



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 2, 2017 – 05:06 AM EDT

PDB ID : 3AE6  
Title : Crystal structure of porcine heart mitochondrial complex II bound with N-(3-Isopropoxy-phenyl)-phthalamicacid  
Authors : Harada, S.; Sasaki, T.; Shindo, M.; Kido, Y.; Inaoka, D.K.; Omori, J.; Osanai, A.; Sakamoto, K.; Mao, J.; Matsuoka, S.; Inoue, M.; Honma, T.; Tanaka, A.; Kita, K.  
Deposited on : unknown  
Resolution : 3.40 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](mailto: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.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030345
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030345

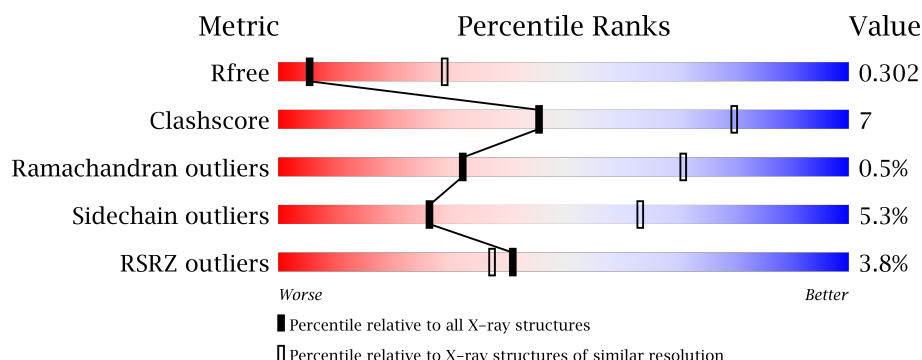
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.40 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))
$R_{free}$	100719	1679 (3.50-3.30)
Clashscore	112137	1832 (3.50-3.30)
Ramachandran outliers	110173	1789 (3.50-3.30)
Sidechain outliers	110143	1789 (3.50-3.30)
RSRZ outliers	101464	1709 (3.50-3.30)

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  $\geq 3$ , 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.

Mol	Chain	Length	Quality of chain
1	A	622	<div> <div>5%</div> <div> <div></div> <div>75%</div> <div>22%</div> <div>..</div> </div> </div>
2	B	252	<div> <div>3%</div> <div> <div></div> <div>77%</div> <div>15%</div> <div>5%</div> </div> </div>
3	C	140	<div> <div>2%</div> <div> <div></div> <div>91%</div> <div>7%</div> <div>..</div> </div> </div>
4	D	103	<div> <div>3%</div> <div> <div></div> <div>88%</div> <div>11%</div> <div>.</div> </div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	EPH	D	1306	X	-	-	X
5	FAD	A	700	-	-	-	X
9	HEM	C	1305	-	-	-	X

## 2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 8661 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 Succinate dehydrogenase [ubiquinone] flavoprotein subunit, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	613	Total	C	N	O	S	0	0	0
			4729	2954	848	895	32			

- Molecule 2 is a protein called Succinate dehydrogenase [ubiquinone] iron-sulfur subunit, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	239	Total	C	N	O	S	0	0	0
			1922	1214	326	360	22			

- Molecule 3 is a protein called Succinate dehydrogenase cytochrome b560 subunit, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	138	Total	C	N	O	S	0	0	0
			1064	695	179	183	7			

- Molecule 4 is a protein called Succinate dehydrogenase [ubiquinone] cytochrome b small subunit, mitochondrial.

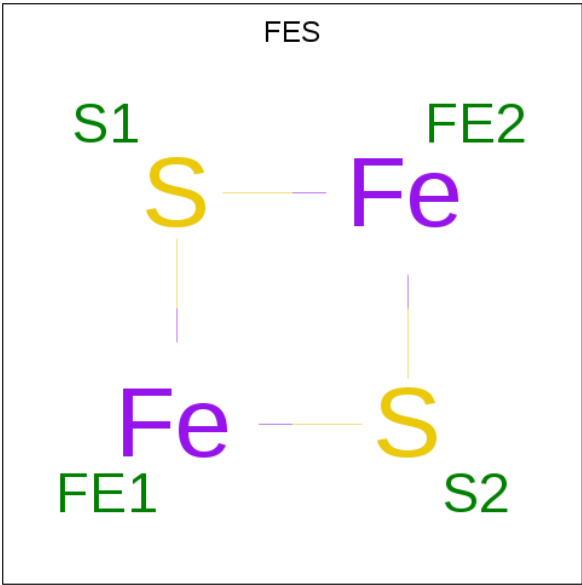
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	102	Total	C	N	O	S	0	0	0
			765	499	128	133	5			

- Molecule 5 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C<sub>27</sub>H<sub>33</sub>N<sub>9</sub>O<sub>15</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 6 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe<sub>2</sub>S<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 7 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



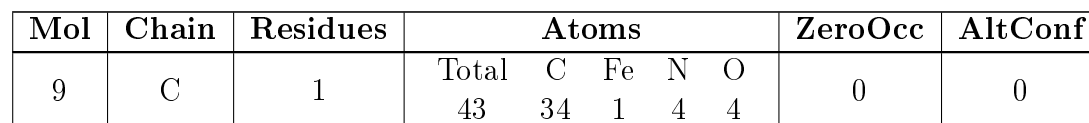
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 8 is FE3-S4 CLUSTER (three-letter code: F3S) (formula:  $\text{Fe}_3\text{S}_4$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	Fe	S	0	0
			7	3	4		

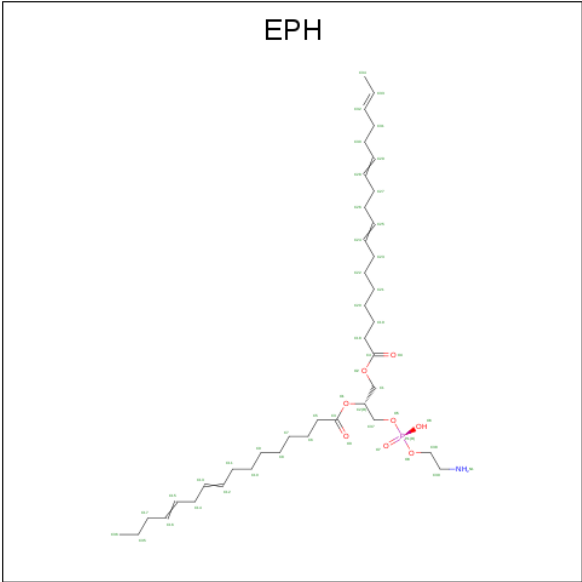
- Molecule 9 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $\text{C}_{34}\text{H}_{32}\text{FeN}_4\text{O}_4$ ).



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- The chemical structure is labeled **JMP**. It features a central imidazole ring with a carbonyl group at position 3. One nitrogen atom is bonded to a phenyl ring, and the other is bonded to an isopropoxy group. The carbonyl oxygen is also bonded to a phenyl ring. The atoms are labeled with green text: C1, C2, C3, C4, C5, C6, C7, C8, C9, C10, C11, C12, C13, C14, C15, C16, C17 for carbon; O1, O2, O3, O4 for oxygen; and N for nitrogen. The isopropoxy group consists of an oxygen atom (O2) bonded to a central carbon (C15), which is further bonded to two methyl groups (C16 and C17).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	C	1	Total	C	N	O	0	0
			22	17	1	4		

- WORLDWIDE  
**PDB**  
PROTEIN DATA BANK




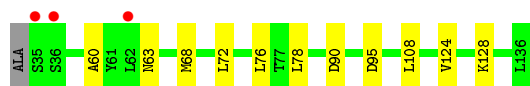
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	D	1	Total	C	N	O	P	0	0
			44	34	1	8	1		





- Molecule 4: Succinate dehydrogenase [ubiquinone] cytochrome b small subunit, mitochondrial

Chain D:  3% 88% 11%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	71.12Å 84.12Å 293.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.49 – 3.40 47.49 – 3.40	Depositor EDS
% Data completeness (in resolution range)	98.2 (47.49-3.40) 98.2 (47.49-3.40)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.37 (at 3.40Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.250 , 0.299 0.252 , 0.302	Depositor DCC
$R_{free}$ test set	1251 reflections (5.36%)	DCC
Wilson B-factor (Å <sup>2</sup> )	81.3	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 26.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	8661	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.36% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 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: SF4, F3S, FES, EPH, HEM, JMP, FAD

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	0.32	0/4828	0.49	0/6531
2	B	0.32	0/1964	0.49	0/2648
3	C	0.33	0/1091	0.45	0/1483
4	D	0.30	0/784	0.45	0/1066
All	All	0.32	0/8667	0.49	0/11728

There are no bond length outliers.

There are no bond angle outliers.

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	4729	0	4618	90	0
2	B	1922	0	1904	27	0
3	C	1064	0	1104	10	0
4	D	765	0	773	3	0
5	A	53	0	31	10	0
6	B	4	0	0	0	0
7	B	8	0	0	1	0
8	B	7	0	0	1	0
9	C	43	0	30	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	C	22	0	16	2	0
11	D	44	0	53	0	0
All	All	8661	0	8529	125	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 7.

The worst 5 of 125 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:57:HIS:NE2	5:A:700:FAD:HM82	1.28	1.40
1:A:57:HIS:CE1	5:A:700:FAD:HM82	1.62	1.35
1:A:61:ALA:HB3	1:A:155:GLY:HA3	1.47	0.97
2:B:164:CYS:HB2	7:B:303:SF4:S1	2.06	0.95
1:A:57:HIS:HE1	1:A:226:SER:HA	1.35	0.92

There are no symmetry-related clashes.

## 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	611/622 (98%)	568 (93%)	40 (6%)	3 (0%)	32	71
2	B	237/252 (94%)	216 (91%)	20 (8%)	1 (0%)	38	75
3	C	136/140 (97%)	130 (96%)	6 (4%)	0	100	100
4	D	100/103 (97%)	95 (95%)	4 (4%)	1 (1%)	18	59
All	All	1084/1117 (97%)	1009 (93%)	70 (6%)	5 (0%)	32	71

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	29	GLY
1	A	516	TRP
2	B	164	CYS
1	A	260	GLY
4	D	95	ASP

### 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	499/506 (99%)	474 (95%)	25 (5%)	28	65
2	B	214/220 (97%)	198 (92%)	16 (8%)	16	51
3	C	117/118 (99%)	114 (97%)	3 (3%)	51	80
4	D	76/76 (100%)	72 (95%)	4 (5%)	26	63
All	All	906/920 (98%)	858 (95%)	48 (5%)	26	63

5 of 48 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	556	LYS
2	B	39	ASN
4	D	63	ASN
1	A	561	GLU
1	A	597	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	474	GLN
1	A	550	HIS
3	C	29	HIS
1	A	535	GLN
1	A	571	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules 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 ⓘ

7 ligands are modelled in this entry.

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	FAD	A	700	1	51,58,58	1.36	7 (13%)	54,89,89	2.00	7 (12%)
6	FES	B	302	2	0,4,4	0.00	-	0,4,4	0.00	-
7	SF4	B	303	2	0,12,12	0.00	-	0,24,24	0.00	-
8	F3S	B	304	2	0,9,9	0.00	-	0,15,15	0.00	-
10	JMP	C	1201	-	20,23,23	1.53	2 (10%)	27,31,31	0.92	1 (3%)
9	HEM	C	1305	3,4	28,50,50	2.20	7 (25%)	17,82,82	1.64	4 (23%)
11	EPH	D	1306	-	43,43,48	1.51	6 (13%)	45,48,53	1.48	6 (13%)

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	FAD	A	700	1	-	0/28/50/50	0/6/6/6
6	FES	B	302	2	-	0/0/4/4	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	SF4	B	303	2	-	0/0/48/48	0/6/5/5
8	F3S	B	304	2	-	0/0/24/24	0/0/3/3
10	JMP	C	1201	-	-	0/12/16/16	0/2/2/2
9	HEM	C	1305	3,4	-	0/6/54/54	0/0/8/8
11	EPH	D	1306	-	1/1/4/14	0/47/47/52	0/0/0/0

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	C	1305	HEM	C3B-C2B	-4.48	1.34	1.40
9	C	1305	HEM	C3C-C2C	-3.98	1.35	1.40
10	C	1201	JMP	C9-N	-2.46	1.36	1.41
9	C	1305	HEM	CAA-C2A	2.23	1.55	1.52
5	A	700	FAD	C5X-N5	2.27	1.38	1.35

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	700	FAD	N3A-C2A-N1A	-10.92	119.35	128.86
11	D	1306	EPH	C30-C29-C28	-3.80	110.70	127.03
9	C	1305	HEM	CAA-CBA-CGA	-3.06	107.44	112.66
11	D	1306	EPH	O1-C3-O3	-2.53	117.36	123.68
9	C	1305	HEM	CAD-CBD-CGD	-2.48	108.43	112.66

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
11	D	1306	EPH	C2

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	700	FAD	10	0
7	B	303	SF4	1	0
8	B	304	F3S	1	0
10	C	1201	JMP	2	0
9	C	1305	HEM	3	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](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	613/622 (98%)	0.28	29 (4%) 32 30	65, 86, 121, 137	0
2	B	239/252 (94%)	0.17	7 (2%) 52 48	64, 80, 112, 130	0
3	C	138/140 (98%)	0.14	3 (2%) 62 57	72, 89, 125, 137	0
4	D	102/103 (99%)	-0.09	3 (2%) 52 48	73, 91, 116, 138	0
All	All	1092/1117 (97%)	0.21	42 (3%) 41 37	64, 86, 120, 138	0

The worst 5 of 42 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	82	LEU	4.5
2	B	11	ILE	4.2
1	A	622	TYR	3.9
1	A	357	PRO	3.8
3	C	81	CYS	3.6

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors

of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
11	EPH	D	1306	44/49	0.78	0.69	5.04	116,121,128,128	0
9	HEM	C	1305	43/43	0.95	0.27	2.09	80,81,82,82	0
5	FAD	A	700	53/53	0.88	0.43	0.89	71,72,73,74	0
10	JMP	C	1201	22/22	0.90	0.26	0.28	74,75,75,76	0
8	F3S	B	304	7/7	0.98	0.18	-0.70	74,75,75,75	0
7	SF4	B	303	8/8	0.99	0.17	-1.55	64,64,65,65	0
6	FES	B	302	4/4	0.99	0.21	-1.60	59,59,59,60	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.