wwPDB X-ray Structure Validation Summary Report (i)

Feb 19, 2016 – 07:24 PM GMT

PDB ID	:	3X2Q
Title	:	X-ray structure of cyanide-bound bovine heart cytochrome c oxidase in the fully oxidized state at 2.0 angstrom resolution
Authors	:	Yano, N.; Muramoto, K.; Mochizuki, M.; Shinzawa-Itoh, K.; Yamashita, E.; Yoshikawa, S.; Tsukihara, T.
Deposited on	:	2014-12-26
Resolution	:	2.00 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 (i) symbol.

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

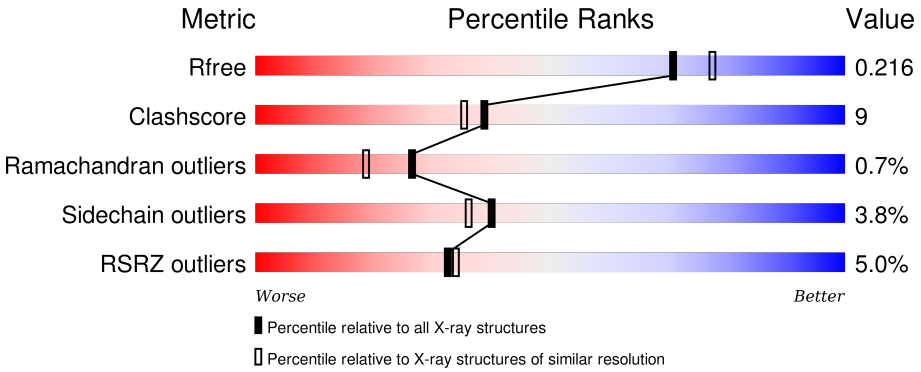
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982

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 2.00 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	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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 <=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	514	81% 18%
1	N	514	84% 14%
2	B	227	78% 19%
2	O	227	80% 18%
3	C	261	83% 16%

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Mol	Chain	Length	Quality of chain
3	P	261	2% 84% 14%
4	D	147	% 79% 16%
4	Q	147	14% 82% 12%
5	E	109	2% 82% 13%
5	R	109	4% 86% 7%
6	F	98	8% 79% 18%
6	S	98	10% 76% 17% 7%
7	G	85	19% 72% 16% 11%
7	T	85	20% 68% 20% 11%
8	H	85	9% 76% 12% 7%
8	U	85	11% 74% 14% 7%
9	I	73	5% 86% 10%
9	V	73	11% 85% 12%
10	J	59	14% 90% 7%
10	W	59	14% 93%
11	K	56	79% 9% 13%
11	X	56	30% 77% 9% 13%
12	L	47	79% 17%
12	Y	47	2% 77% 19%
13	M	46	11% 74% 17% 7%
13	Z	46	17% 78% 15% 7%

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
15	HEA	A	602	X	-	-	-
15	HEA	A	603	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	HEA	N	602	X	-	-	-
15	HEA	N	603	X	-	-	-
17	MG	A	605	-	-	-	X
17	MG	N	605	-	-	-	X
18	NA	A	606	-	-	-	X
18	NA	N	606	-	-	-	X
19	TGL	A	607	-	-	-	X
19	TGL	D	201	-	-	-	X
19	TGL	L	101	-	-	-	X
19	TGL	N	609	-	-	-	X
19	TGL	N	610	-	-	-	X
19	TGL	Q	201	-	-	-	X
20	PGV	A	609	-	-	-	X
20	PGV	C	307	-	-	-	X
20	PGV	N	607	-	-	-	X
20	PGV	P	302	-	-	-	X
22	CHD	C	304	-	-	-	X
24	CDL	C	303	-	-	-	X
24	CDL	G	103	-	-	X	X
24	CDL	P	306	-	-	-	X
24	CDL	T	102	-	-	X	X
25	PEK	G	104	-	-	-	X
25	PEK	T	101	-	-	X	X
26	PSC	E	201	-	-	-	X
26	PSC	O	303	-	-	-	X
28	DMU	G	101	-	-	-	X
28	DMU	P	301	-	-	-	X
28	DMU	Z	101	-	-	-	X

2 Entry composition

There are 29 unique types of molecules in this entry. The entry contains 32060 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 c oxidase subunit 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	514	Total	C	N	O	S	0	3	0
			4051	2708	626	681	36			
1	N	514	Total	C	N	O	S	0	3	0
			4051	2708	626	681	36			

- Molecule 2 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	227	Total	C	N	O	S	0	0	0
			1824	1185	281	340	18			
2	O	227	Total	C	N	O	S	0	0	0
			1824	1185	281	340	18			

- Molecule 3 is a protein called Cytochrome c oxidase subunit 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	259	Total	C	N	O	S	0	3	0
			2134	1427	339	353	15			
3	P	259	Total	C	N	O	S	0	3	0
			2134	1427	339	353	15			

- Molecule 4 is a protein called Cytochrome c oxidase subunit 4 isoform 1, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	144	Total	C	N	O	S	0	0	0
			1195	777	196	218	4			
4	Q	144	Total	C	N	O	S	0	0	0
			1195	777	196	218	4			

- Molecule 5 is a protein called Cytochrome c oxidase subunit 5A, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	105	Total	C	N	O	S	0	0	0
			852	544	144	162	2			
5	R	105	Total	C	N	O	S	0	0	0
			852	544	144	162	2			

- Molecule 6 is a protein called Cytochrome c oxidase subunit 5B, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	98	Total	C	N	O	S	0	0	0
			748	464	134	145	5			
6	S	98	Total	C	N	O	S	0	0	0
			748	464	134	145	5			

- Molecule 7 is a protein called Cytochrome c oxidase subunit 6A2, mitochondrial.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
7	G	84	Total	C	N	O	P	S	0	0	0
			675	431	129	113	1	1			
7	T	84	Total	C	N	O	P	S	0	0	0
			675	431	129	113	1	1			

- Molecule 8 is a protein called Cytochrome c oxidase subunit 6B1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	79	Total	C	N	O	S	0	0	0
			662	417	121	119	5			
8	U	79	Total	C	N	O	S	0	0	0
			662	417	121	119	5			

- Molecule 9 is a protein called Cytochrome c oxidase subunit 6C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	73	Total	C	N	O	S	0	0	0
			601	390	107	100	4			
9	V	73	Total	C	N	O	S	0	0	0
			601	390	107	100	4			

- Molecule 10 is a protein called Cytochrome c oxidase subunit 7A1, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	58	Total	C	N	O	S	0	0	0
			460	297	78	82	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	W	58	Total	C	N	O	S	0	0	0
			460	297	78	82	3			

- Molecule 11 is a protein called Cytochrome c oxidase subunit 7B, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	49	Total	C	N	O	S	0	0	0
			384	250	65	67	2			
11	X	49	Total	C	N	O	S	0	0	0
			384	250	65	67	2			

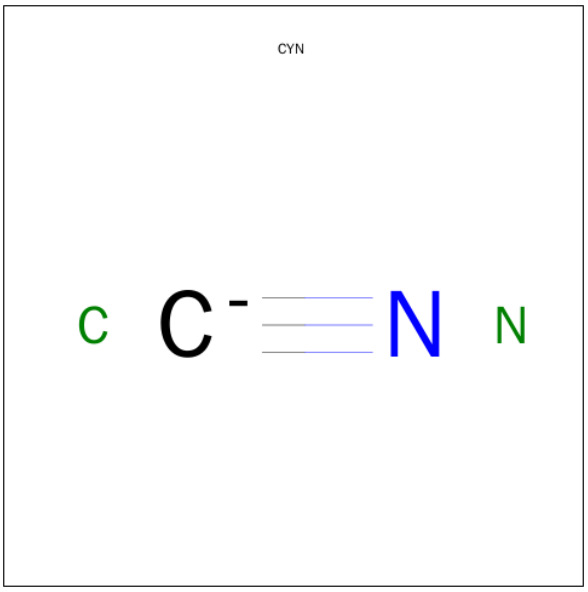
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	46	Total	C	N	O	S	0	0	0
			380	254	64	60	2			
12	Y	46	Total	C	N	O	S	0	0	0
			380	254	64	60	2			

- Molecule 13 is a protein called Cytochrome c oxidase subunit 8B, mitochondrial.

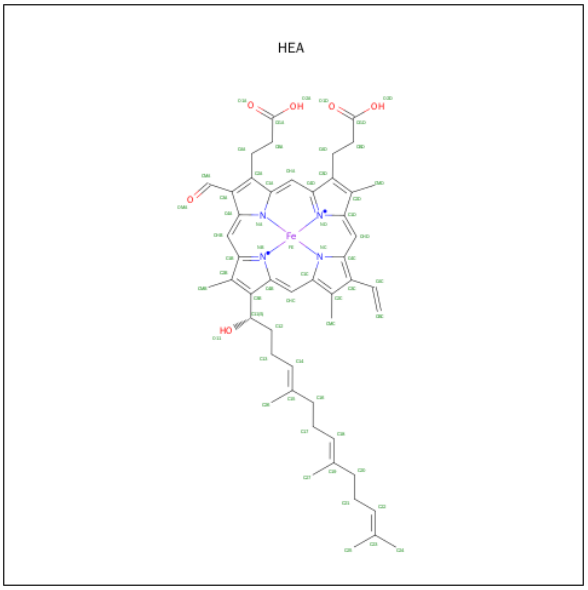
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	M	43	Total	C	N	O	0	0	0
			335	223	53	59			
13	Z	43	Total	C	N	O	0	0	0
			335	223	53	59			

- Molecule 14 is CYANIDE ION (three-letter code: CYN) (formula: CN).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	A	1	Total C N 2 1 1	0	0
14	N	1	Total C N 2 1 1	0	0

- Molecule 15 is HEME-A (three-letter code: HEA) (formula: $C_{49}H_{56}FeN_4O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	A	1	Total C Fe N O 60 49 1 4 6	0	0
15	A	1	Total C Fe N O 60 49 1 4 6	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
15	N	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
15	N	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		

- Molecule 16 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	1	Total	Cu	0	0
			1	1		
16	N	1	Total	Cu	0	0
			1	1		

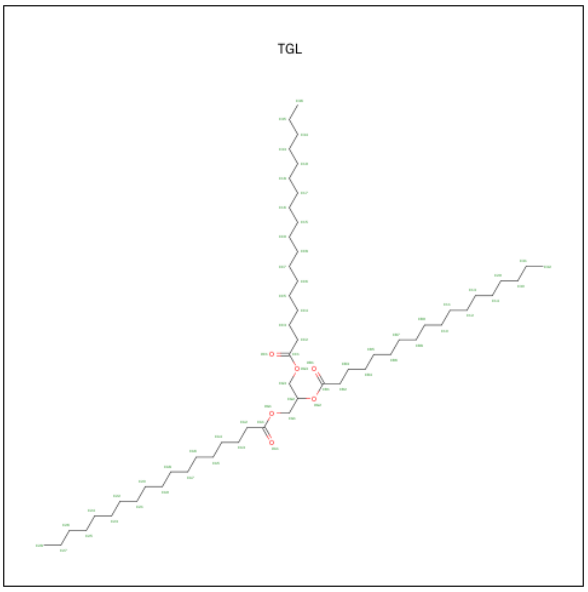
- Molecule 17 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	1	Total	Mg	0	0
			1	1		
17	N	1	Total	Mg	0	0
			1	1		

- Molecule 18 is SODIUM ION (three-letter code: NA) (formula: Na).

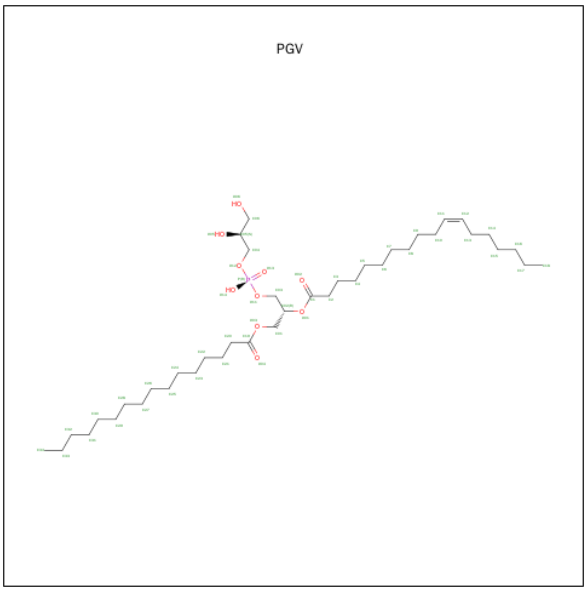
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	A	1	Total	Na	0	0
			1	1		
18	N	1	Total	Na	0	0
			1	1		

- Molecule 19 is TRISTEAROYLGLYCEROL (three-letter code: TGL) (formula: $C_{57}H_{110}O_6$).



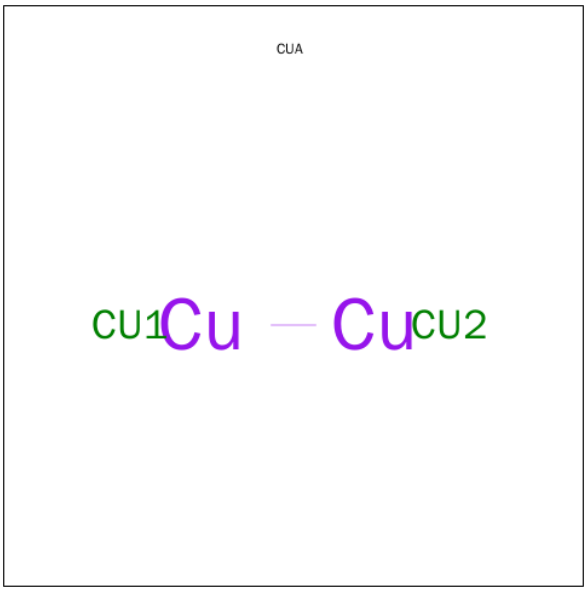
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	A	1	Total C O 63 57 6	0	0
19	D	1	Total C O 63 57 6	0	0
19	L	1	Total C O 63 57 6	0	0
19	N	1	Total C O 63 57 6	0	0
19	N	1	Total C O 63 57 6	0	0
19	Q	1	Total C O 63 57 6	0	0

- Molecule 20 is (1R)-2-{[{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (three-letter code: PGV) (formula: $C_{40}H_{77}O_{10}P$).



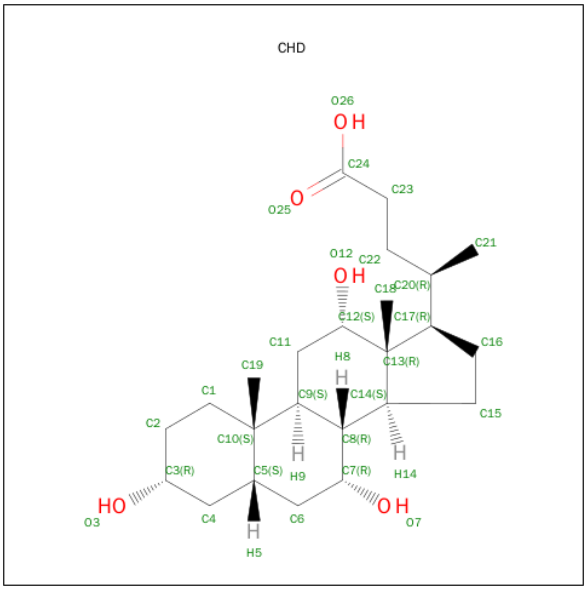
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
20	A	1	Total	C	O	P	0	0
			51	40	10	1		
20	A	1	Total	C	O	P	0	0
			51	40	10	1		
20	C	1	Total	C	O	P	0	0
			51	40	10	1		
20	C	1	Total	C	O	P	0	0
			51	40	10	1		
20	N	1	Total	C	O	P	0	0
			51	40	10	1		
20	N	1	Total	C	O	P	0	0
			51	40	10	1		
20	P	1	Total	C	O	P	0	0
			51	40	10	1		
20	P	1	Total	C	O	P	0	0
			51	40	10	1		

- Molecule 21 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu_2).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	B	1	Total Cu 2 2	0	0
21	O	1	Total Cu 2 2	0	0

- Molecule 22 is CHOLIC ACID (three-letter code: CHD) (formula: $C_{24}H_{40}O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	B	1	Total C O 29 24 5	0	0
22	C	1	Total C O 29 24 5	0	0

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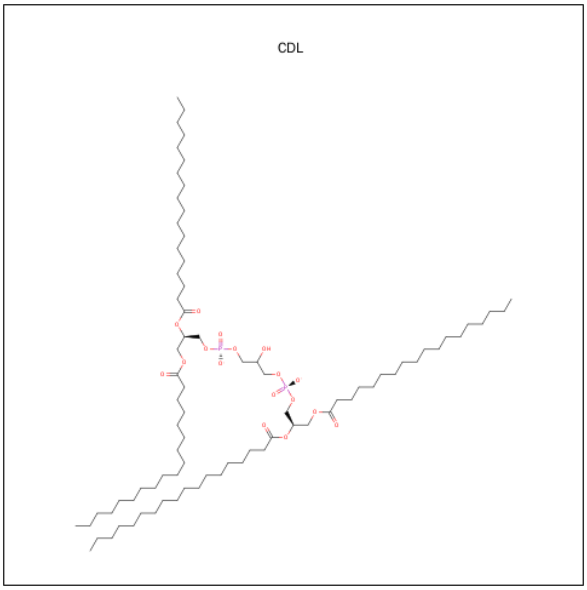
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	C	1	Total C O 29 24 5	0	0
22	O	1	Total C O 29 24 5	0	0
22	P	1	Total C O 29 24 5	0	0
22	P	1	Total C O 29 24 5	0	0

- Molecule 23 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	P	1	Total X 1 1	0	0
23	C	1	Total X 1 1	0	0

- Molecule 24 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	C	1	Total C O P 100 81 17 2	0	0
24	G	1	Total C O P 100 81 17 2	0	0
24	P	1	Total C O P 100 81 17 2	0	0

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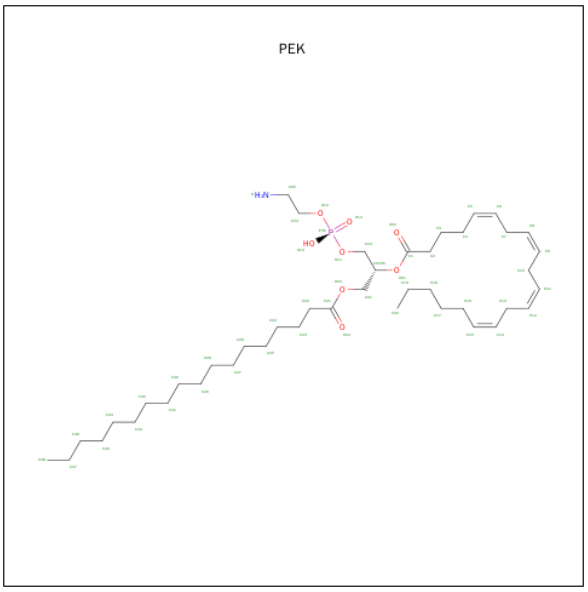
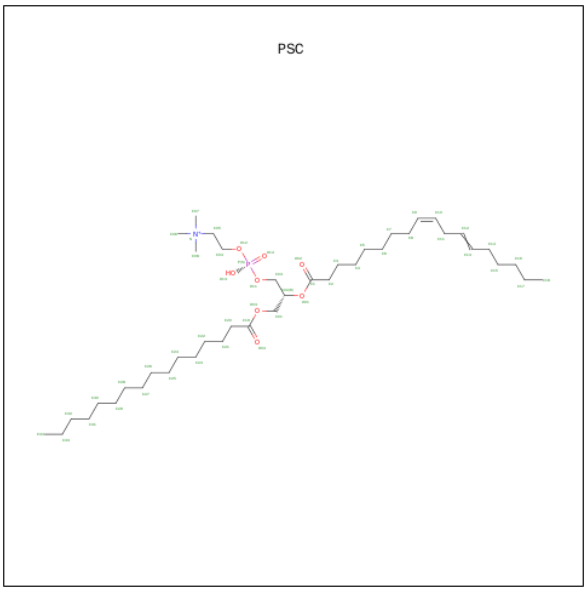
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
24	T	1	Total	C	O	P	0	0
			100	81	17	2		

- Molecule 25 is (1S)-2-{[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(STEAROYLOXY)METHYL]ETHYL (5E,8E,11E,14E)-ICOSA-5,8,11,14-TETRAENOATE (three-letter code: PEK) (formula: $C_{43}H_{78}NO_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	G	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	G	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	P	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	P	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	T	1	Total	C	N	O	P	0	0
			53	43	1	8	1		

- Molecule 26 is (7R,17E,20E)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSA-17,20-DIEN-1-AMINIUM 4-OXIDE (three-letter code: PSC) (formula: $C_{42}H_{81}NO_8P$).

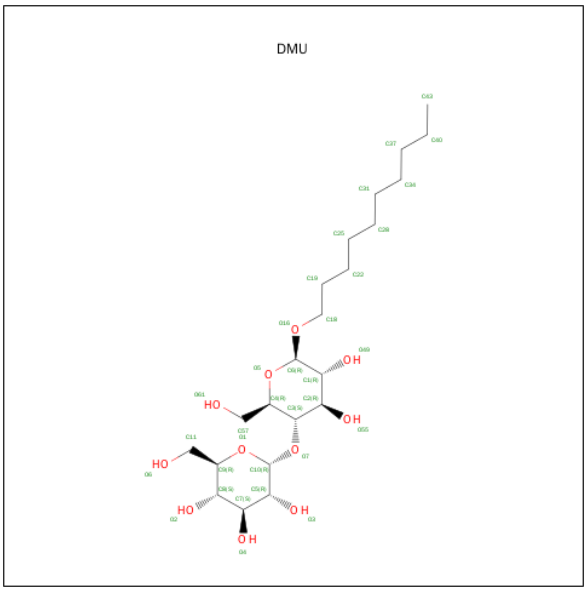


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
26	E	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
26	O	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

- Molecule 27 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
27	S	1	Total	Zn	0	0
			1	1		
27	F	1	Total	Zn	0	0
			1	1		

- Molecule 28 is SUGAR (DECYL-BETA-D-MALTOPYRANOSIDE) (three-letter code: DMU) (formula: $C_{22}H_{42}O_{11}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	G	1	Total C O 33 22 11	0	0
28	M	1	Total C O 33 22 11	0	0
28	P	1	Total C O 33 22 11	0	0
28	Z	1	Total C O 33 22 11	0	0

- Molecule 29 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	A	188	Total O 188 188	0	0
29	B	121	Total O 121 121	0	0
29	C	77	Total O 77 77	0	0
29	D	78	Total O 78 78	0	0
29	E	58	Total O 58 58	0	0
29	F	58	Total O 58 58	0	0
29	G	27	Total O 27 27	0	0
29	H	34	Total O 34 34	0	0

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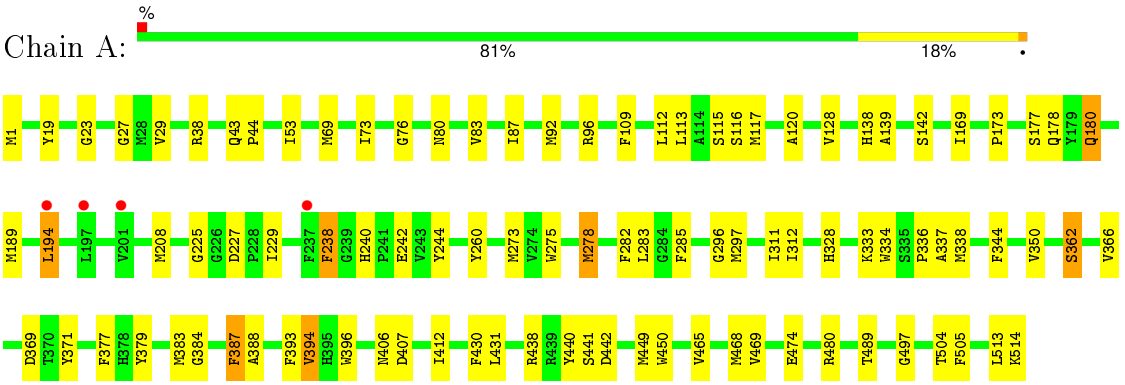
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	I	29	Total O 29 29	0	0
29	J	15	Total O 15 15	0	0
29	K	20	Total O 20 20	0	0
29	L	16	Total O 16 16	0	0
29	M	14	Total O 14 14	0	0
29	N	156	Total O 156 156	0	0
29	O	91	Total O 91 91	0	0
29	P	76	Total O 76 76	0	0
29	Q	46	Total O 46 46	0	0
29	R	42	Total O 42 42	0	0
29	S	38	Total O 38 38	0	0
29	T	23	Total O 23 23	0	0
29	U	28	Total O 28 28	0	0
29	V	14	Total O 14 14	0	0
29	W	4	Total O 4 4	0	0
29	X	15	Total O 15 15	0	0
29	Y	11	Total O 11 11	0	0
29	Z	7	Total O 7 7	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.

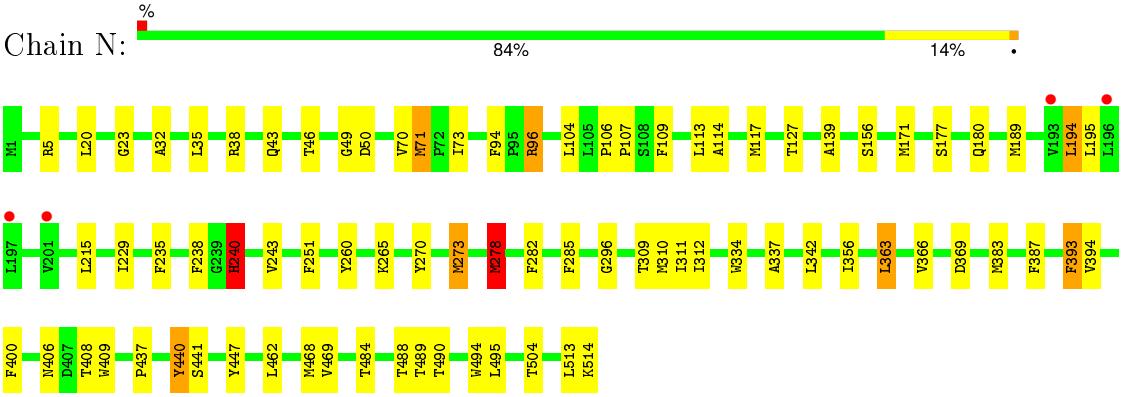
- Molecule 1: Cytochrome c oxidase subunit 1

Chain A:



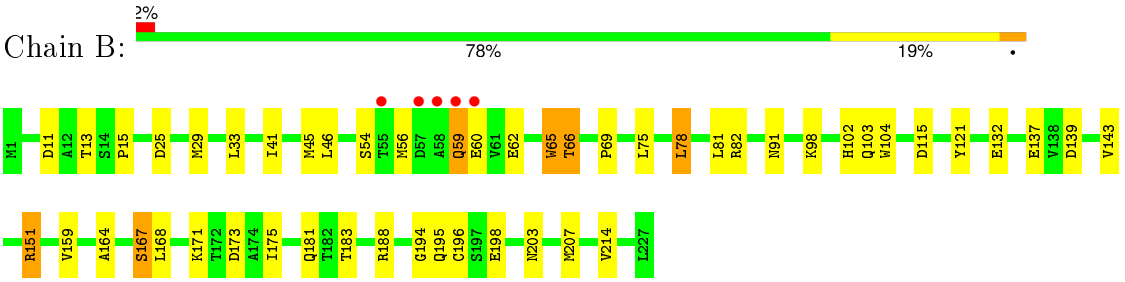
- Molecule 1: Cytochrome c oxidase subunit 1

Chain N:



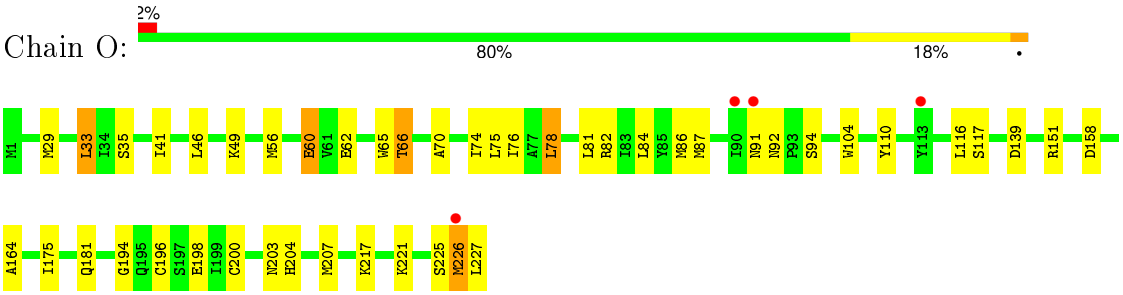
- Molecule 2: Cytochrome c oxidase subunit 2

Chain B:



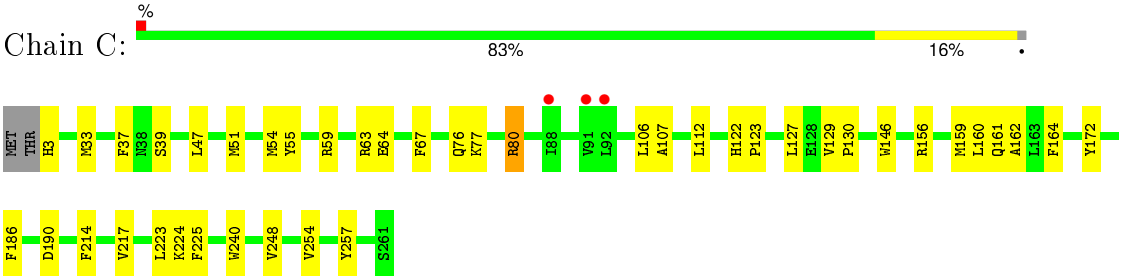
- Molecule 2: Cytochrome c oxidase subunit 2

Chain O:



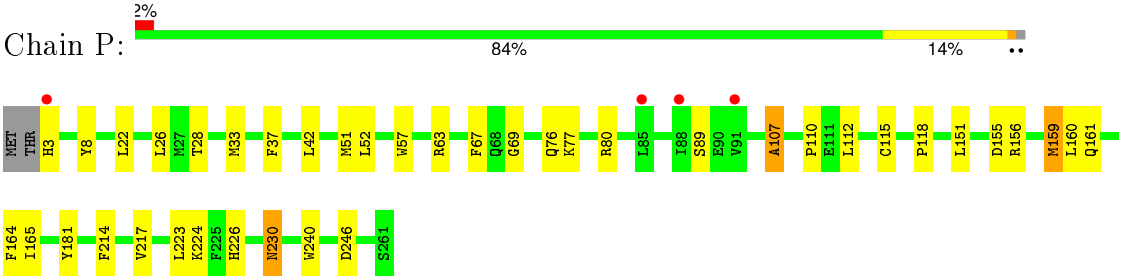
• Molecule 3: Cytochrome c oxidase subunit 3

Chain C:



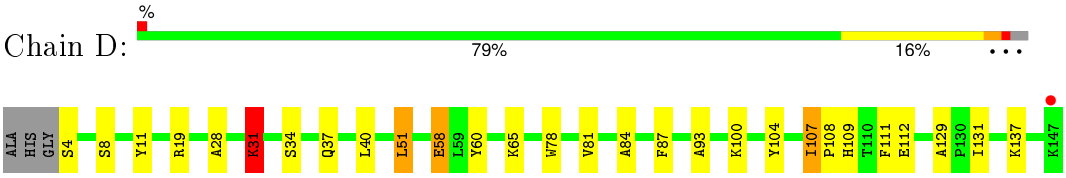
• Molecule 3: Cytochrome c oxidase subunit 3

Chain P:



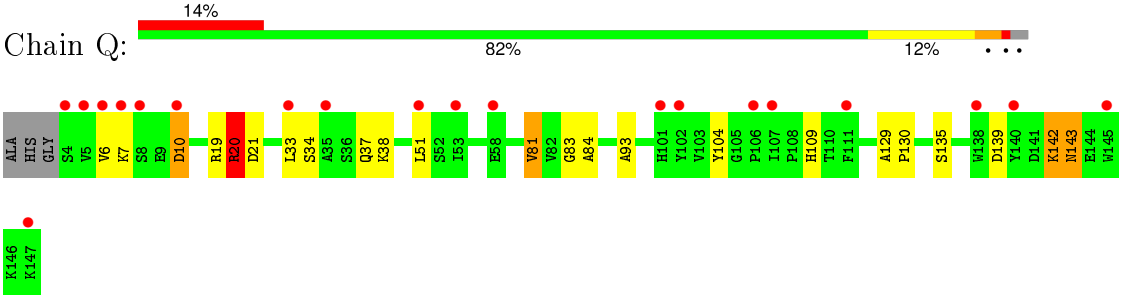
• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

Chain D:



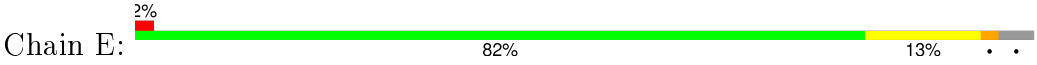
• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

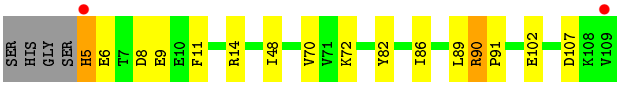
Chain Q:



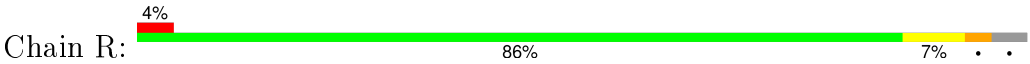
• Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial

Chain E:

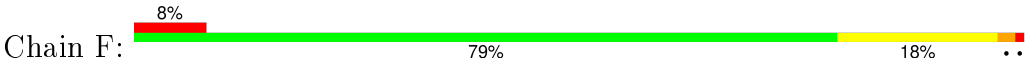


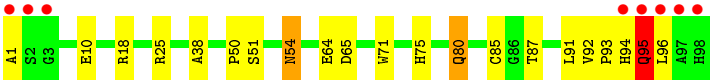


• Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial

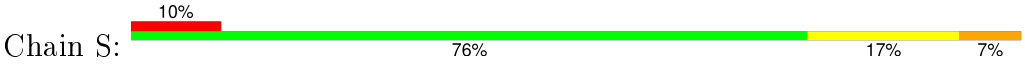


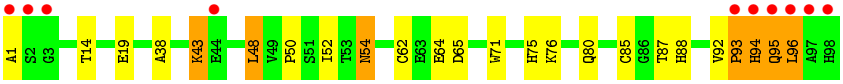
• Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



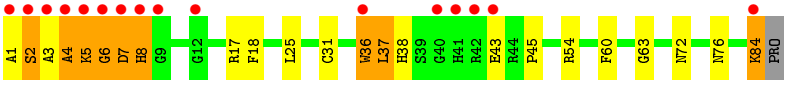


• Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial

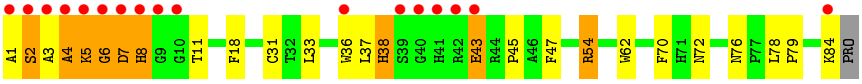




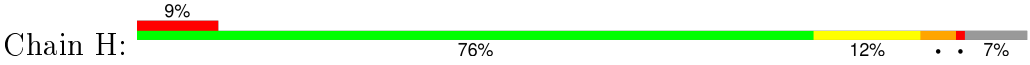
• Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial

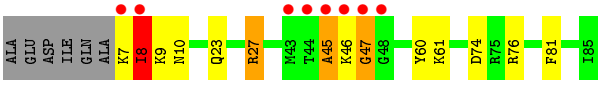


• Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial

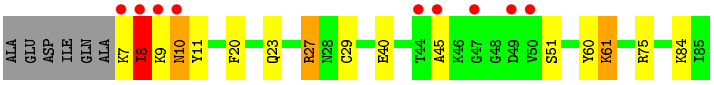


• Molecule 8: Cytochrome c oxidase subunit 6B1

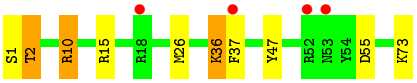




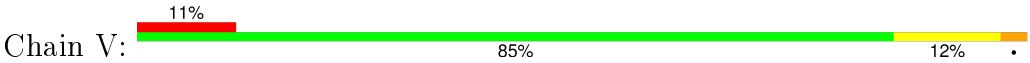
• Molecule 8: Cytochrome c oxidase subunit 6B1

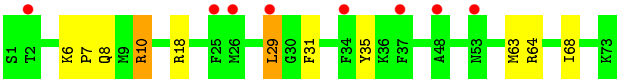


• Molecule 9: Cytochrome c oxidase subunit 6C

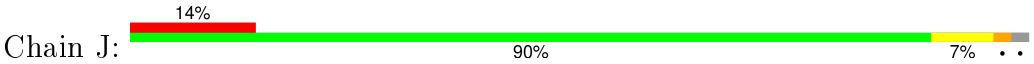


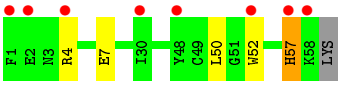
• Molecule 9: Cytochrome c oxidase subunit 6C



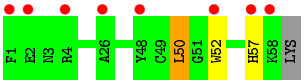


• Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial

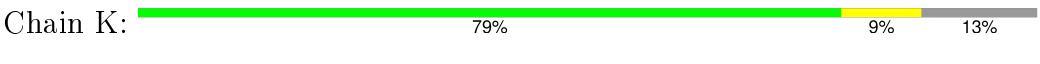


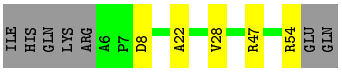


• Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial

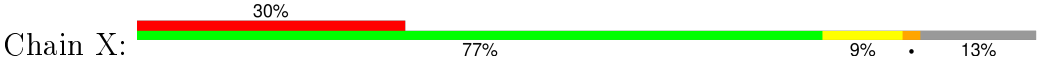


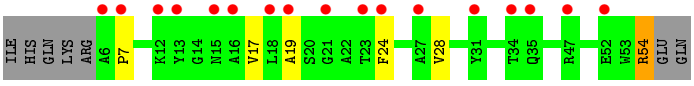
• Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial



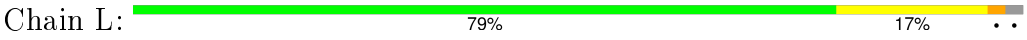


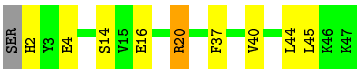
• Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial



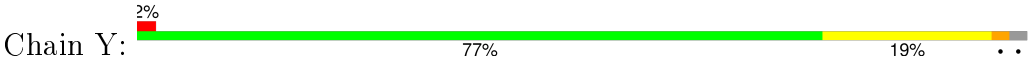


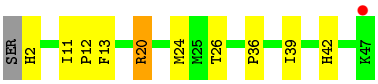
• Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial



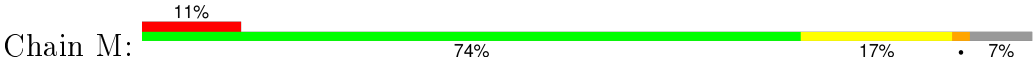


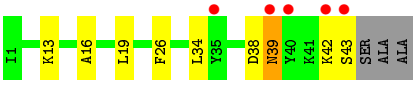
• Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial



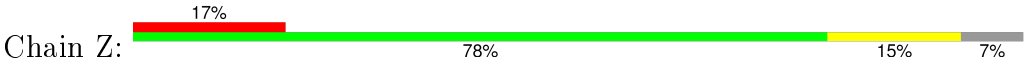


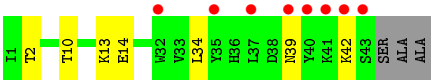
• Molecule 13: Cytochrome c oxidase subunit 8B, mitochondrial





• Molecule 13: Cytochrome c oxidase subunit 8B, mitochondrial





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	183.68Å 206.68Å 178.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.00 81.64 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (40.00-2.00) 99.9 (81.64-2.00)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.85 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.187 , 0.214 0.188 , 0.216	Depositor DCC
R_{free} test set	22863 reflections (5.33%)	DCC
Wilson B-factor (Å^2)	31.7	Xtriage
Anisotropy	0.465	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 58.5	EDS
Estimated twinning fraction	0.004 for l,-k,h	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	1 of 451733 reflections (0.000%)	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	32060	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.61% 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: ZN, CHD, HEA, SAC, CDL, PSC, PEK, MG, TGL, PGV, TPO, UNX, CUA, NA, FME, CYN, CU, DMU

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	1.51	29/4180 (0.7%)	1.15	18/5710 (0.3%)
1	N	1.34	15/4180 (0.4%)	0.99	10/5710 (0.2%)
2	B	1.45	11/1860 (0.6%)	1.16	13/2534 (0.5%)
2	O	1.14	3/1860 (0.2%)	1.01	3/2534 (0.1%)
3	C	1.35	5/2221 (0.2%)	0.96	1/3035 (0.0%)
3	P	1.31	6/2221 (0.3%)	0.93	2/3035 (0.1%)
4	D	1.48	10/1229 (0.8%)	1.14	6/1658 (0.4%)
4	Q	1.03	1/1229 (0.1%)	0.92	3/1658 (0.2%)
5	E	1.27	3/871 (0.3%)	1.11	3/1182 (0.3%)
5	R	1.15	3/871 (0.3%)	0.97	2/1182 (0.2%)
6	F	1.31	0/765	1.08	2/1038 (0.2%)
6	S	1.20	0/765	1.02	0/1038
7	G	1.33	3/690 (0.4%)	1.01	4/937 (0.4%)
7	T	1.31	4/690 (0.6%)	1.07	2/937 (0.2%)
8	H	1.26	1/682 (0.1%)	1.01	3/921 (0.3%)
8	U	1.04	0/682	0.91	1/921 (0.1%)
9	I	1.36	0/605	1.11	2/802 (0.2%)
9	V	1.09	0/605	1.06	3/802 (0.4%)
10	J	1.21	0/471	0.94	0/636
10	W	1.07	0/471	0.92	0/636
11	K	1.38	1/398 (0.3%)	1.11	2/546 (0.4%)
11	X	1.07	1/398 (0.3%)	0.85	0/546
12	L	1.38	3/393 (0.8%)	1.02	1/526 (0.2%)
12	Y	1.16	0/393	0.82	0/526
13	M	1.38	2/345 (0.6%)	1.04	0/470
13	Z	1.05	0/345	0.87	0/470
All	All	1.32	101/29420 (0.3%)	1.03	81/39990 (0.2%)

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
1	N	0	1
6	F	0	1
6	S	0	1
10	J	0	1
10	W	0	1
All	All	0	6

The worst 5 of 101 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	R	80	GLU	CG-CD	9.50	1.66	1.51
2	B	167	SER	CB-OG	-8.83	1.30	1.42
1	A	371	TYR	CD1-CE1	8.27	1.51	1.39
7	T	36	TRP	CB-CG	8.23	1.65	1.50
5	R	80	GLU	CB-CG	8.14	1.67	1.52

The worst 5 of 81 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	69	MET	CG-SD-CE	-19.27	69.37	100.20
4	D	19	ARG	NE-CZ-NH1	-13.36	113.62	120.30
1	A	96	ARG	NE-CZ-NH2	-11.58	114.51	120.30
4	Q	20	ARG	NE-CZ-NH2	-10.39	115.10	120.30
1	A	278	MET	CG-SD-CE	-9.12	85.61	100.20

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	240	HIS	Sidechain
6	F	93	PRO	Peptide
10	J	57	HIS	Peptide
1	N	240	HIS	Sidechain
6	S	93	PRO	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	4051	0	4029	55	0
1	N	4051	0	4029	56	0
2	B	1824	0	1833	26	0
2	O	1824	0	1833	31	0
3	C	2134	0	2051	31	0
3	P	2134	0	2051	36	0
4	D	1195	0	1183	15	0
4	Q	1195	0	1183	20	0
5	E	852	0	845	11	0
5	R	852	0	845	8	0
6	F	748	0	728	16	0
6	S	748	0	728	29	0
7	G	675	0	643	27	0
7	T	675	0	643	45	0
8	H	662	0	623	7	0
8	U	662	0	623	12	0
9	I	601	0	613	12	0
9	V	601	0	613	10	0
10	J	460	0	459	4	0
10	W	460	0	459	2	0
11	K	384	0	366	2	0
11	X	384	0	366	4	0
12	L	380	0	380	10	0
12	Y	380	0	380	15	0
13	M	335	0	352	2	0
13	Z	335	0	352	2	0
14	A	2	0	0	0	0
14	N	2	0	0	0	0
15	A	120	0	108	9	0
15	N	120	0	108	8	0
16	A	1	0	0	0	0
16	N	1	0	0	0	0
17	A	1	0	0	0	0
17	N	1	0	0	0	0
18	A	1	0	0	1	0
18	N	1	0	0	0	0
19	A	63	0	110	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	D	63	0	110	12	0
19	L	63	0	110	14	0
19	N	126	0	220	22	0
19	Q	63	0	110	2	0
20	A	102	0	152	8	0
20	C	102	0	152	5	0
20	N	102	0	152	10	0
20	P	102	0	152	5	0
21	B	2	0	0	0	0
21	O	2	0	0	0	0
22	B	29	0	39	2	0
22	C	58	0	78	6	0
22	O	29	0	39	1	0
22	P	58	0	78	8	0
23	C	1	0	0	0	0
23	P	1	0	0	0	0
24	C	100	0	156	17	0
24	G	100	0	156	26	0
24	P	100	0	156	20	0
24	T	100	0	156	27	0
25	C	53	0	77	6	0
25	G	106	0	154	13	0
25	P	106	0	154	13	0
25	T	53	0	77	22	0
26	E	52	0	80	16	0
26	O	52	0	80	17	0
27	F	1	0	0	0	0
27	S	1	0	0	0	0
28	G	33	0	41	4	0
28	M	33	0	42	0	0
28	P	33	0	42	3	0
28	Z	33	0	42	0	0
29	A	188	0	0	10	0
29	B	121	0	0	3	0
29	C	77	0	0	1	0
29	D	78	0	0	4	0
29	E	58	0	0	2	0
29	F	58	0	0	4	0
29	G	27	0	0	3	0
29	H	34	0	0	0	0
29	I	29	0	0	4	0
29	J	15	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	K	20	0	0	1	0
29	L	16	0	0	2	0
29	M	14	0	0	0	0
29	N	156	0	0	3	0
29	O	91	0	0	3	0
29	P	76	0	0	9	0
29	Q	46	0	0	4	0
29	R	42	0	0	1	0
29	S	38	0	0	3	0
29	T	23	0	0	2	0
29	U	28	0	0	3	0
29	V	14	0	0	0	0
29	W	4	0	0	0	0
29	X	15	0	0	1	0
29	Y	11	0	0	0	0
29	Z	7	0	0	0	0
All	All	32060	0	31341	561	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 9.

The worst 5 of 561 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)
25:P:309:PEK:H383	24:T:102:CDL:C27	1.43	1.46
1:A:297:MET:SD	1:A:297:MET:CE	2.04	1.45
25:C:306:PEK:H383	24:G:103:CDL:C27	1.49	1.38
1:A:312[A]:ILE:HD12	29:A:740:HOH:O	1.21	1.31
6:S:43:LYS:CD	6:S:43:LYS:H	1.43	1.26

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	515/514 (100%)	502 (98%)	12 (2%)	1 (0%)	52	48
1	N	515/514 (100%)	501 (97%)	14 (3%)	0	100	100
2	B	225/227 (99%)	216 (96%)	9 (4%)	0	100	100
2	O	225/227 (99%)	218 (97%)	6 (3%)	1 (0%)	39	33
3	C	260/261 (100%)	256 (98%)	4 (2%)	0	100	100
3	P	260/261 (100%)	255 (98%)	5 (2%)	0	100	100
4	D	142/147 (97%)	138 (97%)	4 (3%)	0	100	100
4	Q	142/147 (97%)	132 (93%)	10 (7%)	0	100	100
5	E	103/109 (94%)	102 (99%)	1 (1%)	0	100	100
5	R	103/109 (94%)	103 (100%)	0	0	100	100
6	F	96/98 (98%)	90 (94%)	4 (4%)	2 (2%)	9	3
6	S	96/98 (98%)	91 (95%)	2 (2%)	3 (3%)	5	1
7	G	81/85 (95%)	70 (86%)	6 (7%)	5 (6%)	2	0
7	T	81/85 (95%)	66 (82%)	10 (12%)	5 (6%)	2	0
8	H	77/85 (91%)	70 (91%)	3 (4%)	4 (5%)	2	0
8	U	77/85 (91%)	71 (92%)	2 (3%)	4 (5%)	2	0
9	I	71/73 (97%)	70 (99%)	1 (1%)	0	100	100
9	V	71/73 (97%)	69 (97%)	2 (3%)	0	100	100
10	J	56/59 (95%)	56 (100%)	0	0	100	100
10	W	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
11	K	47/56 (84%)	46 (98%)	1 (2%)	0	100	100
11	X	47/56 (84%)	46 (98%)	1 (2%)	0	100	100
12	L	44/47 (94%)	42 (96%)	2 (4%)	0	100	100
12	Y	44/47 (94%)	42 (96%)	2 (4%)	0	100	100
13	M	41/46 (89%)	41 (100%)	0	0	100	100
13	Z	41/46 (89%)	38 (93%)	3 (7%)	0	100	100
All	All	3516/3614 (97%)	3386 (96%)	105 (3%)	25 (1%)	26	19

5 of 25 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	94	HIS
7	G	4	ALA
7	G	7	ASP
8	H	8	ILE
8	H	45	ALA

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	429/426 (101%)	418 (97%)	11 (3%)	54	54
1	N	429/426 (101%)	421 (98%)	8 (2%)	65	67
2	B	210/210 (100%)	198 (94%)	12 (6%)	25	19
2	O	210/210 (100%)	200 (95%)	10 (5%)	31	26
3	C	227/226 (100%)	224 (99%)	3 (1%)	76	79
3	P	227/226 (100%)	223 (98%)	4 (2%)	66	69
4	D	128/129 (99%)	123 (96%)	5 (4%)	39	35
4	Q	128/129 (99%)	122 (95%)	6 (5%)	32	27
5	E	92/95 (97%)	91 (99%)	1 (1%)	80	83
5	R	92/95 (97%)	88 (96%)	4 (4%)	35	30
6	F	81/81 (100%)	77 (95%)	4 (5%)	31	25
6	S	81/81 (100%)	77 (95%)	4 (5%)	31	25
7	G	67/68 (98%)	61 (91%)	6 (9%)	12	7
7	T	67/68 (98%)	61 (91%)	6 (9%)	12	7
8	H	71/75 (95%)	67 (94%)	4 (6%)	26	20
8	U	71/75 (95%)	64 (90%)	7 (10%)	10	5
9	I	57/57 (100%)	54 (95%)	3 (5%)	28	22
9	V	57/57 (100%)	55 (96%)	2 (4%)	43	40
10	J	49/50 (98%)	48 (98%)	1 (2%)	63	65
10	W	49/50 (98%)	48 (98%)	1 (2%)	63	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
11	K	39/46 (85%)	38 (97%)	1 (3%)	54 54
11	X	39/46 (85%)	37 (95%)	2 (5%)	29 23
12	L	39/40 (98%)	39 (100%)	0	100 100
12	Y	39/40 (98%)	36 (92%)	3 (8%)	16 10
13	M	37/38 (97%)	32 (86%)	5 (14%)	5 2
13	Z	37/38 (97%)	33 (89%)	4 (11%)	8 4
All	All	3052/3082 (99%)	2935 (96%)	117 (4%)	40 36

5 of 117 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	M	34	LEU
2	O	60	GLU
11	X	7	PRO
13	M	39	ASN
1	N	238	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 41 such sidechains are listed below:

Mol	Chain	Res	Type
7	G	76	ASN
1	N	178	GLN
6	S	94	HIS
10	J	29	ASN
10	J	57	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

8 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	FME	A	1	1	8,9,10	1.18	1 (12%)	5,9,11	2.39	3 (60%)
2	FME	B	1	2	8,9,10	2.14	2 (25%)	5,9,11	5.84	3 (60%)
7	TPO	G	11	7	7,10,11	1.78	2 (28%)	10,14,16	1.58	2 (20%)
9	SAC	I	1	9	7,8,9	3.25	2 (28%)	7,9,11	3.70	4 (57%)
1	FME	N	1	1	8,9,10	1.55	1 (12%)	5,9,11	3.56	3 (60%)
2	FME	O	1	2	8,9,10	0.97	0	5,9,11	2.60	2 (40%)
7	TPO	T	11	7	7,10,11	2.00	3 (42%)	10,14,16	1.86	2 (20%)
9	SAC	V	1	9	7,8,9	2.33	2 (28%)	7,9,11	2.18	4 (57%)

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
1	FME	A	1	1	-	1/6/9/11	0/0/0/0
2	FME	B	1	2	-	1/6/9/11	0/0/0/0
7	TPO	G	11	7	-	0/8/11/13	0/0/0/0
9	SAC	I	1	9	-	0/6/8/10	0/0/0/0
1	FME	N	1	1	-	1/6/9/11	0/0/0/0
2	FME	O	1	2	-	1/6/9/11	0/0/0/0
7	TPO	T	11	7	-	0/8/11/13	0/0/0/0
9	SAC	V	1	9	-	0/6/8/10	0/0/0/0

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	FME	O1-CN	-2.43	1.14	1.22
1	A	1	FME	O1-CN	-2.24	1.15	1.22
7	T	11	TPO	CB-CA	2.04	1.57	1.54
7	G	11	TPO	P-O2P	2.08	1.61	1.54
7	T	11	TPO	P-O3P	2.16	1.62	1.54

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	I	1	SAC	C2A-C1A-N	-6.84	102.98	116.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1	FME	CG-CB-CA	-4.96	98.15	113.07
9	I	1	SAC	OG-CB-CA	-4.78	100.16	111.18
2	O	1	FME	O1-CN-N	-4.11	118.51	124.80
2	O	1	FME	CG-CB-CA	-2.85	104.50	113.07

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	N	1	FME	O1-CN-N-CA
2	B	1	FME	O1-CN-N-CA
1	A	1	FME	O1-CN-N-CA
2	O	1	FME	O1-CN-N-CA

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1	FME	1	0
9	I	1	SAC	2	0
7	T	11	TPO	1	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 54 ligands modelled in this entry, 2 are unknown and 8 are monoatomic - leaving 44 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	$\#\|Z\|>2$
14	CYN	A	601	16	0,1,1	0.00	-	0,0,0	0.00	-
15	HEA	A	602	1	40,67,67	1.67	9 (22%)	36,103,103	2.95	10 (27%)
15	HEA	A	603	1	40,67,67	1.32	5 (12%)	36,103,103	2.78	11 (30%)
19	TGL	A	607	-	62,62,62	1.34	7 (11%)	65,65,65	2.29	16 (24%)
20	PGV	A	608	-	50,50,50	0.95	2 (4%)	51,56,56	1.45	5 (9%)
20	PGV	A	609	-	50,50,50	1.21	2 (4%)	51,56,56	1.50	9 (17%)
21	CUA	B	301	2	0,1,1	0.00	-	0,0,0	0.00	-
22	CHD	B	302	-	29,32,32	1.07	3 (10%)	48,51,51	1.68	9 (18%)
20	PGV	C	302	-	50,50,50	0.91	3 (6%)	51,56,56	1.09	5 (9%)
24	CDL	C	303	-	99,99,99	1.37	12 (12%)	101,111,111	1.43	13 (12%)
22	CHD	C	304	-	29,32,32	0.66	0	48,51,51	2.77	22 (45%)
22	CHD	C	305	-	29,32,32	1.16	3 (10%)	48,51,51	1.79	11 (22%)
25	PEK	C	306	-	51,52,52	1.13	2 (3%)	52,57,57	1.29	5 (9%)
20	PGV	C	307	-	50,50,50	1.39	4 (8%)	51,56,56	1.47	6 (11%)
19	TGL	D	201	-	62,62,62	1.42	7 (11%)	65,65,65	1.49	11 (16%)
26	PSC	E	201	-	51,51,51	1.27	3 (5%)	55,59,59	1.28	4 (7%)
28	DMU	G	101	-	34,34,34	0.83	2 (5%)	45,45,45	2.45	12 (26%)
25	PEK	G	102	-	51,52,52	0.97	3 (5%)	52,57,57	1.67	9 (17%)
24	CDL	G	103	-	99,99,99	1.39	12 (12%)	101,111,111	1.44	16 (15%)
25	PEK	G	104	-	51,52,52	1.11	2 (3%)	52,57,57	1.21	6 (11%)
19	TGL	L	101	-	62,62,62	1.49	7 (11%)	65,65,65	1.67	15 (23%)
28	DMU	M	101	-	34,34,34	0.59	0	45,45,45	1.92	12 (26%)
14	CYN	N	601	16	0,1,1	0.00	-	0,0,0	0.00	-
15	HEA	N	602	1	40,67,67	1.17	6 (15%)	36,103,103	2.98	10 (27%)
15	HEA	N	603	1	40,67,67	1.15	3 (7%)	36,103,103	2.31	13 (36%)
20	PGV	N	607	-	50,50,50	1.00	2 (4%)	51,56,56	1.57	6 (11%)
20	PGV	N	608	-	50,50,50	1.01	2 (4%)	51,56,56	1.27	5 (9%)
19	TGL	N	609	-	62,62,62	1.27	6 (9%)	65,65,65	1.47	9 (13%)
19	TGL	N	610	-	62,62,62	1.50	6 (9%)	65,65,65	1.68	15 (23%)
21	CUA	O	301	2	0,1,1	0.00	-	0,0,0	0.00	-
22	CHD	O	302	-	29,32,32	1.08	3 (10%)	48,51,51	1.69	8 (16%)
26	PSC	O	303	-	51,51,51	1.17	3 (5%)	55,59,59	1.36	6 (10%)
28	DMU	P	301	-	34,34,34	0.90	1 (2%)	45,45,45	2.60	12 (26%)
20	PGV	P	302	-	50,50,50	1.12	2 (4%)	51,56,56	1.27	3 (5%)
25	PEK	P	304	-	51,52,52	0.84	2 (3%)	52,57,57	1.79	9 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
20	PGV	P	305	-	50,50,50	0.87	2 (4%)	51,56,56	1.15	4 (7%)
24	CDL	P	306	-	99,99,99	1.37	12 (12%)	101,111,111	1.40	11 (10%)
22	CHD	P	307	-	29,32,32	0.71	0	48,51,51	3.12	23 (47%)
22	CHD	P	308	-	29,32,32	1.13	3 (10%)	48,51,51	2.03	17 (35%)
25	PEK	P	309	-	51,52,52	1.19	2 (3%)	52,57,57	1.22	4 (7%)
19	TGL	Q	201	-	62,62,62	1.30	6 (9%)	65,65,65	1.48	8 (12%)
25	PEK	T	101	-	51,52,52	1.21	2 (3%)	52,57,57	1.31	6 (11%)
24	CDL	T	102	-	99,99,99	1.33	12 (12%)	101,111,111	1.38	12 (11%)
28	DMU	Z	101	-	34,34,34	0.63	0	45,45,45	1.92	10 (22%)

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	CYN	A	601	16	-	0/0/0/0	0/0/0/0
15	HEA	A	602	1	2/2/7/16	0/24/76/76	0/0/8/8
15	HEA	A	603	1	2/2/7/16	0/24/76/76	0/0/8/8
19	TGL	A	607	-	-	0/65/65/65	0/0/0/0
20	PGV	A	608	-	-	0/55/55/55	0/0/0/0
20	PGV	A	609	-	-	2/55/55/55	0/0/0/0
21	CUA	B	301	2	-	0/0/0/0	0/0/0/0
22	CHD	B	302	-	-	0/7/74/74	0/4/4/4
20	PGV	C	302	-	-	0/55/55/55	0/0/0/0
24	CDL	C	303	-	-	0/110/110/110	0/0/0/0
22	CHD	C	304	-	-	0/7/74/74	0/4/4/4
22	CHD	C	305	-	-	0/7/74/74	0/4/4/4
25	PEK	C	306	-	-	0/56/56/56	0/0/0/0
20	PGV	C	307	-	-	0/55/55/55	0/0/0/0
19	TGL	D	201	-	-	0/65/65/65	0/0/0/0
26	PSC	E	201	-	-	0/55/55/55	0/0/0/0
28	DMU	G	101	-	-	0/19/59/59	0/2/2/2
25	PEK	G	102	-	-	0/56/56/56	0/0/0/0
24	CDL	G	103	-	-	0/110/110/110	0/0/0/0
25	PEK	G	104	-	-	0/56/56/56	0/0/0/0
19	TGL	L	101	-	-	0/65/65/65	0/0/0/0
28	DMU	M	101	-	-	0/19/59/59	0/2/2/2
14	CYN	N	601	16	-	0/0/0/0	0/0/0/0
15	HEA	N	602	1	3/3/7/16	0/24/76/76	0/0/8/8

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	HEA	N	603	1	2/2/7/16	0/24/76/76	0/0/8/8
20	PGV	N	607	-	-	1/55/55/55	0/0/0/0
20	PGV	N	608	-	-	0/55/55/55	0/0/0/0
19	TGL	N	609	-	-	0/65/65/65	0/0/0/0
19	TGL	N	610	-	-	0/65/65/65	0/0/0/0
21	CUA	O	301	2	-	0/0/0/0	0/0/0/0
22	CHD	O	302	-	-	0/7/74/74	0/4/4/4
26	PSC	O	303	-	-	0/55/55/55	0/0/0/0
28	DMU	P	301	-	-	0/19/59/59	0/2/2/2
20	PGV	P	302	-	-	0/55/55/55	0/0/0/0
25	PEK	P	304	-	-	0/56/56/56	0/0/0/0
20	PGV	P	305	-	-	0/55/55/55	0/0/0/0
24	CDL	P	306	-	-	0/110/110/110	0/0/0/0
22	CHD	P	307	-	-	0/7/74/74	0/4/4/4
22	CHD	P	308	-	-	0/7/74/74	0/4/4/4
25	PEK	P	309	-	-	0/56/56/56	0/0/0/0
19	TGL	Q	201	-	-	0/65/65/65	0/0/0/0
25	PEK	T	101	-	-	0/56/56/56	0/0/0/0
24	CDL	T	102	-	-	0/110/110/110	0/0/0/0
28	DMU	Z	101	-	-	0/19/59/59	0/2/2/2

The worst 5 of 163 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	L	101	TGL	C20-CA9	-3.76	1.30	1.51
15	A	602	HEA	C3A-C2A	-3.50	1.35	1.40
25	P	304	PEK	O03-C01	-3.43	1.37	1.45
19	N	610	TGL	C20-CA9	-3.41	1.32	1.51
24	C	303	CDL	C59-C58	-3.40	1.32	1.51

The worst 5 of 398 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	A	602	HEA	C20-C19-C18	-11.33	99.87	120.98
15	N	602	HEA	C17-C18-C19	-11.15	103.15	127.75
15	A	603	HEA	C13-C12-C11	-10.99	101.82	114.74
22	C	304	CHD	C6-C5-C4	-7.60	102.91	111.07
15	N	602	HEA	C27-C19-C18	-6.76	110.48	123.58

5 of 9 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
15	N	602	HEA	ND
15	N	602	HEA	NA
15	N	602	HEA	NB
15	A	603	HEA	ND
15	A	603	HEA	NB

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
20	A	609	PGV	C02-O01-C1-O02
20	N	607	PGV	C02-O01-C1-C2
20	A	609	PGV	C02-O01-C1-C2

There are no ring outliers.

37 monomers are involved in 286 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	A	602	HEA	7	0
15	A	603	HEA	2	0
19	A	607	TGL	6	0
20	A	609	PGV	8	0
22	B	302	CHD	2	0
20	C	302	PGV	2	0
24	C	303	CDL	17	0
22	C	304	CHD	5	0
22	C	305	CHD	1	0
25	C	306	PEK	6	0
20	C	307	PGV	3	0
19	D	201	TGL	12	0
26	E	201	PSC	16	0
28	G	101	DMU	4	0
25	G	102	PEK	2	0
24	G	103	CDL	26	0
25	G	104	PEK	11	0
19	L	101	TGL	14	0
15	N	602	HEA	6	0
15	N	603	HEA	2	0
20	N	607	PGV	9	0
20	N	608	PGV	1	0
19	N	609	TGL	8	0
19	N	610	TGL	14	0
22	O	302	CHD	1	0
26	O	303	PSC	17	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	P	301	DMU	3	0
20	P	302	PGV	2	0
25	P	304	PEK	5	0
20	P	305	PGV	3	0
24	P	306	CDL	20	0
22	P	307	CHD	7	0
22	P	308	CHD	1	0
25	P	309	PEK	8	0
19	Q	201	TGL	2	0
25	T	101	PEK	22	0
24	T	102	CDL	27	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	513/514 (99%)	-0.05	4 (0%) 87 88	21, 27, 35, 67	0
1	N	513/514 (99%)	-0.06	4 (0%) 87 88	26, 35, 47, 76	0
2	B	226/227 (99%)	-0.39	5 (2%) 65 66	24, 33, 55, 80	0
2	O	226/227 (99%)	-0.17	4 (1%) 71 72	34, 45, 69, 95	0
3	C	259/261 (99%)	-0.27	3 (1%) 81 81	25, 33, 44, 64	0
3	P	259/261 (99%)	-0.21	4 (1%) 76 77	29, 37, 49, 69	0
4	D	144/147 (97%)	-0.44	1 (0%) 89 89	28, 36, 52, 69	0
4	Q	144/147 (97%)	1.08	20 (13%) 4 4	41, 58, 83, 130	0
5	E	105/109 (96%)	-0.20	2 (1%) 70 70	29, 36, 59, 99	0
5	R	105/109 (96%)	0.23	4 (3%) 44 45	36, 47, 66, 104	0
6	F	98/98 (100%)	0.70	8 (8%) 14 15	29, 39, 97, 134	0
6	S	98/98 (100%)	0.71	10 (10%) 9 9	31, 45, 103, 128	0
7	G	83/85 (97%)	1.02	16 (19%) 2 2	31, 39, 110, 123	0
7	T	83/85 (97%)	0.98	17 (20%) 1 1	32, 47, 104, 119	0
8	H	79/85 (92%)	0.14	8 (10%) 9 10	30, 40, 88, 113	0
8	U	79/85 (92%)	0.45	9 (11%) 7 7	39, 50, 97, 125	0
9	I	72/73 (98%)	0.16	4 (5%) 28 29	34, 44, 65, 71	0
9	V	72/73 (98%)	0.71	8 (11%) 7 8	35, 60, 75, 102	0
10	J	58/59 (98%)	0.62	8 (13%) 4 4	33, 43, 72, 103	0
10	W	58/59 (98%)	0.71	8 (13%) 4 4	41, 52, 85, 125	0
11	K	49/56 (87%)	-0.29	0 100 100	34, 40, 52, 57	0
11	X	49/56 (87%)	1.52	17 (34%) 0 1	47, 59, 76, 84	0
12	L	46/47 (97%)	-0.32	0 100 100	28, 33, 55, 83	0
12	Y	46/47 (97%)	-0.05	1 (2%) 65 66	38, 50, 74, 97	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å^2)	Q<0.9
13	M	43/46 (93%)	0.18	5 (11%)	6 7	29, 34, 90, 114	0
13	Z	43/46 (93%)	0.53	8 (18%)	2 2	46, 54, 122, 136	0
All	All	3550/3614 (98%)	0.10	178 (5%)	32 34	21, 38, 72, 136	0

The worst 5 of 178 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	Q	5	VAL	25.4
4	Q	6	VAL	23.8
6	S	97	ALA	17.4
6	F	97	ALA	14.5
6	S	96	LEU	13.6

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
2	FME	B	1	10/11	0.97	0.12	-	32,34,43,59	0
2	FME	O	1	10/11	0.98	0.14	-	45,47,58,65	0
1	FME	A	1	10/11	0.93	0.14	-	44,53,74,81	0
7	TPO	G	11	11/12	0.53	0.38	-	83,91,111,114	0
7	TPO	T	11	11/12	0.56	0.35	-	87,95,113,113	0
9	SAC	I	1	9/10	0.80	0.18	-	68,71,73,74	0
9	SAC	V	1	9/10	0.25	0.59	-	113,117,118,119	0
1	FME	N	1	10/11	0.95	0.18	-	52,58,75,76	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
28	DMU	G	101	33/33	0.53	0.29	19.75	103,146,153,154	0
28	DMU	P	301	33/33	0.31	0.45	15.97	132,165,171,171	0
18	NA	A	606	1/1	0.87	0.29	11.89	45,45,45,45	0
20	PGV	A	609	51/51	0.73	0.28	10.14	34,78,100,106	0
19	TGL	N	610	63/63	0.66	0.32	7.48	57,80,98,100	0
24	CDL	P	306	100/100	0.67	0.37	6.82	57,103,125,132	0
19	TGL	L	101	63/63	0.77	0.27	6.69	38,61,82,85	0
24	CDL	T	102	100/100	0.61	0.35	6.57	68,101,133,137	0
18	NA	N	606	1/1	0.85	0.32	5.97	53,53,53,53	0
24	CDL	C	303	100/100	0.74	0.39	5.57	44,96,128,130	0
19	TGL	N	609	63/63	0.83	0.22	5.37	57,84,100,103	0
19	TGL	D	201	63/63	0.75	0.22	5.15	46,69,82,83	0
19	TGL	A	607	63/63	0.84	0.21	4.53	49,77,97,100	0
20	PGV	N	607	51/51	0.72	0.32	4.36	54,92,119,123	0
17	MG	N	605	1/1	0.84	0.15	3.82	39,39,39,39	0
19	TGL	Q	201	63/63	0.71	0.25	3.81	64,87,97,100	0
24	CDL	G	103	100/100	0.57	0.37	3.32	73,101,133,138	0
26	PSC	E	201	52/52	0.72	0.34	2.86	53,106,127,129	0
17	MG	A	605	1/1	0.97	0.13	2.31	27,27,27,27	0
26	PSC	O	303	52/52	0.58	0.34	2.30	57,105,133,136	0
25	PEK	T	101	53/53	0.52	0.48	2.19	62,105,129,130	0
20	PGV	C	307	51/51	0.65	0.41	2.12	62,90,111,112	0
28	DMU	Z	101	33/33	0.81	0.30	2.08	57,70,87,91	0
20	PGV	P	302	51/51	0.64	0.42	1.94	74,105,119,121	0
22	CHD	C	304	29/29	0.70	0.48	1.79	92,125,126,127	0
22	CHD	P	307	29/29	0.71	0.37	1.55	91,121,122,124	0
25	PEK	G	104	53/53	0.58	0.51	1.54	60,112,135,137	0
25	PEK	P	304	53/53	0.93	0.17	1.42	38,60,93,95	0
21	CUA	B	301	2/2	0.99	0.13	1.31	26,26,26,27	0
25	PEK	P	309	53/53	0.55	0.36	1.28	47,97,125,127	0
28	DMU	M	101	33/33	0.91	0.16	1.24	43,49,68,70	0
25	PEK	G	102	53/53	0.95	0.14	1.12	29,50,79,81	0
20	PGV	P	305	51/51	0.95	0.14	1.12	31,47,86,89	0
22	CHD	C	305	29/29	0.90	0.15	0.84	37,44,47,48	0
25	PEK	C	306	53/53	0.48	0.30	0.84	53,92,130,133	0
27	ZN	F	101	1/1	1.00	0.09	0.81	35,35,35,35	0
14	CYN	N	601	2/2	0.99	0.15	0.72	30,30,30,31	0
20	PGV	A	608	51/51	0.96	0.13	0.58	24,41,65,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
20	PGV	C	302	51/51	0.96	0.12	0.57	26,37,79,82	0
20	PGV	N	608	51/51	0.96	0.14	0.46	30,49,74,76	0
14	CYN	A	601	2/2	0.99	0.15	0.27	20,20,20,24	0
21	CUA	O	301	2/2	0.99	0.10	0.25	38,38,38,38	0
15	HEA	N	603	60/60	0.99	0.13	0.20	25,30,39,42	0
22	CHD	P	308	29/29	0.92	0.13	0.04	41,47,50,50	0
15	HEA	A	602	60/60	0.98	0.13	-0.15	17,23,51,55	0
15	HEA	A	603	60/60	0.99	0.12	-0.33	18,23,33,35	0
22	CHD	O	302	29/29	0.97	0.10	-0.34	33,37,43,45	0
22	CHD	B	302	29/29	0.97	0.09	-0.43	33,37,42,53	0
15	HEA	N	602	60/60	0.97	0.10	-0.60	15,31,57,63	0
27	ZN	S	101	1/1	1.00	0.08	-0.66	40,40,40,40	0
23	UNX	C	301	1/1	0.73	0.24	-	38,38,38,38	0
23	UNX	P	303	1/1	0.92	0.30	-	35,35,35,35	0
16	CU	A	604	1/1	1.00	0.13	-	25,25,25,25	0
16	CU	N	604	1/1	1.00	0.13	-	30,30,30,30	0

6.5 Other polymers (i)

There are no such residues in this entry.