wwPDB X-ray Structure Validation Summary Report (i)

Oct 16, 2016 – 05:13 AM EDT

PDB ID	:	4U3F
Title	:	Cytochrome bc1 complex from chicken with designed inhibitor bound
Authors	:	Huang, L.-S.; Zhu, X.-L.; Yang, G.F.; Berry, E.A.
Deposited on	:	2014-07-21
Resolution	:	3.23 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

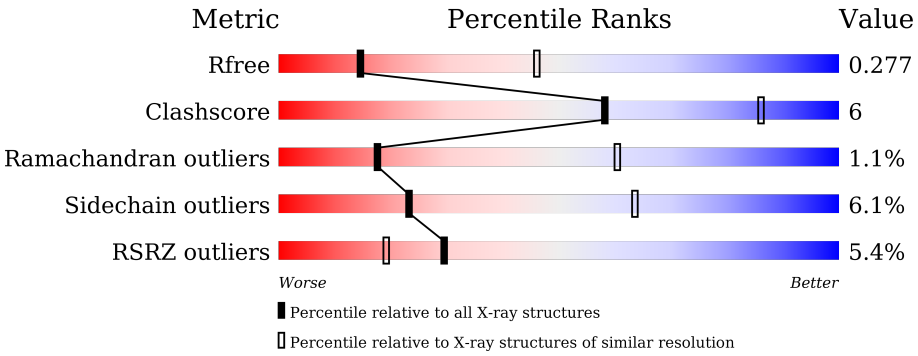
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027939
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027939

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.23 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	1092 (3.28-3.20)
Clashscore	102246	1227 (3.28-3.20)
Ramachandran outliers	100387	1204 (3.28-3.20)
Sidechain outliers	100360	1203 (3.28-3.20)
RSRZ outliers	91569	1097 (3.28-3.20)

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 <=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	2% 81% 16%
1	N	446	2% 81% 16%
2	B	441	2% 72% 21% 5%
2	O	441	2% 73% 20%
3	C	380	% 84% 14%
3	P	380	% 83% 15%

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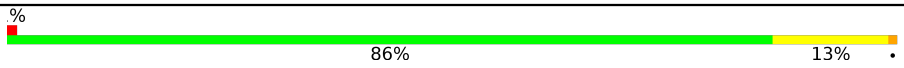
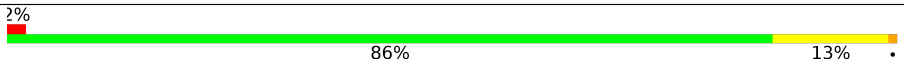
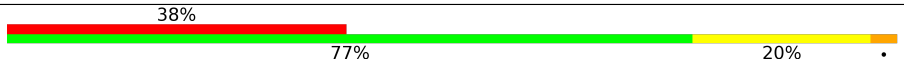
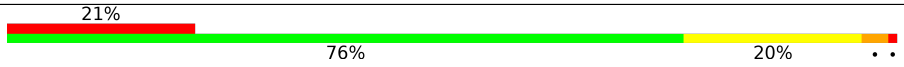
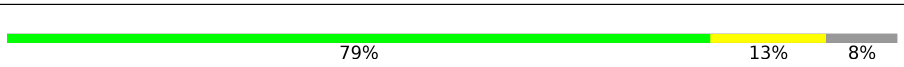
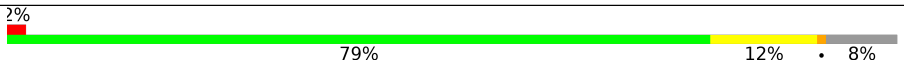
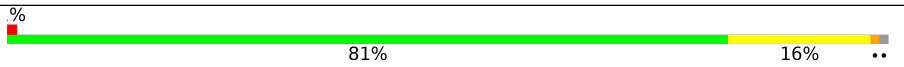
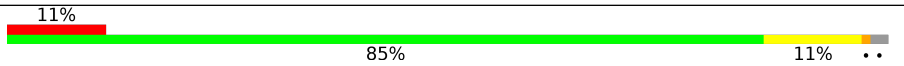
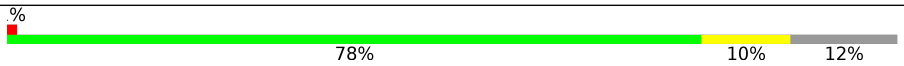
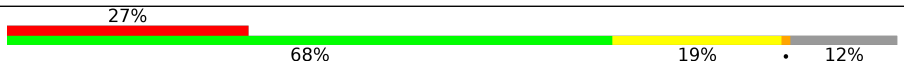
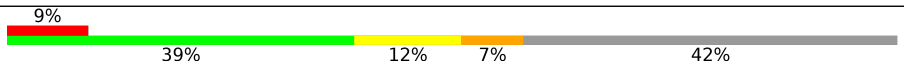
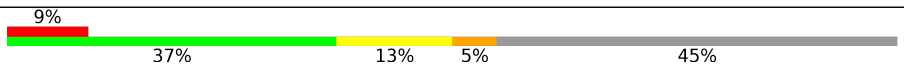
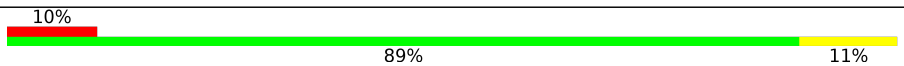
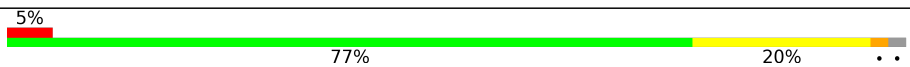
Mol	Chain	Length	Quality of chain
4	D	241	
4	Q	241	
5	E	196	
5	R	196	
6	F	110	
6	S	110	
7	G	81	
7	T	81	
8	H	77	
8	U	77	
9	I	76	
9	V	76	
10	J	61	
10	W	61	

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
11	PEE	A	501	-	-	-	X
11	PEE	C	509	-	-	-	X
11	PEE	E	503	-	-	-	X
11	PEE	P	401	-	-	-	X
11	PEE	P	409	-	-	-	X
11	PEE	P	411	-	-	-	X
11	PEE	R	502	-	-	-	X
14	U10	C	504	-	-	-	X
14	U10	P	405	-	-	-	X
18	CDL	D	502	-	-	-	X
18	CDL	Q	502	-	-	-	X
19	BOG	D	503	-	-	-	X
19	BOG	P	406	-	-	-	X

2 Entry composition

There are 21 unique types of molecules in this entry. The entry contains 32790 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 Mitochondrial ubiquinol-cytochrome-c reductase complex core protein i.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	443	Total	C	N	O	S	0	0	0
			3442	2157	606	658	21			
1	N	442	Total	C	N	O	S	0	0	0
			3437	2154	605	657	21			

- Molecule 2 is a protein called Mitochondrial ubiquinol-cytochrome-c reductase complex core protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	421	Total	C	N	O	S	0	0	0
			3137	1971	544	613	9			
2	O	422	Total	C	N	O	S	0	0	0
			3143	1974	545	614	10			

- Molecule 3 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	380	Total	C	N	O	S	0	0	0
			3021	2025	478	505	13			
3	P	379	Total	C	N	O	S	0	1	0
			3022	2025	480	505	12			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1	FME	-	expression tag	UNP P18946
P	1	FME	-	expression tag	UNP P18946

- Molecule 4 is a protein called Mitochondrial cytochrome c1, heme protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	241	Total	C	N	O	S	0	0	0
			1898	1212	327	347	12			
4	Q	241	Total	C	N	O	S	0	0	0
			1898	1212	327	347	12			

- 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	N	O	S	0	0	0
			1513	952	263	292	6			
5	R	196	Total	C	N	O	S	0	0	0
			1509	950	263	290	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	101	Total	C	N	O	S	0	0	0
			891	570	159	159	3			
6	S	101	Total	C	N	O	S	0	0	0
			891	570	159	159	3			

- Molecule 7 is a protein called Mitochondrial ubiquinol-cytochrome c reductase ubiquinone-binding protein qp-c.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	G	80	Total	C	N	O	0	0	0
			672	437	119	116			
7	T	79	Total	C	N	O	0	0	0
			662	432	117	113			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	68	Total	C	N	O	S	0	0	0
			562	343	104	110	5			
8	U	68	Total	C	N	O	S	0	0	0
			558	341	104	108	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	44	Total	C	N	O	S	0	0	1
			266	157	54	53	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	V	42	Total	C	N	O	S	0	0	1
			265	157	55	51	2			

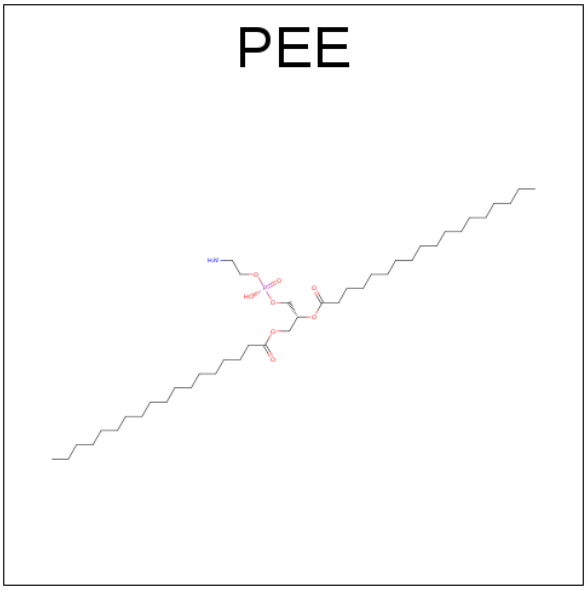
There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	1	AME	-	expression tag	UNP Q5ZLR5
I	29	UNK	LEU	see remark 999	UNP Q5ZLR5
I	30	UNK	ALA	see remark 999	UNP Q5ZLR5
I	31	UNK	PRO	see remark 999	UNP Q5ZLR5
I	32	UNK	ALA	see remark 999	UNP Q5ZLR5
I	33	UNK	ALA	see remark 999	UNP Q5ZLR5
I	37	UNK	LEU	see remark 999	UNP Q5ZLR5
I	38	UNK	ARG	see remark 999	UNP Q5ZLR5
I	39	UNK	ALA	see remark 999	UNP Q5ZLR5
I	40	UNK	GLU	see remark 999	UNP Q5ZLR5
I	41	UNK	LYS	see remark 999	UNP Q5ZLR5
I	42	UNK	VAL	see remark 999	UNP Q5ZLR5
I	43	UNK	VAL	see remark 999	UNP Q5ZLR5
I	44	UNK	LEU	see remark 999	UNP Q5ZLR5
I	45	UNK	ASP	see remark 999	UNP Q5ZLR5
V	-1	AME	-	expression tag	UNP Q5ZLR5
V	27	UNK	LEU	see remark 999	UNP Q5ZLR5
V	28	UNK	ALA	see remark 999	UNP Q5ZLR5
V	29	UNK	PRO	see remark 999	UNP Q5ZLR5
V	30	UNK	ALA	see remark 999	UNP Q5ZLR5
V	31	UNK	ALA	see remark 999	UNP Q5ZLR5
V	32	UNK	LEU	see remark 999	UNP Q5ZLR5
V	33	UNK	ARG	see remark 999	UNP Q5ZLR5
V	37	UNK	ALA	see remark 999	UNP Q5ZLR5
V	38	UNK	GLU	see remark 999	UNP Q5ZLR5
V	39	UNK	LYS	see remark 999	UNP Q5ZLR5
V	40	UNK	VAL	see remark 999	UNP Q5ZLR5
V	41	UNK	VAL	see remark 999	UNP Q5ZLR5
V	42	UNK	LEU	see remark 999	UNP Q5ZLR5
V	43	UNK	ASP	see remark 999	UNP Q5ZLR5

- Molecule 10 is a protein called Mitochondrial ubiquinol-cytochrome c reductase 7.2 kda protein.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
10	J	61	Total C N O 497 321 87 89	0	0	0
10	W	60	Total C N O 479 311 86 82	0	0	1

- Molecule 11 is 1,2-Dioleoyl-sn-glycero-3-phosphoethanolamine (three-letter code: PEE) (formula: $C_{41}H_{83}NO_8P$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	1	Total C N O P 26 16 1 8 1	0	0
11	C	1	Total C N O P 49 39 1 8 1	0	0
11	C	1	Total C N O P 11 5 1 4 1	0	0
11	C	1	Total C N O P 47 37 1 8 1	0	0
11	C	1	Total C O 15 13 2	0	0
11	E	1	Total C N O P 48 38 1 8 1	0	0
11	E	1	Total C 15 15	0	0
11	N	1	Total C N O P 8 2 1 4 1	0	0
11	P	1	Total C O 15 13 2	0	0

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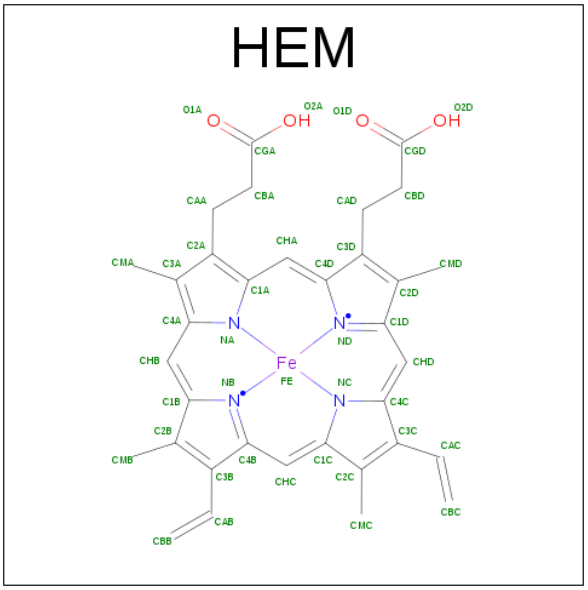
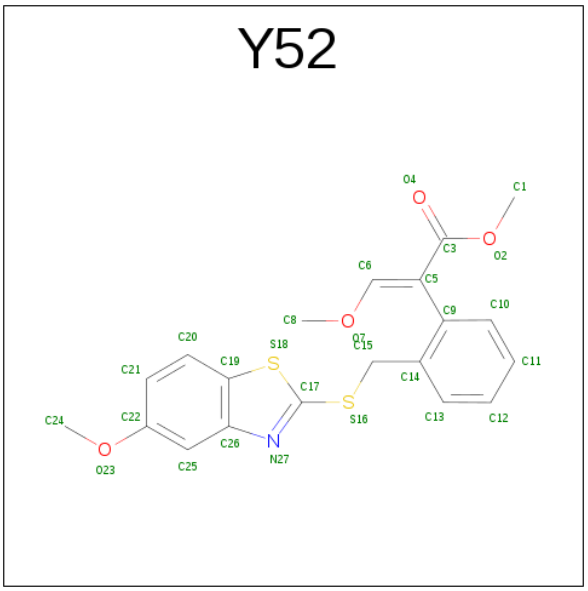
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	P	1	Total C N O P 49 39 1 8 1	0	0
11	P	1	Total C N O P 41 31 1 8 1	0	0
11	P	1	Total C O 12 10 2	0	0
11	P	1	Total C N O P 25 15 1 8 1	0	0
11	R	1	Total C N O P 49 39 1 8 1	0	0

- Molecule 12 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



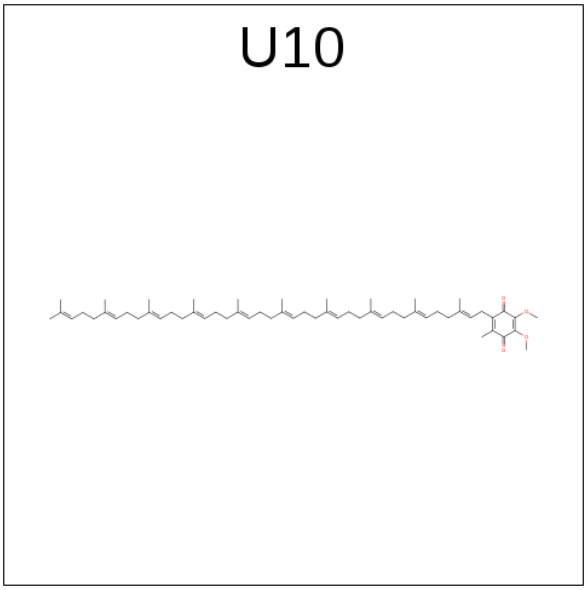
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	C	1	Total C Fe N O 43 34 1 4 4	0	0
12	C	1	Total C Fe N O 43 34 1 4 4	0	0
12	P	1	Total C Fe N O 43 34 1 4 4	0	0
12	P	1	Total C Fe N O 43 34 1 4 4	0	0

- Molecule 13 is methyl (2E)-3-methoxy-2-(2-{[(5-methoxy-1,3-benzothiazol-2-yl)sulfanyl]methyl}phenyl)prop-2-enoate (three-letter code: Y52) (formula: $C_{20}H_{19}NO_4S_2$).



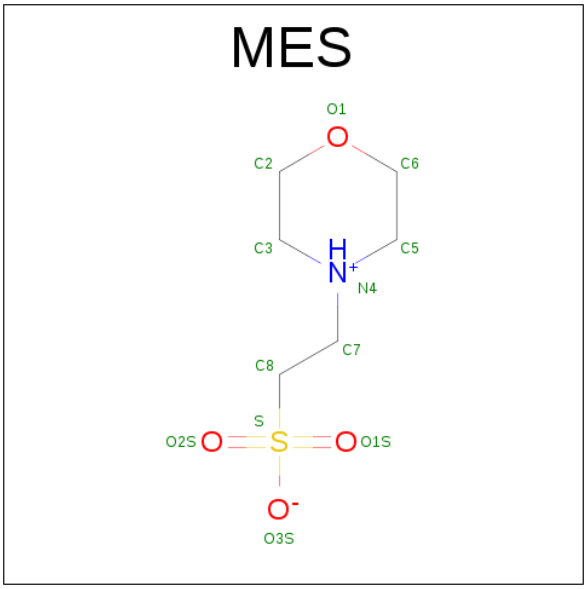
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	C	1	Total	C	N	O	S	0	0
			27	20	1	4	2		
13	P	1	Total	C	N	O	S	0	0
			27	20	1	4	2		

- Molecule 14 is UBIQUINONE-10 (three-letter code: U10) (formula: $C_{59}H_{90}O_4$).



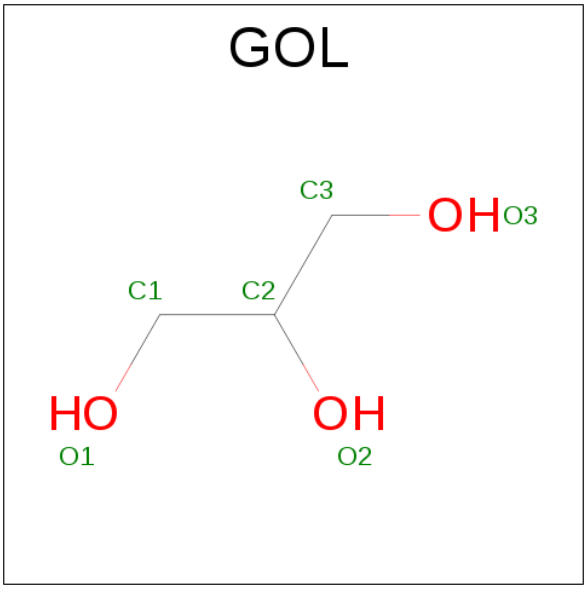
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
14	C	1	Total	C	O		0	0
			19	15	4			
14	P	1	Total	C	O		0	0
			19	15	4			

- Molecule 15 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
15	C	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 16 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
16	C	1	Total	C	O	0	0
			6	3	3		

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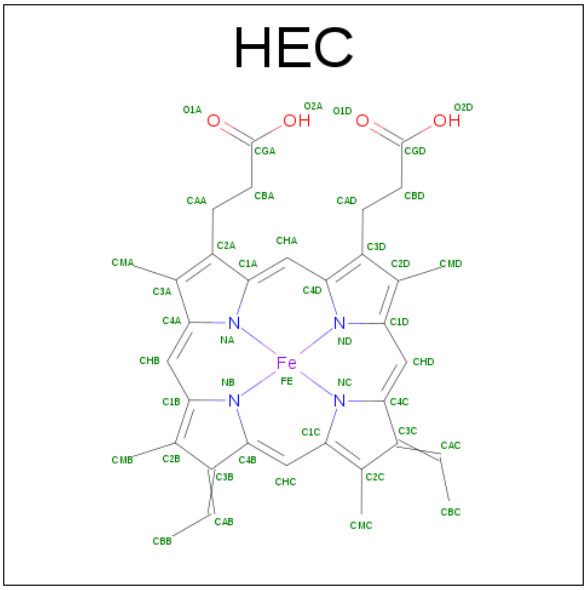
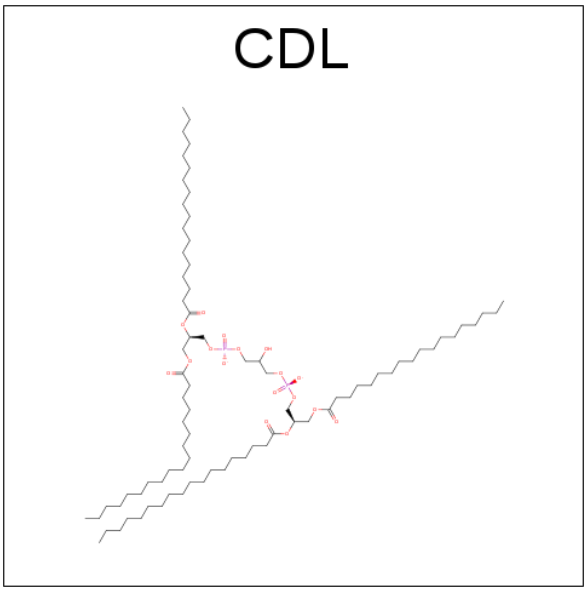
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
16	P	1	Total	C	O	0	0
			6	3	3		

- Molecule 17 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



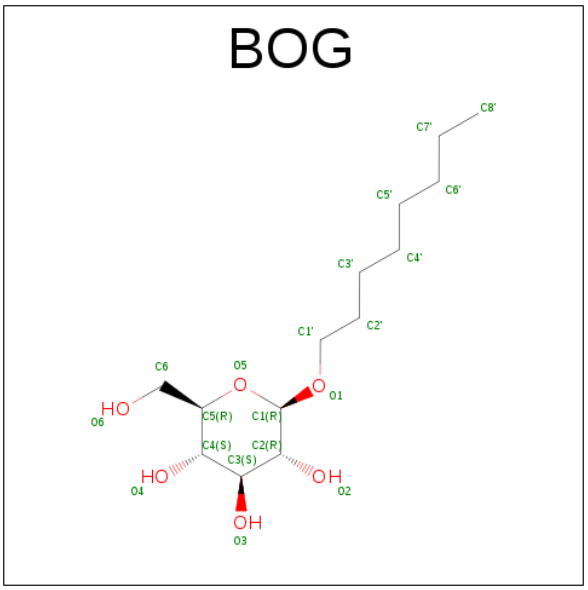
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
17	Q	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 18 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



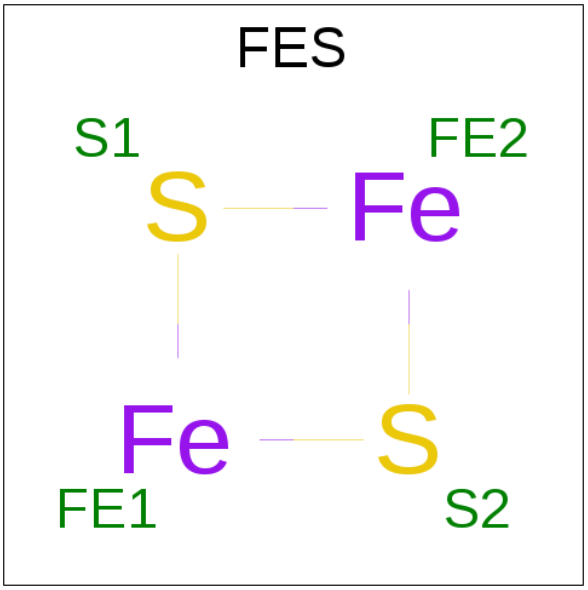
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
18	D	1	Total	C	O	P	0	0
			42	23	17	2		
18	G	1	Total	C	O	P	0	0
			40	21	17	2		
18	Q	1	Total	C	O	P	0	0
			42	23	17	2		
18	T	1	Total	C	O	P	0	0
			40	21	17	2		

- Molecule 19 is B-OCTYLGLUCOSIDE (three-letter code: BOG) (formula: $C_{14}H_{28}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	D	1	Total C O 20 14 6	0	0
19	P	1	Total C O 20 14 6	0	0
19	Q	1	Total C O 20 14 6	0	0

- Molecule 20 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



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

- Molecule 21 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	A	2	Total O 2 2	0	0
21	B	1	Total O 1 1	0	0
21	C	2	Total O 2 2	0	0
21	F	1	Total O 1 1	0	0
21	N	1	Total O 1 1	0	0

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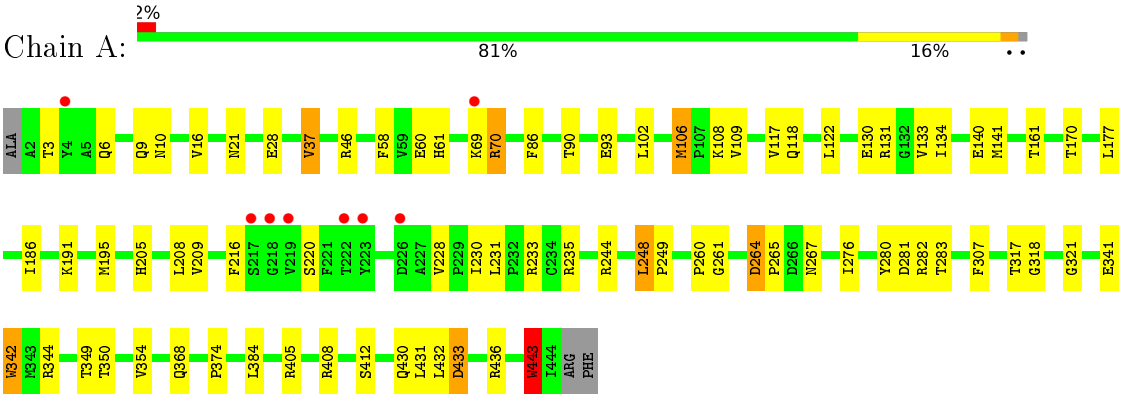
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	O	2	Total O 2 2	0	0
21	P	2	Total O 2 2	0	0

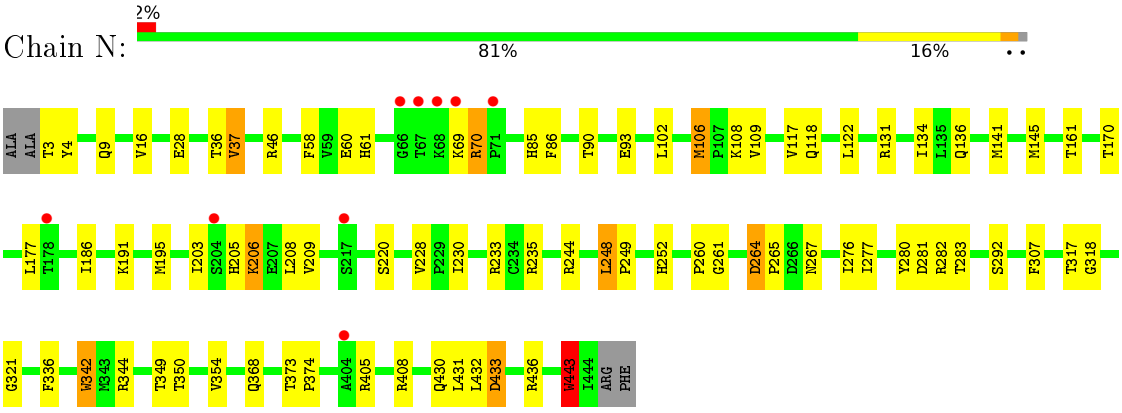
3 Residue-property plots (i)

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.

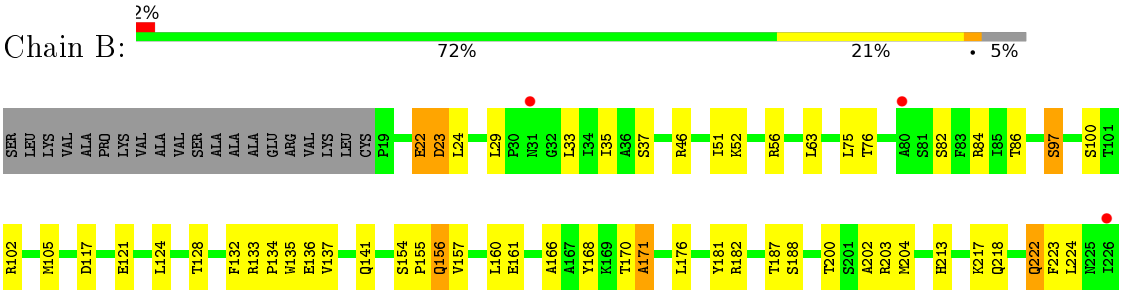
• Molecule 1: Mitochondrial ubiquinol-cytochrome-c reductase complex core protein i

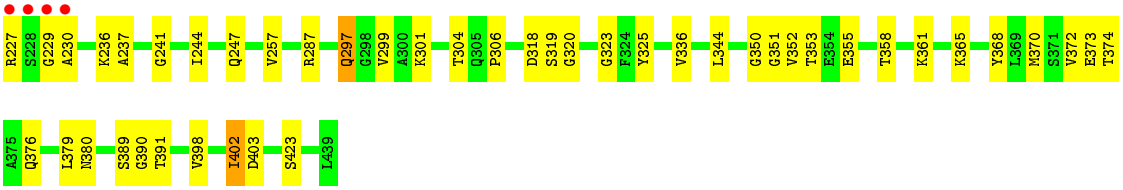


• Molecule 1: Mitochondrial ubiquinol-cytochrome-c reductase complex core protein i



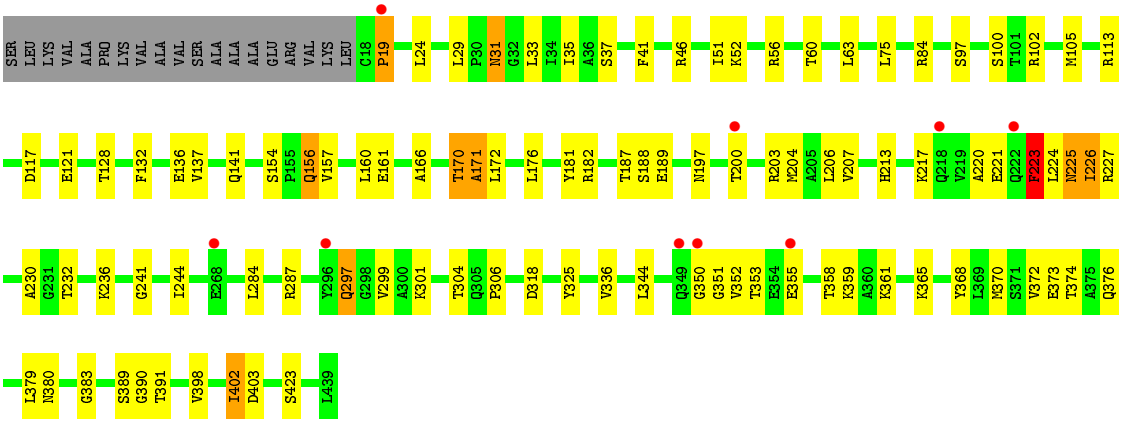
• Molecule 2: Mitochondrial ubiquinol-cytochrome-c reductase complex core protein 2





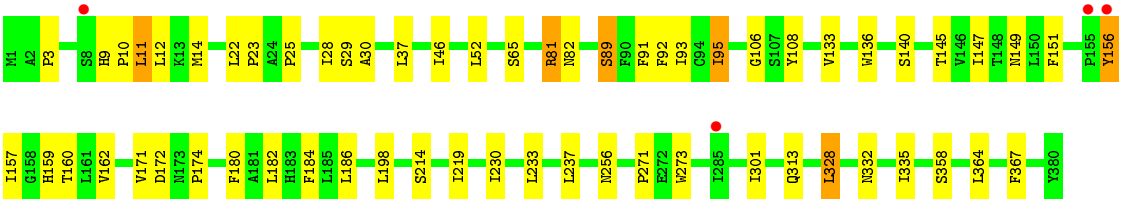
• Molecule 2: Mitochondrial ubiquinol-cytochrome-c reductase complex core protein 2

Chain O:



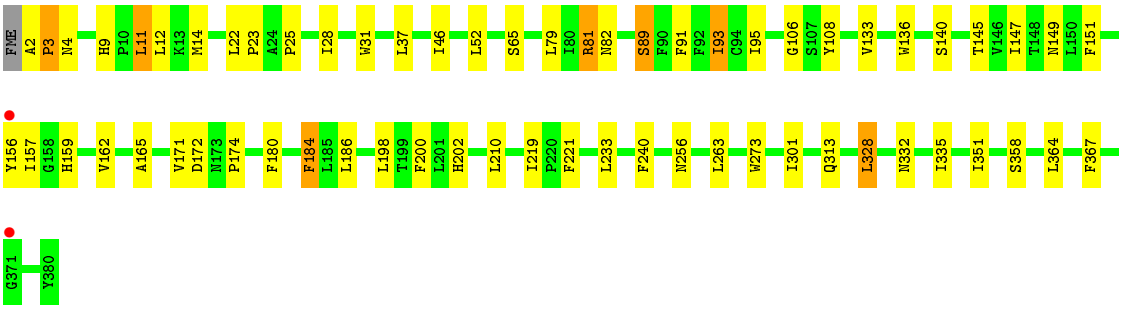
• Molecule 3: Cytochrome b

Chain C:



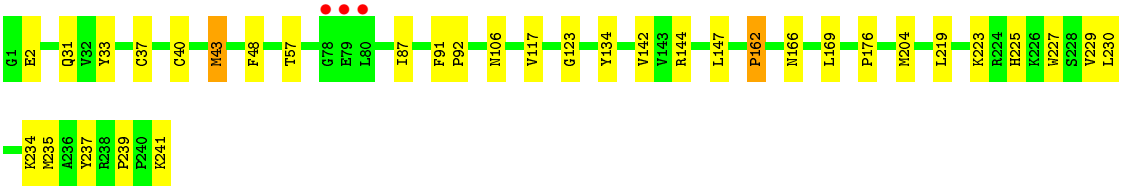
• Molecule 3: Cytochrome b

Chain P:

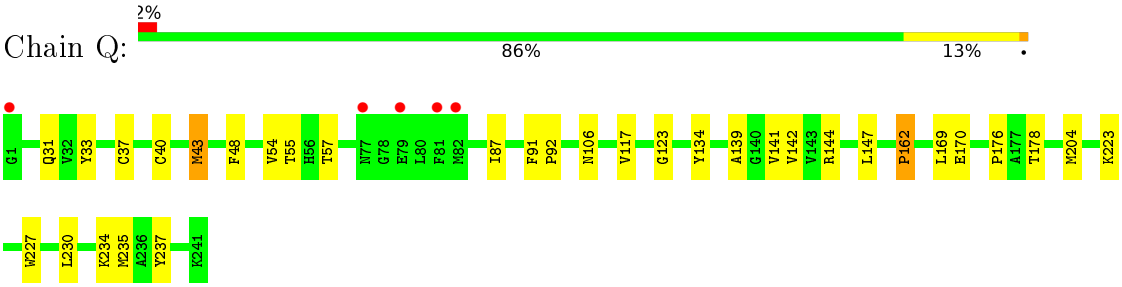


• Molecule 4: Mitochondrial cytochrome c1, heme protein

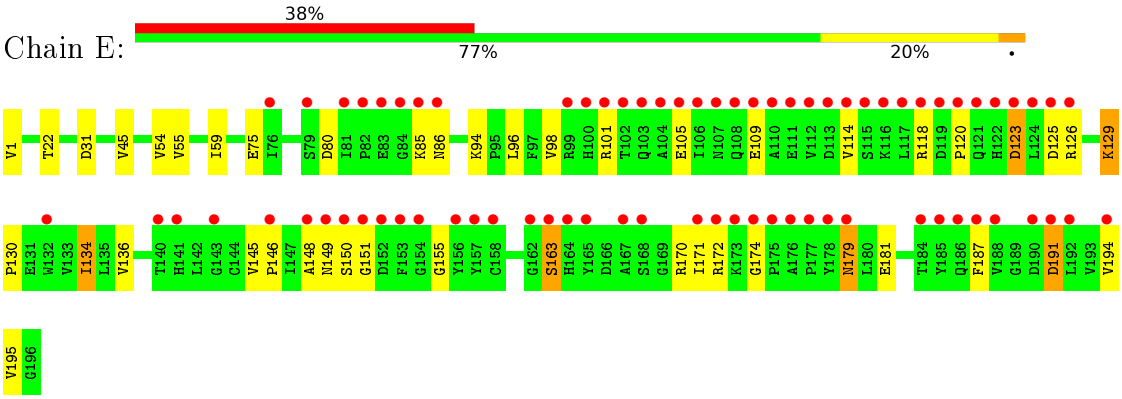
Chain D:



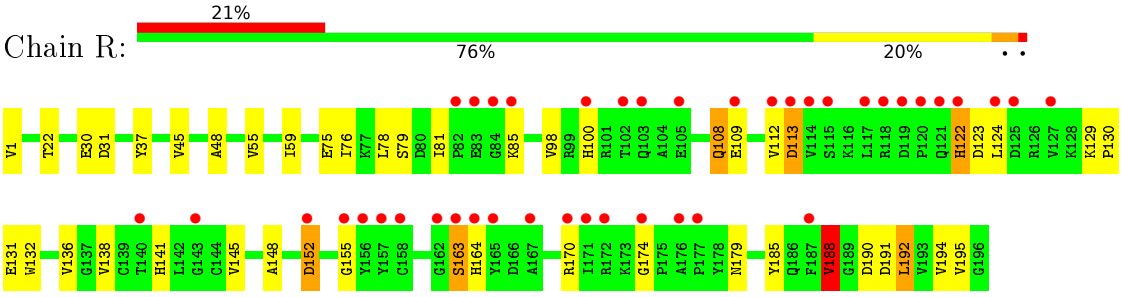
• Molecule 4: Mitochondrial cytochrome c1, heme protein



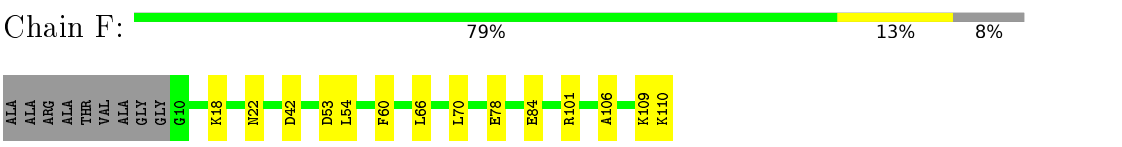
• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial



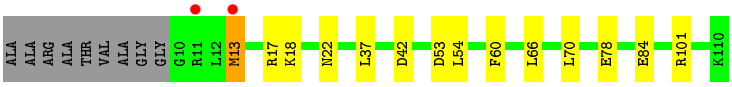
• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial



• Molecule 6: Cytochrome b-c1 complex subunit 7

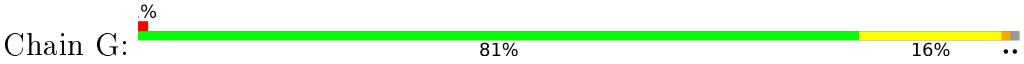


• Molecule 6: Cytochrome b-c1 complex subunit 7



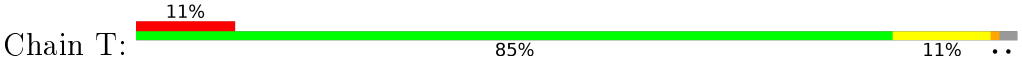
• Molecule 7: Mitochondrial ubiquinol-cytochrome c reductase ubiquinone-binding protein qp-c

Chain G:



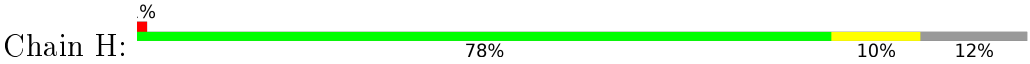
• Molecule 7: Mitochondrial ubiquinol-cytochrome c reductase ubiquinone-binding protein qp-c

Chain T:



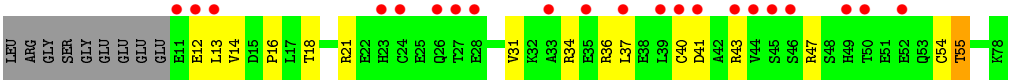
• Molecule 8: Cytochrome b-c1 complex subunit 6

Chain H:



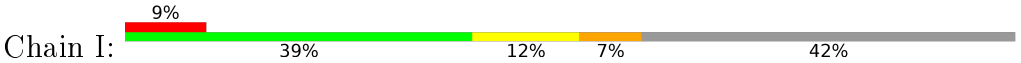
• Molecule 8: Cytochrome b-c1 complex subunit 6

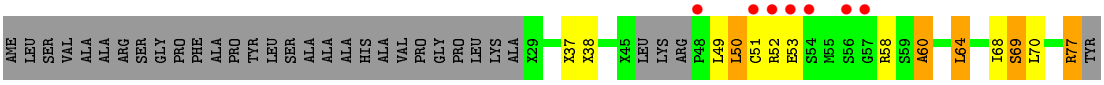
Chain U:



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

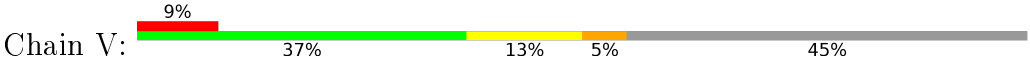
Chain I:

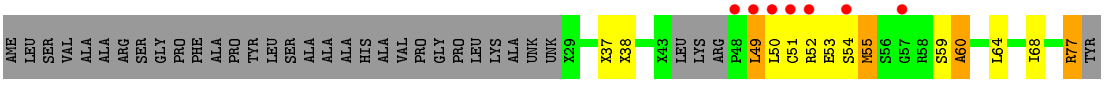




• Molecule 9: Cytochrome b-c1 complex subunit Rieske, mitochondrial

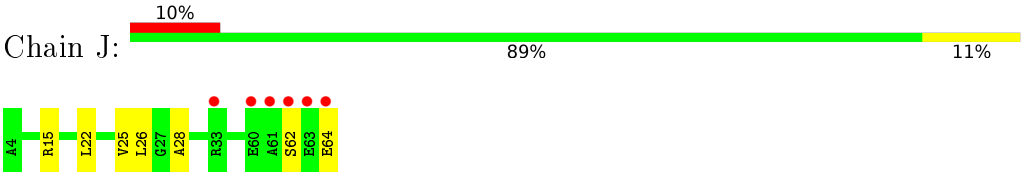
Chain V:





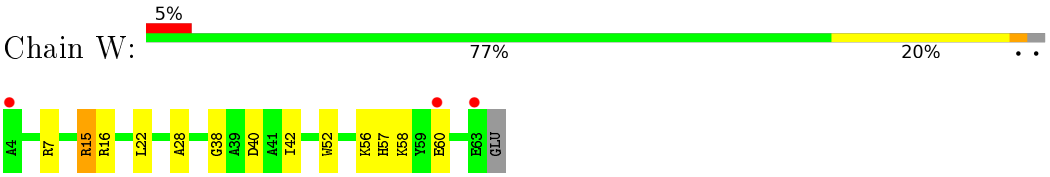
• Molecule 10: Mitochondrial ubiquinol-cytochrome c reductase 7.2 kda protein

Chain J:



• Molecule 10: Mitochondrial ubiquinol-cytochrome c reductase 7.2 kda protein

Chain W:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	167.25Å 181.48Å 239.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 3.23 54.30 – 3.23	Depositor EDS
% Data completeness (in resolution range)	98.3 (15.00-3.23) 82.2 (54.30-3.23)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.30	Depositor
$< I/\sigma(I) >$ [1]	1.88 (at 3.26Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1745)	Depositor
R, R_{free}	0.236 , 0.284 0.235 , 0.277	Depositor DCC
R_{free} test set	2266 reflections (2.42%)	DCC
Wilson B-factor (Å^2)	50.0	Xtriage
Anisotropy	0.460	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 55.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	32790	wwPDB-VP
Average B, all atoms (Å^2)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.04% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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, CDL, Y52, U10, FES, MES, HEC, PEE, FME, HEM, BOG

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	0.21	0/3513	0.40	0/4760
1	N	0.21	0/3508	0.39	0/4753
2	B	0.21	0/3192	0.40	0/4330
2	O	0.22	0/3198	0.40	0/4339
3	C	0.22	0/3114	0.39	0/4263
3	P	0.22	0/3102	0.39	0/4245
4	D	0.20	0/1956	0.37	0/2658
4	Q	0.20	0/1956	0.37	0/2658
5	E	0.20	0/1547	0.38	0/2103
5	R	0.20	0/1543	0.38	0/2098
6	F	0.21	0/911	0.35	0/1219
6	S	0.21	0/911	0.35	0/1219
7	G	0.22	0/694	0.39	0/941
7	T	0.22	0/684	0.39	0/929
8	H	0.21	0/570	0.36	0/763
8	U	0.21	0/566	0.40	0/758
9	I	0.20	0/208	0.48	0/279
9	V	0.21	0/215	0.56	0/288
10	J	0.21	0/508	0.34	0/682
10	W	0.21	0/490	0.35	0/660
All	All	0.21	0/32386	0.39	0/43945

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	216	PHE	Peptide

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	3442	0	3354	41	0
1	N	3437	0	3349	40	0
2	B	3137	0	3131	55	0
2	O	3143	0	3135	56	0
3	C	3021	0	3068	35	0
3	P	3022	0	3064	39	0
4	D	1898	0	1846	17	0
4	Q	1898	0	1846	16	0
5	E	1513	0	1480	21	0
5	R	1509	0	1476	22	0
6	F	891	0	893	6	0
6	S	891	0	893	8	0
7	G	672	0	653	11	0
7	T	662	0	645	10	0
8	H	562	0	545	3	0
8	U	558	0	541	8	0
9	I	266	0	223	14	0
9	V	265	0	239	11	0
10	J	497	0	490	3	0
10	W	479	0	478	6	0
11	A	26	0	26	1	0
11	C	122	0	174	2	0
11	E	63	0	99	5	0
11	N	8	0	7	0	0
11	P	142	0	193	7	0
11	R	49	0	75	5	0
12	C	86	0	60	7	0
12	P	86	0	60	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	C	27	0	19	2	0
13	P	27	0	19	1	0
14	C	19	0	17	1	0
14	P	19	0	17	3	0
15	C	12	0	13	0	0
16	C	6	0	8	1	0
16	P	6	0	8	1	0
17	D	43	0	30	0	0
17	Q	43	0	30	0	0
18	D	42	0	28	1	0
18	G	40	0	24	1	0
18	Q	42	0	28	0	0
18	T	40	0	24	3	0
19	D	20	0	28	0	0
19	P	20	0	28	3	0
19	Q	20	0	28	0	0
20	E	4	0	0	0	0
20	R	4	0	0	0	0
21	A	2	0	0	0	0
21	B	1	0	0	1	0
21	C	2	0	0	0	0
21	F	1	0	0	0	0
21	N	1	0	0	0	0
21	O	2	0	0	1	0
21	P	2	0	0	0	0
All	All	32790	0	32392	385	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 6.

The worst 5 of 385 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)
9:V:37:UNK:HG3	9:V:38:UNK:H	1.37	0.90
9:V:49:LEU:HB2	9:V:55:MET:HB3	1.57	0.85
9:I:37:UNK:HG3	9:I:38:UNK:N	1.94	0.81
9:I:37:UNK:HG3	9:I:38:UNK:H	1.47	0.78
2:B:361:LYS:HD2	2:B:403:ASP:HA	1.67	0.76

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	441/446 (99%)	421 (96%)	16 (4%)	4 (1%)	21	65
1	N	440/446 (99%)	419 (95%)	17 (4%)	4 (1%)	21	65
2	B	419/441 (95%)	397 (95%)	18 (4%)	4 (1%)	19	62
2	O	420/441 (95%)	397 (94%)	17 (4%)	6 (1%)	14	55
3	C	378/380 (100%)	365 (97%)	11 (3%)	2 (0%)	34	75
3	P	378/380 (100%)	364 (96%)	12 (3%)	2 (0%)	34	75
4	D	239/241 (99%)	226 (95%)	11 (5%)	2 (1%)	24	66
4	Q	239/241 (99%)	225 (94%)	12 (5%)	2 (1%)	24	66
5	E	194/196 (99%)	168 (87%)	20 (10%)	6 (3%)	5	32
5	R	194/196 (99%)	175 (90%)	14 (7%)	5 (3%)	7	38
6	F	99/110 (90%)	97 (98%)	2 (2%)	0	100	100
6	S	99/110 (90%)	98 (99%)	1 (1%)	0	100	100
7	G	78/81 (96%)	74 (95%)	4 (5%)	0	100	100
7	T	77/81 (95%)	72 (94%)	5 (6%)	0	100	100
8	H	66/77 (86%)	64 (97%)	2 (3%)	0	100	100
8	U	66/77 (86%)	56 (85%)	9 (14%)	1 (2%)	13	53
9	I	28/76 (37%)	17 (61%)	9 (32%)	2 (7%)	1	9
9	V	28/76 (37%)	19 (68%)	7 (25%)	2 (7%)	1	9
10	J	59/61 (97%)	55 (93%)	3 (5%)	1 (2%)	11	50
10	W	58/61 (95%)	54 (93%)	3 (5%)	1 (2%)	11	50
All	All	4000/4218 (95%)	3763 (94%)	193 (5%)	44 (1%)	17	60

5 of 44 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	390	GLY

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Mol	Chain	Res	Type
2	O	19	PRO
2	O	226	ILE
2	O	390	GLY
9	V	59	SER

5.3.2 Protein sidechains (i)

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	365/368 (99%)	342 (94%)	23 (6%)	22 62
1	N	365/368 (99%)	339 (93%)	26 (7%)	18 56
2	B	331/347 (95%)	312 (94%)	19 (6%)	25 66
2	O	332/347 (96%)	313 (94%)	19 (6%)	25 66
3	C	328/328 (100%)	309 (94%)	19 (6%)	25 65
3	P	327/328 (100%)	310 (95%)	17 (5%)	29 68
4	D	200/200 (100%)	191 (96%)	9 (4%)	34 73
4	Q	200/200 (100%)	190 (95%)	10 (5%)	30 70
5	E	166/166 (100%)	156 (94%)	10 (6%)	24 64
5	R	165/166 (99%)	150 (91%)	15 (9%)	12 41
6	F	93/96 (97%)	89 (96%)	4 (4%)	35 74
6	S	93/96 (97%)	89 (96%)	4 (4%)	35 74
7	G	71/71 (100%)	67 (94%)	4 (6%)	26 67
7	T	70/71 (99%)	67 (96%)	3 (4%)	35 74
8	H	64/71 (90%)	60 (94%)	4 (6%)	22 62
8	U	63/71 (89%)	60 (95%)	3 (5%)	31 71
9	I	22/45 (49%)	18 (82%)	4 (18%)	2 10
9	V	23/45 (51%)	17 (74%)	6 (26%)	0 2
10	J	49/49 (100%)	46 (94%)	3 (6%)	23 63
10	W	47/49 (96%)	42 (89%)	5 (11%)	8 34

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3374/3482 (97%)	3167 (94%)	207 (6%)	23 63

5 of 207 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	I	68	ILE
1	N	248	LEU
7	T	4	PHE
10	J	22	LEU
1	N	70	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
7	G	23	GLN
1	N	136	GLN
5	R	108	GLN
1	N	118	GLN
1	N	173	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	$\#\|Z\| > 2$
3	FME	C	1	3	7,8,10	1.88	1 (14%)	5,8,11	0.84	0

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
3	FME	C	1	3	-	0/4/8/11	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1	FME	CN-N	-4.81	1.33	1.46

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

36 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	$\#\|Z\| > 2$
11	PEE	A	501	-	25,25,50	1.32	2 (8%)	27,30,55	1.57	5 (18%)
12	HEM	C	501	3	24,50,50	1.95	4 (16%)	16,82,82	1.34	1 (6%)
12	HEM	C	502	3	24,50,50	1.92	4 (16%)	16,82,82	1.41	1 (6%)
13	Y52	C	503	-	27,29,29	0.69	0	28,39,39	1.01	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	U10	C	504	-	19,19,63	1.74	2 (10%)	24,26,79	1.28	1 (4%)
11	PEE	C	505	-	48,48,50	0.92	2 (4%)	50,53,55	1.15	4 (8%)
15	MES	C	506	-	12,12,12	2.15	1 (8%)	15,16,16	1.65	3 (20%)
11	PEE	C	507	-	10,10,50	0.51	0	11,12,55	0.51	0
16	GOL	C	508	-	5,5,5	0.35	0	5,5,5	0.27	0
11	PEE	C	509	-	46,46,50	1.00	2 (4%)	48,51,55	1.13	4 (8%)
11	PEE	C	510	-	11,14,50	0.26	0	11,14,55	0.59	0
17	HEC	D	501	4	24,50,50	2.11	2 (8%)	19,82,82	2.89	3 (15%)
18	CDL	D	502	-	41,41,99	1.27	4 (9%)	43,53,111	1.31	5 (11%)
19	BOG	D	503	-	20,20,20	0.53	0	25,25,25	0.68	0
20	FES	E	501	5	0,4,4	0.00	-	0,4,4	0.00	-
11	PEE	E	502	-	47,47,50	0.95	2 (4%)	49,52,55	1.08	4 (8%)
11	PEE	E	503	-	14,14,50	0.23	0	13,13,55	0.68	0
18	CDL	G	101	-	39,39,99	1.30	4 (10%)	41,51,111	1.37	5 (12%)
11	PEE	N	501	-	7,7,50	1.42	1 (14%)	8,9,55	1.43	1 (12%)
11	PEE	P	401	-	11,14,50	0.24	0	11,14,55	0.64	0
12	HEM	P	402	3	24,50,50	1.95	4 (16%)	16,82,82	1.35	1 (6%)
12	HEM	P	403	3	24,50,50	1.92	4 (16%)	16,82,82	1.40	1 (6%)
13	Y52	P	404	-	27,29,29	0.68	0	28,39,39	0.99	2 (7%)
14	U10	P	405	-	19,19,63	1.78	2 (10%)	24,26,79	1.48	3 (12%)
19	BOG	P	406	-	20,20,20	0.50	0	25,25,25	0.66	0
11	PEE	P	407	-	48,48,50	0.94	2 (4%)	50,53,55	1.02	3 (6%)
16	GOL	P	408	-	5,5,5	0.36	0	5,5,5	0.22	0
11	PEE	P	409	-	40,40,50	1.01	2 (5%)	42,45,55	1.16	2 (4%)
11	PEE	P	410	-	8,11,50	0.23	0	8,11,55	0.76	0
11	PEE	P	411	-	24,24,50	1.27	2 (8%)	26,29,55	1.41	4 (15%)
17	HEC	Q	501	4	24,50,50	2.11	3 (12%)	19,82,82	2.89	3 (15%)
18	CDL	Q	502	-	41,41,99	1.27	4 (9%)	43,53,111	1.30	5 (11%)
19	BOG	Q	503	-	20,20,20	0.53	0	25,25,25	0.63	0
20	FES	R	501	5	0,4,4	0.00	-	0,4,4	0.00	-
11	PEE	R	502	-	48,48,50	0.96	2 (4%)	50,53,55	1.11	5 (10%)
18	CDL	T	101	-	39,39,99	1.32	4 (10%)	41,51,111	1.37	4 (9%)

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
11	PEE	A	501	-	-	0/29/29/54	0/0/0/0
12	HEM	C	501	3	-	0/6/54/54	0/0/8/8
12	HEM	C	502	3	-	0/6/54/54	0/0/8/8
13	Y52	C	503	-	-	0/18/20/20	0/3/3/3
14	U10	C	504	-	-	0/11/35/87	0/1/1/1
11	PEE	C	505	-	-	0/52/52/54	0/0/0/0
15	MES	C	506	-	-	0/6/14/14	0/1/1/1
11	PEE	C	507	-	-	0/10/10/54	0/0/0/0
16	GOL	C	508	-	-	0/4/4/4	0/0/0/0
11	PEE	C	509	-	-	0/50/50/54	0/0/0/0
11	PEE	C	510	-	-	0/10/12/54	0/0/0/0
17	HEC	D	501	4	-	0/6/54/54	0/0/8/8
18	CDL	D	502	-	-	0/51/51/110	0/0/0/0
19	BOG	D	503	-	-	0/11/31/31	0/1/1/1
20	FES	E	501	5	-	0/0/4/4	0/1/1/1
11	PEE	E	502	-	-	0/51/51/54	0/0/0/0
11	PEE	E	503	-	-	0/12/12/54	0/0/0/0
18	CDL	G	101	-	-	0/49/49/110	0/0/0/0
11	PEE	N	501	-	-	0/5/5/54	0/0/0/0
11	PEE	P	401	-	-	0/10/12/54	0/0/0/0
12	HEM	P	402	3	-	0/6/54/54	0/0/8/8
12	HEM	P	403	3	-	0/6/54/54	0/0/8/8
13	Y52	P	404	-	-	0/18/20/20	0/3/3/3
14	U10	P	405	-	-	0/11/35/87	0/1/1/1
19	BOG	P	406	-	-	0/11/31/31	0/1/1/1
11	PEE	P	407	-	-	0/52/52/54	0/0/0/0
16	GOL	P	408	-	-	0/4/4/4	0/0/0/0
11	PEE	P	409	-	-	0/44/44/54	0/0/0/0
11	PEE	P	410	-	-	0/7/9/54	0/0/0/0
11	PEE	P	411	-	-	0/28/28/54	0/0/0/0
17	HEC	Q	501	4	-	0/6/54/54	0/0/8/8
18	CDL	Q	502	-	-	0/51/51/110	0/0/0/0
19	BOG	Q	503	-	-	0/11/31/31	0/1/1/1
20	FES	R	501	5	-	0/0/4/4	0/1/1/1
11	PEE	R	502	-	-	0/52/52/54	0/0/0/0
18	CDL	T	101	-	-	0/49/49/110	0/0/0/0

The worst 5 of 59 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	C	506	MES	C8-S	-7.18	1.66	1.77
17	Q	501	HEC	C3B-C2B	-6.05	1.34	1.40
17	D	501	HEC	C3B-C2B	-6.02	1.34	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	Q	501	HEC	C3C-C2C	-5.89	1.34	1.40
17	D	501	HEC	C3C-C2C	-5.85	1.34	1.40

The worst 5 of 72 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	Q	501	HEC	CBC-CAC-C3C	-8.01	109.84	127.34
17	D	501	HEC	CBC-CAC-C3C	-8.00	109.85	127.34
17	Q	501	HEC	CBB-CAB-C3B	-7.69	110.53	127.34
17	D	501	HEC	CBB-CAB-C3B	-7.67	110.58	127.34
14	C	504	U10	C7-C8-C9	-4.30	119.38	126.70

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

23 monomers are involved in 48 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	A	501	PEE	1	0
12	C	501	HEM	4	0
12	C	502	HEM	3	0
13	C	503	Y52	2	0
14	C	504	U10	1	0
16	C	508	GOL	1	0
11	C	509	PEE	2	0
18	D	502	CDL	1	0
11	E	502	PEE	4	0
11	E	503	PEE	2	0
18	G	101	CDL	1	0
11	P	401	PEE	1	0
12	P	402	HEM	5	0
12	P	403	HEM	3	0
13	P	404	Y52	1	0
14	P	405	U10	3	0
19	P	406	BOG	3	0
11	P	407	PEE	2	0
16	P	408	GOL	1	0
11	P	409	PEE	3	0
11	P	411	PEE	1	0
11	R	502	PEE	5	0
18	T	101	CDL	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

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^{th} 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	443/446 (99%)	0.05	8 (1%) 71 60	28, 53, 78, 101	0
1	N	442/446 (99%)	0.15	9 (2%) 68 57	36, 57, 81, 99	0
2	B	421/441 (95%)	0.24	7 (1%) 73 62	47, 67, 102, 123	0
2	O	422/441 (95%)	0.17	9 (2%) 67 55	35, 63, 86, 104	0
3	C	379/380 (99%)	-0.17	4 (1%) 82 73	22, 33, 70, 102	0
3	P	379/380 (99%)	0.03	2 (0%) 91 88	27, 51, 78, 104	0
4	D	241/241 (100%)	-0.15	3 (1%) 81 71	25, 37, 73, 95	0
4	Q	241/241 (100%)	0.14	5 (2%) 67 55	39, 59, 85, 117	0
5	E	196/196 (100%)	1.61	75 (38%) 0 1	28, 114, 166, 182	9 (4%)
5	R	196/196 (100%)	1.00	41 (20%) 1 1	36, 81, 131, 141	8 (4%)
6	F	101/110 (91%)	-0.17	0 100 100	25, 37, 53, 78	0
6	S	101/110 (91%)	0.22	2 (1%) 68 57	46, 59, 86, 102	0
7	G	80/81 (98%)	0.17	1 (1%) 79 69	28, 45, 73, 89	0
7	T	79/81 (97%)	0.65	9 (11%) 7 5	40, 70, 122, 127	0
8	H	68/77 (88%)	0.14	1 (1%) 76 65	35, 50, 68, 101	0
8	U	68/77 (88%)	1.45	21 (30%) 1 1	66, 91, 113, 117	0
9	I	30/76 (39%)	1.02	7 (23%) 1 1	55, 77, 116, 120	0
9	V	30/76 (39%)	1.23	7 (23%) 1 1	47, 78, 119, 130	0
10	J	61/61 (100%)	0.81	6 (9%) 10 7	34, 46, 79, 129	0
10	W	60/61 (98%)	0.74	3 (5%) 32 21	41, 55, 92, 117	0
All	All	4038/4218 (95%)	0.26	220 (5%) 29 19	22, 56, 107, 182	17 (0%)

The worst 5 of 220 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	E	163	SER	14.4
5	R	163	SER	7.6
5	E	162	GLY	7.4
10	J	62	SER	7.2
5	E	172	ARG	6.6

6.2 Non-standard residues in protein, DNA, RNA chains (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^{th} 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(Å^2)	Q<0.9
3	FME	C	1	9/11	0.70	0.41	-	72,88,96,99	0

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^{th} 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(Å^2)	Q<0.9
14	U10	P	405	19/63	0.80	0.40	5.73	60,75,88,91	0
11	PEE	P	411	25/51	0.74	0.41	5.23	36,60,75,80	25
11	PEE	P	401	15/51	0.78	0.37	5.21	41,58,88,89	0
11	PEE	E	503	15/51	0.81	0.33	4.11	22,49,63,68	0
11	PEE	A	501	26/51	0.72	0.33	3.67	27,87,106,123	0
11	PEE	C	509	47/51	0.76	0.32	3.44	22,48,88,107	0
14	U10	C	504	19/63	0.86	0.32	3.36	45,59,67,70	0
18	CDL	Q	502	42/100	0.73	0.36	2.83	40,99,121,136	0
19	BOG	P	406	20/20	0.79	0.27	2.61	39,74,96,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
11	PEE	P	409	41/51	0.72	0.34	2.38	54,69,112,128	0
18	CDL	D	502	42/100	0.83	0.30	2.13	46,80,99,127	0
11	PEE	R	502	49/51	0.76	0.39	2.12	33,64,79,88	0
19	BOG	D	503	20/20	0.88	0.31	2.09	29,46,54,57	0
11	PEE	E	502	48/51	0.81	0.33	1.67	36,55,80,86	0
11	PEE	P	410	12/51	0.86	0.26	1.59	30,37,46,47	0
16	GOL	P	408	6/6	0.93	0.25	1.39	42,43,49,51	0
12	HEM	P	402	43/43	0.96	0.26	0.99	26,32,43,53	0
11	PEE	P	407	49/51	0.86	0.28	0.99	45,68,84,89	0
16	GOL	C	508	6/6	0.91	0.24	0.96	34,35,38,43	0
18	CDL	T	101	40/100	0.81	0.32	0.80	44,85,97,98	0
18	CDL	G	101	40/100	0.86	0.27	0.80	24,56,69,73	0
12	HEM	C	502	43/43	0.97	0.24	0.76	19,24,32,37	0
12	HEM	C	501	43/43	0.96	0.23	0.75	18,24,32,35	0
12	HEM	P	403	43/43	0.96	0.25	0.65	27,33,50,53	0
11	PEE	C	510	15/51	0.87	0.25	0.33	25,54,81,84	0
17	HEC	D	501	43/43	0.96	0.21	0.27	26,34,40,42	0
11	PEE	C	505	49/51	0.91	0.22	0.27	22,43,54,57	0
19	BOG	Q	503	20/20	0.93	0.24	0.13	34,54,62,63	0
13	Y52	P	404	27/27	0.95	0.22	-0.01	38,46,58,63	0
15	MES	C	506	12/12	0.85	0.33	-0.03	45,69,109,122	0
17	HEC	Q	501	43/43	0.96	0.23	-0.25	44,51,63,71	0
13	Y52	C	503	27/27	0.96	0.18	-0.76	25,33,45,51	0
20	FES	E	501	4/4	0.98	0.11	-1.24	92,103,103,106	4
20	FES	R	501	4/4	0.96	0.13	-1.65	71,84,92,107	0
11	PEE	N	501	8/51	0.71	0.28	-	57,79,96,112	0
11	PEE	C	507	11/51	0.76	0.38	-	25,51,62,63	11

6.5 Other polymers (i)

There are no such residues in this entry.