



# wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 29, 2016 – 12:36 AM EST

PDB ID : 5KLV  
Title : Structure of bos taurus cytochrome bc1 with fenamidone inhibited  
Authors : Xia, D.; Esser, L.; Zhou, F.; Zhou, Y.; Xiao, Y.; Tang, W.K.; Yu, C.A.; Qin, Z.  
Deposited on : 2016-06-25  
Resolution : 2.65 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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20028320  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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-20028320

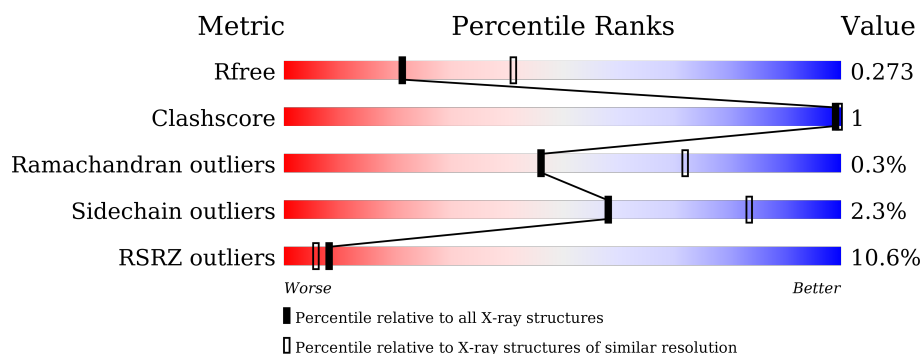
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.65 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.






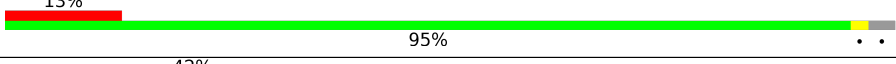

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	3152 (2.70-2.62)
Clashscore	102246	3524 (2.70-2.62)
Ramachandran outliers	100387	3469 (2.70-2.62)
Sidechain outliers	100360	3469 (2.70-2.62)
RSRZ outliers	91569	3161 (2.70-2.62)

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	446	<div> <div>3%</div> <div>96%</div> <div>.</div> </div>
2	B	439	<div> <div>%</div> <div>95%</div> <div>..</div> </div>
3	C	379	<div> <div>3%</div> <div>96%</div> <div>..</div> </div>
4	D	241	<div> <div>17%</div> <div>95%</div> <div>5%</div> </div>
5	E	196	<div> <div>31%</div> <div>96%</div> <div>.</div> </div>
6	F	110	<div> <div>5%</div> <div>92%</div> <div>5%</div> </div>

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Mol	Chain	Length	Quality of chain
7	G	80	
8	H	78	
9	I	78	
10	J	63	
11	K	55	

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
12	6PE	A	501	-	-	-	X
13	CDL	A	502	-	-	-	X
14	GOL	B	501	-	-	-	X
14	GOL	B	503	-	-	-	X
17	8PE	C	1004	-	-	-	X
22	PX4	J	101	-	-	-	X

## 2 Entry composition

There are 23 unique types of molecules in this entry. The entry contains 33655 atoms, of which 16742 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 Cytochrome b-c1 complex subunit 1, mitochondrial.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	446	Total	C	H	N	O	S	0	0	0
			6799	2161	3341	609	668	20			

- Molecule 2 is a protein called Cytochrome b-c1 complex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	425	Total	C	H	N	O	S	0	0	0
			6328	1998	3147	564	612	7			

- Molecule 3 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	377	Total	C	H	N	O	S	0	0	0
			6042	2009	3046	470	499	18			

- Molecule 4 is a protein called Cytochrome c1, heme protein, mitochondrial.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	D	241	Total	C	H	N	O	S	0	0	0
			3778	1225	1859	330	349	15			

- Molecule 5 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
5	E	196	Total	C	H	N	O	S	0	0	0
			3015	957	1497	263	290	8			

- Molecule 6 is a protein called Cytochrome b-c1 complex subunit 7.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
6	F	105	Total	C	H	N	O	S	0	0	0
			1816	576	905	166	167	2			

- Molecule 7 is a protein called Cytochrome b-c1 complex subunit 8.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
7	G	75	Total	C	H	N	O	S	0	0	0
			1261	410	633	118	99	1			

- Molecule 8 is a protein called Cytochrome b-c1 complex subunit 6, mitochondrial.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
8	H	67	Total	C	H	N	O	S	0	0	0
			1075	332	527	99	112	5			

- Molecule 9 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
9	I	34	Total	C	H	N	O	S	0	0	0
			509	149	265	51	43	1			

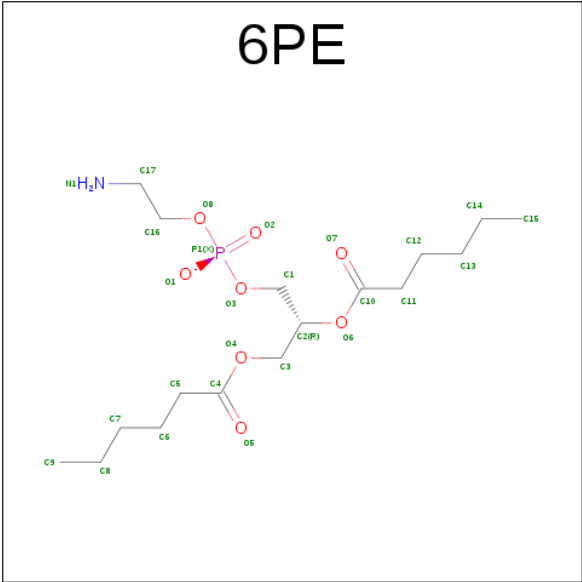
- Molecule 10 is a protein called Cytochrome b-c1 complex subunit 9.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
10	J	61	Total	C	H	N	O	S	0	0	0
			1004	329	502	87	86				

- Molecule 11 is a protein called Cytochrome b-c1 complex subunit 10.

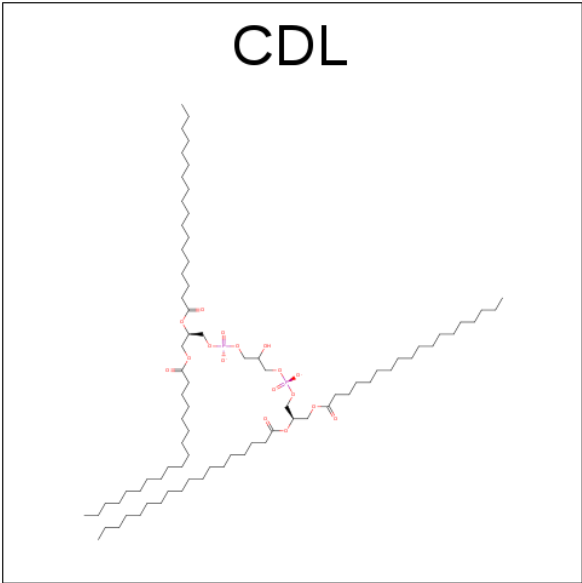
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
11	K	50	Total	C	H	N	O	S	0	0	0
			823	273	413	74	63				

- Molecule 12 is 1,2-DIHEXANOYL-SN-GLYCERO-3-PHOSPHOETHANOLAMINE (three-letter code: 6PE) (formula: C<sub>17</sub>H<sub>33</sub>NO<sub>8</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
12	A	1	Total 60	C 17	H 33	N 1	O 8	P 1	0	0
12	K	1	Total 60	C 17	H 33	N 1	O 8	P 1	0	0

- Molecule 13 is CARDIOLIPIN (three-letter code: CDL) (formula: C<sub>81</sub>H<sub>156</sub>O<sub>17</sub>P<sub>2</sub>).



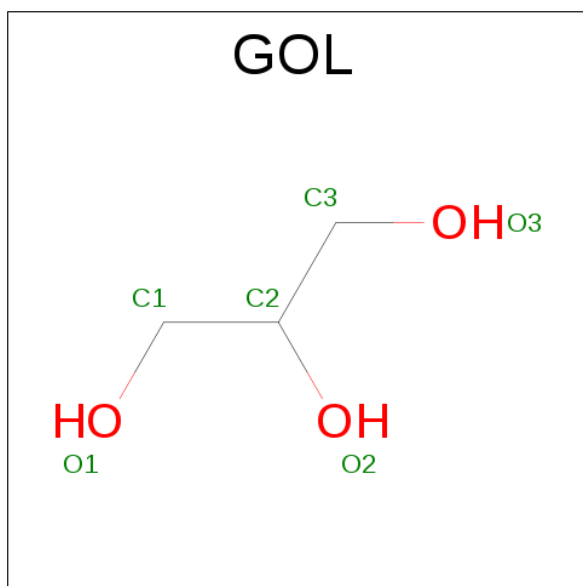
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	A	1	Total	C	H	O	P	0	0
			124	41	64	17	2		
13	D	1	Total	C	H	O	P	0	0
			124	41	64	17	2		

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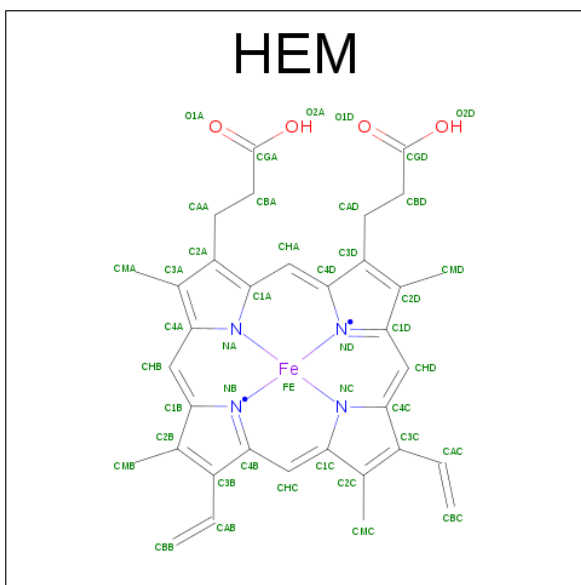
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	G	1	Total	C	H	O	P	0	0
			124	41	64	17	2		

- Molecule 14 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



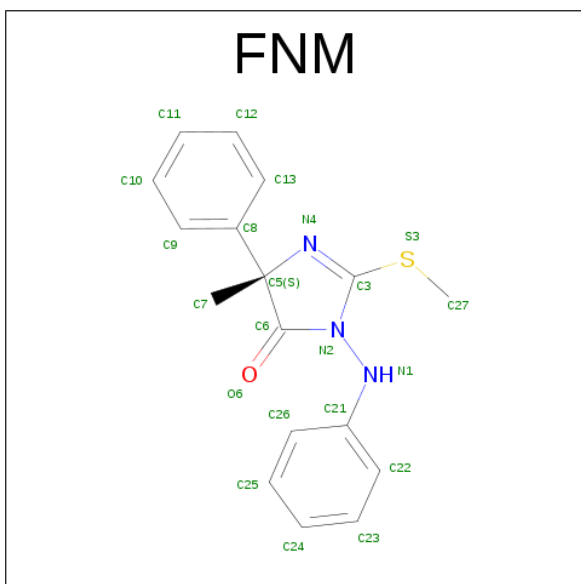
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
14	B	1	Total	C	H	O	0	0
			14	3	8	3		
14	B	1	Total	C	H	O	0	0
			14	3	8	3		
14	B	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 15 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
15	C	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
15	C	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		

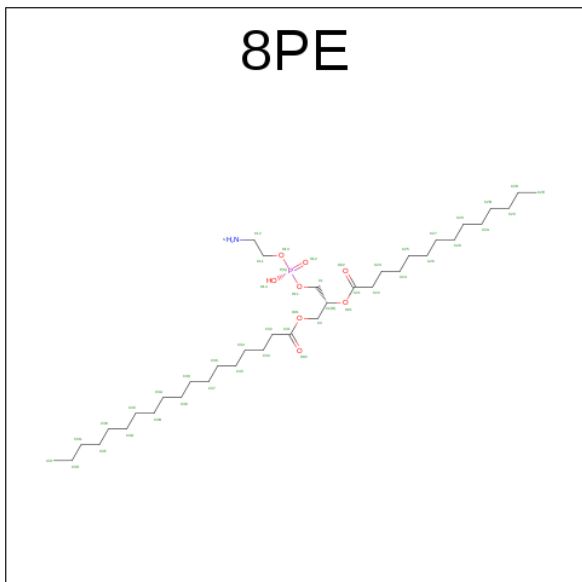
- Molecule 16 is (5S)-5-methyl-2-(methylsulfanyl)-5-phenyl-3-(phenylamino)-3,5-dihydro-4H-imidazol-4-one (three-letter code: FNM) (formula: C<sub>17</sub>H<sub>17</sub>N<sub>3</sub>OS).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
16	C	1	Total	C	H	N	O	S	0	0
			39	17	17	3	1	1		



- Molecule 17 is (2R)-3-{[(S)-(2-aminoethoxy)(hydroxy)phosphoryl]oxy}-2-(tetradecanoyloxy)propyl octadecanoate (three-letter code: 8PE) (formula:  $C_{37}H_{74}NO_8P$ ).

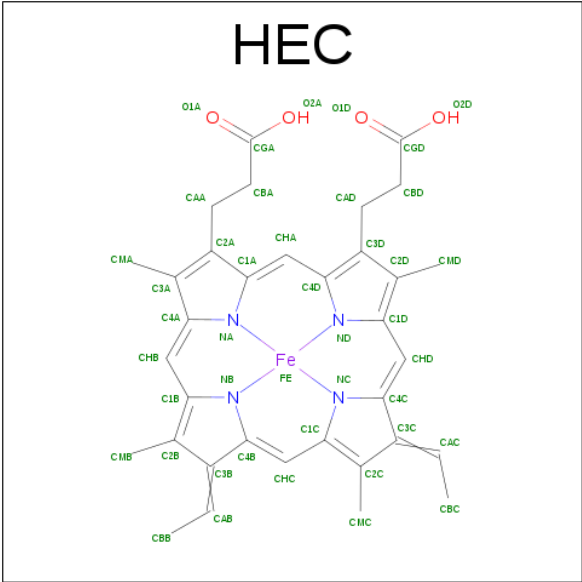


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
17	C	1	Total	C	H	N	O	P	0	0
			120	37	73	1	8	1		

- Molecule 18 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

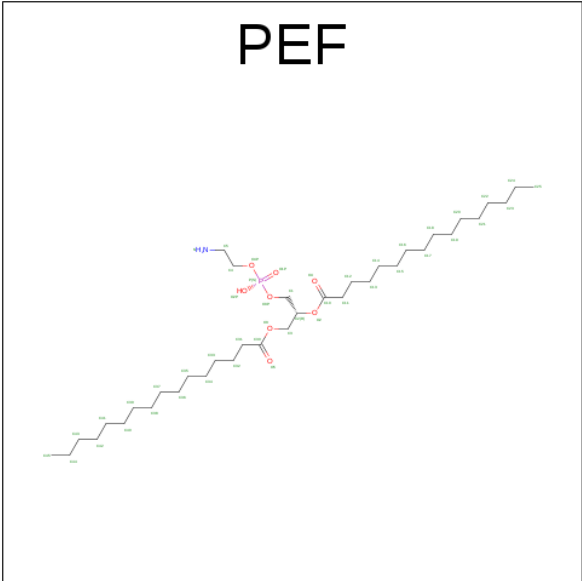
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	C	1	Total	Cl	0	0
			1	1		

- Molecule 19 is HEME C (three-letter code: HEC) (formula:  $C_{34}H_{34}FeN_4O_4$ ).



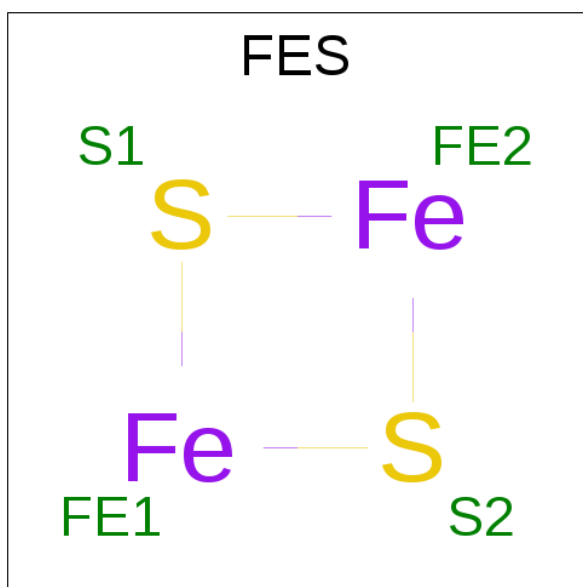
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
19	D	1	Total	C	Fe	H	N	O	0	0
			75	34	1	32	4	4		

- Molecule 20 is DI-PALMITOYL-3-SN-PHOSPHATIDYLETHANOLAMINE (three-letter code: PEF) (formula:  $C_{37}H_{74}NO_8P$ ).



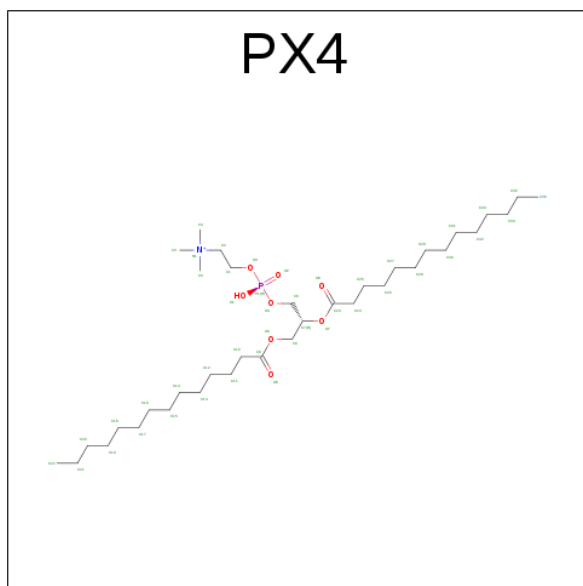
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
20	D	1	Total	C	H	N	O	P	0	0
			118	37	71	1	8	1		

- Molecule 21 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula:  $Fe_2S_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	E	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 22 is 1,2-DIMYRISTOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PX4) (formula:  $C_{36}H_{73}NO_8P$ ).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
22	J	1	Total	C	H	N	O	P	0	0
			118	36	72	1	8	1		

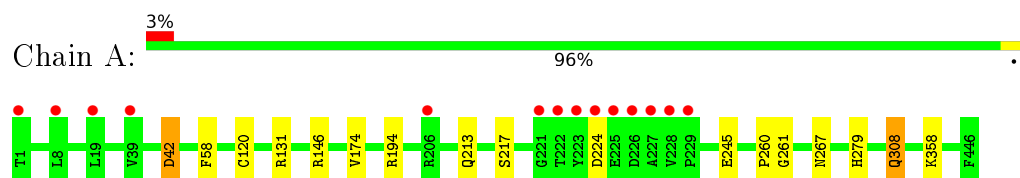
- Molecule 23 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	A	8	Total 8	O 8	0	0
23	B	28	Total 28	O 28	0	0
23	C	4	Total 4	O 4	0	0
23	D	4	Total 4	O 4	0	0
23	F	5	Total 5	O 5	0	0
23	I	1	Total 1	O 1	0	0

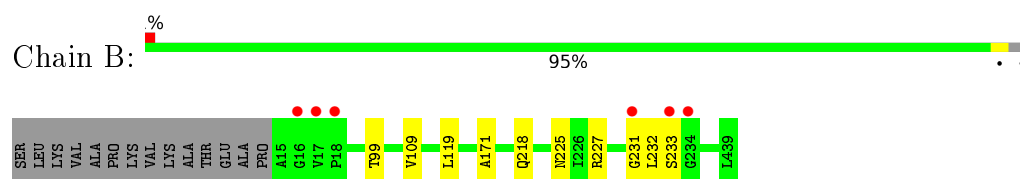
### 3 Residue-property plots [i](#)

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.

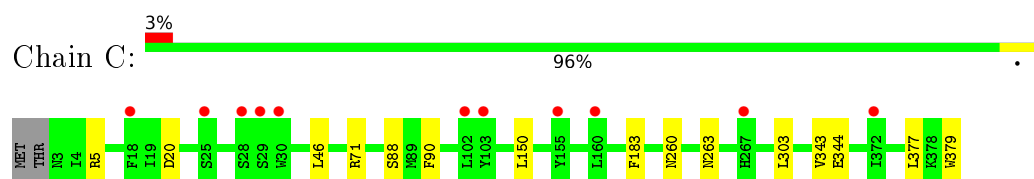
- Molecule 1: Cytochrome b-c1 complex subunit 1, mitochondrial



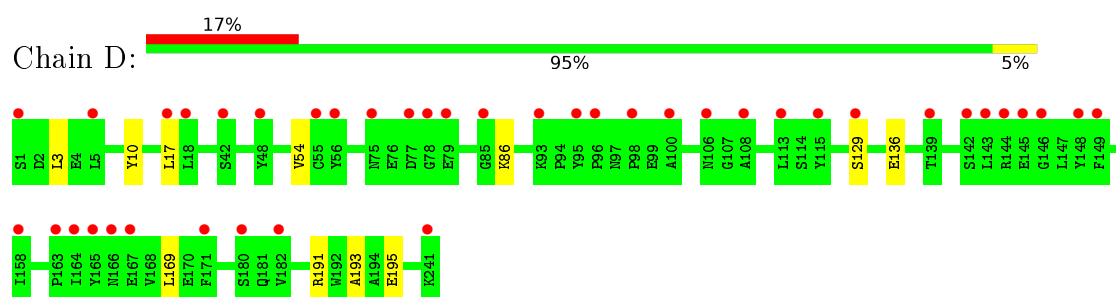
- Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial



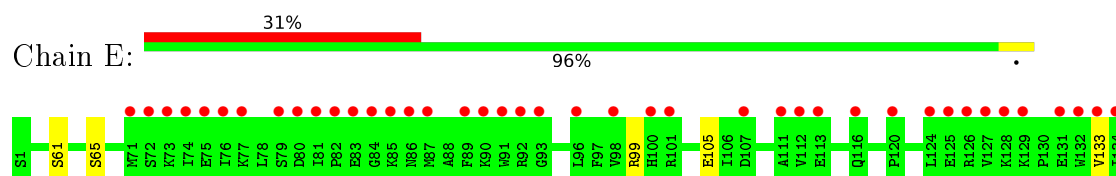
- Molecule 3: Cytochrome b

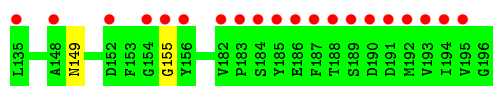


- Molecule 4: Cytochrome c1, heme protein, mitochondrial

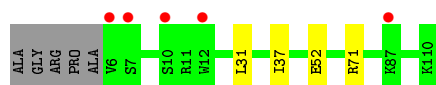
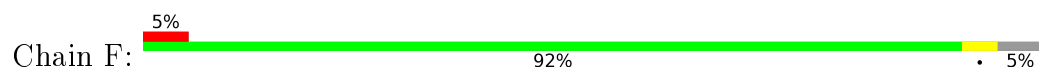


- Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

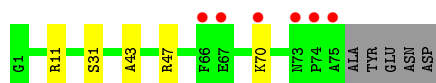
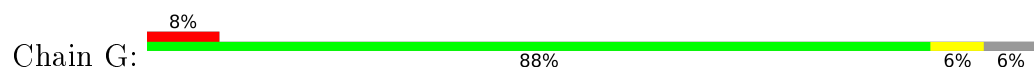




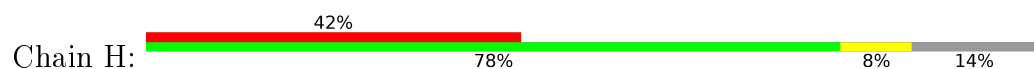
- Molecule 6: Cytochrome b-c1 complex subunit 7



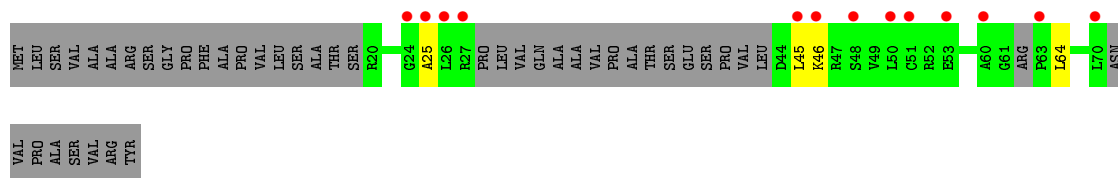
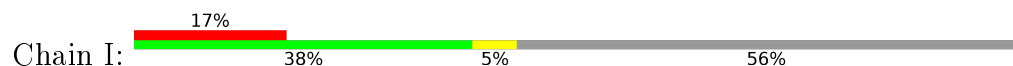
- Molecule 7: Cytochrome b-c1 complex subunit 8



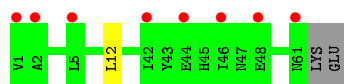
- Molecule 8: Cytochrome b-c1 complex subunit 6, mitochondrial



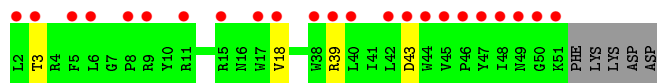
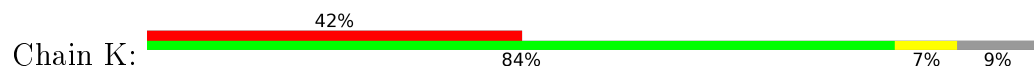
- Molecule 9: Cytochrome b-c1 complex subunit Rieske, mitochondrial



- Molecule 10: Cytochrome b-c1 complex subunit 9



- Molecule 11: Cytochrome b-c1 complex subunit 10



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	153.99Å 153.99Å 592.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.68 – 2.65 40.69 – 2.65	Depositor EDS
% Data completeness (in resolution range)	99.2 (34.68-2.65) 89.2 (40.69-2.65)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.87 (at 2.65Å)	Xtriage
Refinement program	PHENIX (1.11rc1_2513: ???)	Depositor
R, $R_{free}$	0.228 , 0.269 0.230 , 0.273	Depositor DCC
$R_{free}$ test set	1572 reflections (1.65%)	DCC
Wilson B-factor (Å <sup>2</sup> )	56.1	Xtriage
Anisotropy	0.313	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 42.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	33655	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 2.13% 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 ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, CL, CDL, 8PE, PX4, 6PE, FES, HEC, HEM, FNM, PEF

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	0.30	0/3531	0.49	0/4792
2	B	0.30	0/3241	0.51	0/4398
3	C	0.29	0/3093	0.46	0/4232
4	D	0.40	1/1978 (0.1%)	0.59	0/2684
5	E	0.28	0/1552	0.47	0/2100
6	F	0.31	0/930	0.48	0/1246
7	G	0.32	0/649	0.48	0/878
8	H	0.27	0/553	0.50	0/741
9	I	0.31	0/242	0.68	0/319
10	J	0.28	0/515	0.47	0/696
11	K	0.29	0/425	0.51	0/584
All	All	0.31	1/16709 (0.0%)	0.50	0/22670

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	10	TYR	C-N	9.74	1.52	1.34

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	3458	3341	3356	6	0
2	B	3181	3147	3160	2	0
3	C	2996	3046	3058	4	0
4	D	1919	1859	1868	2	0
5	E	1518	1497	1503	2	0
6	F	911	905	906	1	0
7	G	628	633	636	3	0
8	H	548	527	530	2	0
9	I	244	265	265	0	0
10	J	502	502	505	0	0
11	K	410	413	413	1	0
12	A	27	33	33	0	0
12	K	27	33	33	0	0
13	A	60	64	64	0	0
13	D	60	64	64	0	0
13	G	60	64	64	0	0
14	B	18	24	24	0	0
15	C	86	60	60	1	0
16	C	22	17	17	0	0
17	C	47	73	73	0	0
18	C	1	0	0	0	0
19	D	43	32	30	1	0
20	D	47	71	73	0	0
21	E	4	0	0	0	0
22	J	46	72	72	0	0
23	A	8	0	0	1	0
23	B	28	0	0	0	0
23	C	4	0	0	0	0
23	D	4	0	0	0	0
23	F	5	0	0	0	0
23	I	1	0	0	0	0
All	All	16913	16742	16807	22	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 1.

The worst 5 of 22 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:42:ASP:O	1:A:194:ARG:NH2	2.22	0.72
1:A:213:GLN:O	1:A:217:SER:OG	2.09	0.70
5:E:99:ARG:NH2	5:E:105:GLU:OE2	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:191:ARG:NH1	4:D:195:GLU:OE2	2.28	0.67
11:K:39:ARG:NH1	11:K:43:ASP:OD1	2.31	0.63

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	444/446 (100%)	430 (97%)	13 (3%)	1 (0%)	52	77
2	B	423/439 (96%)	407 (96%)	14 (3%)	2 (0%)	34	59
3	C	375/379 (99%)	365 (97%)	9 (2%)	1 (0%)	46	72
4	D	239/241 (99%)	236 (99%)	3 (1%)	0	100	100
5	E	194/196 (99%)	176 (91%)	18 (9%)	0	100	100
6	F	103/110 (94%)	101 (98%)	2 (2%)	0	100	100
7	G	73/80 (91%)	71 (97%)	2 (3%)	0	100	100
8	H	65/78 (83%)	60 (92%)	4 (6%)	1 (2%)	13	28
9	I	28/78 (36%)	25 (89%)	1 (4%)	2 (7%)	1	1
10	J	59/63 (94%)	56 (95%)	3 (5%)	0	100	100
11	K	48/55 (87%)	46 (96%)	2 (4%)	0	100	100
All	All	2051/2165 (95%)	1973 (96%)	71 (4%)	7 (0%)	46	72

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	232	LEU
3	C	343	VAL
9	I	46	LYS
8	H	49	GLN

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Mol	Chain	Res	Type
9	I	25	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	370/370 (100%)	363 (98%)	7 (2%)	65	87
2	B	332/343 (97%)	328 (99%)	4 (1%)	78	92
3	C	325/327 (99%)	317 (98%)	8 (2%)	55	82
4	D	206/206 (100%)	199 (97%)	7 (3%)	44	72
5	E	168/168 (100%)	165 (98%)	3 (2%)	66	88
6	F	96/98 (98%)	93 (97%)	3 (3%)	47	75
7	G	66/70 (94%)	65 (98%)	1 (2%)	72	90
8	H	64/74 (86%)	62 (97%)	2 (3%)	47	75
9	I	25/60 (42%)	23 (92%)	2 (8%)	15	31
10	J	51/53 (96%)	50 (98%)	1 (2%)	63	86
11	K	40/45 (89%)	38 (95%)	2 (5%)	30	56
All	All	1743/1814 (96%)	1703 (98%)	40 (2%)	58	83

5 of 40 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	379	TRP
4	D	86	LYS
9	I	64	LEU
4	D	17	LEU
4	D	129	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	339	GLN
2	B	154	ASN
2	B	313	ASN
1	A	240	GLN
2	B	218	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 ⓘ

Of 17 ligands modelled in this entry, 1 is monoatomic - leaving 16 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
12	6PE	A	501	-	25,26,26	1.69	6 (24%)	26,31,31	1.19	3 (11%)
13	CDL	A	502	-	59,59,99	1.27	7 (11%)	61,71,111	1.10	4 (6%)
14	GOL	B	501	-	5,5,5	0.32	0	5,5,5	0.22	0
14	GOL	B	502	-	5,5,5	0.34	0	5,5,5	0.20	0
14	GOL	B	503	-	5,5,5	0.34	0	5,5,5	0.20	0
15	HEM	C	1001	3	24,50,50	1.93	5 (20%)	16,82,82	1.65	3 (18%)
15	HEM	C	1002	3	24,50,50	1.89	4 (16%)	16,82,82	1.56	3 (18%)
16	FNM	C	1003	-	21,24,24	1.13	3 (14%)	20,34,34	1.07	2 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
17	8PE	C	1004	-	45,46,46	1.65	7 (15%)	46,51,51	1.14	4 (8%)
19	HEC	D	1001	4	24,50,50	2.37	4 (16%)	19,82,82	2.80	3 (15%)
20	PEF	D	1002	-	45,46,46	1.08	4 (8%)	46,51,51	0.82	2 (4%)
13	CDL	D	1003	-	59,59,99	1.29	6 (10%)	61,71,111	1.20	5 (8%)
21	FES	E	1001	5	0,4,4	0.00	-	0,4,4	0.00	-
13	CDL	G	101	-	59,59,99	1.25	6 (10%)	61,71,111	1.05	4 (6%)
22	PX4	J	101	-	45,45,45	1.26	3 (6%)	49,53,53	0.94	3 (6%)
12	6PE	K	101	-	25,26,26	1.68	6 (24%)	26,31,31	1.25	2 (7%)

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
12	6PE	A	501	-	-	0/30/30/30	0/0/0/0
13	CDL	A	502	-	-	0/70/70/110	0/0/0/0
14	GOL	B	501	-	-	0/4/4/4	0/0/0/0
14	GOL	B	502	-	-	0/4/4/4	0/0/0/0
14	GOL	B	503	-	-	0/4/4/4	0/0/0/0
15	HEM	C	1001	3	-	0/6/54/54	0/0/8/8
15	HEM	C	1002	3	-	0/6/54/54	0/0/8/8
16	FNM	C	1003	-	-	0/12/31/31	0/3/3/3
17	8PE	C	1004	-	-	0/50/50/50	0/0/0/0
19	HEC	D	1001	4	-	0/6/54/54	0/0/8/8
20	PEF	D	1002	-	-	0/50/50/50	0/0/0/0
13	CDL	D	1003	-	-	1/70/70/110	0/0/0/0
21	FES	E	1001	5	-	0/0/4/4	0/1/1/1
13	CDL	G	101	-	-	0/70/70/110	0/0/0/0
22	PX4	J	101	-	-	0/49/49/49	0/0/0/0
12	6PE	K	101	-	-	0/30/30/30	0/0/0/0

The worst 5 of 61 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	D	1001	HEC	C3B-C2B	-5.97	1.34	1.40
19	D	1001	HEC	C3C-C2C	-5.66	1.34	1.40
15	C	1002	HEM	C3C-C2C	-3.81	1.35	1.40
15	C	1002	HEM	C3B-C2B	-3.47	1.35	1.40
15	C	1001	HEM	C3C-C2C	-3.47	1.36	1.40

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
19	D	1001	HEC	CBB-CAB-C3B	-9.36	106.87	127.34
19	D	1001	HEC	CBC-CAC-C3C	-5.35	115.64	127.34
16	C	1003	FNM	C27-S3-C3	-3.26	96.18	100.47
15	C	1002	HEM	CBD-CAD-C3D	-3.14	106.96	112.47
17	C	1004	8PE	O31-C31-O32	-2.94	115.79	123.51

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	D	1003	CDL	CA4-OA6-CA5-C11

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	C	1002	HEM	1	0
19	D	1001	HEC	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 ⓘ

### 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	446/446 (100%)	0.37	14 (3%)	52	51	40, 64, 101, 189	0
2	B	425/439 (96%)	0.17	6 (1%)	78	76	31, 47, 82, 180	0
3	C	377/379 (99%)	0.38	11 (2%)	55	53	48, 70, 101, 129	0
4	D	241/241 (100%)	0.96	41 (17%)	2	1	48, 112, 153, 188	0
5	E	196/196 (100%)	1.61	61 (31%)	1	0	66, 119, 197, 246	0
6	F	105/110 (95%)	0.41	5 (4%)	34	32	38, 60, 110, 166	0
7	G	75/80 (93%)	0.36	6 (8%)	15	12	42, 79, 127, 161	0
8	H	67/78 (85%)	2.19	33 (49%)	0	0	108, 140, 175, 211	0
9	I	34/78 (43%)	1.69	13 (38%)	0	0	45, 78, 105, 111	0
10	J	61/63 (96%)	0.92	8 (13%)	5	3	74, 96, 137, 166	0
11	K	50/55 (90%)	1.61	23 (46%)	0	0	72, 92, 146, 167	0
All	All	2077/2165 (95%)	0.65	221 (10%)	8	6	31, 72, 151, 246	0

The worst 5 of 221 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
10	J	1	VAL	11.0
5	E	190	ASP	10.0
5	E	187	PHE	9.3
11	K	44	TRP	9.2
5	E	76	ILE	8.7

### 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 [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
14	GOL	B	501	6/6	0.64	0.38	9.39	75,91,92,92	0
14	GOL	B	503	6/6	0.84	0.58	6.76	82,99,100,100	0
17	8PE	C	1004	47/47	0.88	0.36	2.69	50,81,106,109	0
22	PX4	J	101	46/46	0.82	0.34	2.37	86,107,120,120	0
12	6PE	A	501	27/27	0.88	0.33	2.26	80,97,116,116	0
13	CDL	A	502	60/100	0.90	0.35	2.09	70,100,123,124	0
13	CDL	D	1003	60/100	0.69	0.34	1.95	76,101,123,124	0
13	CDL	G	101	60/100	0.74	0.36	1.88	77,96,114,115	0
15	HEM	C	1001	43/43	0.97	0.24	1.08	71,79,96,104	0
15	HEM	C	1002	43/43	0.97	0.23	0.69	55,61,75,75	0
12	6PE	K	101	27/27	0.84	0.34	0.56	102,123,132,132	0
20	PEF	D	1002	47/47	0.89	0.27	0.46	69,88,106,106	0
16	FNM	C	1003	22/22	0.94	0.20	0.24	79,88,107,108	0
18	CL	C	1005	1/1	0.92	0.24	0.06	62,62,62,62	0
14	GOL	B	502	6/6	0.92	0.20	-0.02	60,72,74,74	0
19	HEC	D	1001	43/43	0.96	0.23	-0.33	101,125,151,156	0
21	FES	E	1001	4/4	0.98	0.13	-1.15	104,105,106,106	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.