wwPDB X-ray Structure Validation Summary Report (i)

Nov 5, 2023 – 07:28 AM EST

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 (i) 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 (1)) were used in the production of this report:

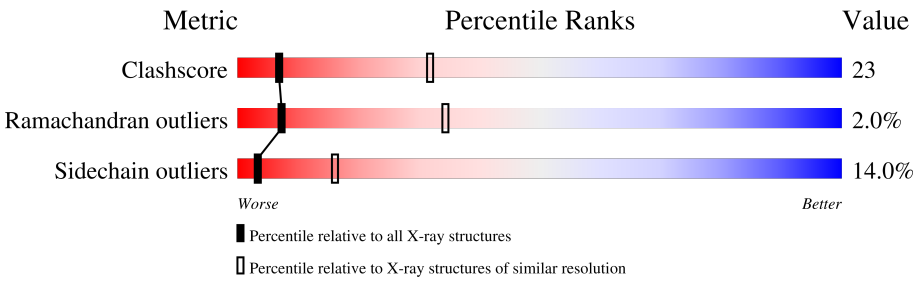
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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 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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	1231	56% 36% 8%
1	B	1231	56% 36% 8%

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 (i)

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
			Total	C	N	O	S			
1	A	1231	9382	5941	1599	1783	59	25	0	0
1	B	1231	9382	5941	1599	1783	59	25	0	0

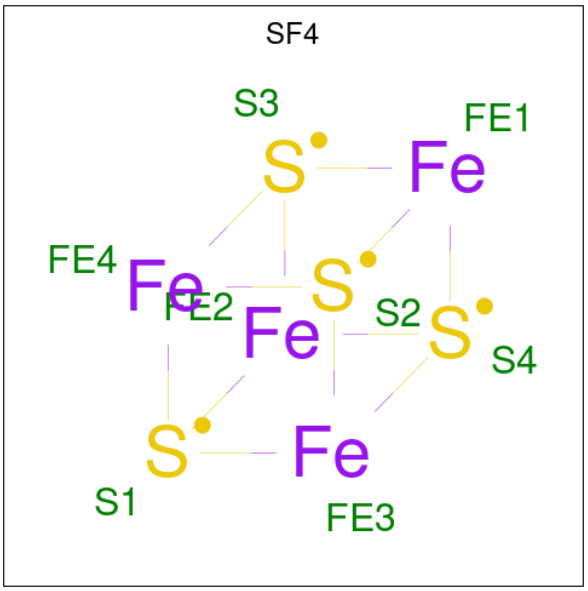
- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

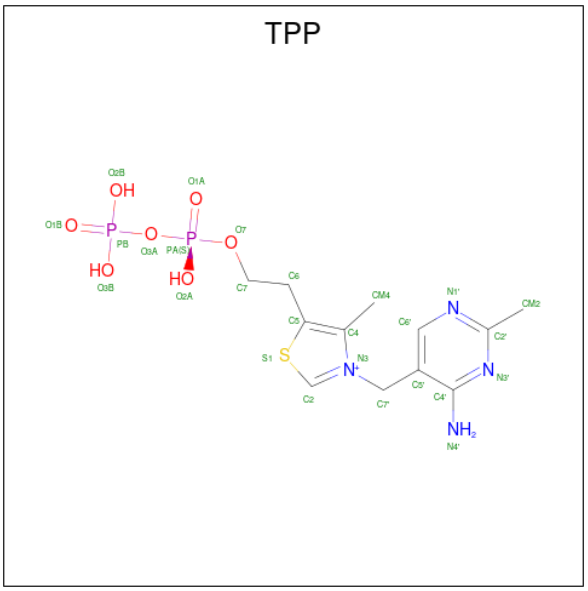
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
3	A	1	1	1	0	0
3	B	1	1	1	0	0

- Molecule 4 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



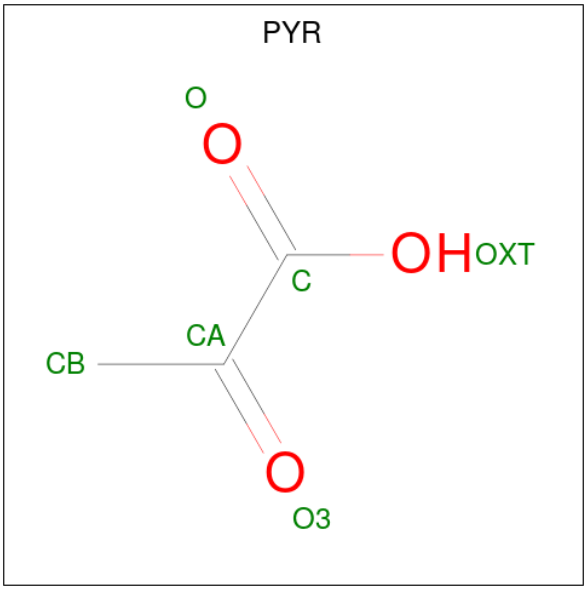
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
4	A	1	8	4	4	0	0
			Total	Fe	S		
4	A	1	8	4	4	0	0
			Total	Fe	S		
4	A	1	8	4	4	0	0
			Total	Fe	S		
4	B	1	8	4	4	0	0
			Total	Fe	S		
4	B	1	8	4	4	0	0
			Total	Fe	S		
4	B	1	8	4	4	0	0

- Molecule 5 is THIAMINE DIPHOSPHATE (three-letter code: TPP) (formula: $C_{12}H_{19}N_4O_7P_2S$).



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

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



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

- Molecule 7 is water.

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

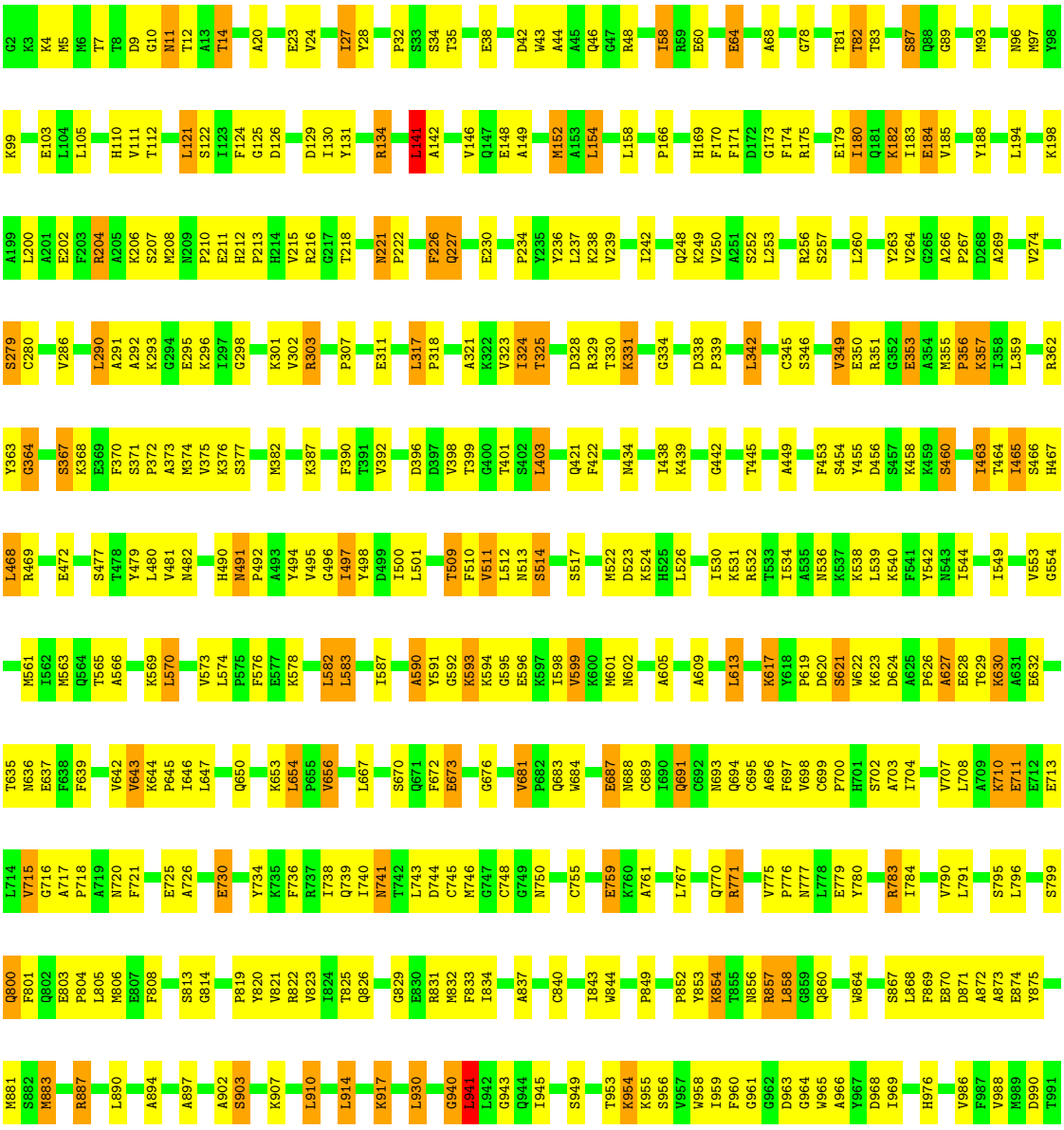
3 Residue-property plots (i)

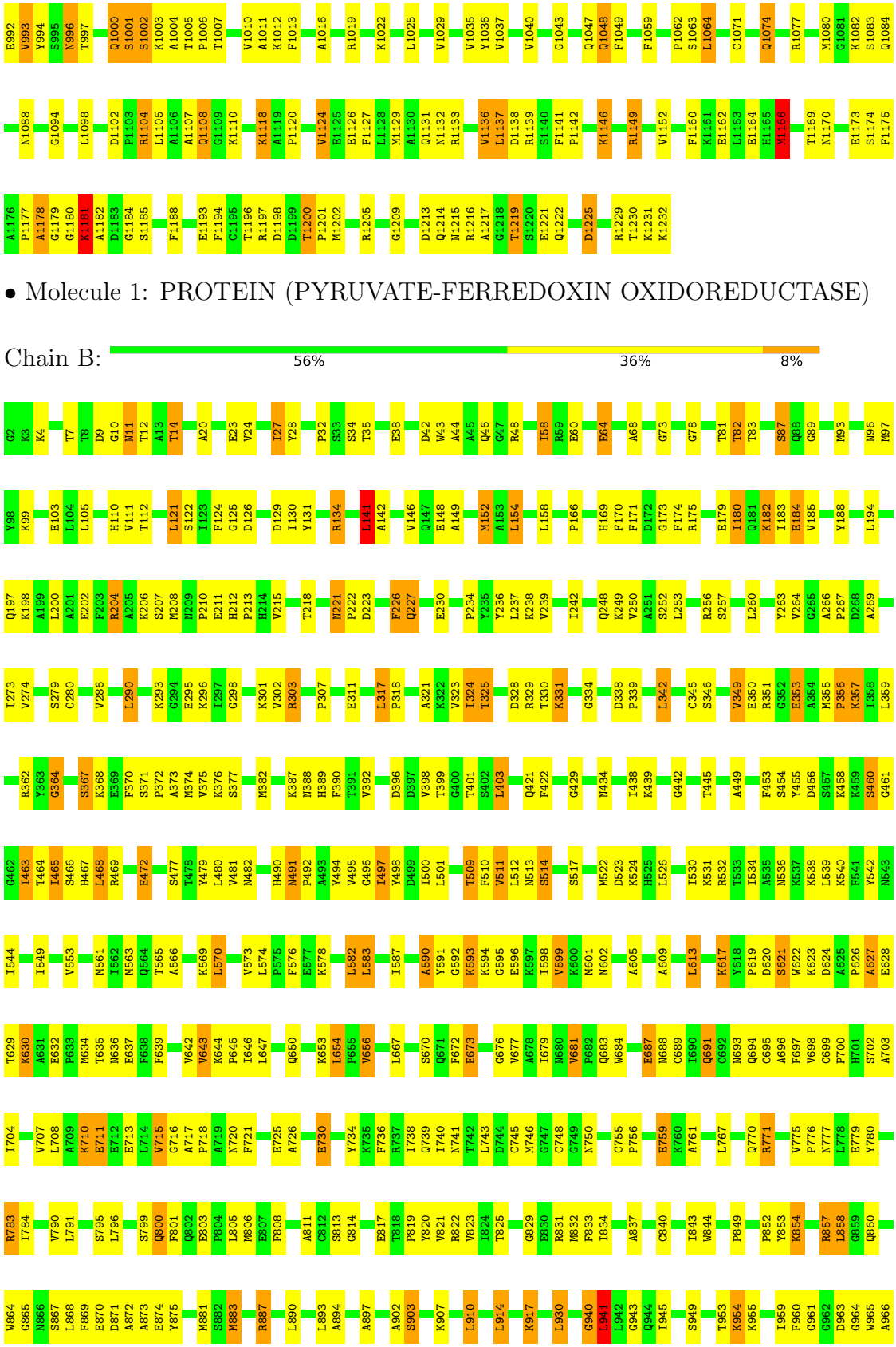
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

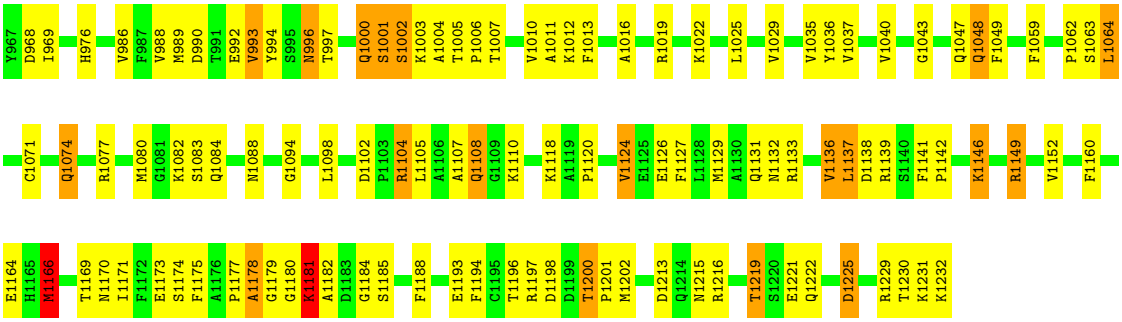
Chain A: 56% 36% 8%





- Molecule 1: PROTEIN (PYRUVATE-FERREDOXIN OXIDOREDUCTASE)

Chain B:


Y967
D968
I969
H976
V986
F987
V988
M989
D990
T991
E992
V993
Y994
S995
N996
T997
Q1000
S1001
S1002
K1003
A1004
T1005
P1006
T1007
V1010
A1011
K1012
F1013
A1016
R1019
K1022
L1025
V1029
V1035
Y1036
V1037
V1040
G1043
Q1047
Q1048
F1049
F1059
P1062
S1063
L1064
C1071
Q1074
R1077
M1080
G1081
K1082
S1083
Q1084
N1088
G1094
L1098
D1102
P1103
R1104
L1105
A1106
A1107
Q1108
G1109
K1110
K1118
A1119
P1120
V1124
E1125
E1126
F1127
L1128
M1129
A1130
Q1131
N1132
R1133
V1136
L1137
D1138
R1139
S1140
F1141
P1142
K1146
R1149
V1152
F1160
E1164
H1165
M1166
T1169
N1170
I1171
F1172
E1173
S1174
F1175
A1176
P1177
A1178
G1179
G1180
K1181
A1182
D1183
G1184
S1185
F1188
E1193
F1194
G1195
T1196
R1197
D1198
D1199
T1200
P1201
M1202
D1213
Q1214
N1215
R1216
T1219
S1220
E1221
Q1222
D1225
R1229
T1230
K1231
K1232

4 Data and refinement statistics (i)

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	86.00Å 146.30Å 211.90Å 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: TPP, SF4, MG, CA, PYR

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(^{o})	Ideal(^{o})
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 (i)

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	457	4
1	B	9382	0	9263	453	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	0	2	0
6	B	6	0	0	2	0
7	A	7	0	0	0	0
7	B	7	0	0	0	0
All	All	18894	0	18558	862	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 862 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 (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	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 (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	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	B	823	VAL
1	B	914	LEU
1	B	1136	VAL
1	A	858	LEU
1	A	823	VAL

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

such sidechains are listed below:

Mol	Chain	Res	Type
1	B	467	HIS
1	B	739	GLN
1	B	513	ASN
1	B	671	GLN
1	B	800	GLN

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 monosaccharides 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	$\#\|Z\| > 2$
4	SF4	B	1240	1	0,12,12	-	-	-		
4	SF4	B	1242	1	0,12,12	-	-	-		
5	TPP	A	1236	2	22,27,27	2.17	5 (22%)	29,40,40	1.93	6 (20%)
5	TPP	B	1243	2	22,27,27	2.16	5 (22%)	29,40,40	1.93	6 (20%)
4	SF4	A	1234	1	0,12,12	-	-	-		
4	SF4	A	1233	1	0,12,12	-	-	-		
4	SF4	A	1235	1	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	PYR	A	1239	-	5,5,5	4.14	3 (60%)	3,6,6	2.80	2 (66%)
6	PYR	B	1246	-	5,5,5	4.13	3 (60%)	3,6,6	2.80	2 (66%)
4	SF4	B	1241	1	0,12,12	-	-	-		

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	B	1240	1	-	-	0/6/5/5
4	SF4	B	1242	1	-	-	0/6/5/5
5	TPP	B	1243	2	-	8/16/17/17	0/2/2/2
5	TPP	A	1236	2	-	8/16/17/17	0/2/2/2
4	SF4	A	1234	1	-	-	0/6/5/5
4	SF4	A	1233	1	-	-	0/6/5/5
4	SF4	A	1235	1	-	-	0/6/5/5
6	PYR	A	1239	-	-	0/4/4/4	-
6	PYR	B	1246	-	-	0/4/4/4	-
4	SF4	B	1241	1	-	-	0/6/5/5

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1239	PYR	O3-CA	8.03	1.41	1.23
6	B	1246	PYR	O3-CA	8.01	1.40	1.23
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	CA-C	-3.21	1.42	1.54

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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

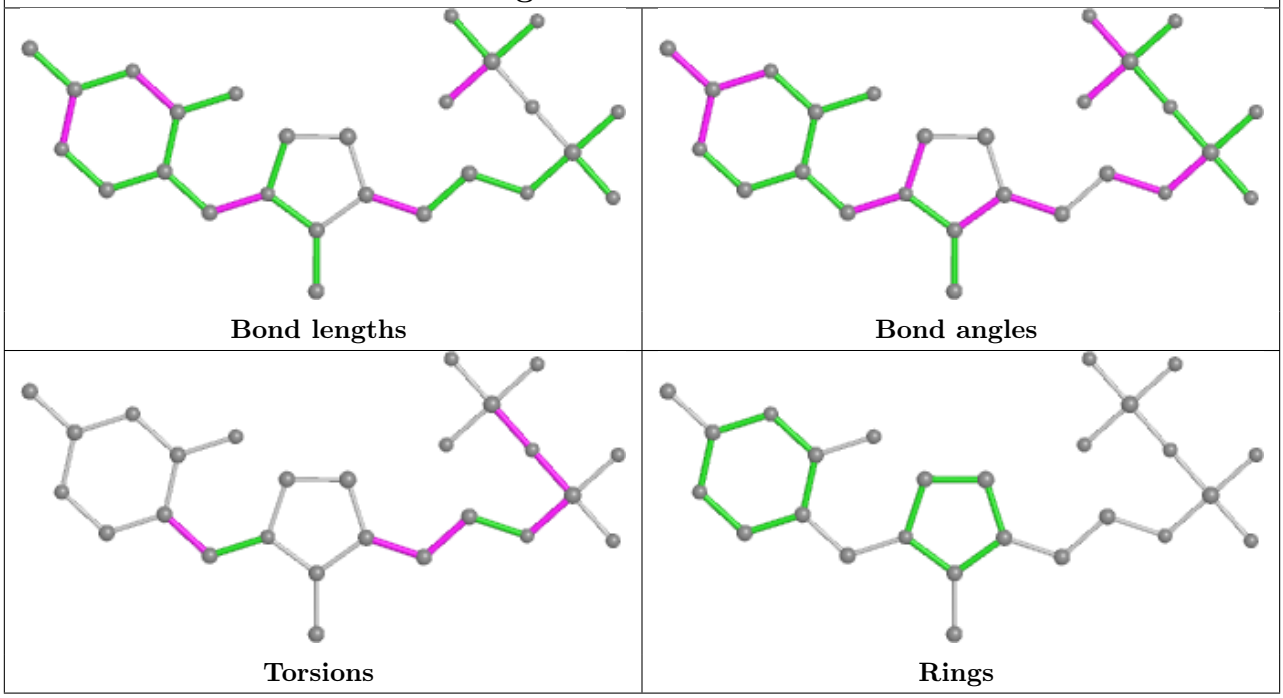
There are no ring outliers.

10 monomers are involved in 22 short contacts:

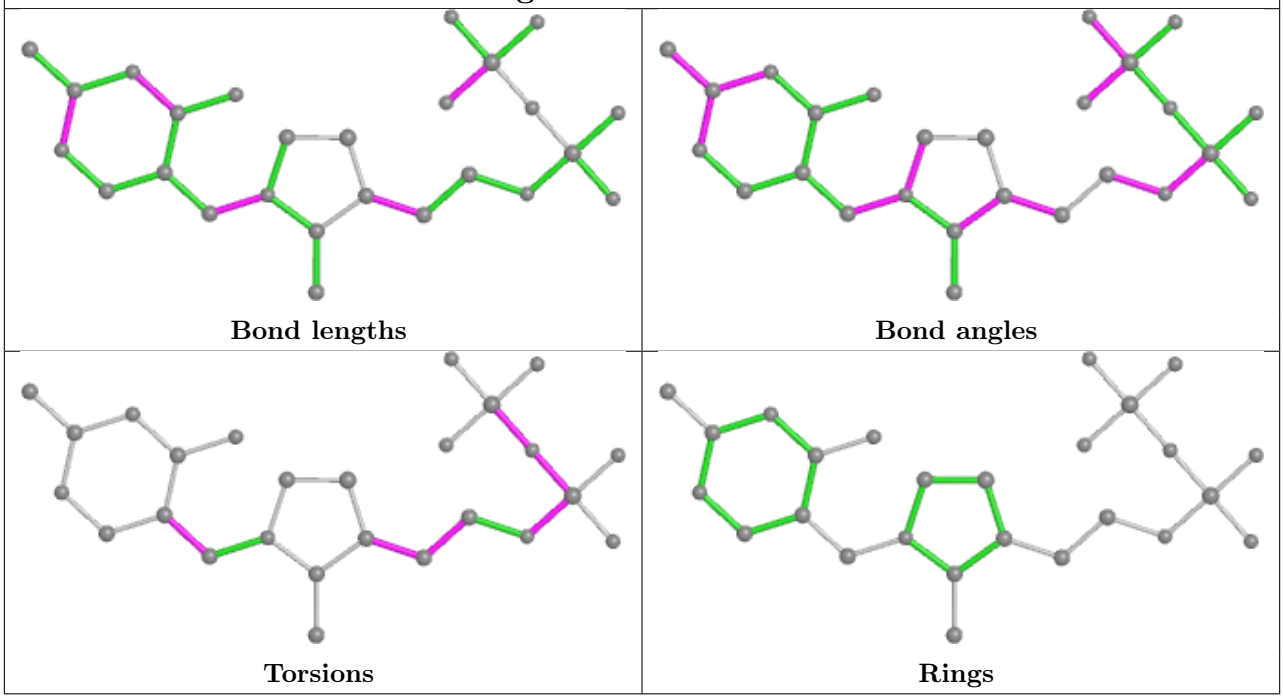
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1240	SF4	1	0
4	B	1242	SF4	1	0
5	A	1236	TPP	7	0
5	B	1243	TPP	7	0
4	A	1234	SF4	2	0
4	A	1233	SF4	1	0
4	A	1235	SF4	1	0
6	A	1239	PYR	2	0
6	B	1246	PYR	2	0
4	B	1241	SF4	2	0

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 then 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.

Ligand TPP A 1236



Ligand TPP B 1243



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.