



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 15, 2017 – 01:09 AM EST

PDB ID : 4PD4
Title : Structural analysis of atovaquone-inhibited cytochrome bc1 complex reveals the molecular basis of antimalarial drug action
Authors : Birth, D.; Kao, W.-C.; Hunte, C.
Deposited on : unknown
Resolution : 3.04 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

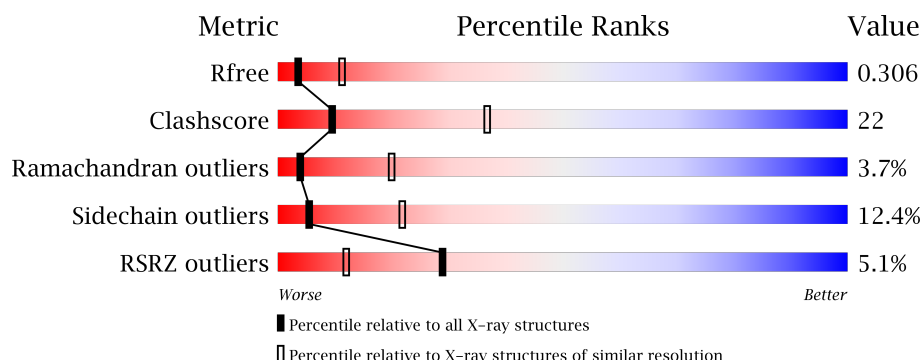
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.04 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	2176 (3.08-3.00)
Clashscore	112137	2542 (3.08-3.00)
Ramachandran outliers	110173	2458 (3.08-3.00)
Sidechain outliers	110143	2461 (3.08-3.00)
RSRZ outliers	101464	2202 (3.08-3.00)

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. 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	431	<div> <div>9%</div> <div>49%</div> <div>45%</div> <div>6%</div> </div>
2	B	352	<div> <div>9%</div> <div>55%</div> <div>41%</div> <div>• •</div> </div>
3	C	385	<div> <div>48%</div> <div>44%</div> <div>8%</div> <div>•</div> </div>
4	D	248	<div> <div>2%</div> <div>48%</div> <div>46%</div> <div>5%</div> <div>•</div> </div>
5	E	185	<div> <div>4%</div> <div>49%</div> <div>42%</div> <div>9%</div> <div>•</div> </div>

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Mol	Chain	Length	Quality of chain
6	F	74	
7	G	126	
8	H	93	
9	I	57	
10	J	127	
11	K	107	

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
16	3PE	C	4004	-	-	-	X
17	UQ6	C	4005	-	-	-	X

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 17646 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 Cytochrome b-c1 complex subunit 1, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	431	Total	C	N	O	S	115	0	0
			3344	2109	576	653	6			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	153	ASP	GLU	conflict	UNP P07256

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	352	Total	C	N	O	S	72	0	0
			2735	1747	453	534	1			

- Molecule 3 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	385	Total	C	N	O	S	10	0	0
			3090	2082	484	503	21			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	248	Total	C	N	O	S	5	0	0
			1961	1249	340	363	9			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	185	Total	C	N	O	S	27	0	0
			1411	893	242	266	10			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	74	Total	C	N	O	S	0	0	0
			624	391	108	123	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	126	Total	C	N	O	S	0	0	0
			1019	653	173	191	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	93	Total	C	N	O	S	98	0	0
			773	510	131	130	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	I	57	Total	C	N	O	0	0	0
			465	310	77	78			

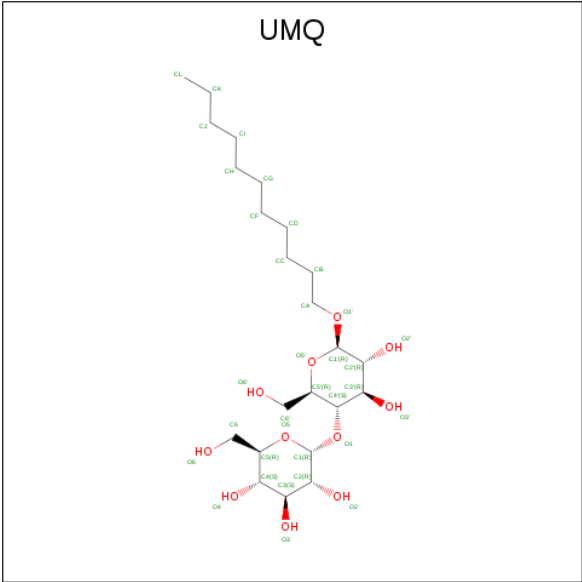
- Molecule 10 is a protein called Igh protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	127	Total	C	N	O	S	0	0	0
			1015	644	167	201	3			

- Molecule 11 is a protein called Ig kappa chain V-V region HP 124E1.

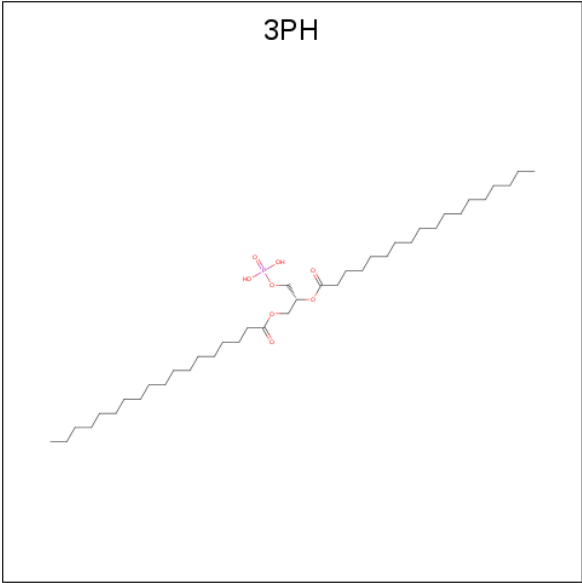
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	107	Total	C	N	O	S	0	0	0
			842	536	141	163	2			

- Molecule 12 is UNDECYL-MALTOSIDE (three-letter code: UMQ) (formula: C₂₃H₄₄O₁₁).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	A	1	Total	C	O	0	0
			34	23	11		

- Molecule 13 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (three-letter code: 3PH) (formula: C₃₉H₇₇O₈P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	A	1	Total	C	O	P	0	0
			31	22	8	1		
13	C	1	Total	C	O	P	0	0
			35	26	8	1		

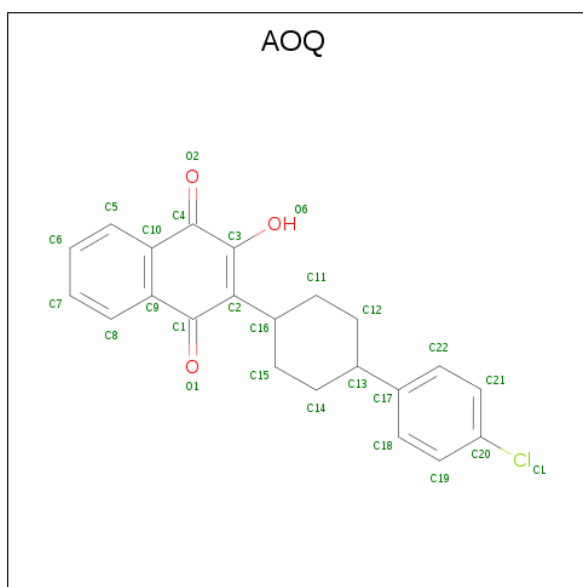
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	E	1	Total	C	O	P	0	0
			38	29	8	1		

- # HEM

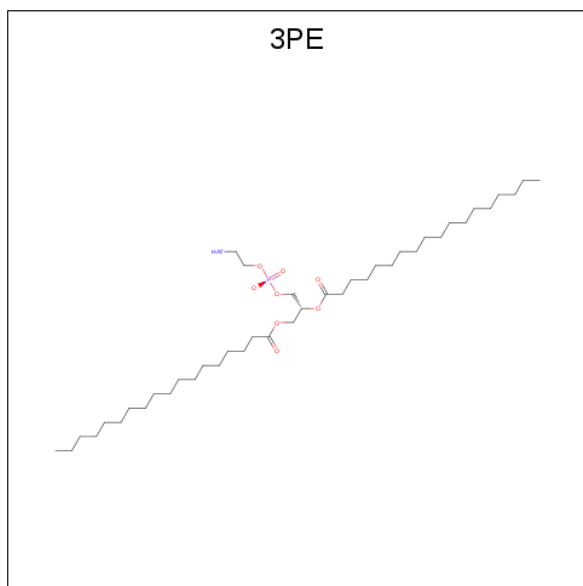
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
14	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
14	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- 



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
15	C	1	Total	C	Cl	O	0	0
			26	22	1	3		

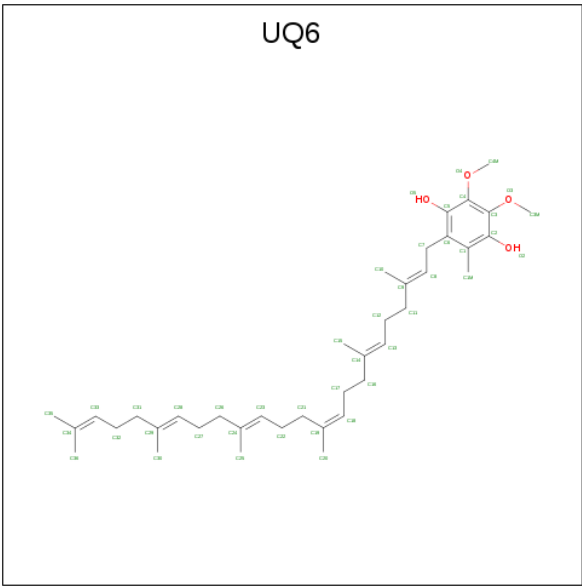
- Molecule 16 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOETHANOLAMINE (three-letter code: 3PE) (formula: $C_{41}H_{82}NO_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
16	C	1	Total	C	N	O	P	0	0
			27	17	1	8	1		

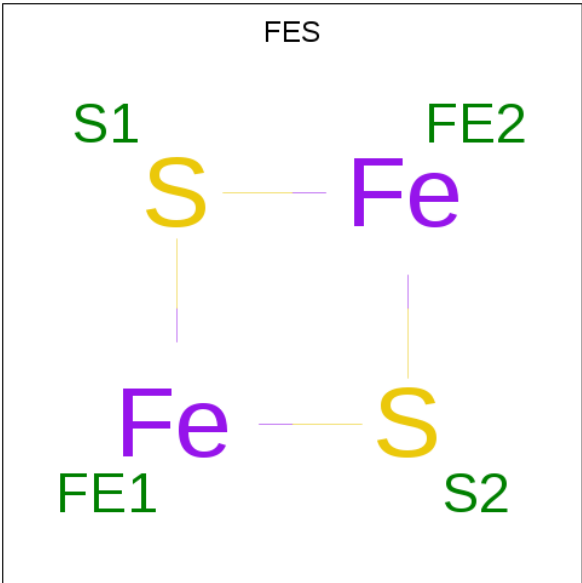
- Molecule 17 is 5-(3,7,11,15,19,23-HEXAMETHYL-TETRACOSA-2,6,10,14,18,22-HEXAENYL)-2,3-DIMETHOXY-6-METHYL-BENZENE-1,4-DIOL (three-letter code: UQ6)

(formula: C₃₉H₆₀O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
17	C	1	Total	C	O	0	0
			43	39	4		

- Molecule 18 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂).

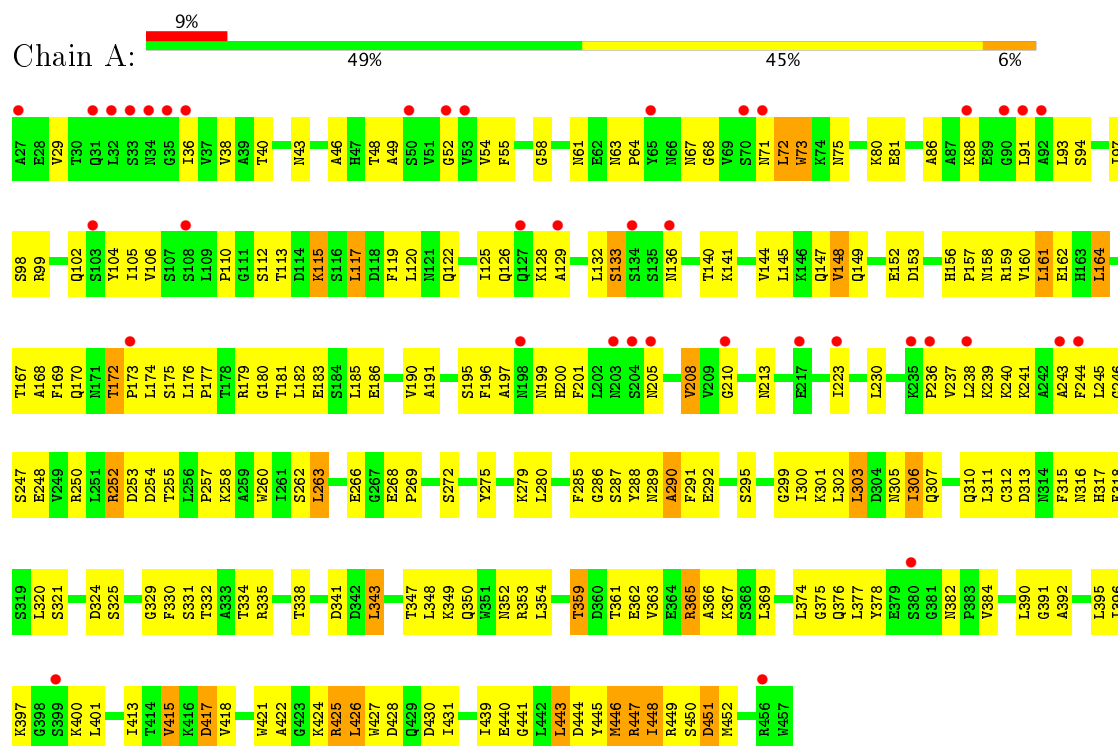


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
18	E	1	Total	Fe	S	0	0
			4	2	2		

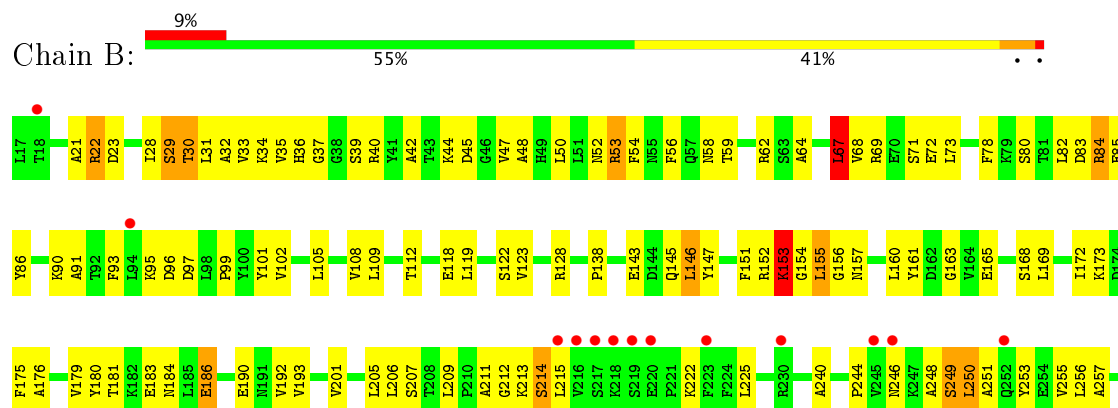
3 Residue-property plots

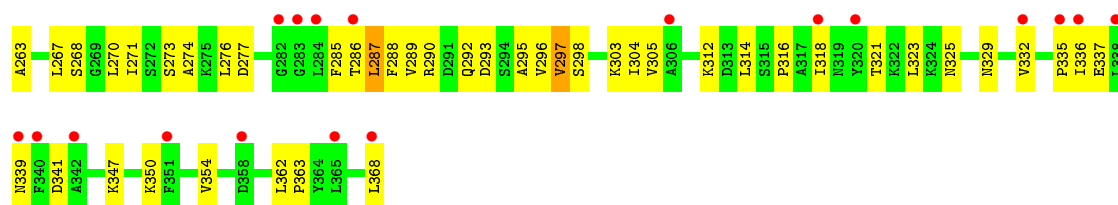
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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

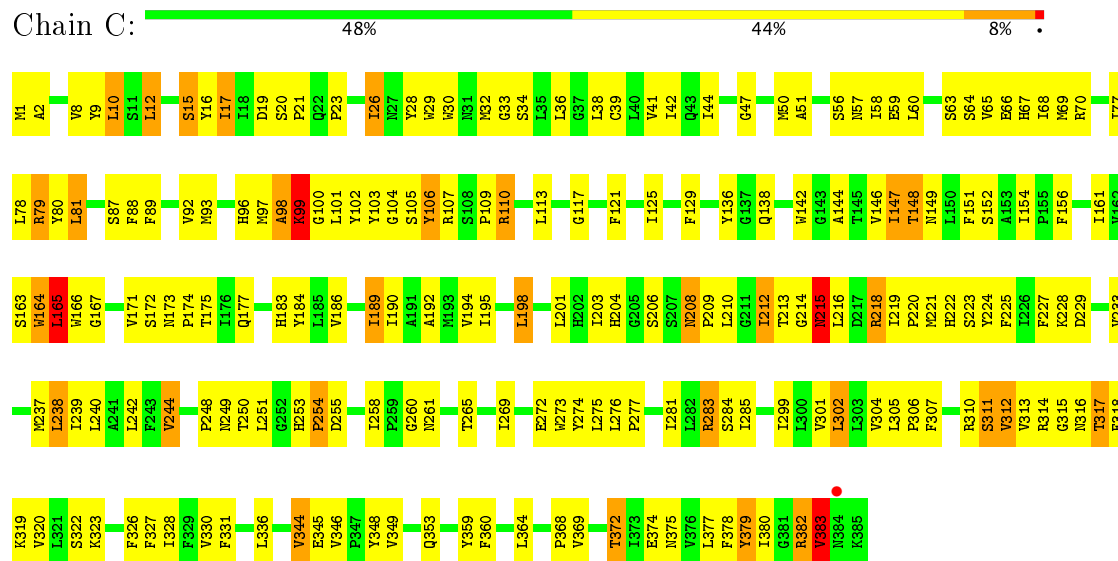


- Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial

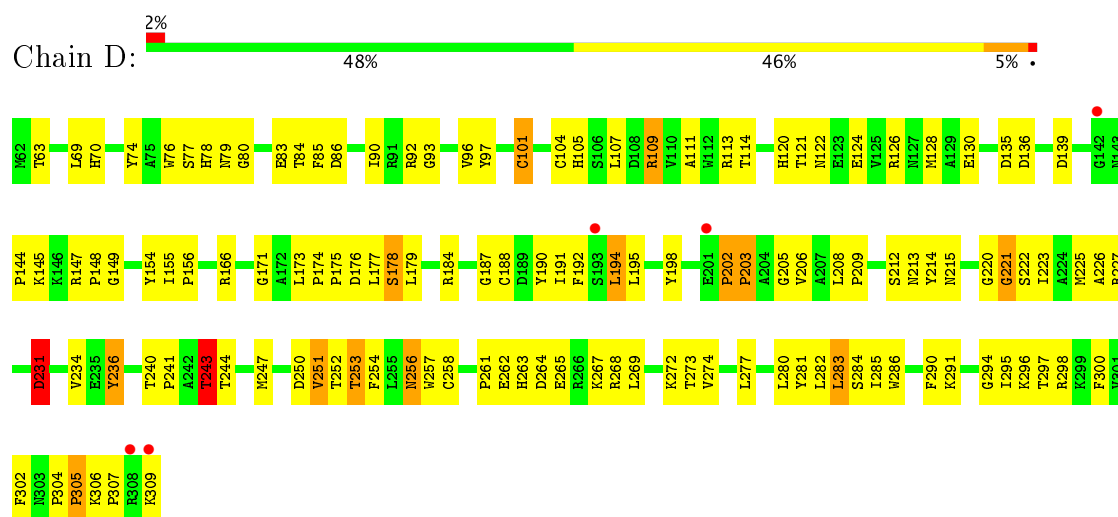




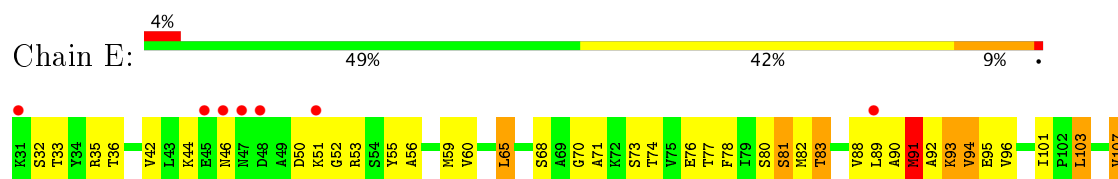
• Molecule 3: Cytochrome b

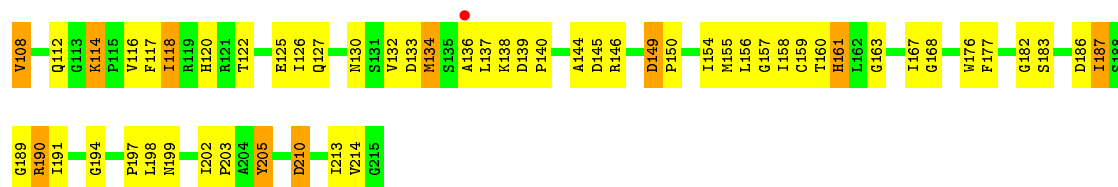


• Molecule 4: Cytochrome c1, heme protein, mitochondrial

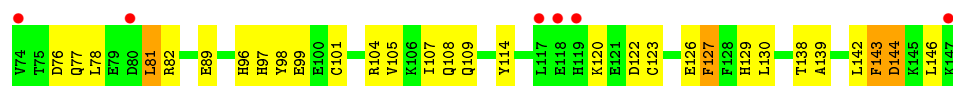


• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

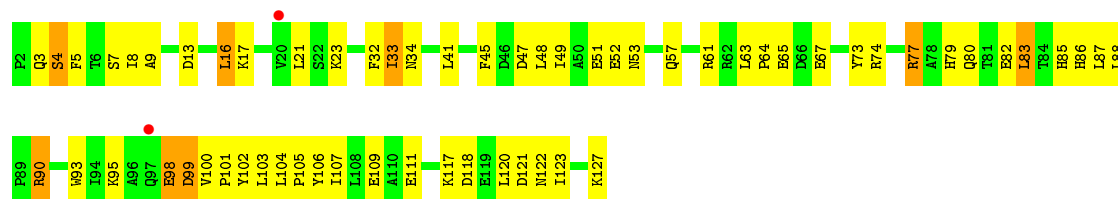




- Molecule 6: Cytochrome b-c1 complex subunit 6



- Molecule 7: Cytochrome b-c1 complex subunit 7



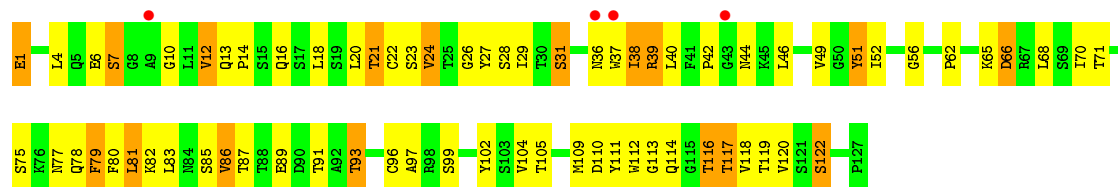
- Molecule 8: Cytochrome b-c1 complex subunit 8



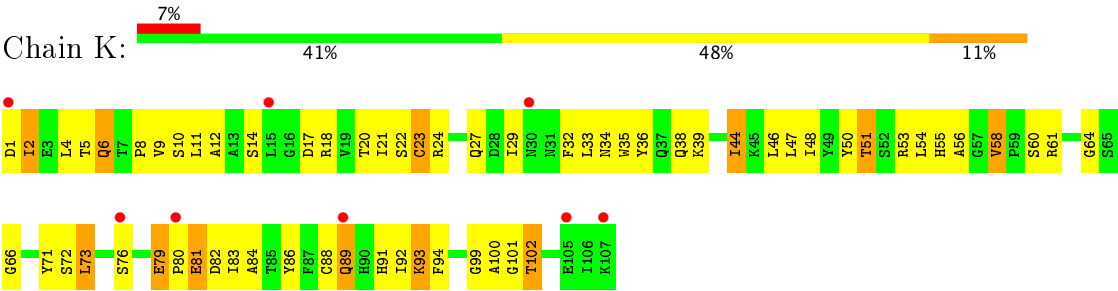
- Molecule 9: Cytochrome b-c1 complex subunit 9



- Molecule 10: Igh protein



- Molecule 11: Ig kappa chain V-V region HP 124E1



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	212.26Å 150.88Å 143.09Å 90.00° 115.18° 90.00°	Depositor
Resolution (Å)	24.99 – 3.04 24.99 – 3.04	Depositor EDS
% Data completeness (in resolution range)	98.4 (24.99-3.04) 98.6 (24.99-3.04)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.48 (at 3.05Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.268 , 0.297 0.280 , 0.306	Depositor DCC
R_{free} test set	2008 reflections (2.67%)	DCC
Wilson B-factor (Å ²)	97.2	Xtriage
Anisotropy	0.052	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 43.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	17646	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.45% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: UMQ, 3PH, FES, AOQ, HEM, 3PE, UQ6

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	0.42	0/3405	0.62	0/4614
2	B	0.37	0/2781	0.58	1/3764 (0.0%)
3	C	0.70	0/3192	0.83	1/4354 (0.0%)
4	D	0.48	0/2022	0.69	0/2751
5	E	0.54	0/1444	0.74	0/1957
6	F	0.40	0/638	0.62	0/858
7	G	0.58	0/1040	0.80	0/1408
8	H	0.55	0/804	0.71	0/1088
9	I	0.43	0/479	0.59	0/646
10	J	0.48	0/1043	0.71	0/1422
11	K	0.38	0/863	0.59	0/1172
All	All	0.51	0/17711	0.69	2/24034 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	B	67	LEU	CA-CB-CG	5.30	127.50	115.30
3	C	110	ARG	NE-CZ-NH2	-5.01	117.79	120.30

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	3344	0	3321	152	0
2	B	2735	0	2774	108	0
3	C	3090	0	3129	167	0
4	D	1961	0	1890	101	0
5	E	1411	0	1386	66	0
6	F	624	0	581	23	0
7	G	1019	0	1034	52	0
8	H	773	0	736	34	0
9	I	465	0	459	18	0
10	J	1015	0	959	57	0
11	K	842	0	820	42	0
12	A	34	0	44	3	0
13	A	31	0	35	2	0
13	C	35	0	46	1	0
13	E	38	0	49	6	0
14	C	86	0	60	15	0
14	D	43	0	30	11	0
15	C	26	0	19	3	0
16	C	27	0	28	1	0
17	C	43	0	58	5	0
18	E	4	0	0	0	0
All	All	17646	0	17458	747	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 22.

The worst 5 of 747 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)
3:C:318:PHE:HD1	7:G:48:LEU:HD21	1.32	0.93
1:A:248:GLU:OE2	1:A:250:ARG:NH2	2.04	0.90
13:A:502:3PH:H321	13:A:502:3PH:H221	1.54	0.89
3:C:32:MET:HE3	3:C:92:VAL:HG13	1.54	0.89
11:K:93:LYS:HD2	11:K:94:PHE:H	1.41	0.83

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	429/431 (100%)	349 (81%)	67 (16%)	13 (3%)	5	25
2	B	350/352 (99%)	284 (81%)	56 (16%)	10 (3%)	5	26
3	C	383/385 (100%)	318 (83%)	49 (13%)	16 (4%)	3	17
4	D	246/248 (99%)	199 (81%)	36 (15%)	11 (4%)	3	15
5	E	183/185 (99%)	142 (78%)	33 (18%)	8 (4%)	3	16
6	F	72/74 (97%)	60 (83%)	10 (14%)	2 (3%)	6	27
7	G	124/126 (98%)	102 (82%)	16 (13%)	6 (5%)	2	14
8	H	91/93 (98%)	61 (67%)	23 (25%)	7 (8%)	1	5
9	I	55/57 (96%)	41 (74%)	13 (24%)	1 (2%)	10	40
10	J	125/127 (98%)	115 (92%)	9 (7%)	1 (1%)	22	61
11	K	105/107 (98%)	76 (72%)	23 (22%)	6 (6%)	2	11
All	All	2163/2185 (99%)	1747 (81%)	335 (16%)	81 (4%)	4	20

5 of 81 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	257	PRO
2	B	153	LYS
3	C	99	LYS
3	C	164	TRP
3	C	165	LEU

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%)	324 (88%)	46 (12%)	5	22
2	B	301/301 (100%)	272 (90%)	29 (10%)	10	34
3	C	338/338 (100%)	295 (87%)	43 (13%)	5	21
4	D	206/206 (100%)	181 (88%)	25 (12%)	6	23
5	E	151/151 (100%)	127 (84%)	24 (16%)	3	13
6	F	67/67 (100%)	59 (88%)	8 (12%)	6	23
7	G	110/110 (100%)	99 (90%)	11 (10%)	9	31
8	H	77/77 (100%)	69 (90%)	8 (10%)	8	29
9	I	47/47 (100%)	41 (87%)	6 (13%)	5	21
10	J	112/112 (100%)	94 (84%)	18 (16%)	3	13
11	K	93/93 (100%)	78 (84%)	15 (16%)	3	13
All	All	1872/1872 (100%)	1639 (88%)	233 (12%)	5	22

5 of 233 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	305	LEU
4	D	234	VAL
10	J	116	THR
3	C	336	LEU
4	D	63	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
4	D	79	ASN
11	K	89	GLN
7	G	79	HIS
3	C	141	HIS
5	E	127	GLN

5.3.3 RNA ⓘ

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

11 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
12	UMQ	A	501	-	35,35,35	0.47	0	46,46,46	1.27	6 (13%)
13	3PH	A	502	-	30,30,47	1.21	2 (6%)	34,35,52	1.18	4 (11%)
14	HEM	C	4001	3	28,50,50	2.49	11 (39%)	17,82,82	2.02	6 (35%)
14	HEM	C	4002	3	28,50,50	2.07	7 (25%)	17,82,82	2.44	7 (41%)
15	AOQ	C	4003	-	29,29,29	1.73	7 (24%)	41,42,42	1.74	11 (26%)
16	3PE	C	4004	-	26,26,50	1.35	2 (7%)	28,31,55	1.48	5 (17%)
17	UQ6	C	4005	-	43,43,43	1.19	3 (6%)	52,55,55	2.21	20 (38%)
13	3PH	C	4006	-	34,34,47	1.15	2 (5%)	38,39,52	1.68	8 (21%)
14	HEM	D	401	4	28,50,50	2.28	7 (25%)	17,82,82	2.07	6 (35%)
18	FES	E	301	5	0,4,4	0.00	-	0,4,4	0.00	-
13	3PH	E	302	-	37,37,47	1.08	2 (5%)	41,42,52	1.31	3 (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	UMQ	A	501	-	-	0/20/60/60	0/2/2/2
13	3PH	A	502	-	-	0/32/32/49	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	HEM	C	4001	3	-	0/6/54/54	0/0/8/8
14	HEM	C	4002	3	-	0/6/54/54	0/0/8/8
15	AOQ	C	4003	-	-	0/8/38/38	0/4/4/4
16	3PE	C	4004	-	-	0/30/30/54	0/0/0/0
17	UQ6	C	4005	-	-	0/39/39/39	0/1/1/1
13	3PH	C	4006	-	-	0/36/36/49	0/0/0/0
14	HEM	D	401	4	-	0/6/54/54	0/0/8/8
18	FES	E	301	5	-	0/0/4/4	0/1/1/1
13	3PH	E	302	-	-	0/39/39/49	0/0/0/0

The worst 5 of 43 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	D	401	HEM	C3B-C2B	-5.21	1.33	1.40
17	C	4005	UQ6	O5-C5	-4.54	1.26	1.37
15	C	4003	AOQ	C9-C1	-4.46	1.39	1.48
17	C	4005	UQ6	O2-C2	-4.24	1.27	1.37
15	C	4003	AOQ	C10-C4	-4.20	1.39	1.48

The worst 5 of 76 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	C	4001	HEM	CBA-CAA-C2A	-4.98	102.97	112.48
14	C	4002	HEM	CAA-CBA-CGA	-4.91	104.27	112.66
15	C	4003	AOQ	C16-C2-C3	-4.53	114.39	123.51
17	C	4005	UQ6	C17-C18-C19	-4.13	117.30	127.68
14	C	4002	HEM	CBD-CAD-C3D	-4.12	104.61	112.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 47 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	A	501	UMQ	3	0
13	A	502	3PH	2	0
14	C	4001	HEM	7	0
14	C	4002	HEM	8	0
15	C	4003	AOQ	3	0
16	C	4004	3PE	1	0
17	C	4005	UQ6	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	C	4006	3PH	1	0
14	D	401	HEM	11	0
13	E	302	3PH	6	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, 95th 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 ²)	Q<0.9
1	A	417/431 (96%)	0.43	39 (9%) 9 3	17, 69, 116, 122	0
2	B	344/352 (97%)	0.55	31 (9%) 10 4	29, 71, 104, 127	0
3	C	384/385 (99%)	-0.25	1 (0%) 93 82	0, 7, 18, 69	0
4	D	248/248 (100%)	0.14	5 (2%) 65 36	16, 40, 63, 83	1 (0%)
5	E	182/185 (98%)	0.03	8 (4%) 35 15	4, 26, 70, 112	0
6	F	74/74 (100%)	0.35	6 (8%) 13 5	38, 61, 92, 94	0
7	G	126/126 (100%)	-0.19	2 (1%) 72 44	6, 27, 48, 67	0
8	H	82/93 (88%)	0.20	4 (4%) 30 12	7, 29, 67, 88	1 (1%)
9	I	57/57 (100%)	0.02	2 (3%) 44 20	24, 45, 78, 102	0
10	J	127/127 (100%)	0.14	4 (3%) 49 22	27, 44, 63, 68	0
11	K	107/107 (100%)	0.37	8 (7%) 15 6	36, 67, 105, 116	0
All	All	2148/2185 (98%)	0.18	110 (5%) 29 12	0, 42, 102, 127	2 (0%)

The worst 5 of 110 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	27	ALA	8.7
9	I	58	ALA	8.1
3	C	384	ASN	7.6
2	B	282	GLY	5.8
6	F	119	HIS	5.5

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, 95th 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(\AA^2)	Q<0.9
17	UQ6	C	4005	43/43	0.83	0.35	3.30	6,12,21,24	0
16	3PE	C	4004	27/51	0.93	0.27	2.33	4,8,12,14	0
14	HEM	C	4002	43/43	0.98	0.26	0.97	2,5,10,11	0
13	3PH	C	4006	35/48	0.88	0.25	0.92	3,17,29,39	0
13	3PH	E	302	38/48	0.91	0.26	0.72	7,15,21,23	0
13	3PH	A	502	31/48	0.91	0.22	0.56	13,20,33,38	0
14	HEM	C	4001	43/43	0.98	0.25	0.09	0,2,7,20	0
14	HEM	D	401	43/43	0.94	0.25	0.06	22,31,37,43	0
12	UMQ	A	501	34/34	0.89	0.24	0.05	13,31,43,48	0
18	FES	E	301	4/4	0.99	0.18	-0.24	6,7,7,13	0
15	AOQ	C	4003	26/26	0.96	0.17	-1.59	7,12,16,22	0

6.5 Other polymers [i](#)

There are no such residues in this entry.