



wwPDB X-ray Structure Validation Summary Report ⓘ

May 25, 2020 – 12:22 am BST

PDB ID : 2PDA
Title : CRYSTAL STRUCTURE OF THE COMPLEX BETWEEN PYRUVATE-FERREDOXIN OXIDOREDUCTASE FROM DESULFOVIBRIO AFRICANUS AND PYRUVATE.
Authors : Chabriere, E.; Charon, M.H.
Deposited on : 1998-11-10
Resolution : 3.00 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

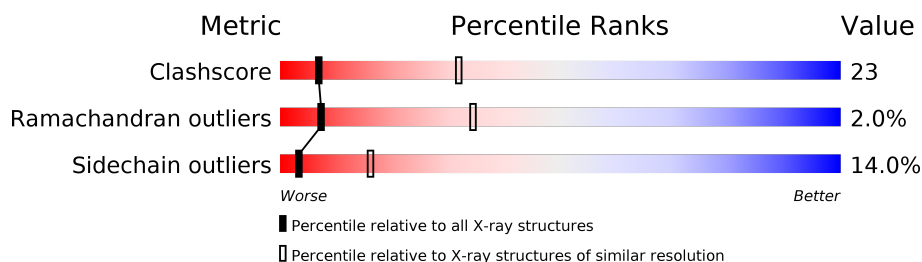
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)

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	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SF4	A	1234	-	-	X	-
4	SF4	B	1241	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 18894 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	25	0	0
			9382	5941	1599	1783	59			
1	B	1231	Total	C	N	O	S	25	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).

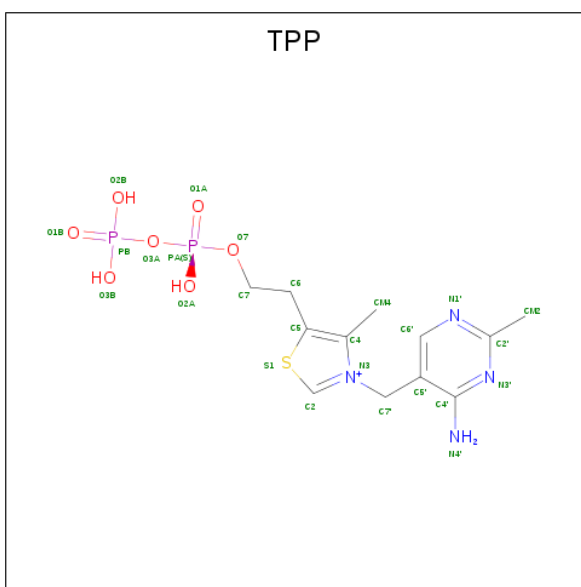
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Ca	0	0
			1	1		
3	A	1	Total	Ca	0	0
			1	1		

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



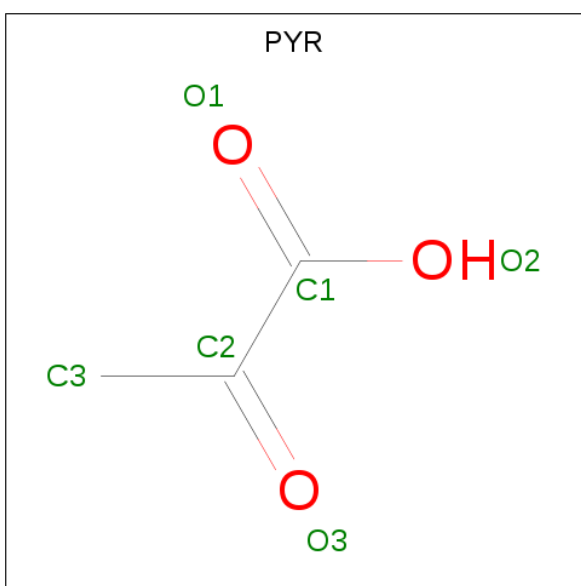
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	Fe	S	0	0
			8	4	4		
4	A	1	Total	Fe	S	0	0
			8	4	4		
4	A	1	Total	Fe	S	0	0
			8	4	4		
4	B	1	Total	Fe	S	0	0
			8	4	4		
4	B	1	Total	Fe	S	0	0
			8	4	4		
4	B	1	Total	Fe	S	0	0
			8	4	4		

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



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

- Molecule 6 is PYRUVIC ACID (three-letter code: PYR) (formula: $C_3H_4O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is water.

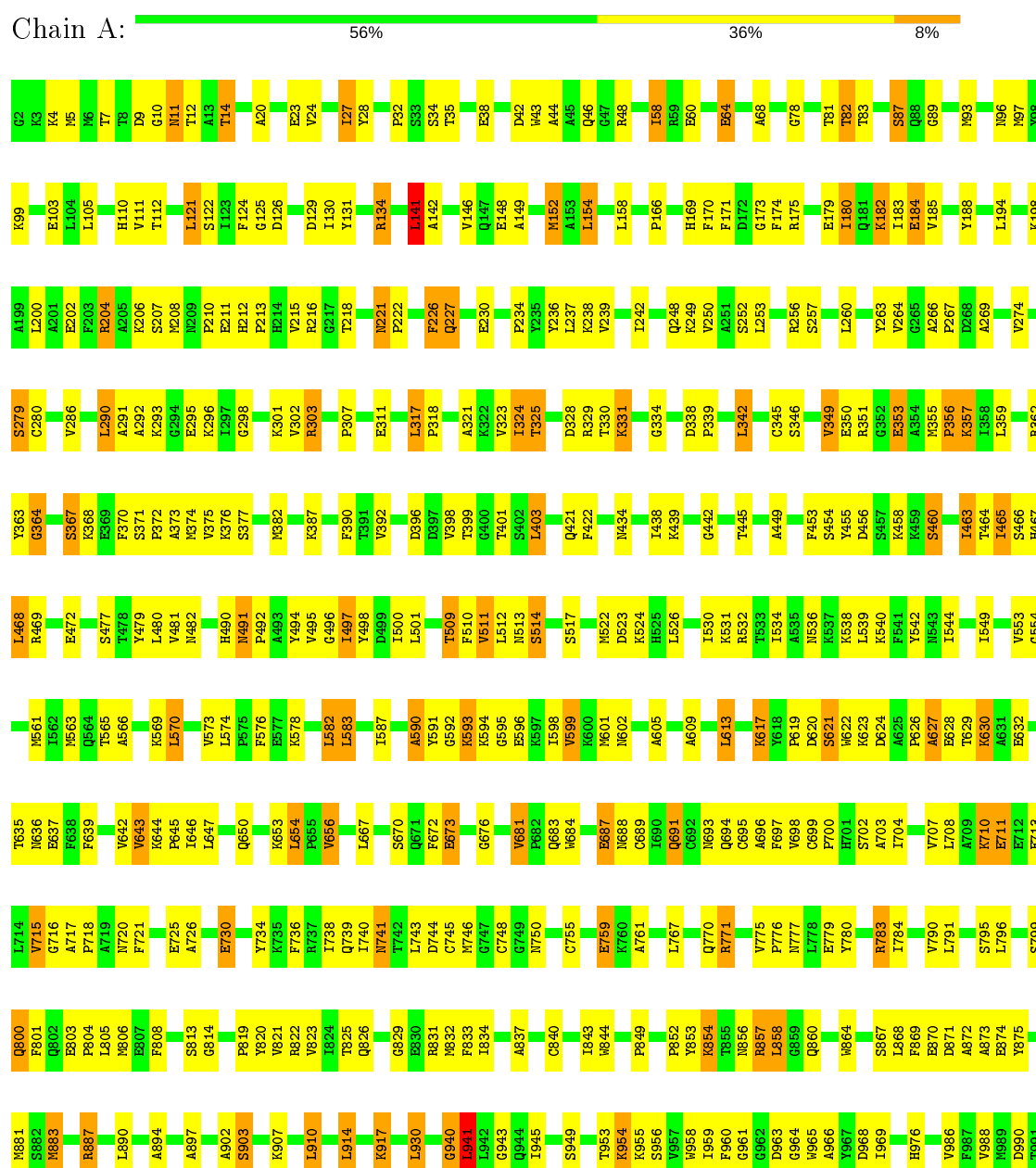
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	7	Total 7	O 7	0	0
7	B	7	Total 7	O 7	0	0

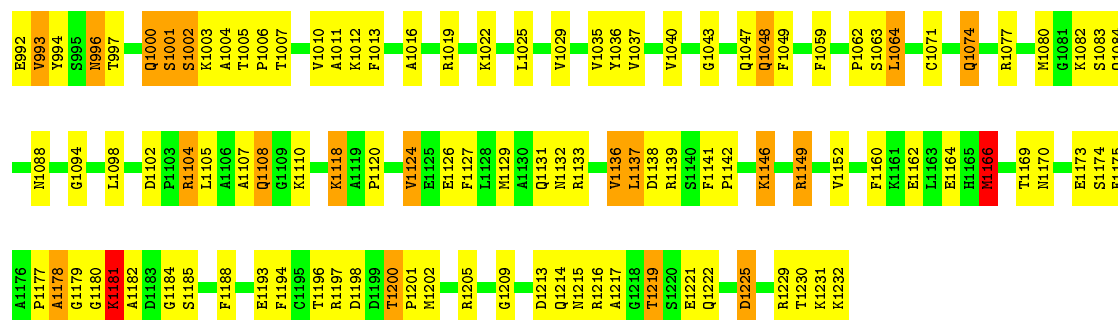
3 Residue-property plots

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.

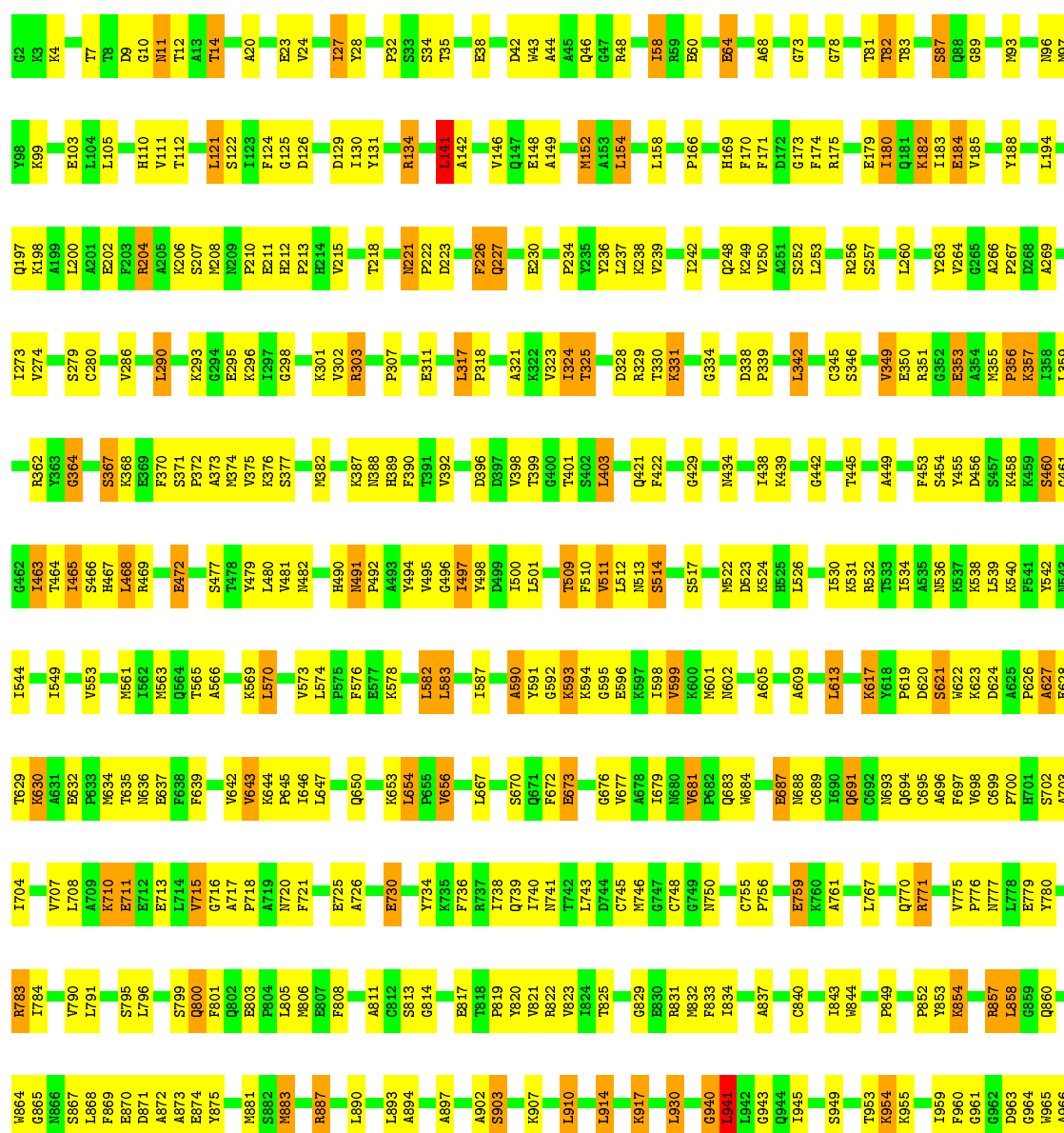
• Molecule 1: PROTEIN (PYRUVATE-FERREDOXIN OXIDOREDUCTASE)





• Molecule 1: PROTEIN (PYRUVATE-FERREDOXIN OXIDOREDUCTASE)

Chain B:  56%  36% 8%



Y967	C1071	E1164
D968	Q1074	H1165
Y969		M1166
H976	R1077	T1169
		N1170
Y986		I1171
F987	M1080	F1172
Y988	G1081	E1173
Y989	K1082	S1174
D990	S1083	F1175
T991	Q1084	A1176
E992		P1177
Y993	M1088	A1178
Y994		G1179
S995	G1094	G1180
Y996		K1181
T997	L1098	A1182
		D1183
Q1000	D1102	G1184
S1001	P1103	S1185
S1002	R1104	
K1003	L1105	F1188
A1004	A1106	
T1005	A1107	E1193
P1006	Q1108	F1194
T1007	G1109	G1195
	K1110	T1196
V1010		R1197
A1011	K1118	D1198
K1012	A1119	D1199
F1013	P1120	T1200
		P1201
A1016	V1124	M1202
	E1125	
R1019	E1126	D1213
	F1127	Q1214
K1022	L1128	N1215
	M1129	R1216
L1025	A1130	
V1029	Q1131	T1219
	N1132	S1220
	R1133	E1221
		Q1222
V1035	V1136	
Y1036	L1137	D1225
V1037	D1138	
	R1139	R1229
V1040	S1140	T1230
G1043	F1141	K1231
	P1142	K1232
Q1047		
Q1048	K1146	
F1049		
	R1149	
F1059		
	V1152	
P1062		
S1063	F1160	
L1064		

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	86.00 Å 146.30 Å 211.90 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 3.00	Depositor
% Data completeness (in resolution range)	94.2 (10.00-3.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
Refinement program	X-PLOR 3.854	Depositor
R, R_{free}	0.234 , 0.297	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	18894	wwPDB-VP
Average B, all atoms (Å ²)	12.0	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: MG, SF4, PYR, CA, 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	0.66	0/9584	0.89	13/12954 (0.1%)
1	B	0.66	0/9584	0.89	13/12954 (0.1%)
All	All	0.66	0/19168	0.89	26/25908 (0.1%)

There are no bond length outliers.

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1166	MET	N-CA-C	-6.13	94.45	111.00
1	B	1166	MET	N-CA-C	-6.13	94.45	111.00
1	A	364	GLY	N-CA-C	5.78	127.55	113.10
1	B	364	GLY	N-CA-C	5.78	127.54	113.10
1	A	141	LEU	CA-CB-CG	5.72	128.46	115.30

There are no chirality outliers.

There are no planarity outliers.

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	9263	458	4
1	B	9382	0	9263	454	4
2	A	1	0	0	0	0
2	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	24	0	0	4	0
4	B	24	0	0	4	0
5	A	26	0	16	7	0
5	B	26	0	16	7	0
6	A	6	0	3	3	0
6	B	6	0	3	3	0
7	A	7	0	0	0	0
7	B	7	0	0	0	0
All	All	18894	0	18564	864	4

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 23.

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:A:1184:GLY:HA3	1:B:1141:PHE:HZ	1.17	1.08
1:B:805:LEU:HA	1:B:854:LYS:HZ2	1.17	1.06
1:A:124:PHE:HB3	1:A:367:SER:HB2	1.37	1.04
1:B:124:PHE:HB3	1:B:367:SER:HB2	1.37	1.02
1:A:68:ALA:HB2	1:A:93:MET:HG2	1.46	0.97

All (4) 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:292:ALA:N	1:B:634:MET:CE[3_445]	2.01	0.19
1:A:292:ALA:CA	1:B:634:MET:CE[3_445]	2.05	0.15
1:A:291:ALA:C	1:B:634:MET:CE[3_445]	2.12	0.08
1:A:291:ALA:O	1:B:634:MET:CE[3_445]	2.18	0.02

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%)	1101 (90%)	103 (8%)	25 (2%)	7	34
1	B	1229/1231 (100%)	1102 (90%)	102 (8%)	25 (2%)	7	34
All	All	2458/2462 (100%)	2203 (90%)	205 (8%)	50 (2%)	7	34

5 of 50 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	87	SER
1	A	218	THR
1	A	595	GLY
1	A	626	PRO
1	A	627	ALA

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%)	841 (86%)	137 (14%)	3	16
1	B	978/978 (100%)	841 (86%)	137 (14%)	3	16
All	All	1956/1956 (100%)	1682 (86%)	274 (14%)	3	16

5 of 274 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1136	VAL
1	B	184	GLU
1	B	1088	ASN
1	A	1166	MET
1	B	14	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 85 such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	1088	ASN
1	B	169	HIS
1	B	976	HIS
1	A	1132	ASN
1	B	16	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 4 are monoatomic - leaving 10 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	2.17	5 (22%)	29,40,40	1.93	6 (20%)
4	SF4	B	1240	1	0,12,12	0.00	-	-		
4	SF4	A	1235	1	0,12,12	0.00	-	-		
4	SF4	A	1234	1	0,12,12	0.00	-	-		
5	TPP	B	1243	2	22,27,27	2.16	5 (22%)	29,40,40	1.93	6 (20%)
4	SF4	B	1242	1	0,12,12	0.00	-	-		
6	PYR	A	1239	-	2,5,5	4.20	1 (50%)	2,6,6	0.74	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SF4	A	1233	1	0,12,12	0.00	-	-		
6	PYR	B	1246	-	2,5,5	4.19	1 (50%)	2,6,6	0.73	0
4	SF4	B	1241	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	-	8/16/17/17	0/2/2/2
4	SF4	B	1240	1	-	-	0/6/5/5
4	SF4	A	1235	1	-	-	0/6/5/5
4	SF4	A	1234	1	-	-	0/6/5/5
5	TPP	B	1243	2	-	8/16/17/17	0/2/2/2
4	SF4	B	1242	1	-	-	0/6/5/5
6	PYR	A	1239	-	-	0/0/4/4	-
4	SF4	A	1233	1	-	-	0/6/5/5
6	PYR	B	1246	-	-	0/0/4/4	-
4	SF4	B	1241	1	-	-	0/6/5/5

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1236	TPP	C6-C5	-7.58	1.47	1.50
5	B	1243	TPP	C6-C5	-7.56	1.47	1.50
6	A	1239	PYR	O3-C2	5.87	1.41	1.22
6	B	1246	PYR	O3-C2	5.86	1.40	1.22
5	B	1243	TPP	C4'-N3'	2.98	1.39	1.35

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1236	TPP	C7'-N3-C2	6.03	136.25	125.35
5	B	1243	TPP	C7'-N3-C2	6.03	136.24	125.35
5	B	1243	TPP	O3B-PB-O2B	3.77	122.06	107.64
5	A	1236	TPP	O3B-PB-O2B	3.77	122.04	107.64
5	A	1236	TPP	CM2-C2'-N1'	3.58	121.08	117.14

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

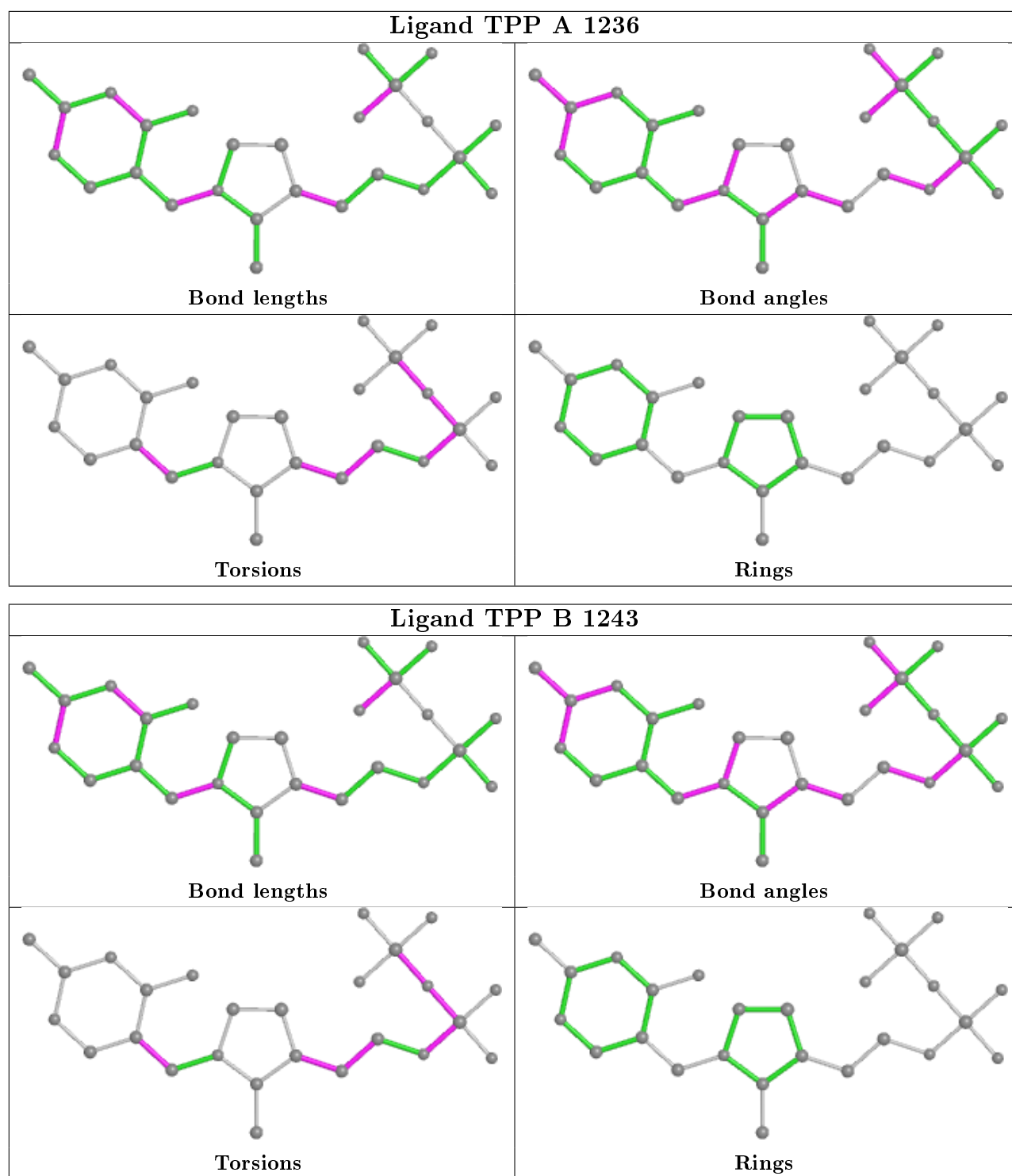
Mol	Chain	Res	Type	Atoms
5	A	1236	TPP	C4-C5-C6-C7
5	A	1236	TPP	C5-C6-C7-O7
5	A	1236	TPP	C7-O7-PA-O2A
5	A	1236	TPP	C7-O7-PA-O3A
5	A	1236	TPP	PA-O3A-PB-O3B

There are no ring outliers.

10 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1236	TPP	7	0
4	B	1240	SF4	1	0
4	A	1235	SF4	1	0
4	A	1234	SF4	2	0
5	B	1243	TPP	7	0
4	B	1242	SF4	1	0
6	A	1239	PYR	3	0
4	A	1233	SF4	1	0
6	B	1246	PYR	3	0
4	B	1241	SF4	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 [\(i\)](#)

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.