



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 06:29 PM GMT

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
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

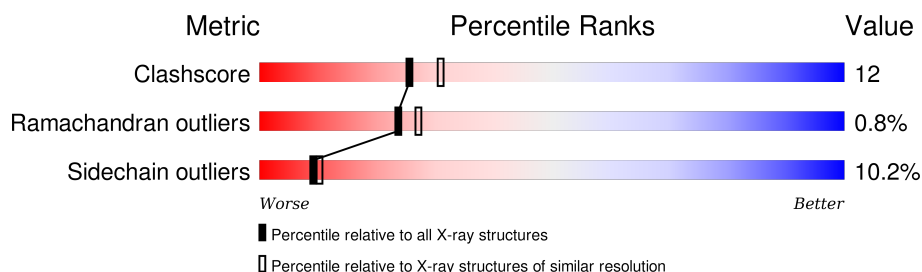
1 Overall quality at a glance

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	102246	5057 (2.34-2.30)
Ramachandran outliers	100387	5008 (2.34-2.30)
Sidechain outliers	100360	5007 (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. 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

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).

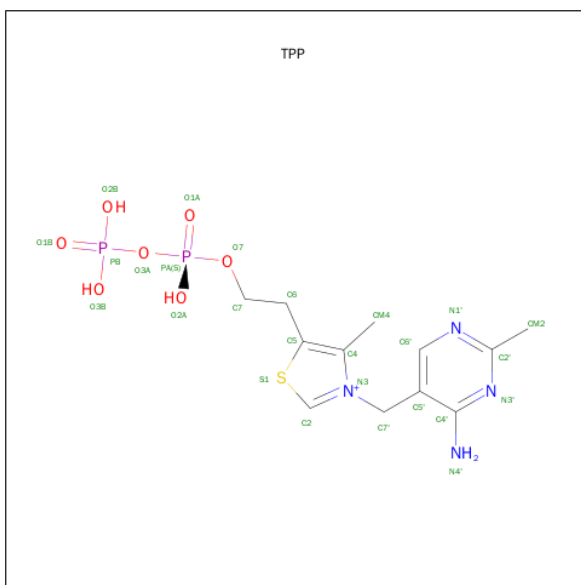
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Ca	0	0
			1	1		
3	A	1	Total	Ca	0	0
			1	1		

- 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.

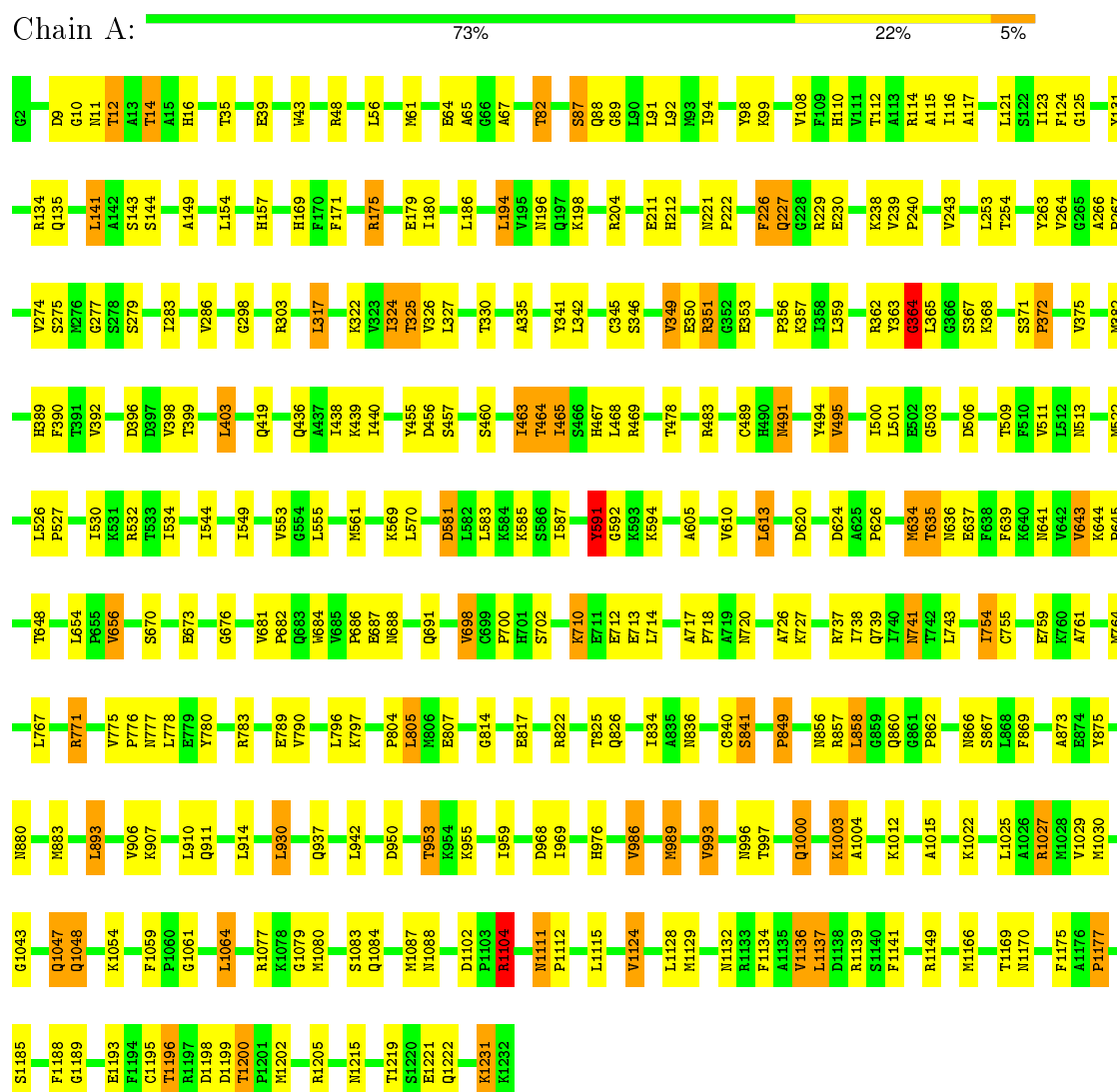
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	273	Total O 273 273	0	0
6	B	270	Total O 270 270	0	0

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 errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($\text{RSRZ} > 2$). 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)



G1189	K1054	Q937	E789	G668	L570	D446	D338	H212	H110	H2
E1190	L1064	L942	V790	E673	A571	L447	P339	V215	R114	D9
T1196	L1072	D950	L796	K674	V572	F448	L342	G217	A115	G10
T1200	L1076	L951	K797	P682	D561	S454	C345	V221	A117	T11
P1201	L1077	Y952	L805	Q683	L582	Y455	S346	P222	F124	A13
M1202	R1077	Y953	F808	W684	L583	D456	V349	F226	G125	T14
Q1214	M1080	K954	V685	V685	I587	S457	E350	Q227	D126	A15
M1215	S1083	K955	E817	E687	A580	S460	R351	Q227	H127	H16
T1219	Q1084	L959	V821	Q691	Y591	G461	G352	V233	Q128	A20
S1220	D1085	G960	T825	C692	G592	G462	E353	P234	Y131	E23
E1221	V1086	G961	M832	C694	K594	T464	P356	Y236	R134	A26
K1228	M1087	W965	C695	C695	G595	S466	K357	V239	M140	I27
K1231	M1088	D968	M836	V698	E596	L467	L358	P240	L141	E39
K1232	D1102	I969	S841	I704	K597	L468	L359	G241	A142	D42
	P1103	H976	P849	K710	V599	R469	R362	I242	S143	W43
	R1104	V986	P849	E711	A605	P474	Y363	L253	S144	W44
	K1110	V987	E712	E713	D607	T478	L365	Y258	Q147	A45
	M1111	V988	E714	L714	Q608	V487	G366	Y264	E148	O46
	P1112	M989	L715	L716	A609	V491	S367	Y264	A149	E47
	L1115	E992	E717	E718	V610	V495	K368	Y274	L154	R48
	V1124	V993	E719	E720	T611	V495	P372	Y274	H157	I51
	M1132	M996	E721	E722	L612	L501	Y379	G277	S163	L56
	V1136	Q1000	E723	E724	L613	D506	M382	S278	M164	M61
	L1137	K1003	E725	E726	Q614	P619	R389	S279	M168	Q62
	D1138	A1004	E727	E728	W622	W622	F390	E284	S63	E64
	R1139	T1005	E729	E730	K623	K623	T391	E284	F170	E64
	S1140	G1008	E731	E732	D624	D624	V392	E284	F171	A67
	F1141	K1012	E733	E734	A625	A625	D396	E284	R175	V71
	P1142	K1018	E735	E736	P626	P626	D397	E284	E179	T82
	E1143	K1022	E737	E738	A627	A627	V398	E284	I180	T83
	K1146	K1026	E739	E740	M634	M634	G400	E284	Q181	F84
	R1147	L1027	E741	E742	T635	T635	L403	E284	E184	S87
	L1148	K1030	E743	E744	M636	M636	V185	E284	V185	Q88
	M1166	L1034	E745	E746	F639	F639	Q419	E284	L186	G89
	T1169	Y1034	E747	E748	K640	K640	Q421	E284	D187	L90
	F1172	V1040	E749	E750	V643	V643	G426	E284	Y188	L91
	F1175	V1047	E751	E752	K644	K644	Q426	E284	A189	L92
	A1176	Q1048	E753	E754	P645	P645	V431	E284	D190	G93
	P1177	V1048	E755	E756	T648	T648	W435	E284	L194	I94
	S1185	V1049	E757	E758	G651	G651	K435	E284	K198	G97
	V1186	Q1049	E759	E760	L654	L654	I438	E284	R204	K99
	D1187	Q1049	E761	E762	P655	P655	K439	E284	E211	V108
	F1188	Q1048	E763	E764	V656	V656	K439	E284	F109	F109

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be 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:B:635:THR:HG23	1:B:639:PHE:HB3	1.48	0.95
1:A:64:GLU:HG3	1:A:89:GLY:HA2	1.46	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%)	26	31
1	B	1229/1231 (100%)	1184 (96%)	35 (3%)	10 (1%)	24	27
All	All	2458/2462 (100%)	2361 (96%)	78 (3%)	19 (1%)	24	27

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

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
4	SF4	A	1233	1	0,12,12	0.00	-	0,24,24	0.00	-
4	SF4	A	1234	1	0,12,12	0.00	-	0,24,24	0.00	-
4	SF4	A	1235	1	0,12,12	0.00	-	0,24,24	0.00	-
5	TPP	A	1236	2	20,27,27	1.19	3 (15%)	31,40,40	1.55	7 (22%)
4	SF4	B	1233	1	0,12,12	0.00	-	0,24,24	0.00	-
4	SF4	B	1234	1	0,12,12	0.00	-	0,24,24	0.00	-
4	SF4	B	1235	1	0,12,12	0.00	-	0,24,24	0.00	-
5	TPP	B	1236	2	20,27,27	1.60	4 (20%)	31,40,40	1.37	5 (16%)

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
4	SF4	A	1233	1	-	0/0/48/48	0/6/5/5
4	SF4	A	1234	1	-	0/0/48/48	0/6/5/5
4	SF4	A	1235	1	-	0/0/48/48	0/6/5/5
5	TPP	A	1236	2	-	0/16/17/17	0/2/2/2
4	SF4	B	1233	1	-	0/0/48/48	0/6/5/5
4	SF4	B	1234	1	-	0/0/48/48	0/6/5/5
4	SF4	B	1235	1	-	0/0/48/48	0/6/5/5
5	TPP	B	1236	2	-	0/16/17/17	0/2/2/2

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1236	TPP	PB-O3B	-3.93	1.40	1.54
5	A	1236	TPP	PA-O2A	-2.54	1.44	1.54
5	A	1236	TPP	PB-O3B	-2.36	1.46	1.54
5	B	1236	TPP	C2'-N1'	2.24	1.38	1.34
5	A	1236	TPP	C7'-N3	2.29	1.53	1.48

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1236	TPP	C5'-C7'-N3	-3.55	107.40	113.33
5	A	1236	TPP	N1'-C2'-N3'	-2.50	120.98	125.60
5	B	1236	TPP	N1'-C2'-N3'	-2.20	121.54	125.60
5	A	1236	TPP	CM4-C4-C5	-2.01	124.38	128.90
5	A	1236	TPP	C6-C5-C4	2.09	129.44	127.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 4 short contacts:

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

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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.