



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 09:06 AM GMT

PDB ID : 3H1J
Title : Stigmatellin-bound cytochrome bc1 complex from chicken
Authors : Zhang, Z.; Huang, L.; Shulmeister, V.M.; Chi, Y.-I.; Kim, K.K.; Hung, L.-W.; Crofts, A.R.; Berry, E.A.; Kim, S.-H.
Deposited on : 2009-04-12
Resolution : 3.00 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 (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

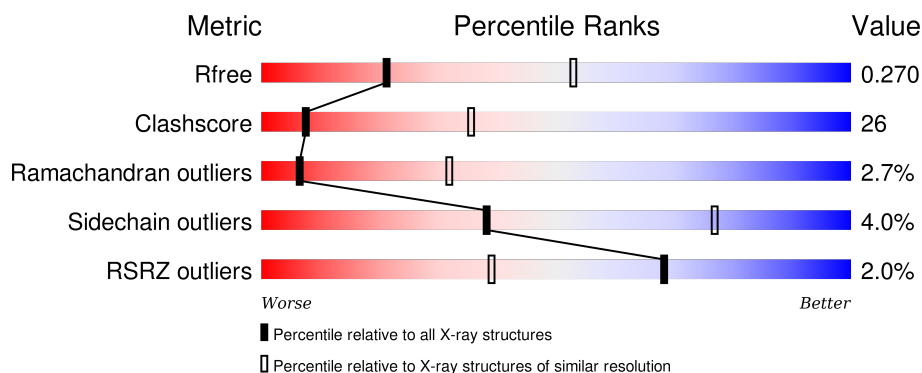
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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.




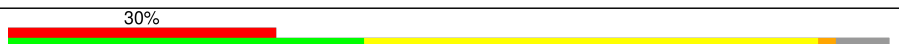
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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	446	
1	N	446	
2	B	441	
2	O	441	
3	C	380	

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Mol	Chain	Length	Quality of chain
3	P	380	
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	47	
9	V	47	
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	UNL	A	3016	-	-	-	X
11	UNL	C	2010	-	-	-	X
11	UNL	E	3103	-	-	-	X
11	UNL	R	2103	-	-	-	X
14	UQ	C	2002	-	-	-	X
14	UQ	P	3002	-	-	-	X
15	PEE	C	2007	-	-	-	X
15	PEE	C	2008	-	-	-	X
15	PEE	E	2005	-	-	-	X
15	PEE	N	3008	-	X	-	-
15	PEE	P	3007	-	-	-	X
15	PEE	R	3005	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
16	GOL	C	2011	-	-	-	X
16	GOL	P	3011	-	-	-	X
18	CDL	G	2004	-	-	-	X
18	CDL	S	3003	-	-	-	X
20	PLC	E	2009	-	-	-	X
20	PLC	R	3009	-	-	-	X

2 Entry composition

There are 21 unique types of molecules in this entry. The entry contains 32679 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	1
			3440	2155	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
			3141	1974	545	613	9			
2	O	422	Total	C	N	O	S	0	0	0
			3147	1977	546	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
			3020	2024	478	505	13			
3	P	379	Total	C	N	O	S	0	0	0
			3012	2019	477	504	12			

- 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
			1513	952	263	292	6			

- Molecule 6 is a protein called MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 14 KDA PROTEIN.

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	81	Total	C	N	O	0	0	0
			676	439	120	117			
7	T	79	Total	C	N	O	0	0	0
			658	430	117	111			

- Molecule 8 is a protein called MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 11 KDA PROTEIN, COMPLEX III SUBUNIT VIII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	70	Total	C	N	O	S	0	0	0
			574	350	105	114	5			
8	U	67	Total	C	N	O	S	0	0	0
			553	338	103	107	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	46	Total	C	N	O	S	0	0	0
			285	169	58	56	2			
9	V	44	Total	C	N	O	S	0	0	1
			275	164	56	53	2			

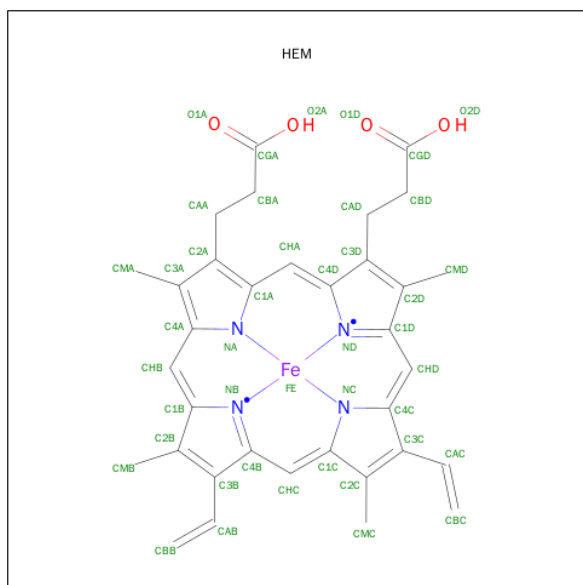
- Molecule 10 is a protein called MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 7.2 KDA PROTEIN.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	J	61	Total	C	N	O	0	0	0
			497	321	87	89			
10	W	59	Total	C	N	O	0	0	0
			478	311	85	82			

- Molecule 11 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	P	3	Total	O	0	0
			3	3		
11	R	1	Total	O	0	0
			1	1		
11	A	1	Total	O	0	0
			1	1		
11	C	3	Total	O	0	0
			3	3		
11	E	2	Total	O	0	0
			2	2		

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



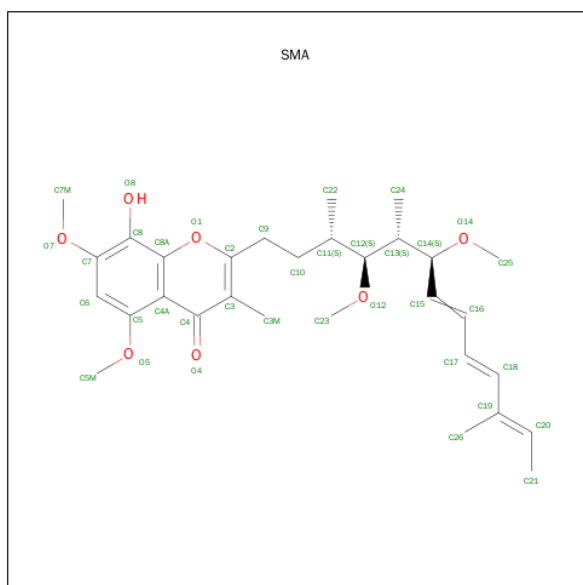
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	0
12	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	0

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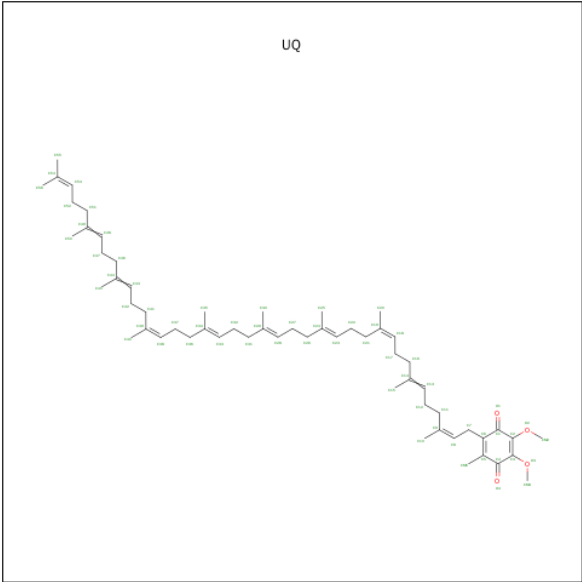
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	P	1	Total	C	Fe	N	O	
			43	34	1	4	4	0
12	P	1	Total	C	Fe	N	O	
			43	34	1	4	4	0

- Molecule 13 is STIGMATELLIN A (three-letter code: SMA) (formula: C₃₀H₄₂O₇).



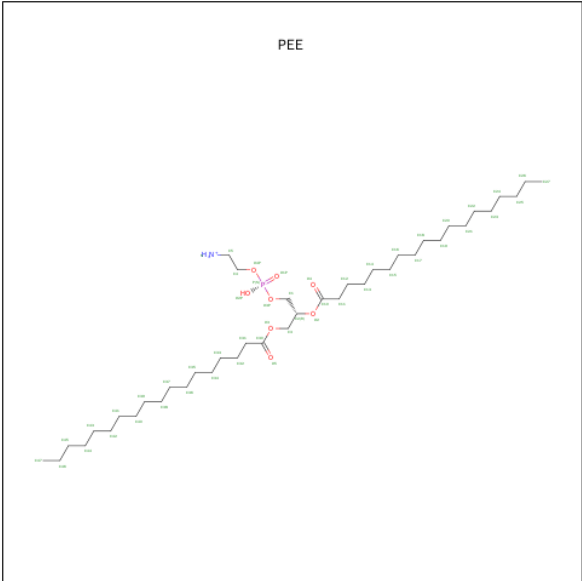
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	C	1	Total	C	O		
			37	30	7	0	0
13	P	1	Total	C	O		
			37	30	7	0	0

- Molecule 14 is COENZYME Q10, (2Z,6E,10Z,14E,18E,22E,26Z)-ISOMER (three-letter code: UQ) (formula: C₅₉H₉₀O₄).



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 PHOSPHATIDYLETHANOLAMINE (three-letter code: PEE) (formula: C₄₁H₈₃NO₈P).



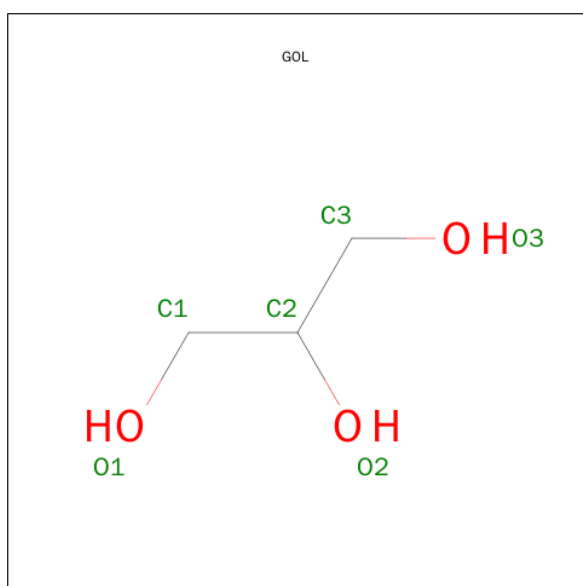
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
15	C	1	Total	C	N	O	P	0	0
			49	39	1	8	1		

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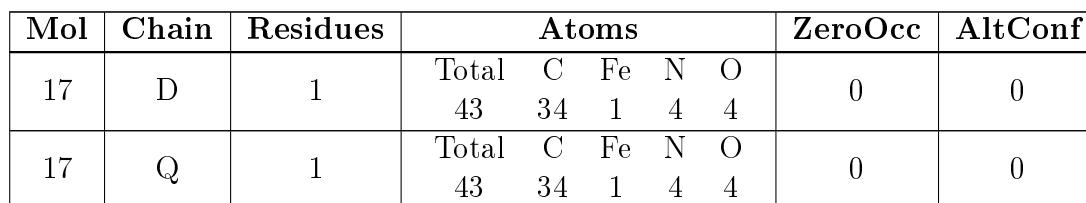
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	C	1	Total C O P 21 12 8 1	0	0
15	E	1	Total C N O P 50 40 1 8 1	0	0
15	N	1	Total O P 5 4 1	0	0
15	P	1	Total C N O P 49 39 1 8 1	0	0
15	R	1	Total C N O P 50 40 1 8 1	0	0

- 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 6 3 3	0	0
16	P	1	Total C O 6 3 3	0	0

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



- CDL
-
- The chemical structure of CDL (1,3-bis(sn-3'-phosphatidyl)-sn-glycerol) is shown. It consists of a glycerol backbone with three fatty acid chains and three phosphate groups. The structure is labeled 'CDL'.

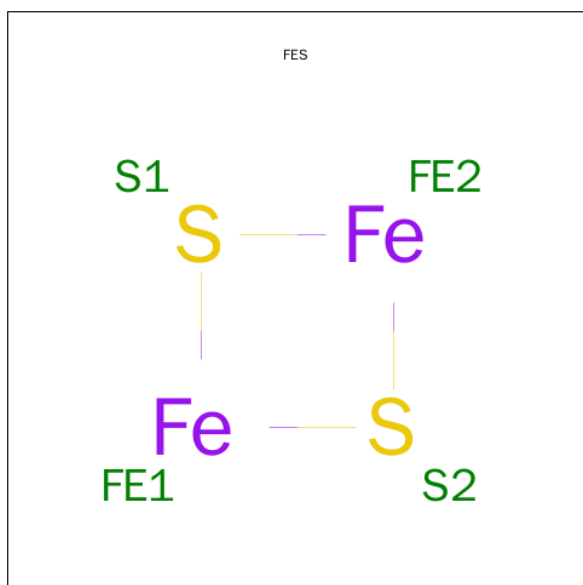
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
18	D	1	Total 50	C 31	O 17	P 2	0	0
18	G	1	Total 40	C 21	O 17	P 2	0	0



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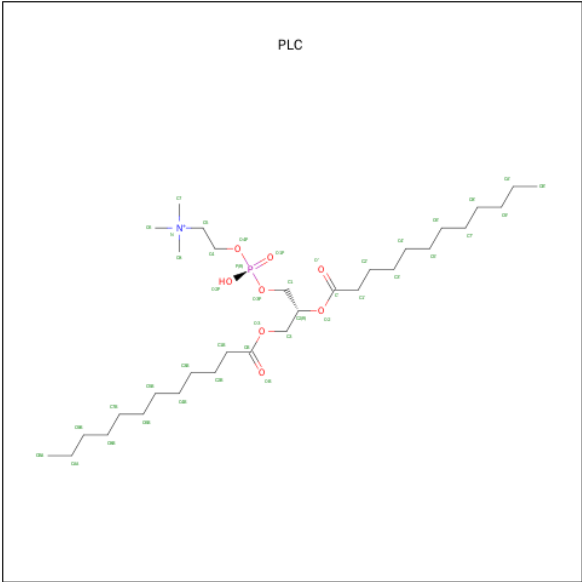
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
18	P	1	Total	C	O	P	0	0
			40	21	17	2		
18	S	1	Total	C	O	P	0	0
			50	31	17	2		

- Molecule 19 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



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

- Molecule 20 is DIUNDECYL PHOSPHATIDYL CHOLINE (three-letter code: PLC) (formula: $\text{C}_{32}\text{H}_{65}\text{NO}_8\text{P}$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	E	1	Total	C	N	O	P	0	0
			32	22	1	8	1		
20	R	1	Total	C	N	O	P	0	0
			32	22	1	8	1		

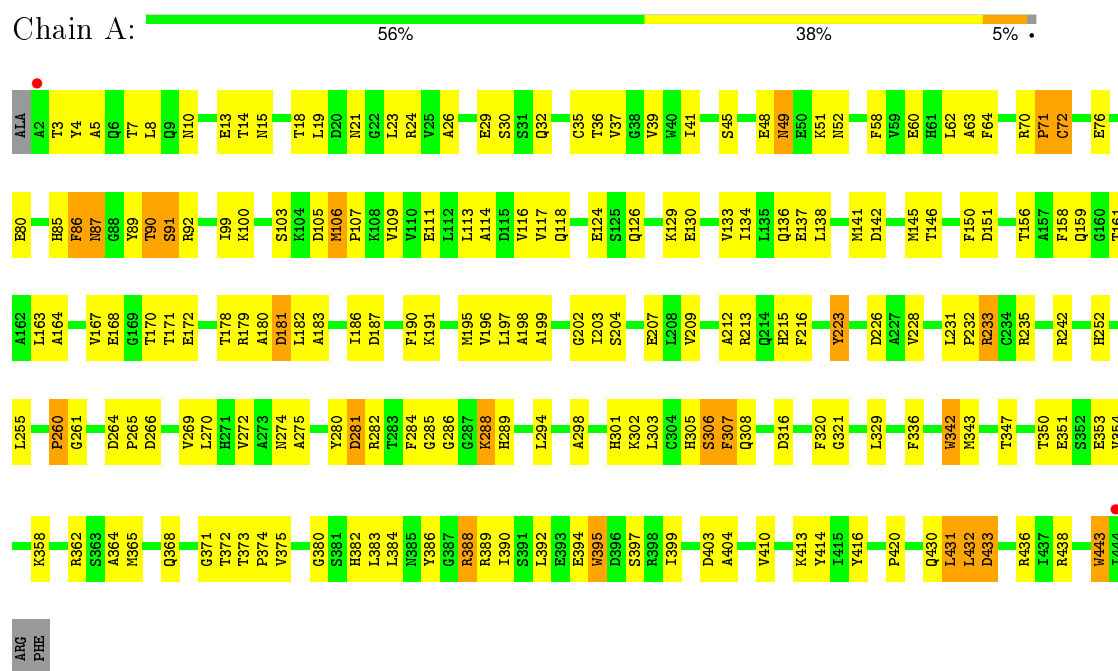
- Molecule 21 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	B	1	Total	O	0	0
			1	1		
21	C	6	Total	O	0	0
			6	6		
21	P	6	Total	O	0	0
			6	6		
21	U	1	Total	O	0	0
			1	1		

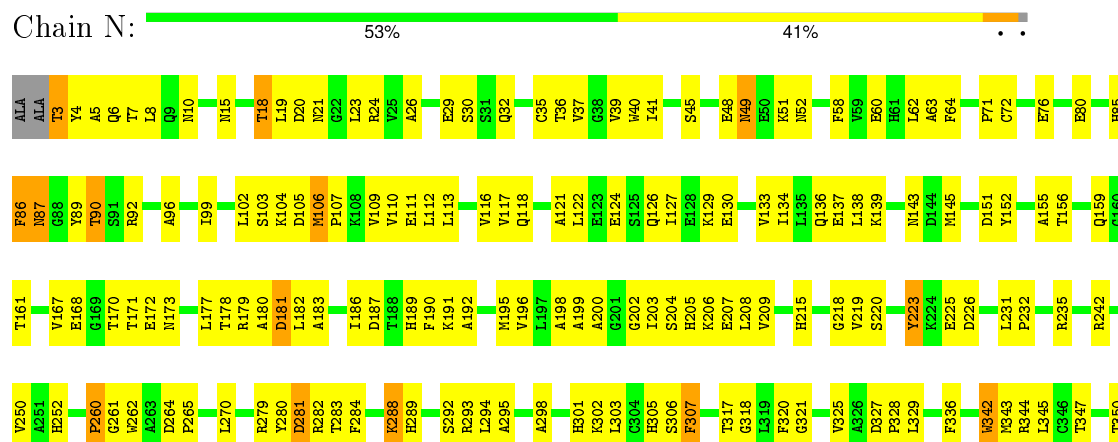
3 Residue-property plots

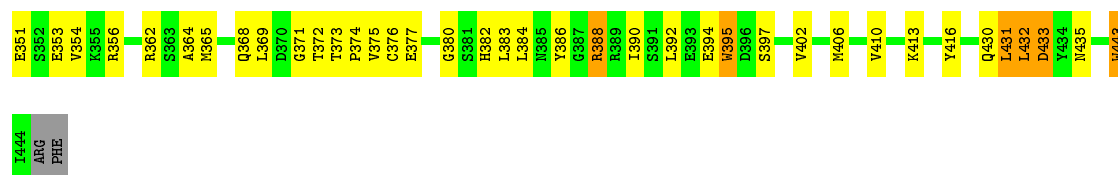
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

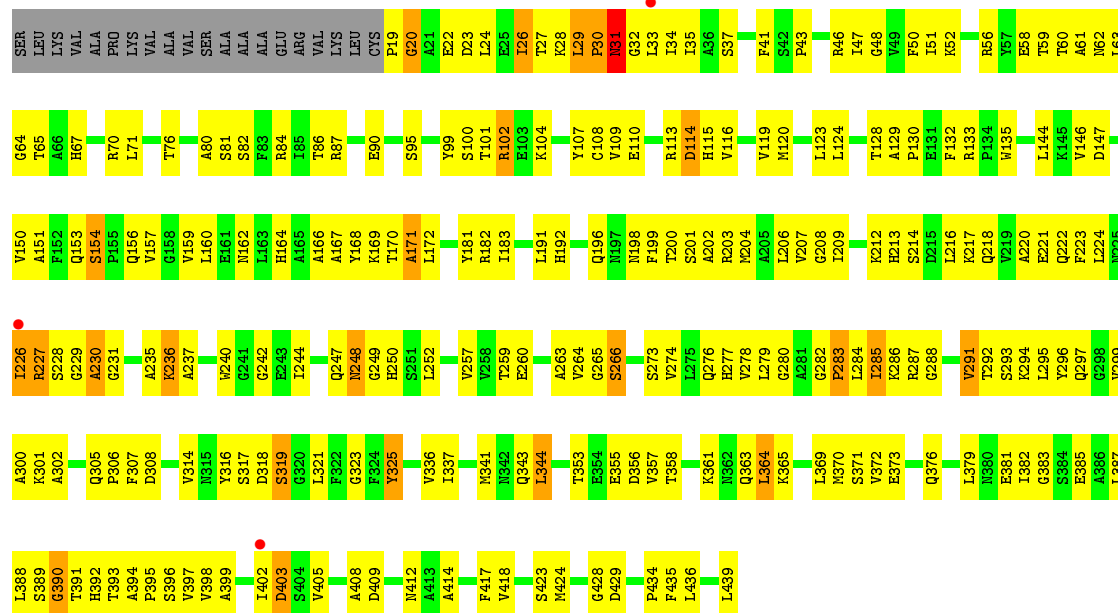
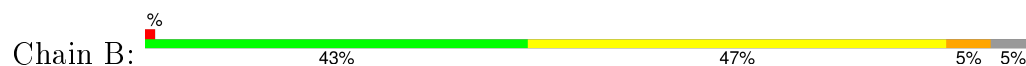


• Molecule 1: MITOCHONDRIAL UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN I

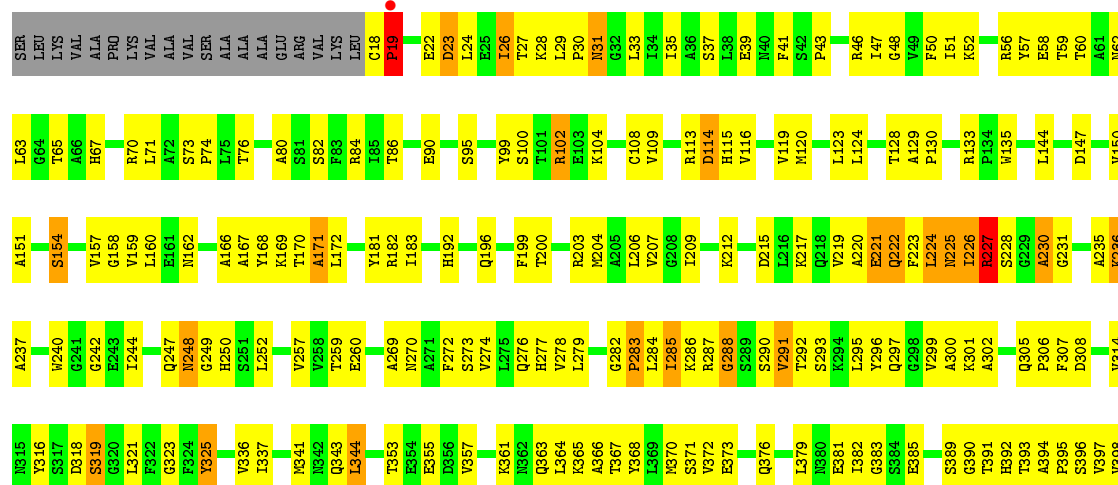


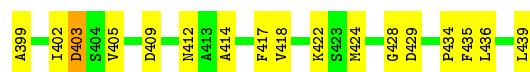


• Molecule 2: MITOCHONDRIAL UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN 2

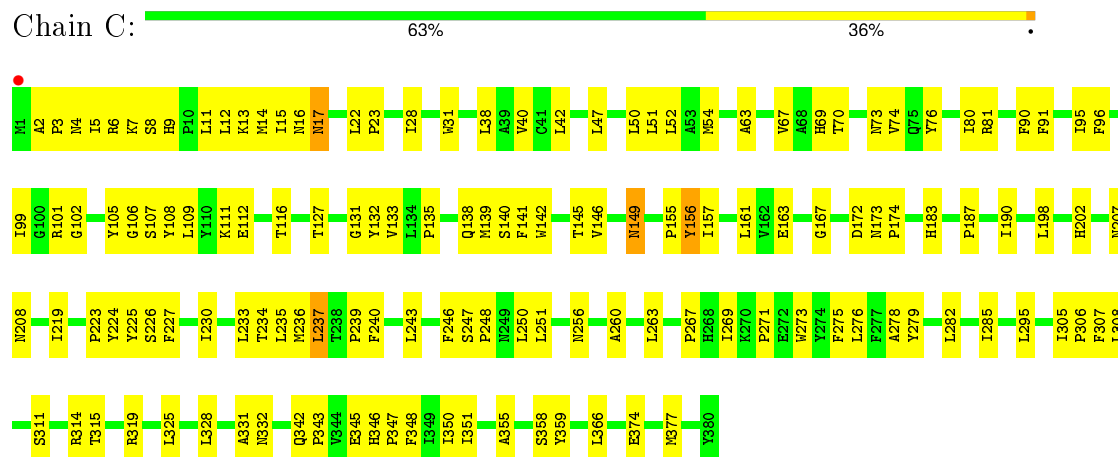


• Molecule 2: MITOCHONDRIAL UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN 2

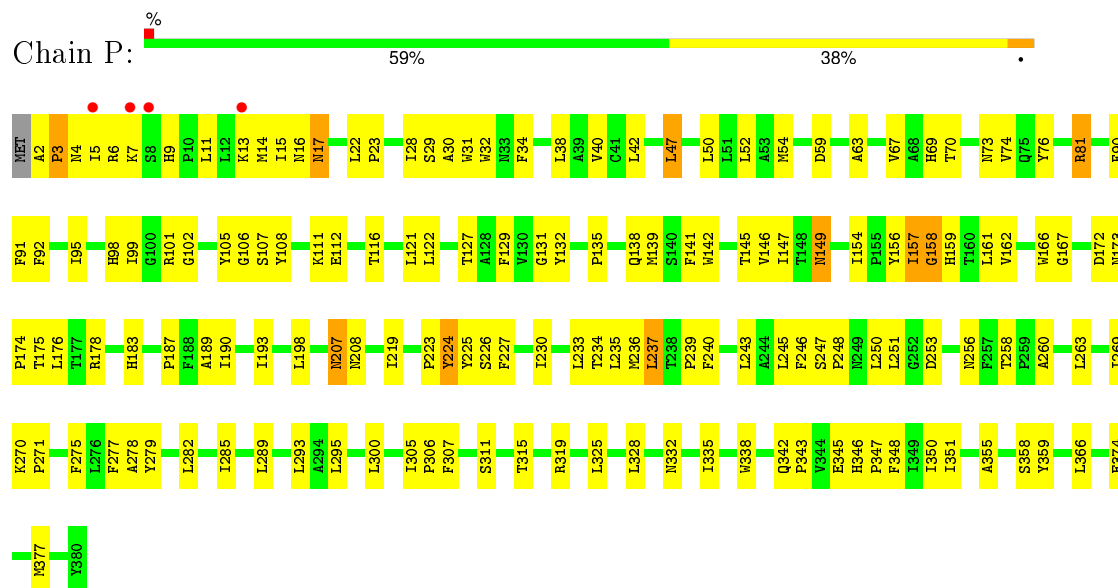




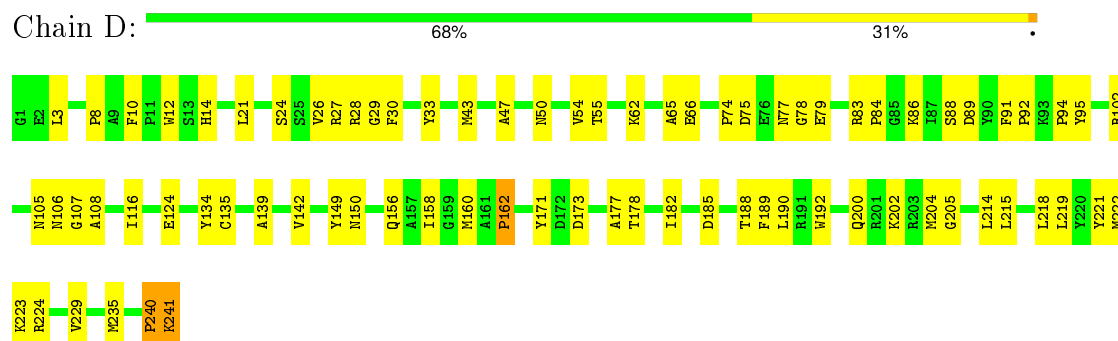
• Molecule 3: Cytochrome b



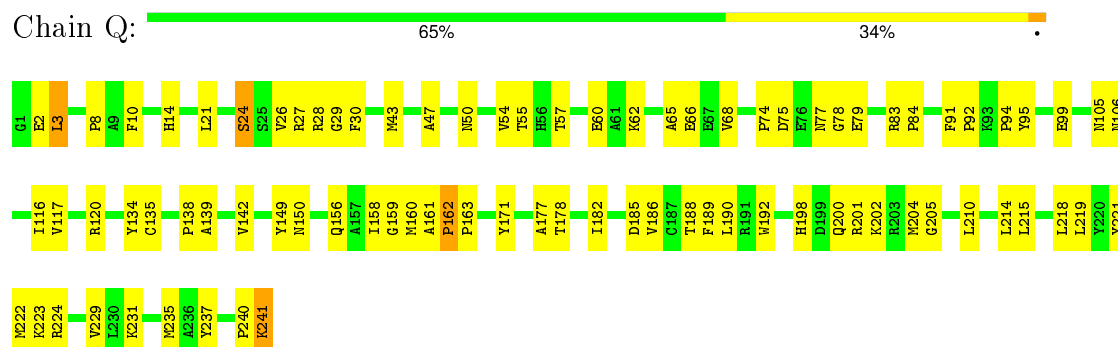
• Molecule 3: Cytochrome b



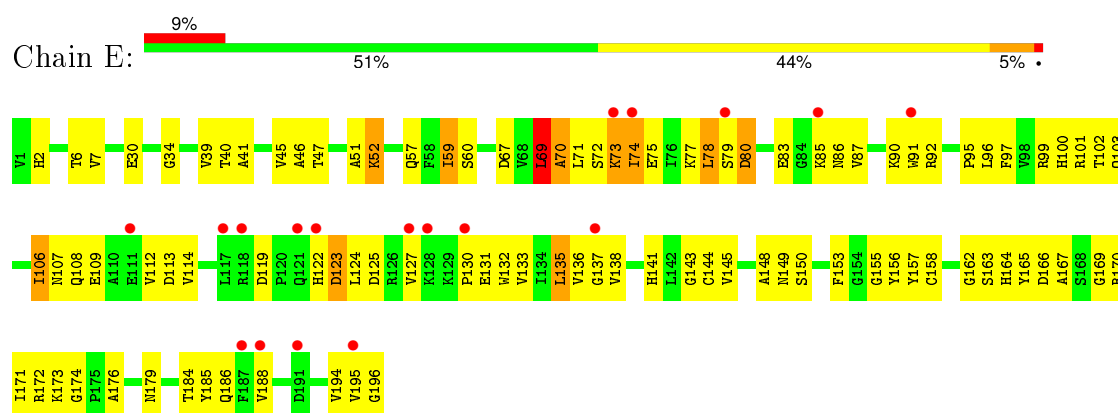
• Molecule 4: MITOCHONDRIAL CYTOCHROME C1, HEME PROTEIN



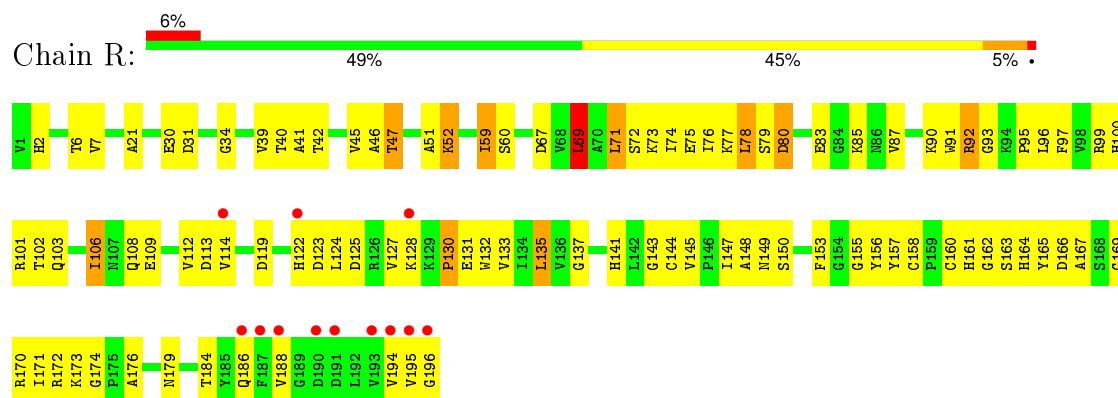
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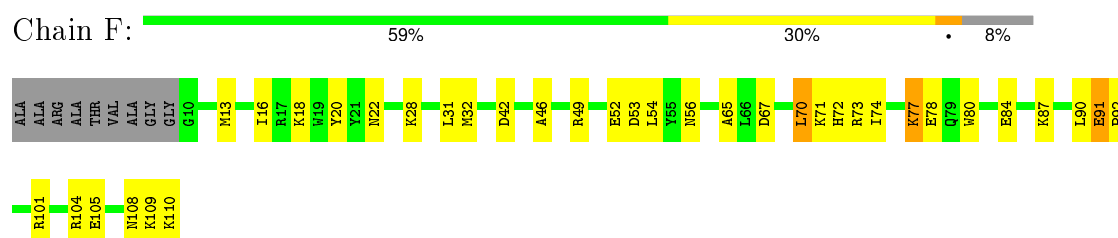
- Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial



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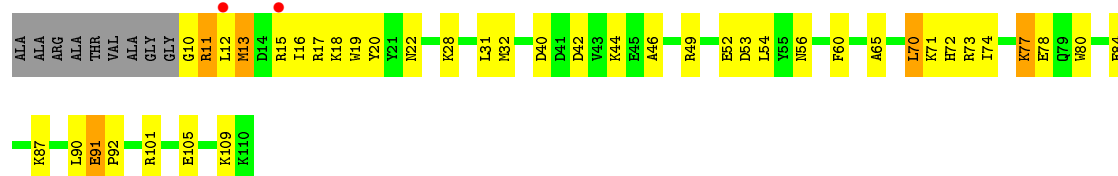


- Molecule 6: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 14 KDA PROTEIN



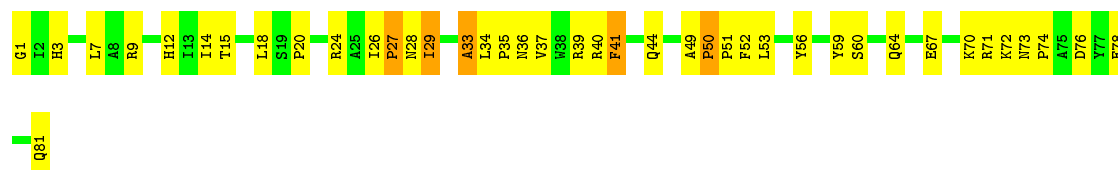
• Molecule 6: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 14 KDA PROTEIN

Chain S: 



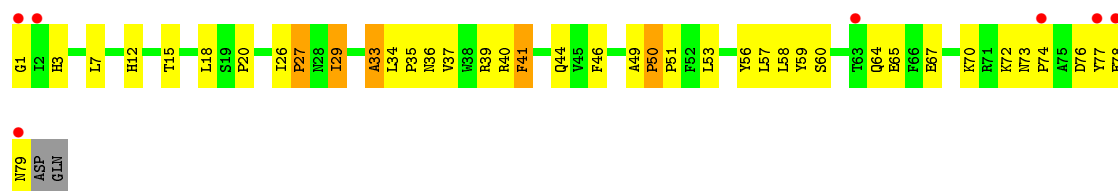
• Molecule 7: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE UBIQUINONE-BINDING PROTEIN QP-C

Chain G: 



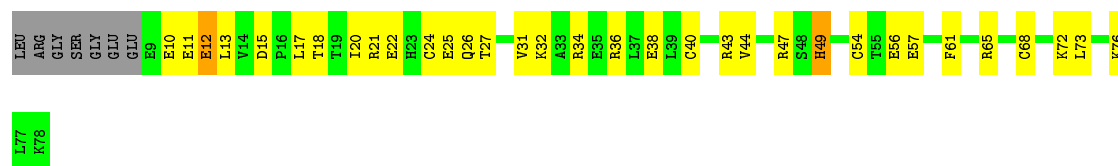
• Molecule 7: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE UBIQUINONE-BINDING PROTEIN QP-C

Chain T: 



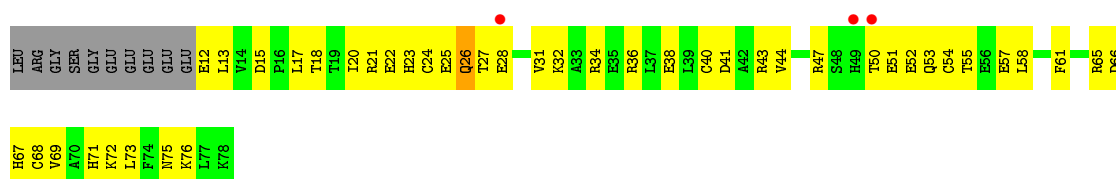
• Molecule 8: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 11 KDA PROTEIN, COMPLEX III SUBUNIT VIII

Chain H: 

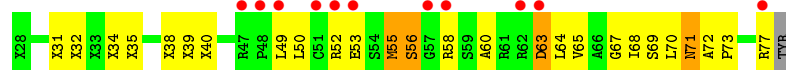


• Molecule 8: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 11 KDA PROTEIN, COMPLEX III SUBUNIT VIII

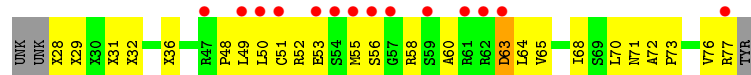
Chain U: 



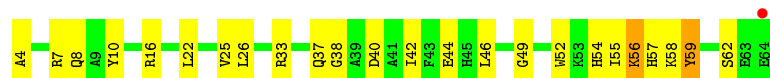
- Molecule 9: Cytochrome b-c1 complex subunit Rieske, mitochondrial



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- Molecule 10: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 7.2 KDA PROTEIN



- Molecule 10: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 7.2 KDA PROTEIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	173.46Å 182.45Å 241.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.68 – 3.00 42.68 – 3.00	Depositor EDS
% Data completeness (in resolution range)	92.8 (42.68-3.00) 92.5 (42.68-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.18	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.32 (at 3.01Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.243 , 0.277 0.236 , 0.270	Depositor DCC
R_{free} test set	2796 reflections (2.01%)	DCC
Wilson B-factor (Å ²)	77.4	Xtriage
Anisotropy	0.418	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 63.2	EDS
Estimated twinning fraction	0.006 for k,h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 141719 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	32679	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.02% 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, 0.375 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: GOL, CDL, UNL, UQ, PLC, FES, HEC, HEM, PEE, 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	0.43	0/3511	0.65	0/4757
1	N	0.43	0/3508	0.65	1/4753 (0.0%)
2	B	0.38	0/3196	0.63	0/4334
2	O	0.40	0/3202	0.63	0/4343
3	C	0.52	0/3122	0.67	0/4273
3	P	0.46	0/3114	0.65	0/4263
4	D	0.45	0/1956	0.64	0/2658
4	Q	0.40	0/1956	0.61	0/2658
5	E	0.37	0/1547	0.64	1/2103 (0.0%)
5	R	0.39	0/1547	0.68	2/2103 (0.1%)
6	F	0.52	0/911	0.71	0/1219
6	S	0.43	0/911	0.63	0/1219
7	G	0.50	0/698	0.68	0/946
7	T	0.44	0/680	0.65	0/923
8	H	0.47	0/582	0.59	0/779
8	U	0.34	0/561	0.57	0/751
9	I	0.40	0/218	0.65	0/293
9	V	0.41	0/218	0.66	0/293
10	J	0.44	0/508	0.63	0/682
10	W	0.41	0/489	0.61	0/658
All	All	0.43	0/32435	0.65	4/44008 (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	P	0	1
4	D	0	1
All	All	0	2

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
5	E	143	GLY	N-CA-C	6.29	128.82	113.10
5	R	143	GLY	N-CA-C	6.28	128.80	113.10
1	N	218	GLY	N-CA-C	-5.19	100.11	113.10
5	R	71	LEU	N-CA-C	5.19	125.02	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	33	TYR	Sidechain
3	P	224	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	3440	0	3353	169	0
1	N	3437	0	3349	192	0
2	B	3141	0	3142	255	0
2	O	3147	0	3146	228	0
3	C	3020	0	3070	136	0
3	P	3012	0	3058	152	0
4	D	1898	0	1846	63	0
4	Q	1898	0	1846	83	0
5	E	1513	0	1478	91	0
5	R	1513	0	1478	93	0
6	F	891	0	893	36	0
6	S	891	0	893	40	0
7	G	676	0	659	46	0
7	T	658	0	647	46	0
8	H	574	0	548	31	0
8	U	553	0	535	46	0
9	I	285	0	237	50	0
9	V	275	0	238	42	0
10	J	497	0	490	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	W	478	0	478	29	0
11	A	1	0	0	0	0
11	C	3	0	0	0	0
11	E	2	0	0	0	0
11	P	3	0	0	0	0
11	R	1	0	0	0	0
12	C	86	0	60	11	0
12	P	86	0	60	11	0
13	C	37	0	42	4	0
13	P	37	0	42	4	0
14	C	19	0	17	5	0
14	P	19	0	17	1	0
15	C	70	0	85	1	0
15	E	50	0	77	4	0
15	N	5	0	0	0	0
15	P	49	0	72	1	0
15	R	50	0	77	4	0
16	C	6	0	8	0	0
16	P	6	0	8	1	0
17	D	43	0	30	1	0
17	Q	43	0	30	1	0
18	D	50	0	44	1	0
18	G	40	0	24	1	0
18	P	40	0	24	3	0
18	S	50	0	44	2	0
19	E	4	0	0	0	0
19	R	4	0	0	1	0
20	E	32	0	38	3	0
20	R	32	0	38	2	0
21	B	1	0	0	0	0
21	C	6	0	0	0	0
21	P	6	0	0	1	0
21	U	1	0	0	1	0
All	All	32679	0	32221	1656	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 26.

The worst 5 of 1656 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:B:353:THR:HG22	2:B:355:GLU:H	1.15	1.08
3:C:17:ASN:HD21	7:G:1:GLY:HA2	0.98	1.07
3:C:328:LEU:HD12	7:G:51:PRO:HB3	1.35	1.06
2:O:353:THR:HG22	2:O:355:GLU:H	1.19	1.06
2:B:203:ARG:HD2	2:B:230:ALA:HA	1.37	1.06

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	441/446 (99%)	393 (89%)	40 (9%)	8 (2%)	11	45
1	N	440/446 (99%)	397 (90%)	36 (8%)	7 (2%)	12	48
2	B	419/441 (95%)	339 (81%)	63 (15%)	17 (4%)	3	20
2	O	420/441 (95%)	336 (80%)	66 (16%)	18 (4%)	3	19
3	C	378/380 (100%)	358 (95%)	18 (5%)	2 (0%)	34	76
3	P	377/380 (99%)	349 (93%)	24 (6%)	4 (1%)	17	58
4	D	239/241 (99%)	217 (91%)	20 (8%)	2 (1%)	24	66
4	Q	239/241 (99%)	214 (90%)	22 (9%)	3 (1%)	15	53
5	E	194/196 (99%)	157 (81%)	24 (12%)	13 (7%)	1	8
5	R	194/196 (99%)	161 (83%)	21 (11%)	12 (6%)	2	10
6	F	99/110 (90%)	94 (95%)	5 (5%)	0	100	100
6	S	99/110 (90%)	93 (94%)	5 (5%)	1 (1%)	19	61
7	G	79/81 (98%)	66 (84%)	9 (11%)	4 (5%)	2	15
7	T	77/81 (95%)	63 (82%)	10 (13%)	4 (5%)	2	15
8	H	68/77 (88%)	57 (84%)	8 (12%)	3 (4%)	3	18
8	U	65/77 (84%)	48 (74%)	16 (25%)	1 (2%)	13	50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	I	29/47 (62%)	19 (66%)	7 (24%)	3 (10%)	1	3
9	V	29/47 (62%)	20 (69%)	7 (24%)	2 (7%)	1	7
10	J	59/61 (97%)	49 (83%)	9 (15%)	1 (2%)	11	46
10	W	57/61 (93%)	45 (79%)	8 (14%)	4 (7%)	1	7
All	All	4002/4160 (96%)	3475 (87%)	418 (10%)	109 (3%)	6	32

5 of 109 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	20	GLY
2	B	26	ILE
2	B	29	LEU
2	B	114	ASP
2	B	171	ALA

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	365/368 (99%)	344 (94%)	21 (6%)	25	63
1	N	365/368 (99%)	344 (94%)	21 (6%)	25	63
2	B	332/347 (96%)	318 (96%)	14 (4%)	36	76
2	O	333/347 (96%)	319 (96%)	14 (4%)	36	76
3	C	329/329 (100%)	323 (98%)	6 (2%)	66	91
3	P	328/329 (100%)	321 (98%)	7 (2%)	61	89
4	D	200/200 (100%)	196 (98%)	4 (2%)	63	89
4	Q	200/200 (100%)	196 (98%)	4 (2%)	63	89
5	E	166/166 (100%)	157 (95%)	9 (5%)	27	66
5	R	166/166 (100%)	157 (95%)	9 (5%)	27	66
6	F	93/96 (97%)	90 (97%)	3 (3%)	46	82
6	S	93/96 (97%)	89 (96%)	4 (4%)	35	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	G	71/71 (100%)	68 (96%)	3 (4%)	36	76
7	T	69/71 (97%)	66 (96%)	3 (4%)	35	75
8	H	65/71 (92%)	63 (97%)	2 (3%)	47	83
8	U	63/71 (89%)	61 (97%)	2 (3%)	46	82
9	I	23/26 (88%)	22 (96%)	1 (4%)	35	75
9	V	23/26 (88%)	22 (96%)	1 (4%)	35	75
10	J	49/49 (100%)	45 (92%)	4 (8%)	14	46
10	W	47/49 (96%)	44 (94%)	3 (6%)	22	59
All	All	3380/3446 (98%)	3245 (96%)	135 (4%)	38	77

5 of 135 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	H	26	GLN
1	N	124	GLU
6	S	77	LYS
9	I	71	ASN
1	N	18	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 101 such sidechains are listed below:

Mol	Chain	Res	Type
7	G	64	GLN
1	N	143	ASN
6	S	56	ASN
7	G	81	GLN
1	N	49	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 36 ligands modelled in this entry, 10 are unknown - leaving 26 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	SMA	C	2001	-	35,38,38	1.91	7 (20%)	40,52,52	1.75	4 (10%)
14	UQ	C	2002	-	19,19,63	2.48	10 (52%)	23,26,79	1.08	3 (13%)
15	PEE	C	2007	-	48,48,50	1.33	7 (14%)	49,53,55	0.96	5 (10%)
15	PEE	C	2008	-	20,20,50	1.71	6 (30%)	21,25,55	0.63	0
16	GOL	C	2011	-	5,5,5	1.24	0	5,5,5	0.60	0
12	HEM	C	501	3	30,50,50	2.58	10 (33%)	24,82,82	2.48	9 (37%)
12	HEM	C	502	3	30,50,50	2.44	8 (26%)	24,82,82	2.11	6 (25%)
18	CDL	D	2003	-	49,49,99	1.11	1 (2%)	51,61,111	1.03	3 (5%)
17	HEC	D	501	4	24,50,50	2.02	6 (25%)	19,82,82	3.36	6 (31%)
15	PEE	E	2005	-	49,49,50	1.39	8 (16%)	50,54,55	0.93	5 (10%)
20	PLC	E	2009	-	31,31,41	1.64	6 (19%)	35,39,49	0.64	1 (2%)
19	FES	E	501	5	0,4,4	0.00	-	0,4,4	0.00	-
18	CDL	G	2004	-	39,39,99	1.31	5 (12%)	41,51,111	1.19	4 (9%)
15	PEE	N	3008	-	4,4,50	3.62	4 (100%)	6,6,55	0.55	0
13	SMA	P	3001	-	35,38,38	2.01	9 (25%)	40,52,52	1.72	4 (10%)
14	UQ	P	3002	-	19,19,63	2.43	9 (47%)	23,26,79	1.10	3 (13%)
18	CDL	P	3004	-	39,39,99	1.22	4 (10%)	41,51,111	1.20	4 (9%)
15	PEE	P	3007	-	48,48,50	1.30	7 (14%)	49,53,55	0.91	4 (8%)
16	GOL	P	3011	-	5,5,5	1.42	1 (20%)	5,5,5	0.71	0
12	HEM	P	501	3	30,50,50	3.00	10 (33%)	24,82,82	2.24	8 (33%)
12	HEM	P	502	3	30,50,50	2.43	8 (26%)	24,82,82	2.12	6 (25%)
17	HEC	Q	501	4	24,50,50	2.18	4 (16%)	19,82,82	3.28	7 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	PEE	R	3005	-	49,49,50	1.41	9 (18%)	50,54,55	0.93	5 (10%)
20	PLC	R	3009	-	31,31,41	1.58	7 (22%)	35,39,49	0.62	1 (2%)
19	FES	R	501	5	0,4,4	0.00	-	0,4,4	0.00	-
18	CDL	S	3003	-	49,49,99	1.10	1 (2%)	51,61,111	1.03	3 (5%)

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
13	SMA	C	2001	-	-	0/33/34/34	0/2/2/2
14	UQ	C	2002	-	-	0/11/35/87	0/1/1/1
15	PEE	C	2007	-	-	0/52/52/54	0/0/0/0
15	PEE	C	2008	-	-	0/24/24/54	0/0/0/0
16	GOL	C	2011	-	-	0/4/4/4	0/0/0/0
12	HEM	C	501	3	-	0/10/54/54	0/0/8/8
12	HEM	C	502	3	-	0/10/54/54	0/0/8/8
18	CDL	D	2003	-	-	0/59/59/110	0/0/0/0
17	HEC	D	501	4	-	0/6/54/54	0/0/8/8
15	PEE	E	2005	-	-	0/53/53/54	0/0/0/0
20	PLC	E	2009	-	-	0/35/35/45	0/0/0/0
19	FES	E	501	5	-	0/0/4/4	0/1/1/1
18	CDL	G	2004	-	-	0/49/49/110	0/0/0/0
15	PEE	N	3008	-	-	0/0/0/54	0/0/0/0
13	SMA	P	3001	-	-	0/33/34/34	0/2/2/2
14	UQ	P	3002	-	-	0/11/35/87	0/1/1/1
18	CDL	P	3004	-	-	0/49/49/110	0/0/0/0
15	PEE	P	3007	-	-	0/52/52/54	0/0/0/0
16	GOL	P	3011	-	-	0/4/4/4	0/0/0/0
12	HEM	P	501	3	-	0/10/54/54	0/0/8/8
12	HEM	P	502	3	-	0/10/54/54	0/0/8/8
17	HEC	Q	501	4	-	0/6/54/54	0/0/8/8
15	PEE	R	3005	-	-	0/53/53/54	0/0/0/0
20	PLC	R	3009	-	-	0/35/35/45	0/0/0/0
19	FES	R	501	5	-	0/0/4/4	0/1/1/1
18	CDL	S	3003	-	-	0/59/59/110	0/0/0/0

The worst 5 of 147 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	Q	501	HEC	C3B-C2B	-7.62	1.32	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	C	502	HEM	C2D-C3D	-6.99	1.33	1.54
12	C	501	HEM	C3B-CAB	-6.97	1.38	1.51
12	P	501	HEM	C3B-CAB	-6.70	1.38	1.51
12	P	501	HEM	C3C-CAC	-6.58	1.39	1.51

The worst 5 of 91 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	D	501	HEC	CBB-CAB-C3B	-9.09	107.14	127.35
17	Q	501	HEC	CBB-CAB-C3B	-8.81	107.77	127.35
17	D	501	HEC	CBC-CAC-C3C	-6.92	111.97	127.35
17	Q	501	HEC	CBC-CAC-C3C	-6.89	112.03	127.35
13	P	3001	SMA	C9-C10-C11	-4.86	109.03	114.75

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

22 monomers are involved in 62 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	C	2001	SMA	4	0
14	C	2002	UQ	5	0
15	C	2007	PEE	1	0
12	C	501	HEM	5	0
12	C	502	HEM	6	0
18	D	2003	CDL	1	0
17	D	501	HEC	1	0
15	E	2005	PEE	4	0
20	E	2009	PLC	3	0
18	G	2004	CDL	1	0
13	P	3001	SMA	4	0
14	P	3002	UQ	1	0
18	P	3004	CDL	3	0
15	P	3007	PEE	1	0
16	P	3011	GOL	1	0
12	P	501	HEM	5	0
12	P	502	HEM	6	0
17	Q	501	HEC	1	0
15	R	3005	PEE	4	0
20	R	3009	PLC	2	0
19	R	501	FES	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	S	3003	CDL	2	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	443/446 (99%)	-0.33	2 (0%) 91 76	44, 77, 105, 114	0
1	N	442/446 (99%)	-0.29	0 100 100	54, 80, 102, 110	0
2	B	421/441 (95%)	-0.24	3 (0%) 89 70	66, 93, 122, 140	0
2	O	422/441 (95%)	-0.27	1 (0%) 95 87	52, 85, 111, 124	0
3	C	380/380 (100%)	-0.48	1 (0%) 94 84	33, 49, 84, 140	0
3	P	379/380 (99%)	-0.29	4 (1%) 82 58	44, 75, 99, 119	0
4	D	241/241 (100%)	-0.50	0 100 100	42, 55, 86, 114	0
4	Q	241/241 (100%)	-0.23	0 100 100	59, 86, 112, 127	0
5	E	196/196 (100%)	0.31	18 (9%) 11 4	48, 114, 165, 172	0
5	R	196/196 (100%)	0.07	12 (6%) 25 9	54, 85, 134, 151	0
6	F	101/110 (91%)	-0.63	0 100 100	37, 53, 67, 99	0
6	S	101/110 (91%)	-0.22	2 (1%) 68 39	64, 84, 112, 141	0
7	G	81/81 (100%)	-0.25	0 100 100	48, 62, 94, 113	0
7	T	79/81 (97%)	0.21	7 (8%) 12 4	69, 95, 147, 164	0
8	H	70/77 (90%)	-0.42	0 100 100	48, 73, 90, 133	0
8	U	67/77 (87%)	0.21	3 (4%) 37 15	102, 125, 148, 154	0
9	I	31/47 (65%)	1.37	11 (35%) 0 0	94, 127, 172, 178	0
9	V	31/47 (65%)	1.65	14 (45%) 0 0	93, 125, 184, 184	0
10	J	61/61 (100%)	-0.41	1 (1%) 74 47	57, 71, 109, 151	0
10	W	59/61 (96%)	0.01	1 (1%) 73 45	69, 85, 101, 117	0
All	All	4042/4160 (97%)	-0.23	80 (1%) 68 39	33, 79, 125, 184	0

The worst 5 of 80 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	T	1	GLY	5.8
8	U	50	THR	5.5
9	V	51	CYS	5.4
7	T	78	GLU	4.9
5	E	187	PHE	4.2

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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(Å ²)	Q<0.9
11	UNL	C	2010	1/-	0.59	1.52	52.71	53,53,53,53	0
11	UNL	R	2103	1/-	0.79	0.62	23.86	45,45,45,45	0
16	GOL	C	2011	6/6	0.84	0.35	7.54	79,81,82,83	0
15	PEE	R	3005	50/51	0.78	0.38	4.79	95,108,116,119	0
15	PEE	E	2005	50/51	0.78	0.34	4.32	76,90,95,95	0
18	CDL	S	3003	50/100	0.75	0.39	4.16	126,140,153,153	0
15	PEE	C	2007	49/51	0.92	0.28	3.92	52,68,87,89	0
20	PLC	E	2009	32/42	0.82	0.32	3.52	67,83,97,98	0
11	UNL	E	3103	1/-	0.65	0.43	3.43	45,45,45,45	0
11	UNL	A	3016	1/-	0.74	0.40	3.29	55,55,55,55	0
15	PEE	P	3007	49/51	0.87	0.34	3.29	73,98,107,108	0
15	PEE	C	2008	21/51	0.76	0.33	3.05	139,142,144,144	0
14	UQ	C	2002	19/63	0.84	0.28	3.00	85,88,90,91	0
16	GOL	P	3011	6/6	0.91	0.27	2.80	69,71,72,72	0
20	PLC	R	3009	32/42	0.82	0.35	2.55	91,99,116,116	0
14	UQ	P	3002	19/63	0.85	0.30	2.26	116,121,122,122	0
18	CDL	G	2004	40/100	0.90	0.26	2.11	81,90,97,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
18	CDL	D	2003	50/100	0.85	0.27	1.59	79,112,130,131	0
13	SMA	P	3001	37/37	0.94	0.23	0.92	67,73,75,78	0
12	HEM	P	501	43/43	0.98	0.21	0.91	56,61,69,75	0
18	CDL	P	3004	40/100	0.85	0.27	0.88	106,114,120,121	0
13	SMA	C	2001	37/37	0.97	0.20	0.79	41,44,46,52	0
12	HEM	C	501	43/43	0.98	0.20	0.71	44,48,50,53	0
12	HEM	P	502	43/43	0.99	0.20	0.16	59,63,71,77	0
12	HEM	C	502	43/43	0.99	0.19	0.02	34,40,50,54	0
19	FES	R	501	4/4	1.00	0.16	0.00	52,54,56,57	0
17	HEC	D	501	43/43	0.98	0.17	-0.29	44,46,50,53	0
17	HEC	Q	501	43/43	0.96	0.19	-0.46	67,71,76,78	0
19	FES	E	501	4/4	0.98	0.15	-1.26	92,93,95,95	0
11	UNL	P	3010	1/-	0.65	0.88	-	67,67,67,67	0
11	UNL	C	2104	1/-	0.67	0.63	-	71,71,71,71	0
15	PEE	N	3008	5/51	0.82	0.34	-	135,135,136,136	0
11	UNL	E	2105	1/-	0.51	0.39	-	62,62,62,62	0
11	UNL	C	3015	1/-	0.72	0.48	-	47,47,47,47	0
11	UNL	P	2015	1/-	0.72	0.39	-	33,33,33,33	0
11	UNL	P	3104	1/-	0.76	0.55	-	59,59,59,59	0

6.5 Other polymers

There are no such residues in this entry.