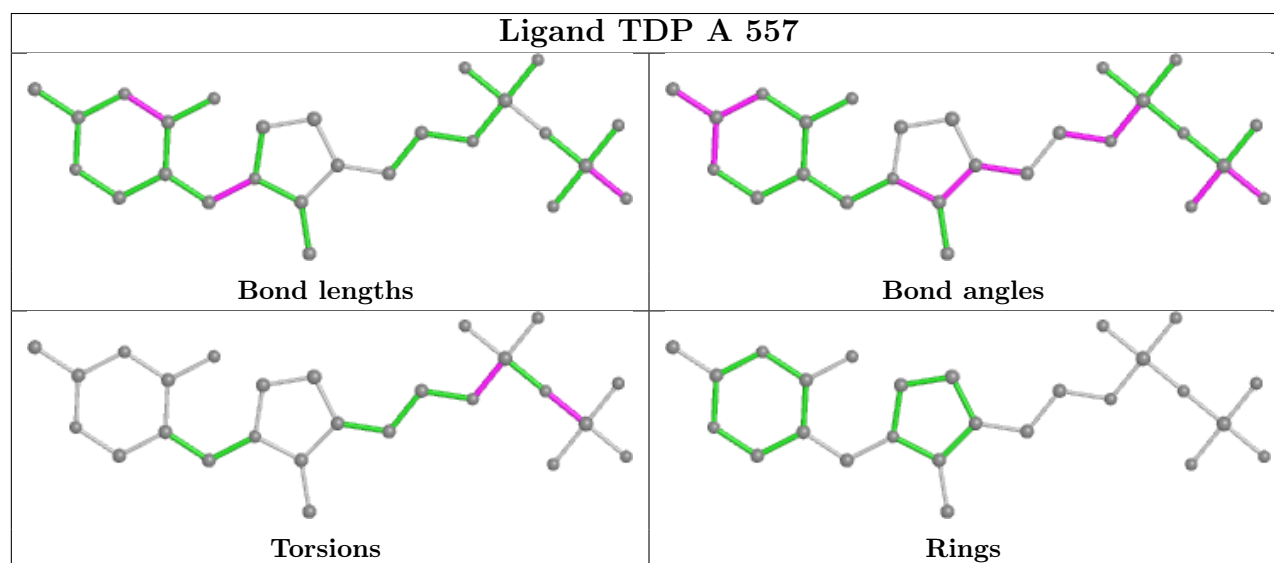
Mol	Chain	Res	Type	Atoms
3	B	557	TDP	C4-C5-C5A-C5B
3	A	557	TDP	C5B-O5G-P1-O13
3	B	557	TDP	P1-O11-P2-O23
3	A	557	TDP	P1-O11-P2-O23
3	A	557	TDP	C5B-O5G-P1-O12

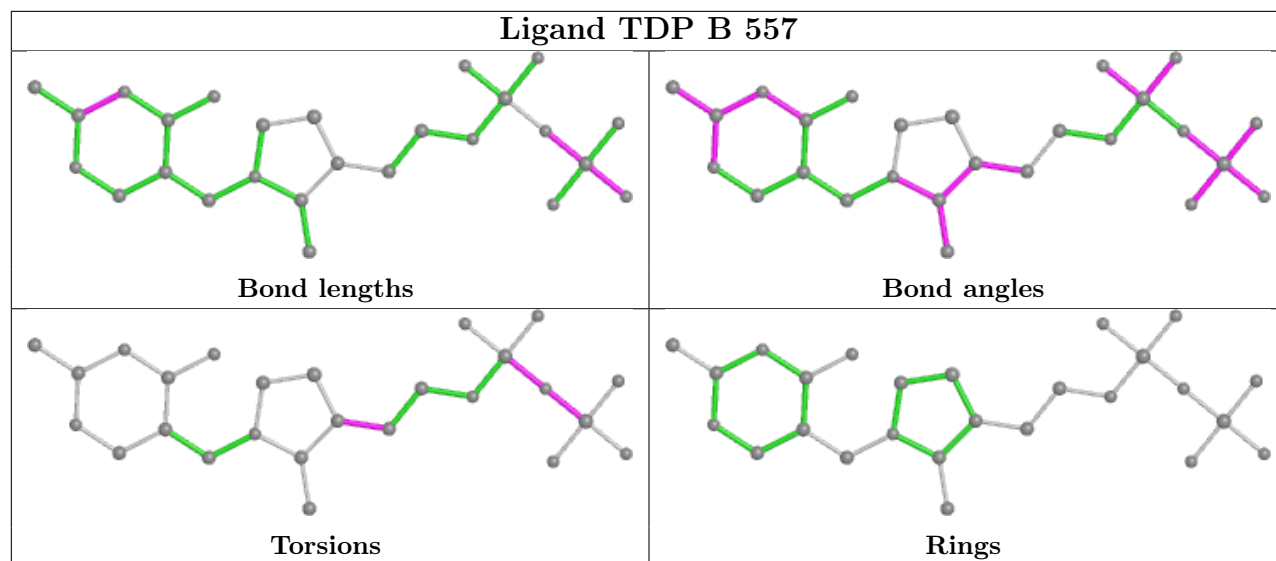
There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	557	TDP	3	0
3	B	557	TDP	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 [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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.