wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 08:04 AM GMT

PDB ID	:	3CXH
Title	:	Structure of yeast complex III with isoform-2 cytochrome c bound and definition of a minimal core interface for electron transfer.
Authors	:	Solmaz, S.R.N.; Hunte, C.
Deposited on	:	2008-04-24
Resolution	:	2.50 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:

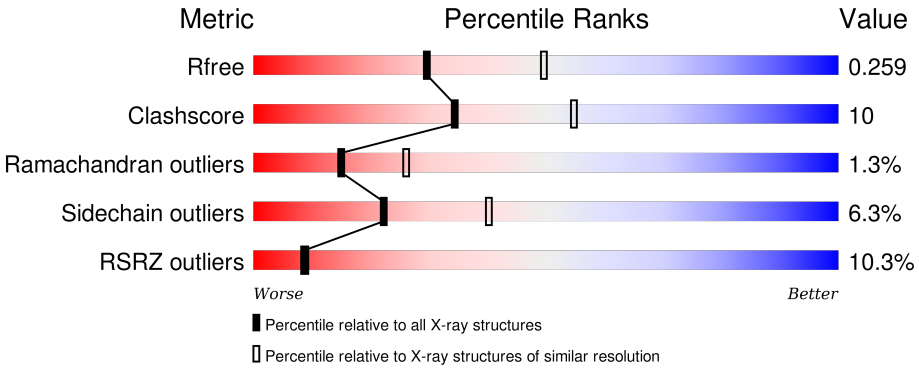
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.50 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	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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	431	9% 68% 27% 5%
1	L	431	10% 75% 21% ·
2	B	352	9% 69% 26% ·
2	M	352	9% 69% 26% 5%
3	C	385	2% 80% 18% ·

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Mol	Chain	Length	Quality of chain
3	N	385	2% 86% 13%
4	D	248	4% 85% 12%
4	O	248	2% 83% 15%
5	E	185	11% 77% 21%
5	P	185	10% 81% 17%
6	F	146	9% 41% 8% 49%
6	Q	146	8% 40% 10% 49%
7	G	126	3% 79% 17%
7	R	126	5% 80% 17%
8	H	93	22% 80% 17%
8	S	93	25% 80% 20%
9	I	65	12% 77% 6% 15%
9	T	65	12% 71% 9% 5% 15%
10	J	127	16% 69% 28%
10	U	127	17% 66% 28% 6%
11	K	107	45% 56% 37% 7%
11	V	107	39% 71% 27%
12	W	112	21% 80% 17%

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
13	SUC	O	4146	-	-	-	X
19	9PE	C	4111	-	-	-	X
19	9PE	N	4011	-	-	-	X

2 Entry composition

There are 23 unique types of molecules in this entry. The entry contains 36805 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	0	0	0
			3344	2109	576	653	6			
1	L	431	Total	C	N	O	S	0	0	0
			3344	2109	576	653	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	153	ASP	GLU	CONFLICT	UNP P07256
L	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	0	0	0
			2735	1747	453	534	1			
2	M	352	Total	C	N	O	S	0	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	0	0	0
			3090	2082	484	503	21			
3	N	385	Total	C	N	O	S	0	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	246	Total	C	N	O	S	0	0	0
			1940	1237	334	360	9			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	O	246	Total	C	N	O	S	0	0	0
			1940	1237	334	360	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	0	0	0
			1411	893	242	266	10			
5	P	185	Total	C	N	O	S	0	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			
6	Q	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	125	Total	C	N	O	S	0	0	0
			1012	648	172	190	2			
7	R	125	Total	C	N	O	S	0	0	0
			1012	648	172	190	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	0	0	0
			773	510	131	130	2			
8	S	93	Total	C	N	O	S	0	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	55	Total	C	N	O	0	0	0
			448	298	75	75			
9	T	55	Total	C	N	O	0	0	0
			448	298	75	75			

- Molecule 10 is a protein called HEAVY CHAIN (VH) OF FV-FRAGMENT.

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

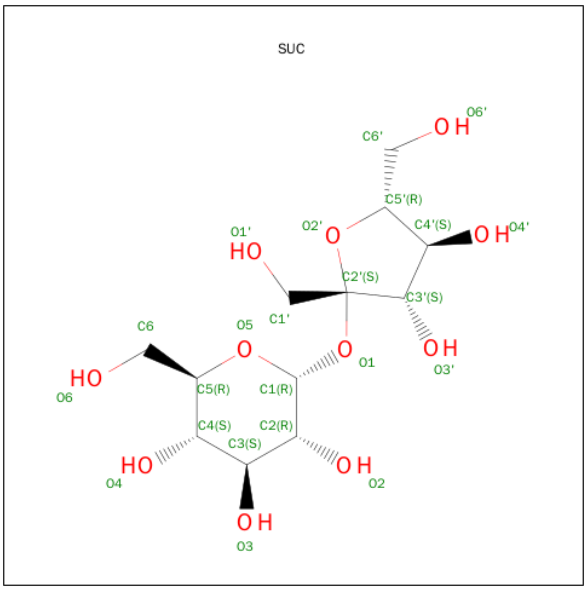
- Molecule 11 is a protein called LIGHT CHAIN (VL) OF FV-FRAGMENT.

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

- Molecule 12 is a protein called Cytochrome c iso-2.

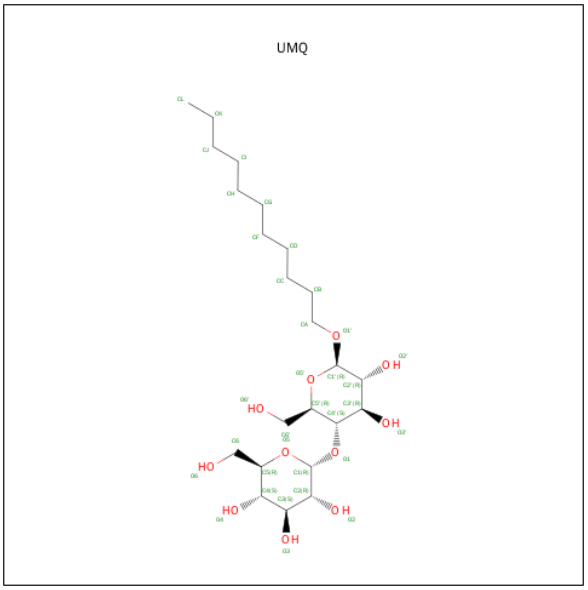
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	W	112	Total	C	N	O	S	0	1	0
			885	555	159	166	5			

- Molecule 13 is SUGAR (SUCROSE) (three-letter code: SUC) (formula: $C_{12}H_{22}O_{11}$).



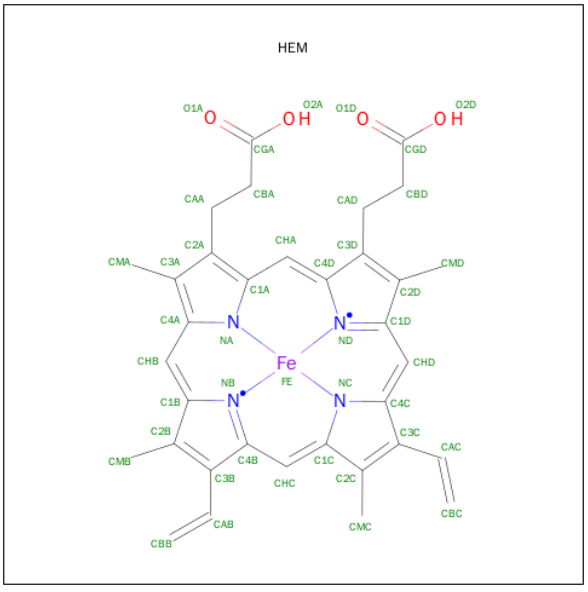
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	O	1	Total	C	O	0	0
			23	12	11		

- Molecule 14 is UNDECYL-MALTOSIDE (three-letter code: UMQ) (formula: $C_{23}H_{44}O_{11}$).



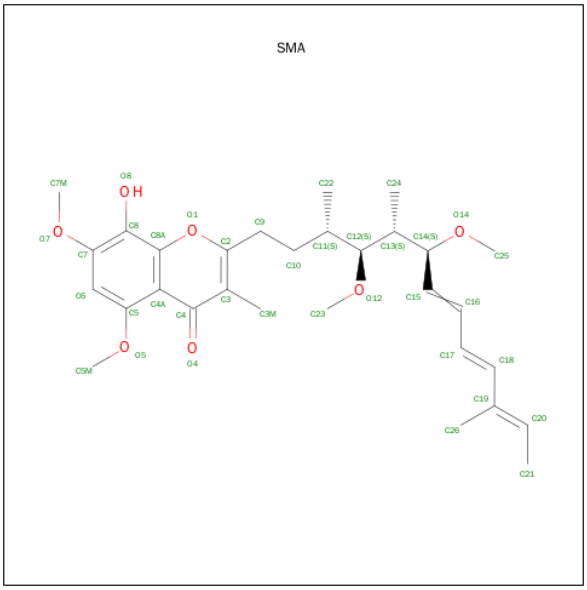
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	A	1	Total C O 34 23 11	0	0
14	L	1	Total C O 34 23 11	0	0

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



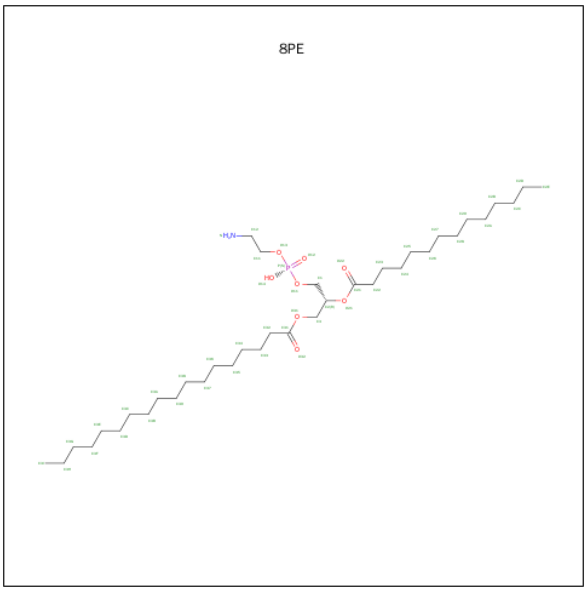
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
15	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
15	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
15	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
15	N	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
15	N	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
15	O	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4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

- Molecule 16 is STIGMATELLIN A (three-letter code: SMA) (formula: $C_{30}H_{42}O_7$).



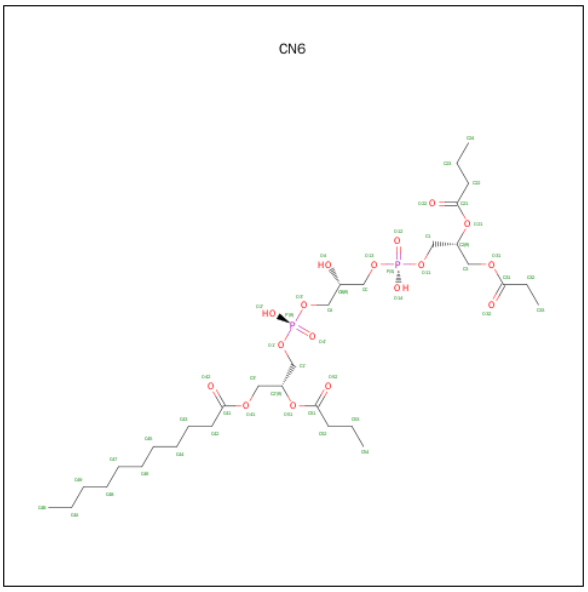
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
16	C	1	Total	C	O	0	0
			37	30	7		
16	N	1	Total	C	O	0	0
			37	30	7		

- 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	N	O	P	0	0
			47	37	1	8	1		
17	N	1	Total	C	N	O	P	0	0
			47	37	1	8	1		

- Molecule 18 is (2R,5R,11S,14R)-2-(BUTANOYLOXY)-5,8,11-TRIHYDROXY-5,11-DIOXIDO-16-OXO-14-[(PROPANOYLOXY)METHYL]-4,6,10,12,15-PENTAOXA-5,11-DIPHOSPHANONADEC-1-YL UNDECANOATE (three-letter code: CN6) (formula: $C_{31}H_{58}O_{17}P_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
18	C	1	Total	C	O	P	0	0
			50	31	17	2		

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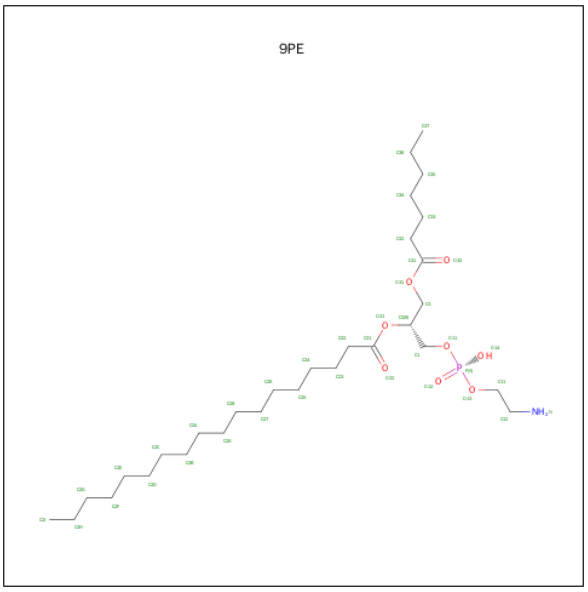
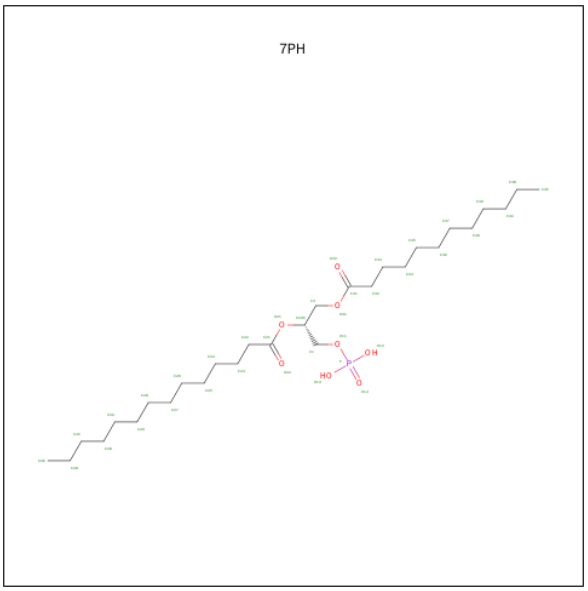
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
18	N	1	Total	C	O	P	0	0
			50	31	17	2		

- Molecule 19 is (1R)-2-{[(S)-(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(HEPTANOYLOXY)METHYL]ETHYL OCTADECANOATE (three-letter code: 9PE) (formula: $C_{30}H_{60}NO_8P$).



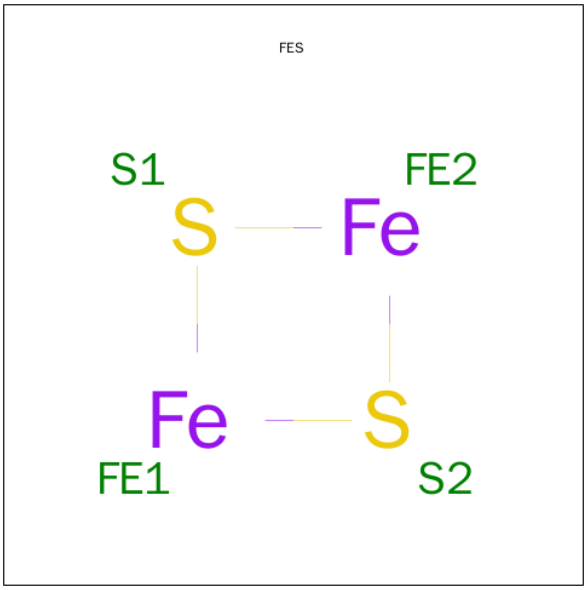
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
19	C	1	Total	C	N	O	P	0	0
			40	30	1	8	1		
19	N	1	Total	C	N	O	P	0	0
			40	30	1	8	1		

- Molecule 20 is (1R)-2-(DODECANOYLOXY)-1-[(PHOSPHONOOXY)METHYL]ETHYL TETRADECANOATE (three-letter code: 7PH) (formula: $C_{29}H_{57}O_8P$).



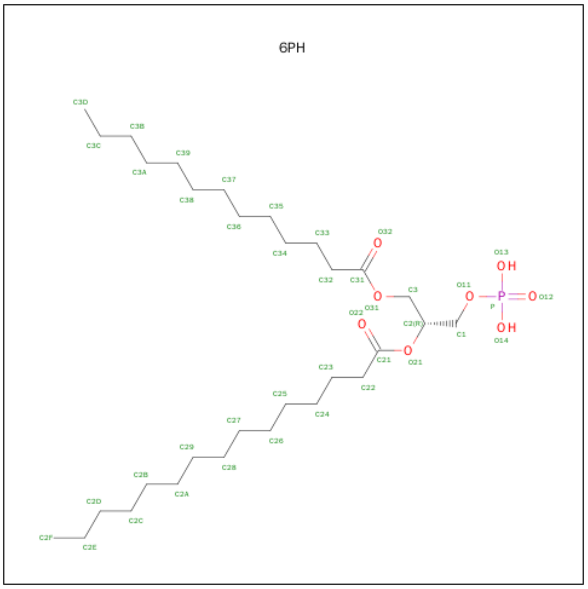
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
20	D	1	Total	C	O	P	0	0
			38	29	8	1		
20	O	1	Total	C	O	P	0	0
			38	29	8	1		

- 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		
21	P	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 22 is (1R)-2-(PHOSPHONOOXY)-1-[(TRIDECANOYLOXY)METHYL]ETHYL PENTADECANOATE (three-letter code: 6PH) (formula: $C_{31}H_{61}O_8P$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	E	1	Total C O P 40 31 8 1	0	0
22	L	1	Total C O P 40 31 8 1	0	0

- Molecule 23 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	A	42	Total O 42 42	0	0
23	B	17	Total O 17 17	0	0
23	C	75	Total O 75 75	0	0
23	D	50	Total O 50 50	0	0
23	E	19	Total O 19 19	0	0
23	F	3	Total O 3 3	0	0
23	G	21	Total O 21 21	0	0
23	H	10	Total O 10 10	0	0

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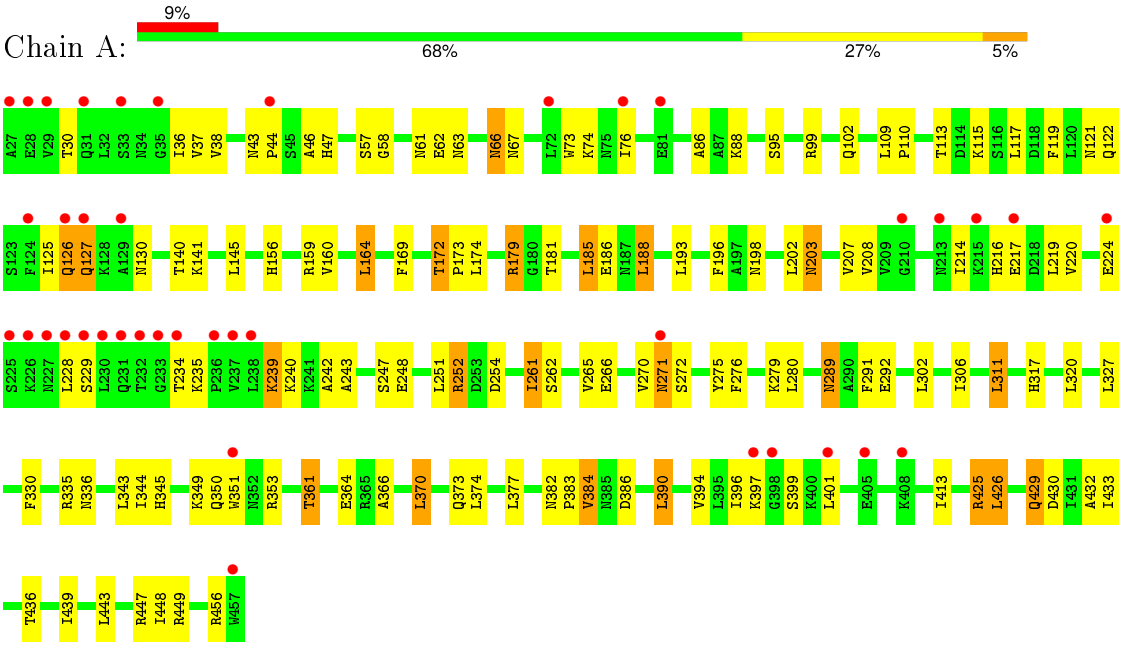
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	I	4	Total O 4 4	0	0
23	J	2	Total O 2 2	0	0
23	K	1	Total O 1 1	0	0
23	L	54	Total O 54 54	0	0
23	M	15	Total O 15 15	0	0
23	N	88	Total O 88 88	0	0
23	O	74	Total O 74 74	0	0
23	P	18	Total O 18 18	0	0
23	Q	3	Total O 3 3	0	0
23	R	22	Total O 22 22	0	0
23	S	13	Total O 13 13	0	0
23	T	5	Total O 5 5	0	0
23	U	2	Total O 2 2	0	0
23	W	10	Total O 10 10	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.

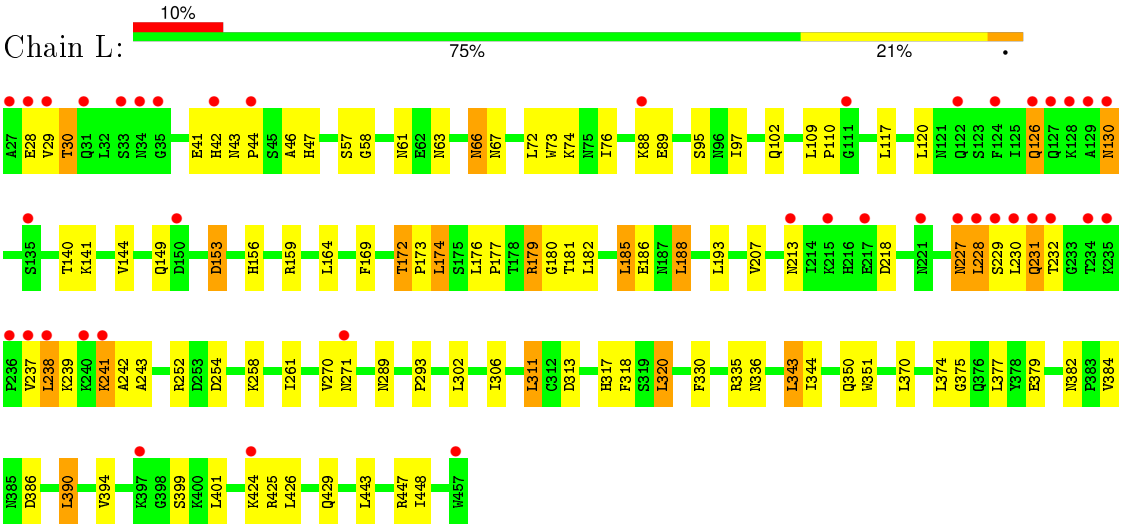
- Molecule 1: Cytochrome b-c1 complex subunit 1, mitochondrial

Chain A:



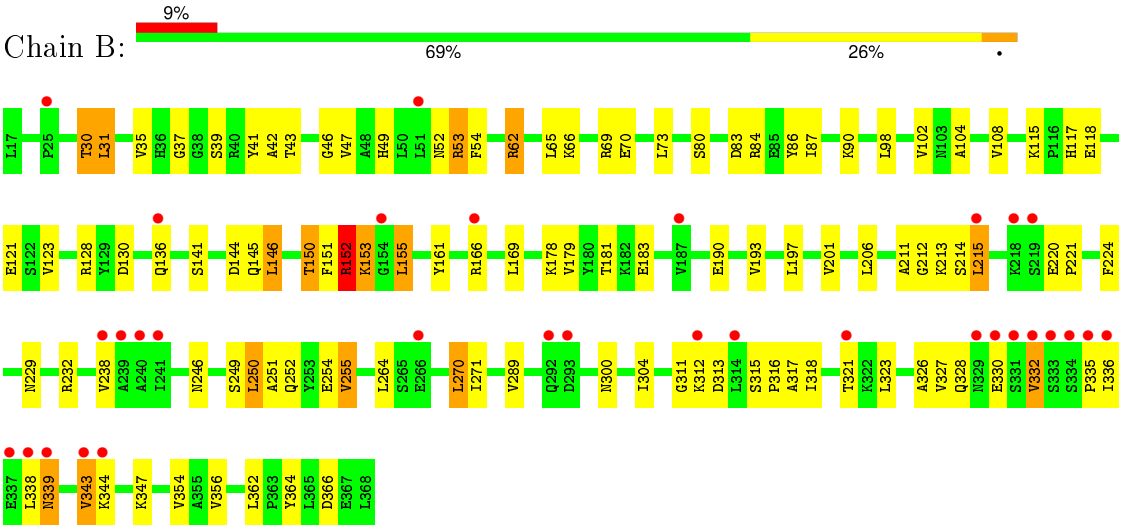
- Molecule 1: Cytochrome b-c1 complex subunit 1, mitochondrial

Chain L:



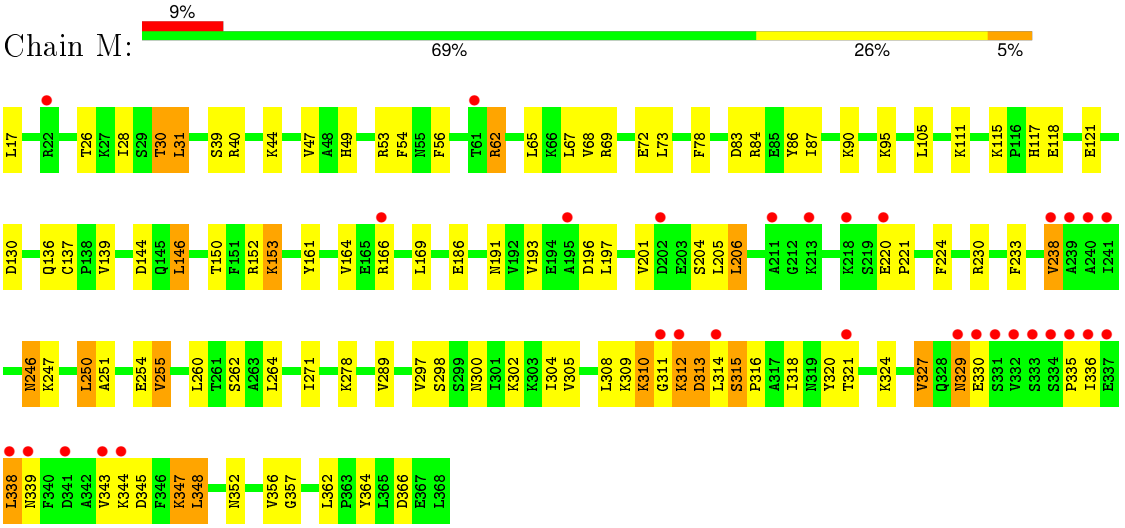
- Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain B:



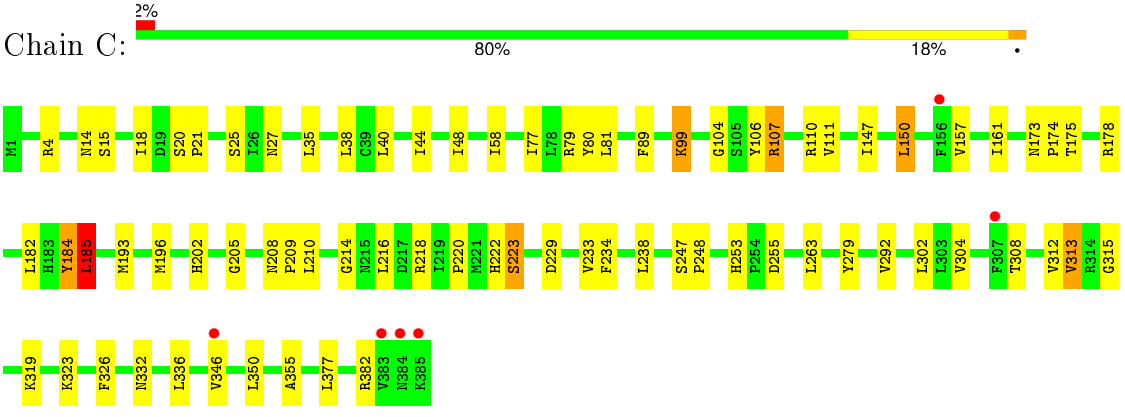
- Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain M:



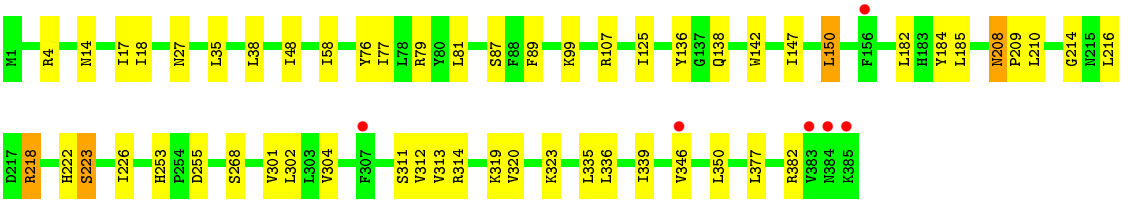
- Molecule 3: Cytochrome b

Chain C:

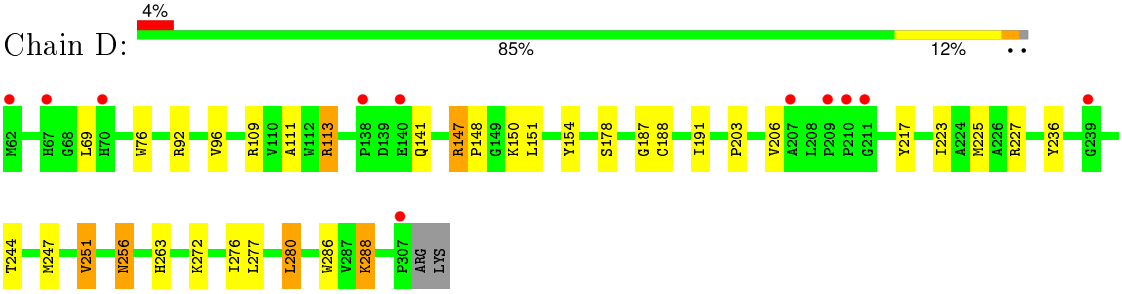


- Molecule 3: Cytochrome b

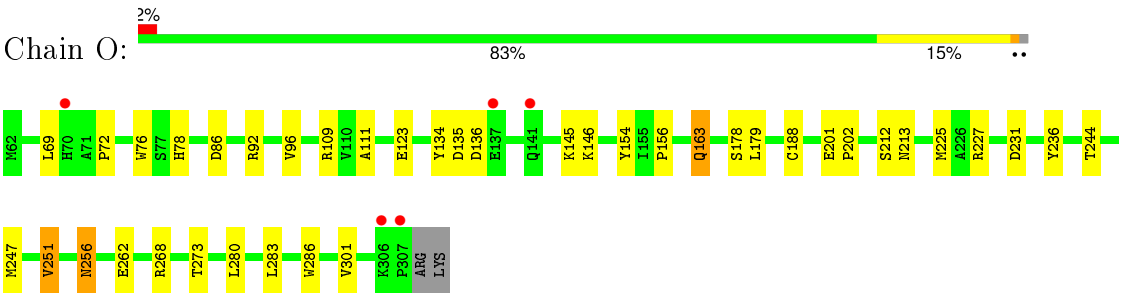
Chain N:



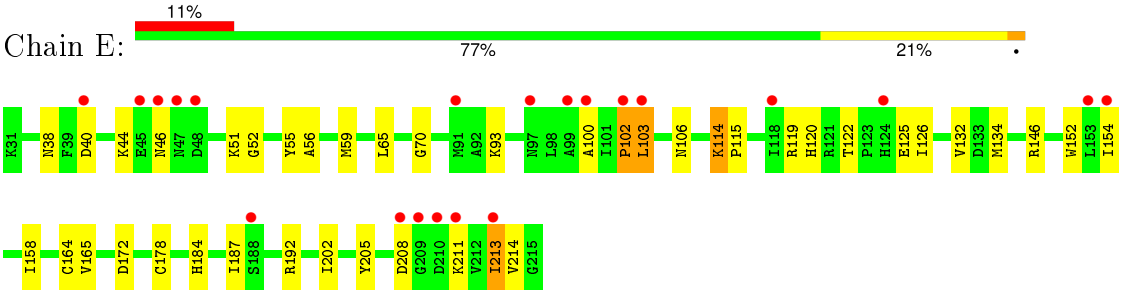
• Molecule 4: Cytochrome c1, heme protein, mitochondrial



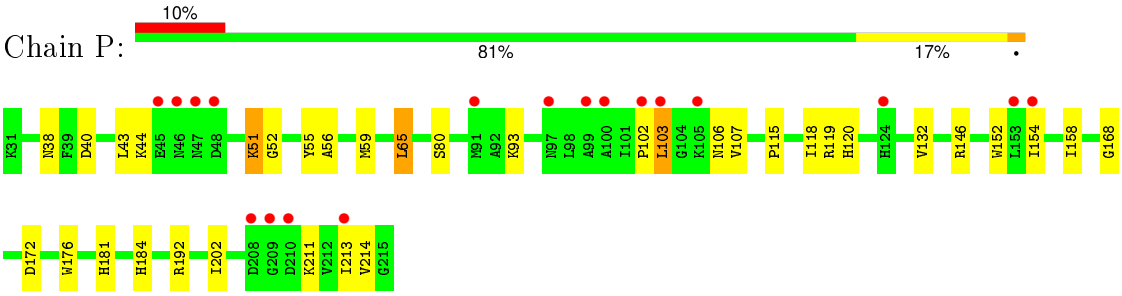
• Molecule 4: Cytochrome c1, heme protein, mitochondrial



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

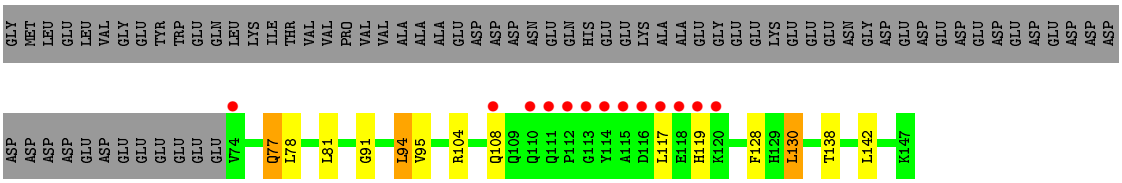


• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial



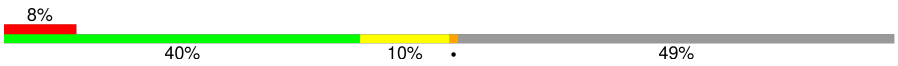
• Molecule 6: Cytochrome b-c1 complex subunit 6

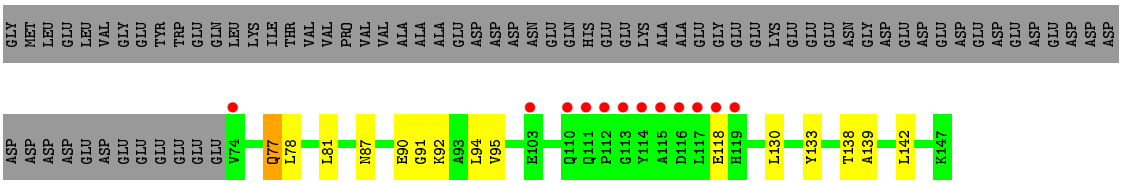
Chain F:



• Molecule 6: Cytochrome b-c1 complex subunit 6

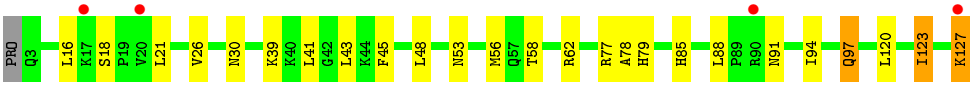
Chain Q:





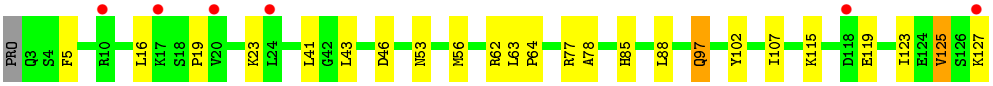
• Molecule 7: Cytochrome b-c1 complex subunit 7

Chain G:



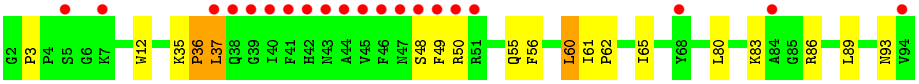
• Molecule 7: Cytochrome b-c1 complex subunit 7

Chain R:



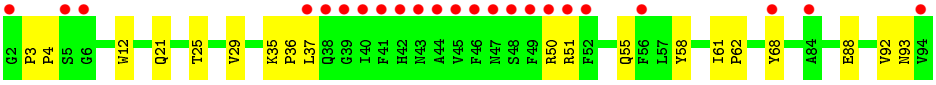
• Molecule 8: Cytochrome b-c1 complex subunit 8

Chain H:



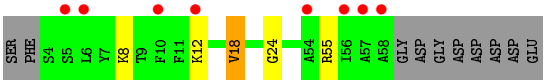
• Molecule 8: Cytochrome b-c1 complex subunit 8

Chain S:

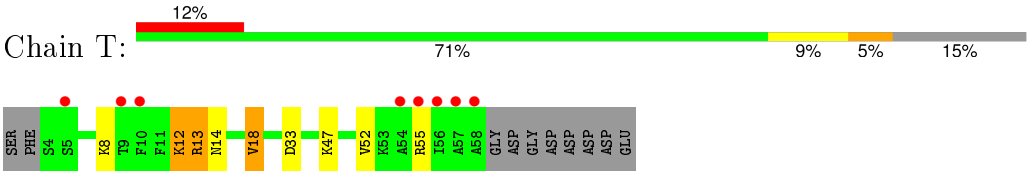


• Molecule 9: Cytochrome b-c1 complex subunit 9

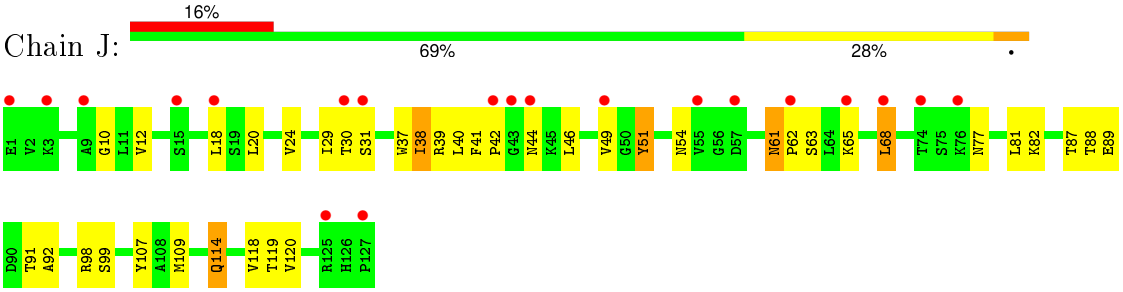
Chain I:



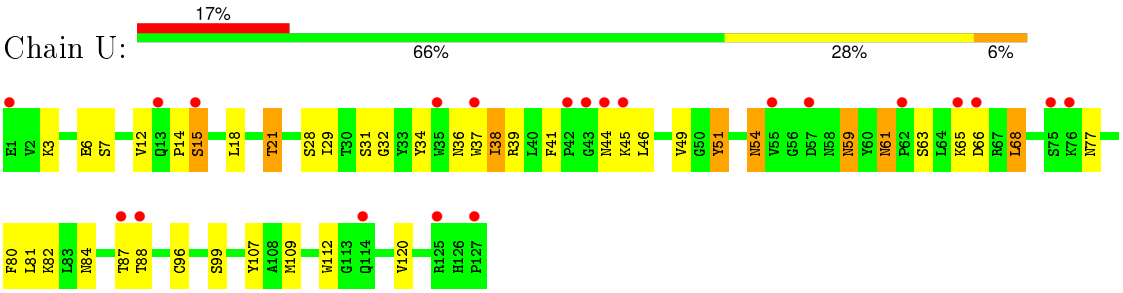
• Molecule 9: Cytochrome b-c1 complex subunit 9



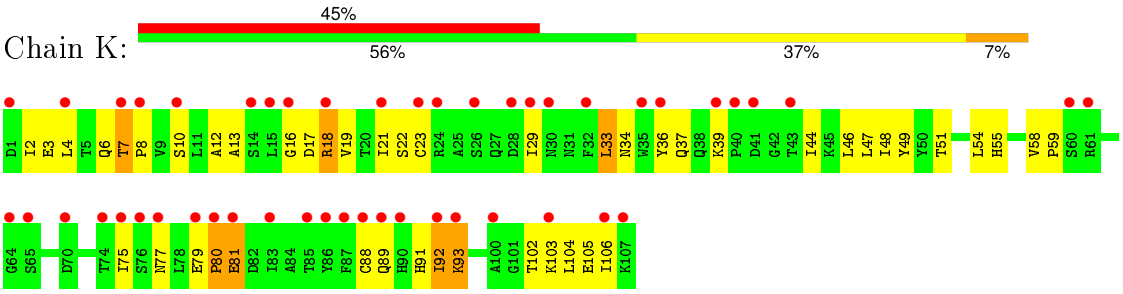
• Molecule 10: HEAVY CHAIN (VH) OF FV-FRAGMENT



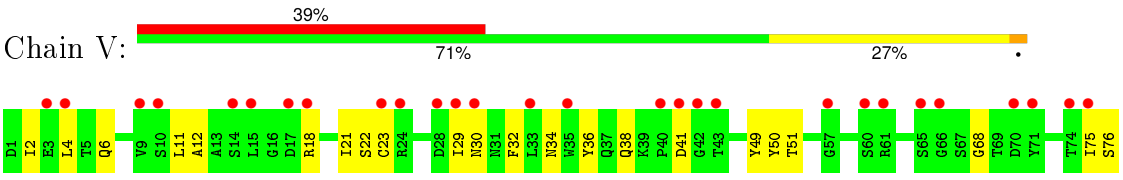
• Molecule 10: HEAVY CHAIN (VH) OF FV-FRAGMENT

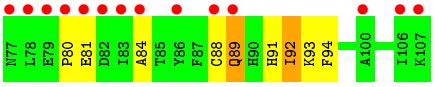


• Molecule 11: LIGHT CHAIN (VL) OF FV-FRAGMENT



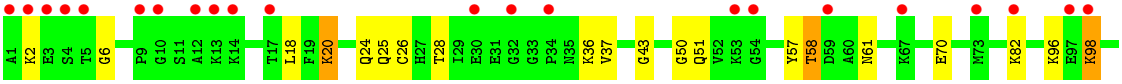
• Molecule 11: LIGHT CHAIN (VL) OF FV-FRAGMENT





- Molecule 12: Cytochrome c iso-2

Chain W:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	145.54Å 162.97Å 194.23Å 90.00° 104.39° 90.00°	Depositor
Resolution (Å)	19.97 – 2.50 19.97 – 2.50	Depositor EDS
% Data completeness (in resolution range)	95.9 (19.97-2.50) 96.0 (19.97-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.66	Depositor
$< I/\sigma(I) >$ [1]	2.01 (at 2.50Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.225 , 0.256 0.227 , 0.259	Depositor DCC
R_{free} test set	14494 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	45.8	Xtriage
Anisotropy	0.430	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 56.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 289897 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	36805	wwPDB-VP
Average B, all atoms (Å^2)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.27% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: CN6, UMQ, 8PE, M3L, 7PH, FES, SUC, 9PE, HEM, 6PH, SMA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.36	0/3405	0.61	1/4614 (0.0%)
1	L	0.37	0/3405	0.63	0/4614
2	B	0.36	0/2781	0.66	2/3764 (0.1%)
2	M	0.37	0/2781	0.65	1/3764 (0.0%)
3	C	0.43	0/3192	0.64	1/4354 (0.0%)
3	N	0.44	0/3192	0.66	0/4354
4	D	0.37	0/2001	0.61	0/2726
4	O	0.40	0/2001	0.63	0/2726
5	E	0.36	0/1444	0.60	0/1957
5	P	0.35	0/1444	0.61	1/1957 (0.1%)
6	F	0.36	0/638	0.53	0/858
6	Q	0.37	0/638	0.58	0/858
7	G	0.37	0/1032	0.62	0/1397
7	R	0.40	0/1032	0.63	0/1397
8	H	0.41	0/804	0.55	0/1088
8	S	0.44	0/804	0.56	0/1088
9	I	0.39	0/461	0.52	0/622
9	T	0.42	0/461	0.51	0/622
10	J	0.35	0/1043	0.60	0/1422
10	U	0.34	0/1043	0.62	0/1422
11	K	0.33	0/863	0.54	0/1172
11	V	0.33	0/863	0.53	0/1172
12	W	0.34	0/891	0.60	0/1191
All	All	0.38	0/36219	0.62	6/49139 (0.0%)

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
3	C	0	1

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	P	65	LEU	CA-CB-CG	6.40	130.03	115.30
2	B	87	ILE	N-CA-C	-6.16	94.38	111.00
2	B	152	ARG	N-CA-C	5.45	125.71	111.00
2	M	87	ILE	N-CA-C	-5.44	96.31	111.00
1	A	251	LEU	CA-CB-CG	5.32	127.54	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	279	TYR	Sidechain

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	99	0
1	L	3344	0	3321	80	0
2	B	2735	0	2774	74	0
2	M	2735	0	2774	77	0
3	C	3090	0	3129	52	0
3	N	3090	0	3129	30	0
4	D	1940	0	1862	30	0
4	O	1940	0	1862	30	0
5	E	1411	0	1386	36	0
5	P	1411	0	1386	25	0
6	F	624	0	581	10	0
6	Q	624	0	581	9	0
7	G	1012	0	1026	22	0
7	R	1012	0	1026	16	0
8	H	773	0	736	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	S	773	0	736	15	0
9	I	448	0	445	5	0
9	T	448	0	445	7	0
10	J	1015	0	959	29	0
10	U	1015	0	959	35	0
11	K	842	0	820	33	0
11	V	842	0	820	23	0
12	W	885	0	890	15	0
13	O	23	0	22	2	0
14	A	34	0	44	4	0
14	L	34	0	44	2	0
15	C	86	0	60	3	0
15	D	43	0	30	0	0
15	N	86	0	60	1	0
15	O	43	0	30	1	0
15	W	43	0	30	2	0
16	C	37	0	42	1	0
16	N	37	0	42	1	0
17	C	47	0	73	2	0
17	N	47	0	73	2	0
18	C	50	0	56	7	0
18	N	50	0	56	5	0
19	C	40	0	59	0	0
19	N	40	0	59	0	0
20	D	38	0	55	3	0
20	O	38	0	55	2	0
21	E	4	0	0	0	0
21	P	4	0	0	1	0
22	E	40	0	59	1	0
22	L	40	0	59	0	0
23	A	42	0	0	0	0
23	B	17	0	0	1	0
23	C	75	0	0	4	0
23	D	50	0	0	0	0
23	E	19	0	0	0	0
23	F	3	0	0	0	0
23	G	21	0	0	1	0
23	H	10	0	0	0	0
23	I	4	0	0	0	0
23	J	2	0	0	1	0
23	K	1	0	0	0	0
23	L	54	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	M	15	0	0	0	0
23	N	88	0	0	3	0
23	O	74	0	0	2	0
23	P	18	0	0	0	0
23	Q	3	0	0	0	0
23	R	22	0	0	1	0
23	S	13	0	0	0	0
23	T	5	0	0	0	0
23	U	2	0	0	0	0
23	W	10	0	0	1	0
All	All	36805	0	35976	721	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 10.

The worst 5 of 721 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)
2:M:347:LYS:H	2:M:347:LYS:HD3	1.19	1.01
1:A:63:ASN:H	1:A:66:ASN:HD21	1.06	1.00
1:A:382:ASN:HD21	1:A:384:VAL:HG22	1.22	0.99
1:L:63:ASN:H	1:L:66:ASN:ND2	1.60	0.99
6:Q:77:GLN:H	6:Q:77:GLN:HE21	1.08	0.98

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	429/431 (100%)	395 (92%)	33 (8%)	1 (0%)	52 75
1	L	429/431 (100%)	393 (92%)	32 (8%)	4 (1%)	21 37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	B	350/352 (99%)	310 (89%)	31 (9%)	9 (3%)	7 10
2	M	350/352 (99%)	320 (91%)	19 (5%)	11 (3%)	5 7
3	C	383/385 (100%)	364 (95%)	17 (4%)	2 (0%)	34 55
3	N	383/385 (100%)	367 (96%)	14 (4%)	2 (0%)	34 55
4	D	244/248 (98%)	231 (95%)	12 (5%)	1 (0%)	39 61
4	O	244/248 (98%)	234 (96%)	10 (4%)	0	100 100
5	E	183/185 (99%)	171 (93%)	9 (5%)	3 (2%)	12 21
5	P	183/185 (99%)	171 (93%)	10 (6%)	2 (1%)	17 31
6	F	72/146 (49%)	68 (94%)	4 (6%)	0	100 100
6	Q	72/146 (49%)	67 (93%)	4 (6%)	1 (1%)	14 24
7	G	123/126 (98%)	121 (98%)	2 (2%)	0	100 100
7	R	123/126 (98%)	119 (97%)	4 (3%)	0	100 100
8	H	91/93 (98%)	78 (86%)	10 (11%)	3 (3%)	5 6
8	S	91/93 (98%)	82 (90%)	6 (7%)	3 (3%)	5 6
9	I	53/65 (82%)	48 (91%)	4 (8%)	1 (2%)	10 16
9	T	53/65 (82%)	50 (94%)	1 (2%)	2 (4%)	4 5
10	J	125/127 (98%)	110 (88%)	14 (11%)	1 (1%)	24 41
10	U	125/127 (98%)	110 (88%)	12 (10%)	3 (2%)	7 11
11	K	105/107 (98%)	80 (76%)	21 (20%)	4 (4%)	4 5
11	V	105/107 (98%)	82 (78%)	20 (19%)	3 (3%)	6 8
12	W	110/112 (98%)	98 (89%)	11 (10%)	1 (1%)	21 37
All	All	4426/4642 (95%)	4069 (92%)	300 (7%)	57 (1%)	15 26

5 of 57 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	152	ARG
2	B	153	LYS
2	B	335	PRO
2	B	343	VAL
3	C	346	VAL

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	370/370 (100%)	338 (91%)	32 (9%)	13	24
1	L	370/370 (100%)	334 (90%)	36 (10%)	10	19
2	B	301/301 (100%)	273 (91%)	28 (9%)	11	21
2	M	301/301 (100%)	274 (91%)	27 (9%)	12	22
3	C	338/338 (100%)	317 (94%)	21 (6%)	23	41
3	N	338/338 (100%)	320 (95%)	18 (5%)	28	50
4	D	204/206 (99%)	197 (97%)	7 (3%)	44	72
4	O	204/206 (99%)	197 (97%)	7 (3%)	44	72
5	E	151/151 (100%)	147 (97%)	4 (3%)	54	81
5	P	151/151 (100%)	147 (97%)	4 (3%)	54	81
6	F	67/130 (52%)	64 (96%)	3 (4%)	34	59
6	Q	67/130 (52%)	64 (96%)	3 (4%)	34	59
7	G	109/110 (99%)	104 (95%)	5 (5%)	33	57
7	R	109/110 (99%)	104 (95%)	5 (5%)	33	57
8	H	77/77 (100%)	76 (99%)	1 (1%)	76	92
8	S	77/77 (100%)	75 (97%)	2 (3%)	54	81
9	I	45/53 (85%)	44 (98%)	1 (2%)	60	84
9	T	45/53 (85%)	43 (96%)	2 (4%)	35	60
10	J	112/112 (100%)	105 (94%)	7 (6%)	22	40
10	U	112/112 (100%)	102 (91%)	10 (9%)	12	23
11	K	93/93 (100%)	86 (92%)	7 (8%)	17	31
11	V	93/93 (100%)	88 (95%)	5 (5%)	27	49
12	W	92/91 (101%)	86 (94%)	6 (6%)	21	39
All	All	3826/3973 (96%)	3585 (94%)	241 (6%)	22	40

5 of 241 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	K	7	THR
1	L	239	LYS
10	U	38	ILE
11	K	77	ASN
1	L	130	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 136 such sidechains are listed below:

Mol	Chain	Res	Type
10	J	44	ASN
1	L	170	GLN
10	U	58	ASN
10	J	61	ASN
1	L	61	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	$\#\|Z\| > 2$
12	M3L	W	81	12	10,11,12	0.82	0	12,14,16	1.19	1 (8%)

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	M3L	W	81	12	-	0/8/10/12	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	W	81	M3L	CM3-NZ-CM1	-2.54	102.43	108.98

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)

24 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	$\#\|Z\| > 2$
14	UMQ	A	4021	-	35,35,35	0.96	1 (2%)	46,46,46	1.69	7 (15%)
15	HEM	C	4001	3	30,50,50	3.14	11 (36%)	24,82,82	1.92	6 (25%)
15	HEM	C	4002	3	30,50,50	2.80	9 (30%)	24,82,82	2.29	8 (33%)
16	SMA	C	4005	-	35,38,38	1.33	4 (11%)	40,52,52	1.51	6 (15%)
17	8PE	C	4010	-	45,46,46	0.94	3 (6%)	46,51,51	1.03	1 (2%)
18	CN6	C	4031	-	49,49,49	1.54	11 (22%)	51,61,61	1.45	5 (9%)
19	9PE	C	4111	-	38,39,39	0.73	0	39,44,44	0.96	1 (2%)
15	HEM	D	4003	4	30,50,50	2.62	7 (23%)	24,82,82	3.23	8 (33%)
20	7PH	D	4014	-	37,37,37	1.02	2 (5%)	40,42,42	1.47	9 (22%)
21	FES	E	4004	5	0,4,4	0.00	-	0,4,4	0.00	-
22	6PH	E	4013	-	39,39,39	0.95	2 (5%)	42,44,44	1.34	4 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	6PH	L	4113	-	39,39,39	0.98	2 (5%)	42,44,44	1.37	4 (9%)
14	UMQ	L	4121	-	35,35,35	0.98	1 (2%)	46,46,46	1.75	5 (10%)
19	9PE	N	4011	-	38,39,39	0.69	0	39,44,44	0.91	1 (2%)
15	HEM	N	4021	3	30,50,50	3.10	11 (36%)	24,82,82	2.24	8 (33%)
15	HEM	N	4022	3	30,50,50	2.98	12 (40%)	24,82,82	2.60	8 (33%)
16	SMA	N	4025	-	35,38,38	1.29	2 (5%)	40,52,52	1.38	4 (10%)
17	8PE	N	4110	-	45,46,46	0.90	2 (4%)	46,51,51	1.21	3 (6%)
18	CN6	N	4131	-	49,49,49	1.59	10 (20%)	51,61,61	1.60	6 (11%)
15	HEM	O	4023	4	30,50,50	2.54	8 (26%)	24,82,82	3.17	10 (41%)
20	7PH	O	4114	-	37,37,37	1.04	2 (5%)	40,42,42	1.51	9 (22%)
13	SUC	O	4146	-	24,24,24	0.62	0	36,36,36	0.68	1 (2%)
21	FES	P	4024	5	0,4,4	0.00	-	0,4,4	0.00	-
15	HEM	W	4026	12	30,50,50	2.65	9 (30%)	24,82,82	3.07	9 (37%)

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
14	UMQ	A	4021	-	-	0/20/60/60	0/2/2/2
15	HEM	C	4001	3	-	0/10/54/54	0/0/8/8
15	HEM	C	4002	3	-	0/10/54/54	0/0/8/8
16	SMA	C	4005	-	-	0/33/34/34	0/2/2/2
17	8PE	C	4010	-	-	0/50/50/50	0/0/0/0
18	CN6	C	4031	-	-	1/60/60/60	0/0/0/0
19	9PE	C	4111	-	-	0/43/43/43	0/0/0/0
15	HEM	D	4003	4	-	0/10/54/54	0/0/8/8
20	7PH	D	4014	-	-	0/39/39/39	0/0/0/0
21	FES	E	4004	5	-	0/0/4/4	0/1/1/1
22	6PH	E	4013	-	-	0/41/41/41	0/0/0/0
22	6PH	L	4113	-	-	0/41/41/41	0/0/0/0
14	UMQ	L	4121	-	-	0/20/60/60	0/2/2/2
19	9PE	N	4011	-	-	0/43/43/43	0/0/0/0
15	HEM	N	4021	3	-	0/10/54/54	0/0/8/8
15	HEM	N	4022	3	-	0/10/54/54	0/0/8/8
16	SMA	N	4025	-	-	0/33/34/34	0/2/2/2
17	8PE	N	4110	-	-	0/50/50/50	0/0/0/0
18	CN6	N	4131	-	-	0/60/60/60	0/0/0/0
15	HEM	O	4023	4	-	0/10/54/54	0/0/8/8

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	7PH	O	4114	-	-	0/39/39/39	0/0/0/0
13	SUC	O	4146	-	-	0/12/51/51	0/2/2/2
21	FES	P	4024	5	-	0/0/4/4	0/1/1/1
15	HEM	W	4026	12	-	0/10/54/54	0/0/8/8

The worst 5 of 109 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	N	4021	HEM	C3B-C4B	-8.39	1.44	1.51
15	C	4001	HEM	C3B-C4B	-7.87	1.44	1.51
15	D	4003	HEM	C3B-C4B	-7.67	1.45	1.51
15	W	4026	HEM	C3B-C4B	-7.61	1.45	1.51
15	N	4022	HEM	C3B-C4B	-7.32	1.45	1.51

The worst 5 of 123 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	D	4003	HEM	C3B-CAB-CBB	-9.56	109.79	124.46
15	O	4023	HEM	C3B-CAB-CBB	-9.40	110.04	124.46
15	D	4003	HEM	C3C-CAC-CBC	-8.55	111.34	124.46
14	L	4121	UMQ	CA-O1'-C1'	-8.36	99.33	113.94
15	W	4026	HEM	C3B-CAB-CBB	-7.99	112.19	124.46

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	C	4031	CN6	C2'-O51-C51-C52

There are no ring outliers.

18 monomers are involved in 39 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	A	4021	UMQ	4	0
15	C	4001	HEM	2	0
15	C	4002	HEM	1	0
16	C	4005	SMA	1	0
17	C	4010	8PE	2	0
18	C	4031	CN6	7	0
20	D	4014	7PH	3	0
22	E	4013	6PH	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	L	4121	UMQ	2	0
15	N	4022	HEM	1	0
16	N	4025	SMA	1	0
17	N	4110	8PE	2	0
18	N	4131	CN6	5	0
15	O	4023	HEM	1	0
20	O	4114	7PH	2	0
13	O	4146	SUC	2	0
21	P	4024	FES	1	0
15	W	4026	HEM	2	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{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	431/431 (100%)	0.41	40 (9%) 11 11	32, 57, 121, 146	0
1	L	431/431 (100%)	0.34	41 (9%) 10 11	29, 53, 114, 140	0
2	B	352/352 (100%)	0.55	32 (9%) 11 12	40, 61, 101, 148	0
2	M	352/352 (100%)	0.51	31 (8%) 12 13	40, 59, 93, 137	0
3	C	385/385 (100%)	-0.30	6 (1%) 74 78	26, 35, 49, 113	0
3	N	385/385 (100%)	-0.26	6 (1%) 74 78	25, 33, 46, 104	0
4	D	246/248 (99%)	0.01	11 (4%) 37 42	32, 48, 70, 79	0
4	O	246/248 (99%)	-0.14	5 (2%) 68 72	25, 42, 64, 80	0
5	E	185/185 (100%)	0.54	21 (11%) 7 6	32, 54, 90, 117	0
5	P	185/185 (100%)	0.44	18 (9%) 10 10	34, 52, 92, 114	0
6	F	74/146 (50%)	0.86	13 (17%) 2 2	44, 62, 112, 114	0
6	Q	74/146 (50%)	0.48	12 (16%) 3 2	39, 57, 108, 110	0
7	G	125/126 (99%)	0.02	4 (3%) 51 56	32, 45, 72, 92	0
7	R	125/126 (99%)	0.00	6 (4%) 34 39	28, 43, 69, 88	0
8	H	93/93 (100%)	1.16	20 (21%) 1 1	29, 57, 147, 154	0
8	S	93/93 (100%)	1.42	23 (24%) 1 1	26, 55, 154, 160	0
9	I	55/65 (84%)	0.65	8 (14%) 3 3	41, 56, 111, 124	0
9	T	55/65 (84%)	0.58	8 (14%) 3 3	37, 49, 112, 124	0
10	J	127/127 (100%)	1.03	20 (15%) 3 2	50, 74, 93, 99	0
10	U	127/127 (100%)	0.99	21 (16%) 2 2	52, 74, 89, 97	0
11	K	107/107 (100%)	1.98	48 (44%) 0 0	70, 105, 135, 141	0
11	V	107/107 (100%)	2.01	42 (39%) 0 0	72, 104, 133, 136	0
12	W	111/112 (99%)	1.23	24 (21%) 1 1	50, 70, 108, 136	0
All	All	4471/4642 (96%)	0.42	460 (10%) 9 9	25, 53, 111, 160	0

The worst 5 of 460 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
8	S	43	ASN	15.5
12	W	4	SER	12.8
8	S	42	HIS	11.5
9	T	58	ALA	11.5
8	S	46	PHE	11.1

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
12	M3L	W	81	12/13	0.89	0.30	-	60,63,64,66	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
19	9PE	N	4011	40/40	0.94	0.19	2.61	50,54,63,64	0
13	SUC	O	4146	23/23	0.80	0.30	2.47	72,77,80,81	0
19	9PE	C	4111	40/40	0.92	0.17	2.28	45,57,75,76	0
20	7PH	D	4014	38/38	0.93	0.21	1.54	48,53,61,62	0
20	7PH	O	4114	38/38	0.93	0.20	1.52	38,44,51,54	0
18	CN6	C	4031	50/50	0.87	0.23	1.46	50,70,78,80	0
22	6PH	L	4113	40/40	0.90	0.17	1.24	49,60,69,69	0
17	8PE	N	4110	47/47	0.91	0.19	0.95	28,65,74,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
22	6PH	E	4013	40/40	0.89	0.17	0.55	56,65,72,72	0
17	8PE	C	4010	47/47	0.91	0.17	0.45	39,59,62,65	0
18	CN6	N	4131	50/50	0.89	0.21	0.26	53,67,77,79	0
16	SMA	C	4005	37/37	0.96	0.14	0.02	29,33,37,37	0
14	UMQ	L	4121	34/34	0.94	0.15	-0.08	39,44,59,60	0
14	UMQ	A	4021	34/34	0.94	0.16	-0.19	42,48,65,67	0
16	SMA	N	4025	37/37	0.97	0.13	-0.23	23,28,31,32	0
15	HEM	D	4003	43/43	0.98	0.13	-0.37	35,39,43,44	0
15	HEM	W	4026	43/43	0.96	0.16	-0.44	47,55,57,58	0
15	HEM	C	4001	43/43	0.99	0.12	-0.61	21,26,32,35	0
15	HEM	O	4023	43/43	0.99	0.10	-0.81	32,37,41,42	0
15	HEM	N	4022	43/43	0.99	0.11	-0.86	21,23,32,35	0
15	HEM	N	4021	43/43	0.99	0.11	-0.98	15,23,30,34	0
21	FES	E	4004	4/4	0.99	0.13	-1.01	30,32,32,37	0
15	HEM	C	4002	43/43	0.99	0.11	-1.13	20,26,37,37	0
21	FES	P	4024	4/4	0.99	0.10	-1.63	32,36,36,37	0

6.5 Other polymers (i)

There are no such residues in this entry.