



# wwPDB X-ray Structure Validation Summary Report i

Mar 1, 2014 – 02:29 AM GMT

PDB ID : 3AE2  
Title : Crystal structure of porcine heart mitochondrial complex II bound with 2-Hydroxy-N-phenyl-benzamide  
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 : 2010-02-04  
Resolution : 3.10 Å(reported)

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A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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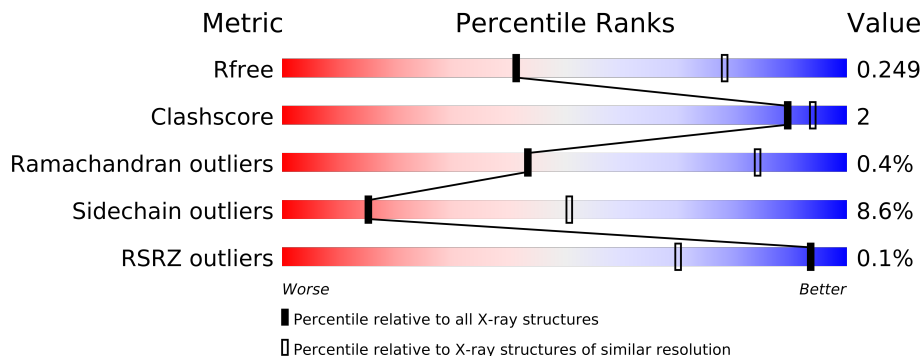
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
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 3.10 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))
$R_{free}$	66092	1007 (3.18-3.02)
Clashscore	79885	1078 (3.16-3.04)
Ramachandran outliers	78287	1044 (3.16-3.04)
Sidechain outliers	78261	1044 (3.16-3.04)
RSRZ outliers	66119	1008 (3.18-3.02)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	622	
2	B	252	
3	C	140	
4	D	103	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
11	EPH	D	1306	-	X
12	SLI	C	1201	-	X

## 2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 8663 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 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.

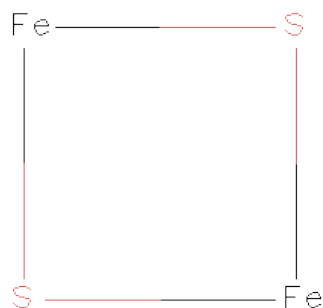
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	102	Total	C	N	O	S	0	0	0
			765	499	128	133	5			

- Molecule 5 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:  $C_{27}H_{33}N_9O_{15}P_2$ ).



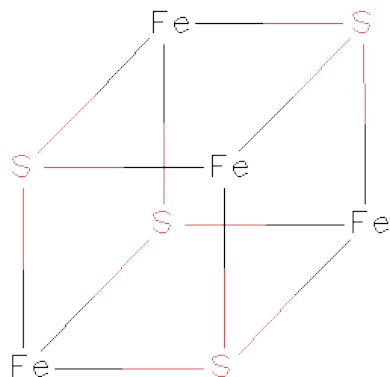
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 6 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula:  $\text{Fe}_2\text{S}_2$ ).



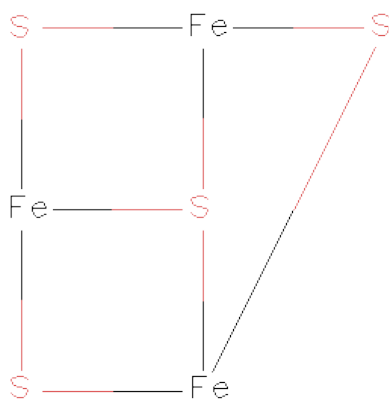
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 7 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula:  $\text{Fe}_4\text{S}_4$ ).



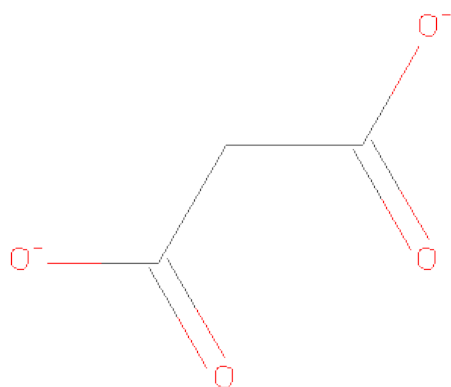
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	Fe	S	0	0
			8	4	4		

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



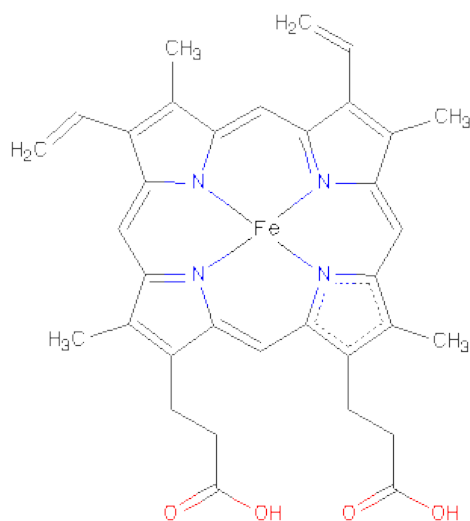
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	Fe	S	0	0
			7	3	4		

- Molecule 9 is MALONATE ION (three-letter code: MLI) (formula:  $\text{C}_3\text{H}_2\text{O}_4$ ).



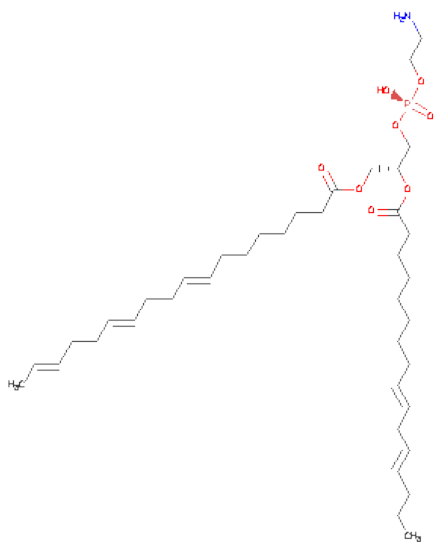
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			7	3	4		

- Molecule 10 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



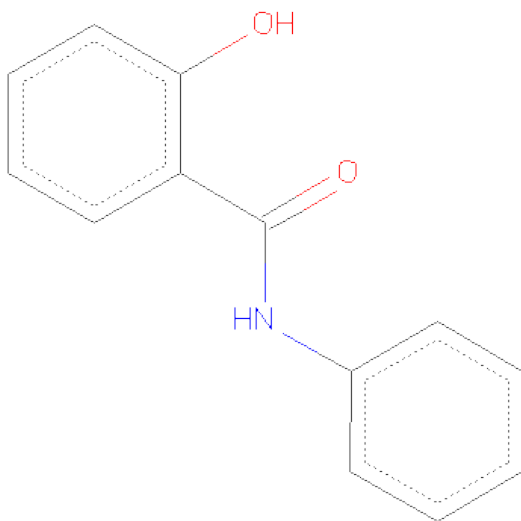
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 11 is L-ALPHA-PHOSPHATIDYL-BETA-OLEOYL-GAMMA-PALMITOYL-PHOSPHATIDYLETHANOLAMINE (three-letter code: EPH) (formula:  $C_{39}H_{68}NO_8P$ ).



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

- Molecule 12 is 2-HYDROXY-N-PHENYLBENZAMIDE (three-letter code: SLI) (formula:  $C_{13}H_{11}NO_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	C	1	Total	C	N	O	0	0
			16	13	1	2		

- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	B	1	Total	O	0	0
			1	1		





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	71.86Å 84.20Å 294.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	27.81 – 3.10 27.81 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.7 (27.81-3.10) 99.6 (27.81-3.10)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.36 (at 3.11Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.204 , 0.248 0.205 , 0.249	Depositor DCC
$R_{free}$ test set	1688 reflections (5.33%)	DCC
Wilson B-factor (Å <sup>2</sup> )	71.1	Xtriage
Anisotropy	0.202	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 27.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 33385 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	8663	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.51% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, MLI, F3S, FES, EPH, HEM, FAD, SLI

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	0.36	0/4828	0.55	1/6531 (0.0%)
2	B	0.36	0/1964	0.52	0/2648
3	C	0.35	0/1091	0.49	0/1483
4	D	0.35	0/784	0.49	0/1066
All	All	0.35	0/8667	0.53	1/11728 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	454	LEU	CA-CB-CG	5.05	126.91	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	4729	0	0	9	0
2	B	1922	0	0	5	0
3	C	1064	0	0	2	0
4	D	765	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	53	0	31	5	0
6	B	4	0	0	0	0
7	B	8	0	0	0	0
8	B	7	0	0	0	0
9	A	7	0	2	2	0
10	C	43	0	30	1	0
11	D	44	0	53	0	0
12	C	16	0	10	2	0
13	B	1	0	0	0	0
All	All	8663	0	126	18	0

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 2.

The worst 5 of 18 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:57:HIS:NE2	5:A:700:FAD:HM82	1.18	1.50
1:A:57:HIS:CE1	5:A:700:FAD:HM82	1.90	1.06
12:C:1201:SLI:O2	12:C:1201:SLI:H9	1.91	0.70
2:B:209:PRO:O	2:B:214:ARG:NH1	2.33	0.61
3:C:46:ARG:NE	10:C:1305:HEM:O2D	2.36	0.57

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	611/622 (98%)	568 (93%)	40 (6%)	3 (0%)	38	81
2	B	237/252 (94%)	227 (96%)	10 (4%)	0	100	100
3	C	136/140 (97%)	134 (98%)	1 (1%)	1 (1%)	30	76
4	D	100/103 (97%)	95 (95%)	5 (5%)	0	100	100
All	All	1084/1117 (97%)	1024 (94%)	56 (5%)	4 (0%)	43	84

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	569	GLN
1	A	260	GLY
3	C	84	PRO
1	A	403	SER

### 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%)	454 (91%)	45 (9%)	14	47
2	B	214/220 (97%)	196 (92%)	18 (8%)	16	52
3	C	117/118 (99%)	108 (92%)	9 (8%)	18	57
4	D	76/76 (100%)	70 (92%)	6 (8%)	18	55
All	All	906/920 (98%)	828 (91%)	78 (9%)	15	51

5 of 78 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	488	SER
1	A	597	LEU
4	D	37	LYS
1	A	514	MET
1	A	556	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 ⓘ

8 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	58,58,58	1.11	5 (8%)	85,89,89	1.98	13 (15%)
9	MLI	A	701	-	2,6,6	2.75	2 (100%)	0,7,7	0.00	-
6	FES	B	302	2	0,4,4	0.00	-	0,4,4	0.00	-
7	SF4	B	303	2	12,12,12	4.36	12 (100%)	0,24,24	0.00	-
8	F3S	B	304	2	3,9,9	18.53	3 (100%)	0,15,15	0.00	-
12	SLI	C	1201	-	17,17,17	1.48	2 (11%)	22,22,22	1.13	2 (9%)
10	HEM	C	1305	3,4	49,50,50	2.27	15 (30%)	46,82,82	1.93	8 (17%)
11	EPH	D	1306	-	42,43,48	2.13	7 (16%)	46,48,53	2.05	9 (19%)

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	-	0/34/50/50	0/1/6/6
9	MLI	A	701	-	-	0/0/4/4	0/0/0/0
6	FES	B	302	2	-	0/0/4/4	0/0/1/1
7	SF4	B	303	2	-	0/0/48/48	0/0/5/5
8	F3S	B	304	2	-	0/0/24/24	0/0/3/3
12	SLI	C	1201	-	-	0/8/8/8	0/2/2/2
10	HEM	C	1305	3,4	-	0/14/114/114	0/0/8/8
11	EPH	D	1306	-	1/1/4/14	0/47/47/52	0/0/0/0

The worst 5 of 46 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	304	F3S	S3-FE4	-19.90	2.19	2.33
8	B	304	F3S	S3-FE1	-19.16	2.20	2.33
8	B	304	F3S	S3-FE3	-16.34	2.22	2.33
11	D	1306	EPH	C31-C30	-8.95	1.51	1.55
7	B	303	SF4	S2-FE3	-5.79	2.29	2.33

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	700	FAD	N3A-C2A-N1A	-11.02	119.49	128.71
11	D	1306	EPH	C14-C15-C16	-9.61	112.03	126.73
10	C	1305	HEM	C3B-C4B-NB	-8.23	108.11	114.00
5	A	700	FAD	C2-N1-C10	6.58	121.61	114.98
10	C	1305	HEM	C4D-ND-C1D	5.73	111.02	105.16

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.

## 5.7 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

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	0	100 100	47, 73, 106, 133	0
2	B	239/252 (94%)	-0.30	0	100 100	49, 66, 104, 124	0
3	C	138/140 (98%)	-0.25	1 (0%)	84 32	51, 76, 122, 145	0
4	D	102/103 (99%)	-0.27	0	100 100	55, 73, 100, 125	0
All	All	1092/1117 (97%)	-0.28	1 (0%)	93 70	47, 72, 108, 145	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	82	LEU	3.4

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

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

### 6.3 Carbohydrates

There are no carbohydrates in this entry.

### 6.4 Ligands

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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
11	EPH	D	1306	44/49	0.35	2.95	95,109,122,123	0
12	SLI	C	1201	16/16	0.29	2.27	95,96,96,96	0
10	HEM	C	1305	43/43	0.18	0.91	60,62,69,71	0
9	MLI	A	701	7/7	0.18	-0.31	80,80,80,81	0
8	F3S	B	304	7/7	0.18	-0.33	56,57,58,59	0
5	FAD	A	700	53/53	0.15	-0.58	51,55,56,57	0
7	SF4	B	303	8/8	0.13	-0.86	48,49,51,53	0
6	FES	B	302	4/4	0.09	-1.09	57,58,59,60	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.