



wwPDB X-ray Structure Validation Summary Report ⓘ

May 15, 2020 – 07:04 am BST

PDB ID : 1B0P
Title : CRYSTAL STRUCTURE OF PYRUVATE-FERREDOXIN OXIDOREDUCTASE FROM DESULFOVIBRIO AFRICANUS
Authors : Chabriere, E.; Charon, M.H.; Volbeda, A.
Deposited on : 1998-11-12
Resolution : 2.31 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

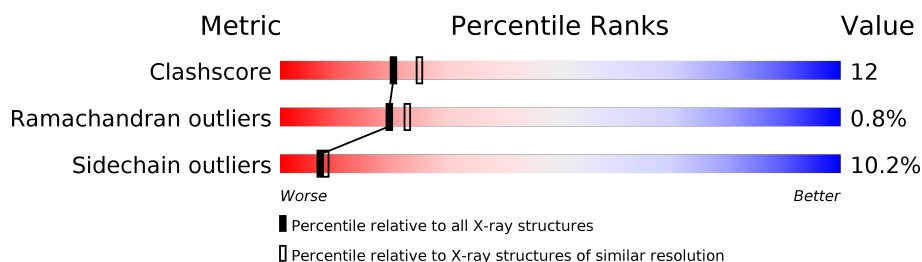
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.31 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	6604 (2.34-2.30)
Ramachandran outliers	138981	6523 (2.34-2.30)
Sidechain outliers	138945	6523 (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 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	1231	
1	B	1231	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 19411 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 PROTEIN (PYRUVATE-FERREDOXIN OXIDOREDUCTASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1231	Total	C	N	O	S	0	0	0
			9382	5941	1599	1783	59			
1	B	1231	Total	C	N	O	S	0	0	0
			9382	5941	1599	1783	59			

- 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 CALCIUM ION (three-letter code: CA) (formula: Ca).

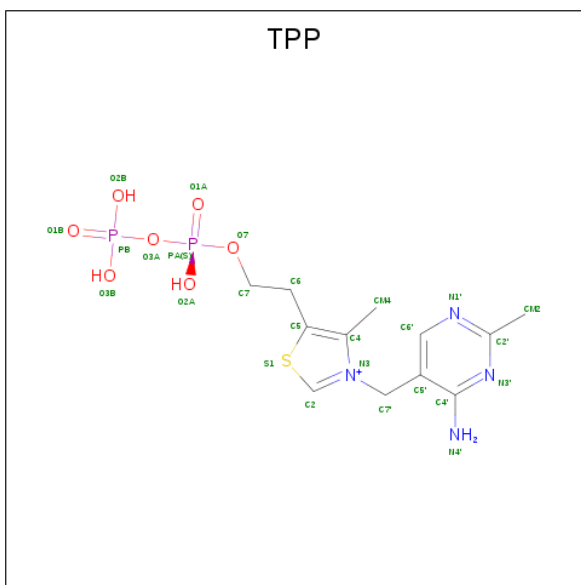
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Ca	0	0
			1	1		
3	A	1	Total	Ca	0	0
			1	1		

- Molecule 4 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	Fe	S	0	0
			8	4	4		
4	A	1	Total	Fe	S	0	0
			8	4	4		
4	A	1	Total	Fe	S	0	0
			8	4	4		
4	B	1	Total	Fe	S	0	0
			8	4	4		
4	B	1	Total	Fe	S	0	0
			8	4	4		
4	B	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 5 is THIAMINE DIPHOSPHATE (three-letter code: TPP) (formula: C₁₂H₁₉N₄O₇P₂S).



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

- Molecule 6 is water.

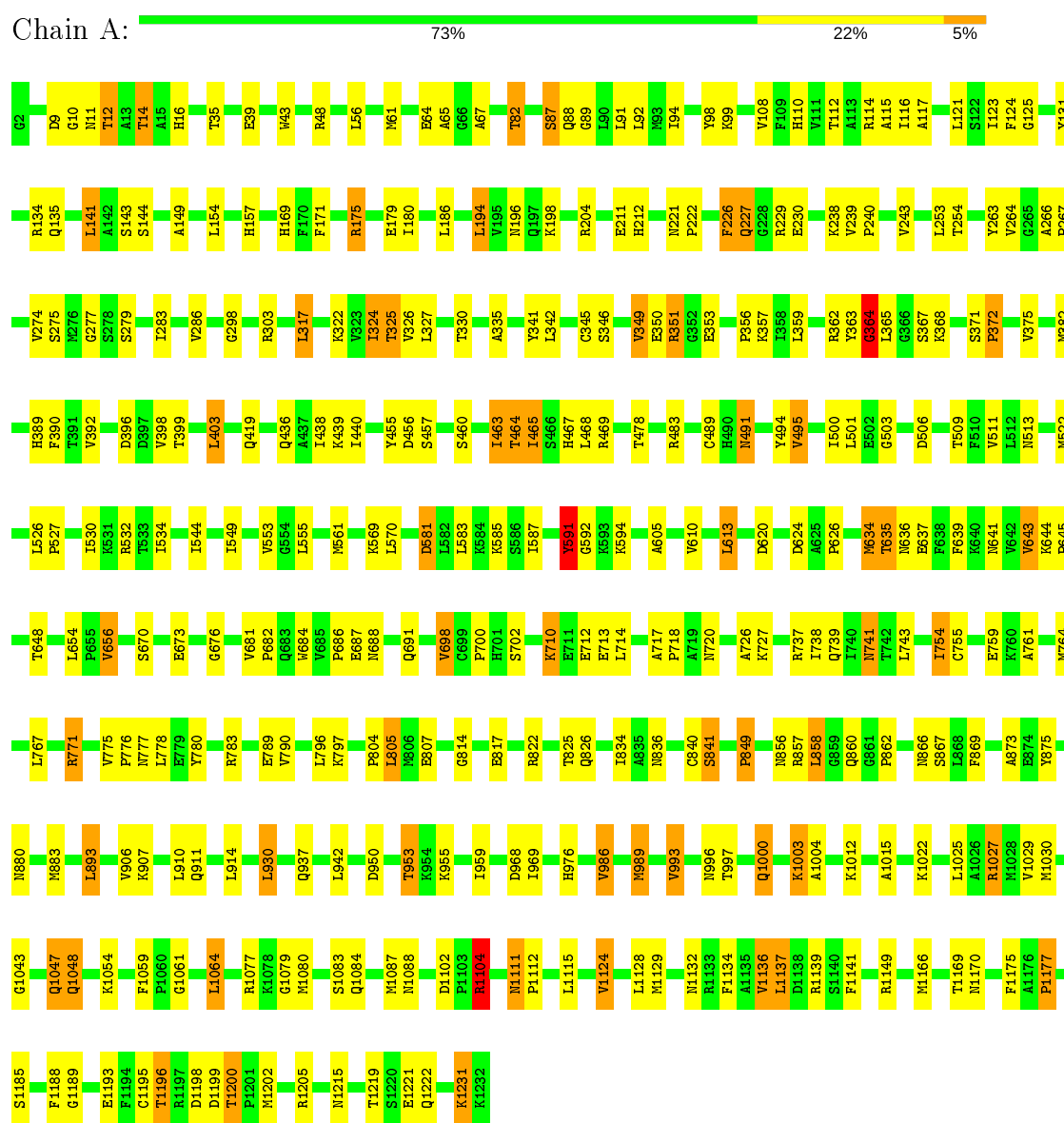
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	273	Total O 273 273	0	0
6	B	270	Total O 270 270	0	0

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: PROTEIN (PYRUVATE-FERREDOXIN OXIDOREDUCTASE)



• Molecule 1: PROTEIN (PYRUVATE-FERREDOXIN OXIDOREDUCTASE)

Chain B:



G1189	K1054	Q937	E789	G668	L570	D446	D338	H212	H110	G2
E1190	L1064	L942	V790	B673	A571	L447	P339	V215	R114	D9
T1196	L1072	D950	L796	K674	V573	A449	L342	G217	T116	N11
T1200	L1076	L951	L805	P682	D581	S454	C945	N221	F124	T12
M1201	R1077	Y952	L805	Q683	L582	Y455	S346	P222	A13	A13
M1202	R1077	T953	L805	Q683	L583	D456	S346	F226	G125	A15
Q1214	K954	K954	F808	V685	I587	S457	V349	Q227	D126	H16
M1215	M1080	K955	E817	P686	A590	S460	E350	H27	H127	
T1219	S1083	I959	V821	E687	A590	G461	R351	N233	Q128	A20
S1220	Q1084	F960	V821	Q691	Y591	G462	G352	N233	Y131	E23
E1221	D1085	G961	T825	C692	K593	T464	E353	P234		
K1228	V1086	W965	N825	N693	K594	L465	P356	Y235	R134	A26
M1087	M1087	W965	N832	C695	G595	S466	K357	Y236		I27
N1088	N1088		W832	C695	G595	H467	P356	V239	M140	
D1102	D1102	D968	N836	V698	K997	L468	L359	P240	L141	E39
P1103	P1103	I969	S841	I704	V599	R469		I242	A142	D42
R1104	H976	H976	S841	I704	V599	P474	Y363	V264	S144	W43
K1110	V986	V986	P849	K710	A605	T478	G364	L253	Q147	A44
N1111	F987	F987	N856	E711	V606	V487	L365	Y258	E148	A45
P1112	V988	V988	R857	E712	D607	N491	S367	K368	A149	Q46
L1115	L1115	L1115	L858	E713	A609	V491	K368	V263		G47
V1124	E932	E932	G859	L714	V610	T611	P372	V264	L154	R48
N1132	V993	V993	Q860	N720	S612	V495		V274		I51
V1136	N996	N996	S867	K727	L613	L501	Y379	G277	H157	L56
L1137	Q1000	Q1000	F869	K729	Q614	D606	N382	S278	S163	M61
D1138	K1003	K1003	A873	F736	P619	T509	H389	I283	N164	Q62
R1139	A1004	A1004	E874	R737	W622	T509	F390	E284	M168	S83
S1140	T1005	T1005	I738	D624	K623	N513	T391	K296	H169	B64
F1141	G1008	G1008	N879	Q739	D624	N513	V392	I297	F171	A67
P1142	M1008	M1008	N880	I740	A625	W622	D396	G298	R175	V71
E1143	E1143	E1143	N881	N741	P626	A627	D397	L299		
K1146	K1012	K1012	S882	S882	M634	L526	V398	G298	E179	T82
R1147	K1018	K1018	N883	I754	T635	P527	T399	G400	I180	T83
L1148	K1022	K1022	R887	C755	N636	S528	G400	R303	Q181	F84
M1166	L1025	L1025	L893	M764	K639	G529	L403	R306		S87
T1169	A1026	A1026	S903	L767	K640	W531	V185	V309	E184	Q88
F1172	M1028	M1028	V906	R771	V643	T533	Q419	L317	L186	Q89
F1175	V1029	V1029	K907	Q774	K644	I534	Q421	K322	D187	L90
A1176	M1030	M1030	Q911	Q774	P645	N536	G426	V323	Y188	L91
P1177	Y1034	Y1034	L778	E779	T648	L555	V431	I324	D190	N93
S1185	V1040	V1040	L914	V780	G651	M561	K435	T325	L194	I94
V1186	D919	D919	R783	E780	L654	F567	I438	L327	L194	N97
D1187	Q1047	Q1047	L784	R783	L654	F567	I438	V326	K198	K99
E1188	E1049	E1049	E785	E785	P655	F568	K439	L327	R204	

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	84.80 Å 144.90 Å 203.00 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.31	Depositor
% Data completeness (in resolution range)	68.6 (6.00-2.31)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
Refinement program	X-PLOR 3.854	Depositor
R, R_{free}	0.199 , 0.271	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	19411	wwPDB-VP
Average B, all atoms (Å ²)	6.0	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, CA, SF4, TPP

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	0.77	1/9584 (0.0%)	0.92	9/12954 (0.1%)
1	B	0.77	0/9584	0.92	14/12954 (0.1%)
All	All	0.77	1/19168 (0.0%)	0.92	23/25908 (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	2
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	489	CYS	CB-SG	-5.80	1.72	1.81

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	317	LEU	CA-CB-CG	6.78	130.90	115.30
1	A	822	ARG	NE-CZ-NH2	-6.65	116.98	120.30
1	B	317	LEU	CA-CB-CG	6.56	130.39	115.30
1	B	1077	ARG	NE-CZ-NH1	6.48	123.54	120.30
1	A	1104	ARG	NE-CZ-NH2	-6.24	117.18	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	591	TYR	Sidechain
1	B	1034	TYR	Sidechain
1	B	591	TYR	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	9382	0	9262	235	0
1	B	9382	0	9262	255	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	24	0	0	1	0
4	B	24	0	0	1	0
5	A	26	0	16	1	0
5	B	26	0	16	1	0
6	A	273	0	0	14	0
6	B	270	0	0	20	0
All	All	19411	0	18556	459	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 12.

The worst 5 of 459 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:A:639:PHE:HA	1:A:643:VAL:HG13	1.41	1.00
1:A:64:GLU:HG3	1:A:89:GLY:HA2	1.46	0.95
1:B:635:THR:HG23	1:B:639:PHE:HB3	1.48	0.95
1:B:64:GLU:HG3	1:B:89:GLY:HA2	1.49	0.93
6:A:1639:HOH:O	1:B:874:GLU:HB3	1.76	0.85

There are no symmetry-related clashes.

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	1229/1231 (100%)	1177 (96%)	43 (4%)	9 (1%)	22	26
1	B	1229/1231 (100%)	1184 (96%)	35 (3%)	10 (1%)	19	23
All	All	2458/2462 (100%)	2361 (96%)	78 (3%)	19 (1%)	19	23

5 of 19 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	87	SER
1	A	1231	LYS
1	B	87	SER
1	B	594	LYS
1	B	1231	LYS

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	978/978 (100%)	883 (90%)	95 (10%)	8	9
1	B	978/978 (100%)	873 (89%)	105 (11%)	6	7
All	All	1956/1956 (100%)	1756 (90%)	200 (10%)	7	8

5 of 200 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1137	LEU

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Mol	Chain	Res	Type
1	B	226	PHE
1	B	1047	GLN
1	A	1200	THR
1	B	143	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 89 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1084	GLN
1	B	128	GLN
1	B	1048	GLN
1	A	1088	ASN
1	A	1215	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 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 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
5	TPP	A	1236	2	22,27,27	2.31	4 (18%)	29,40,40	1.79	7 (24%)
5	TPP	B	1236	2	22,27,27	2.28	5 (22%)	29,40,40	1.64	7 (24%)
4	SF4	A	1235	1	0,12,12	0.00	-	-	-	-
4	SF4	B	1233	1	0,12,12	0.00	-	-	-	-
4	SF4	A	1233	1	0,12,12	0.00	-	-	-	-
4	SF4	A	1234	1	0,12,12	0.00	-	-	-	-
4	SF4	B	1234	1	0,12,12	0.00	-	-	-	-
4	SF4	B	1235	1	0,12,12	0.00	-	-	-	-

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
5	TPP	A	1236	2	-	5/16/17/17	0/2/2/2
5	TPP	B	1236	2	-	5/16/17/17	0/2/2/2
4	SF4	A	1235	1	-	-	0/6/5/5
4	SF4	B	1233	1	-	-	0/6/5/5
4	SF4	A	1233	1	-	-	0/6/5/5
4	SF4	A	1234	1	-	-	0/6/5/5
4	SF4	B	1234	1	-	-	0/6/5/5
4	SF4	B	1235	1	-	-	0/6/5/5

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1236	TPP	C6-C5	-9.32	1.46	1.50
5	B	1236	TPP	C6-C5	-7.74	1.47	1.50
5	B	1236	TPP	PB-O3B	-3.70	1.40	1.54
5	B	1236	TPP	C4'-N3'	3.37	1.39	1.35
5	B	1236	TPP	C7'-N3	2.78	1.53	1.48

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1236	TPP	C7'-N3-C2	-3.70	118.67	125.35
5	A	1236	TPP	C7'-N3-C2	-3.62	118.81	125.35
5	A	1236	TPP	O3B-PB-O2B	3.55	121.19	107.64
5	A	1236	TPP	C5'-C7'-N3	-3.53	107.40	113.28
5	B	1236	TPP	O3B-PB-O2B	3.49	120.96	107.64

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

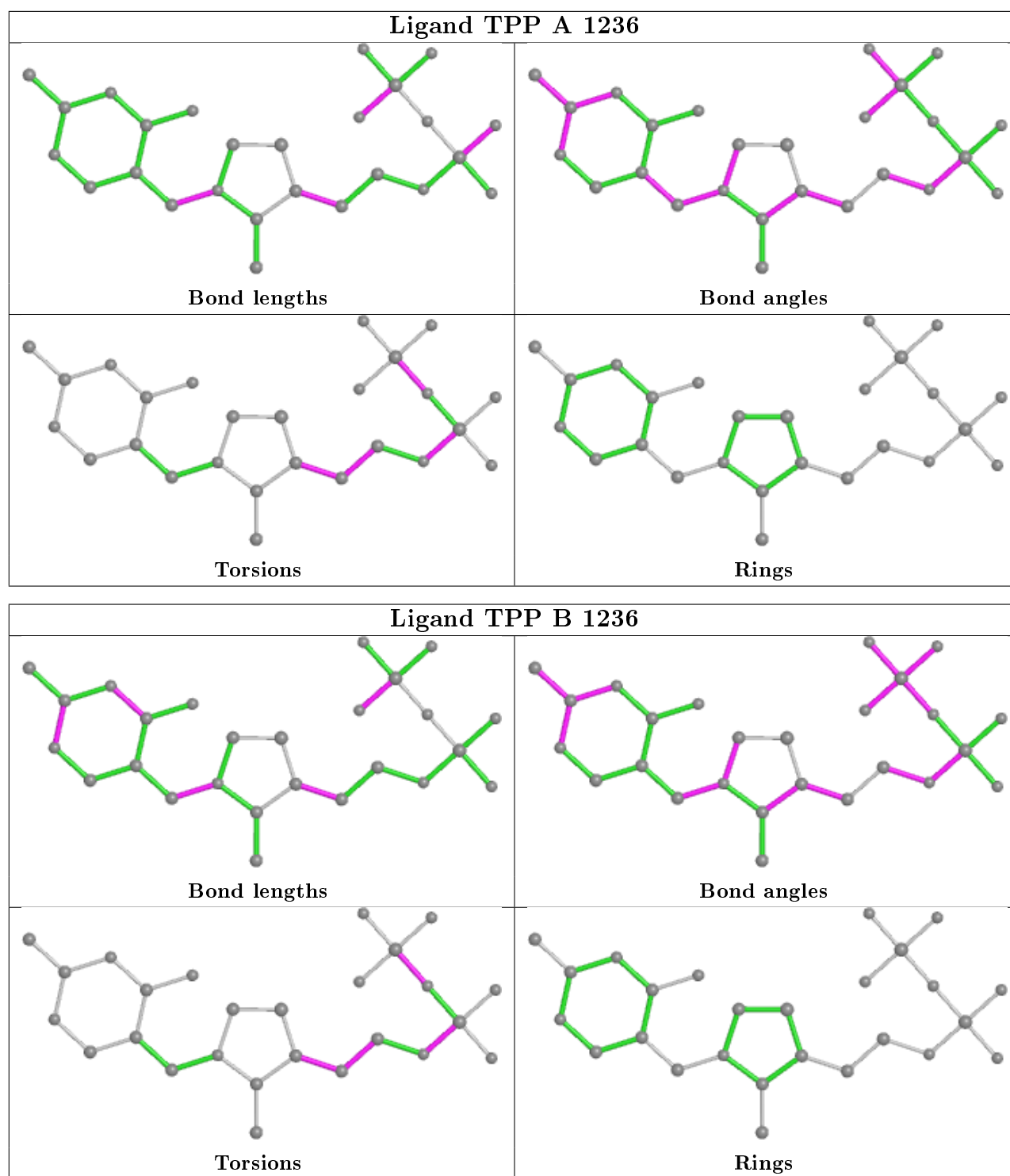
Mol	Chain	Res	Type	Atoms
5	A	1236	TPP	C5-C6-C7-O7
5	B	1236	TPP	C5-C6-C7-O7
5	B	1236	TPP	C7-O7-PA-O1A
5	A	1236	TPP	C7-O7-PA-O3A
5	B	1236	TPP	C7-O7-PA-O3A

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1236	TPP	1	0
5	B	1236	TPP	1	0
4	B	1233	SF4	1	0
4	A	1233	SF4	1	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 ⓘ

There are no chain breaks in this entry.

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.