



wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 02:01 AM GMT

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 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/ValidationPDFNotes.html>

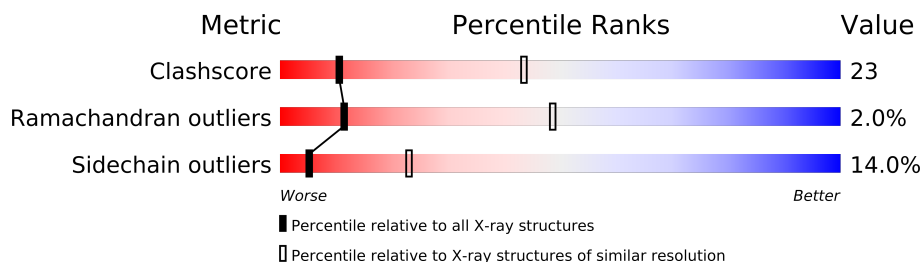
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 21963
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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	79885	1594 (3.00-3.00)
Ramachandran outliers	78287	1537 (3.00-3.00)
Sidechain outliers	78261	1540 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	1231	
1	B	1231	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 18894 atoms, of which 0 are hydrogen and 0 are deuterium.

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).

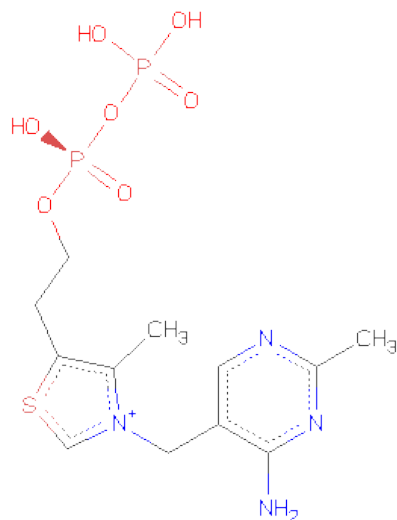
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Ca	0	0
			1	1		
3	A	1	Total	Ca	0	0
			1	1		

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



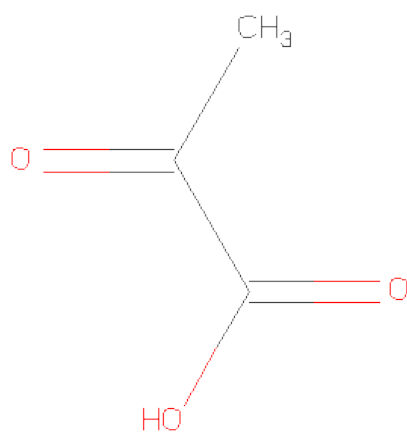
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	Fe	S	0	0
			8	4	4		
4	A	1	Total	Fe	S	0	0
			8	4	4		
4	A	1	Total	Fe	S	0	0
			8	4	4		
4	B	1	Total	Fe	S	0	0
			8	4	4		
4	B	1	Total	Fe	S	0	0
			8	4	4		
4	B	1	Total	Fe	S	0	0
			8	4	4		

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



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: C₃H₄O₃).



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

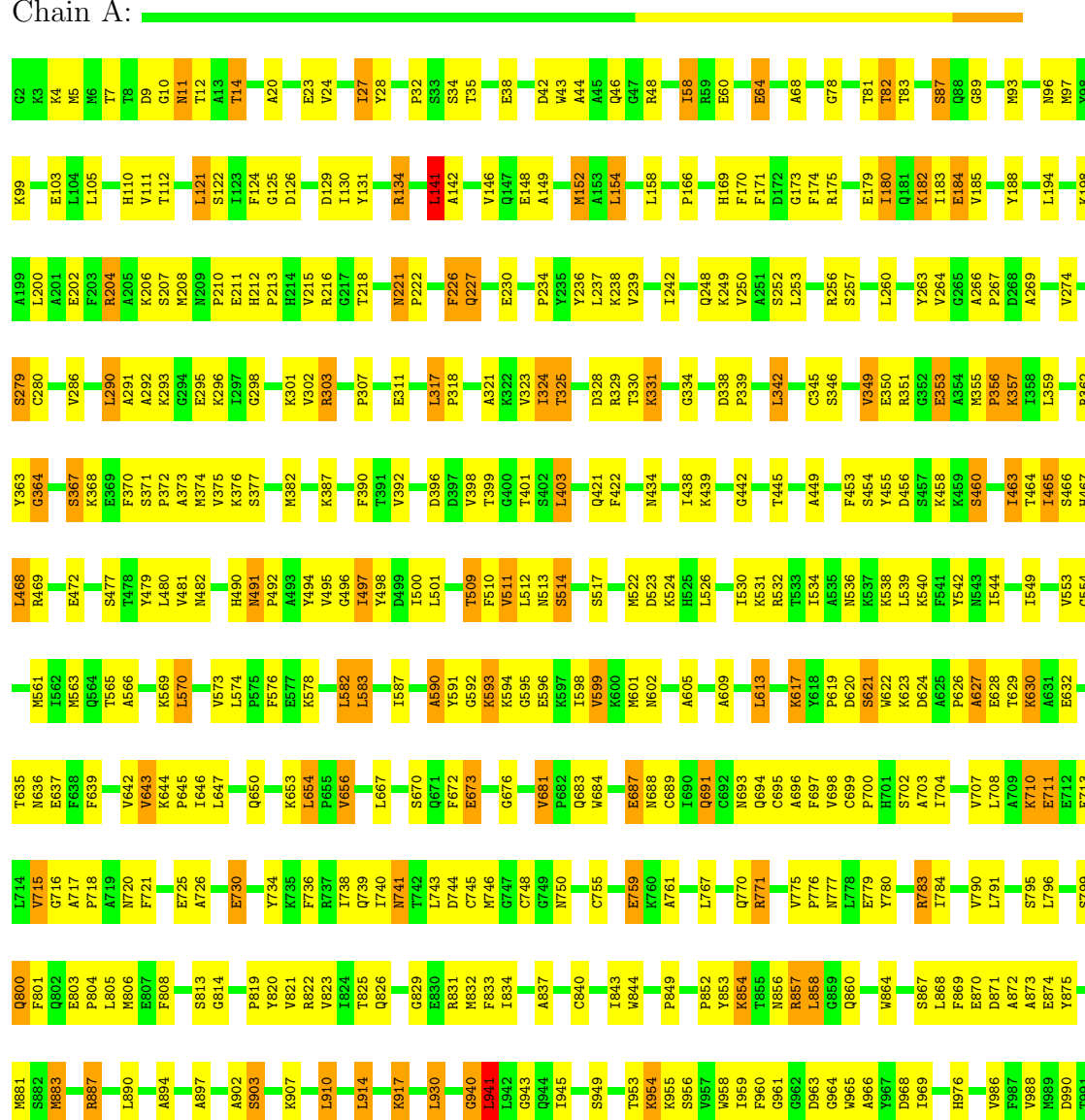
3 Residue-property plots

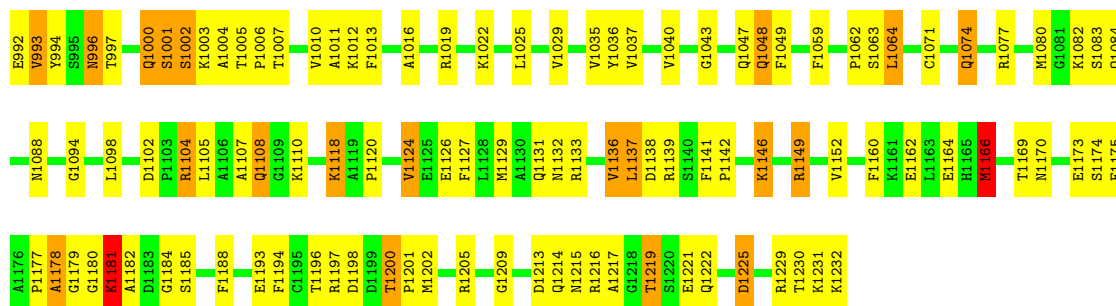
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ($RSRZ > 2$). 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)

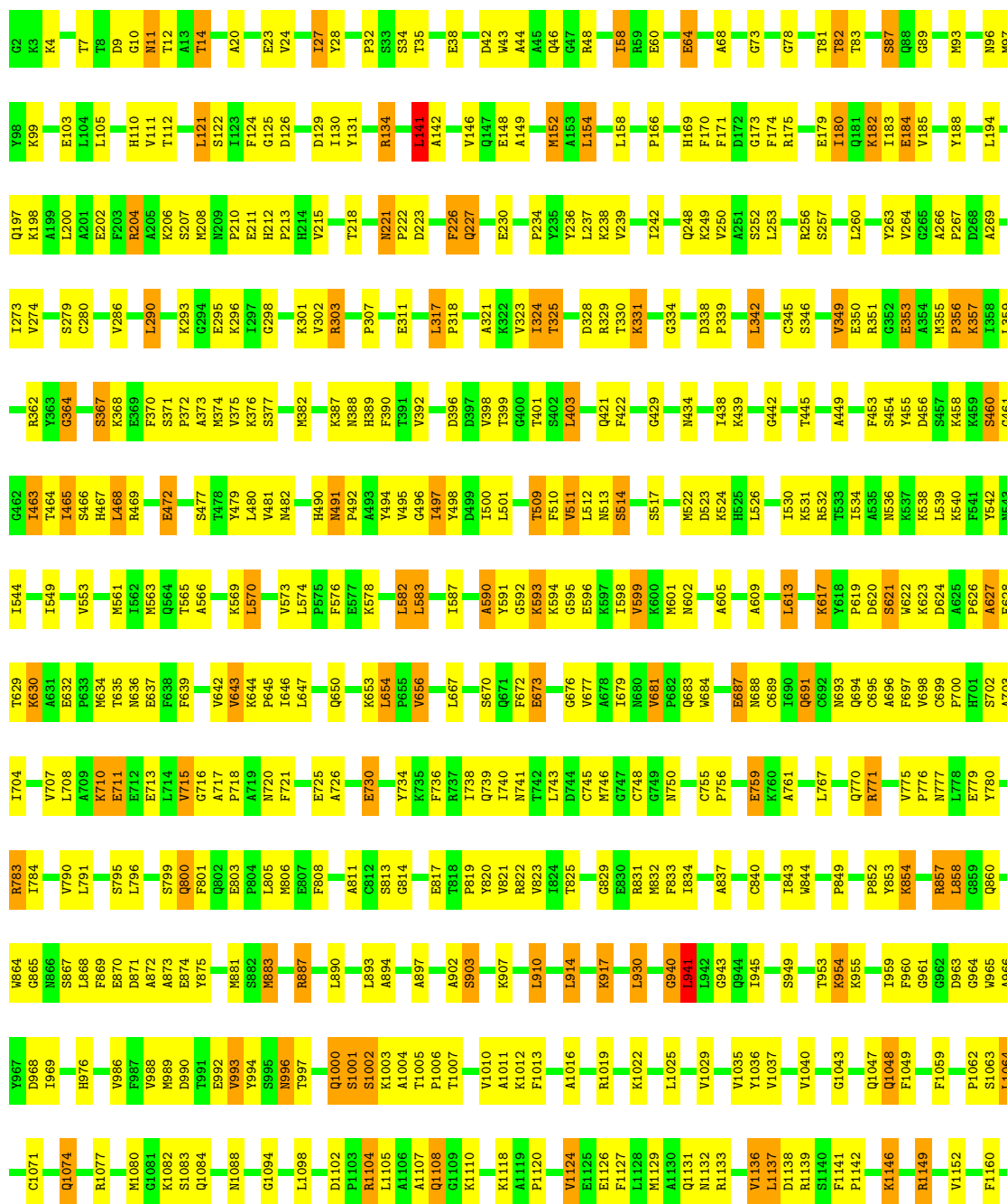
Chain A:





• Molecule 1: PROTEIN (PYRUVATE-FERREDOXIN OXIDOREDUCTASE)

Chain B:



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
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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	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

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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 23.

The worst 5 of 864 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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	Distance(Å)	Clash(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%)	11	48
1	B	1229/1231 (100%)	1102 (90%)	102 (8%)	25 (2%)	11	48
All	All	2458/2462 (100%)	2203 (90%)	205 (8%)	50 (2%)	11	48

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%)	5	23
1	B	978/978 (100%)	841 (86%)	137 (14%)	5	23
All	All	1956/1956 (100%)	1682 (86%)	274 (14%)	5	23

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

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Mol	Chain	Res	Type
1	B	169	HIS
1	B	976	HIS
1	A	1132	ASN
1	B	16	HIS

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	A	1233	1	12,12,12	5.95	9 (75%)	0,24,24	0.00	-
4	SF4	A	1234	1	12,12,12	10.88	11 (91%)	0,24,24	0.00	-
4	SF4	A	1235	1	12,12,12	7.90	11 (91%)	0,24,24	0.00	-
5	TPP	A	1236	2	27,27,27	1.38	5 (18%)	40,40,40	1.95	8 (20%)
6	PYR	A	1239	-	5,5,5	4.34	3 (60%)	6,6,6	2.29	3 (50%)
4	SF4	B	1240	1	12,12,12	5.93	9 (75%)	0,24,24	0.00	-
4	SF4	B	1241	1	12,12,12	10.89	11 (91%)	0,24,24	0.00	-
4	SF4	B	1242	1	12,12,12	7.93	11 (91%)	0,24,24	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	TPP	B	1243	2	27,27,27	1.38	5 (18%)	40,40,40	1.95	8 (20%)
6	PYR	B	1246	-	5,5,5	4.33	3 (60%)	6,6,6	2.30	2 (33%)

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	0/0/5/5
4	SF4	A	1234	1	-	0/0/48/48	0/0/5/5
4	SF4	A	1235	1	-	0/0/48/48	0/0/5/5
5	TPP	A	1236	2	-	0/17/17/17	0/2/2/2
6	PYR	A	1239	-	-	0/4/4/4	0/0/0/0
4	SF4	B	1240	1	-	0/0/48/48	0/0/5/5
4	SF4	B	1241	1	-	0/0/48/48	0/0/5/5
4	SF4	B	1242	1	-	0/0/48/48	0/0/5/5
5	TPP	B	1243	2	-	0/17/17/17	0/2/2/2
6	PYR	B	1246	-	-	0/4/4/4	0/0/0/0

The worst 5 of 78 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1241	SF4	S2-FE3	-20.52	2.19	2.33
4	A	1234	SF4	S2-FE3	-20.49	2.19	2.33
4	B	1241	SF4	S4-FE3	-14.79	2.23	2.33
4	A	1234	SF4	S4-FE3	-14.79	2.23	2.33
4	B	1242	SF4	S4-FE1	-12.95	2.24	2.33

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1236	TPP	C7'-N3-C2	5.28	136.25	125.05
5	B	1243	TPP	C7'-N3-C2	5.28	136.24	125.05
5	A	1236	TPP	C7'-N3-C4	-5.04	114.01	124.34
5	B	1243	TPP	C7'-N3-C4	-5.03	114.02	124.34
6	B	1246	PYR	O2-C1-C2	4.00	123.19	114.37

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

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 will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

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

6.4 Ligands ⓘ

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

6.5 Other polymers ⓘ

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