



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 07:16 AM GMT

PDB ID : 2ZXW  
Title : Bovine heart cytochrome c oxidase at the fully oxidized state (1-s X-ray exposure dataset)  
Authors : Aoyama, H.; Muramoto, K.; Shinzawa-Itoh, K.; Hirata, K.; Yamashita, E.; Tsukihara, T.; Ogura, T.; Yoshikawa, S.  
Deposited on : 2009-01-08  
Resolution : 2.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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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

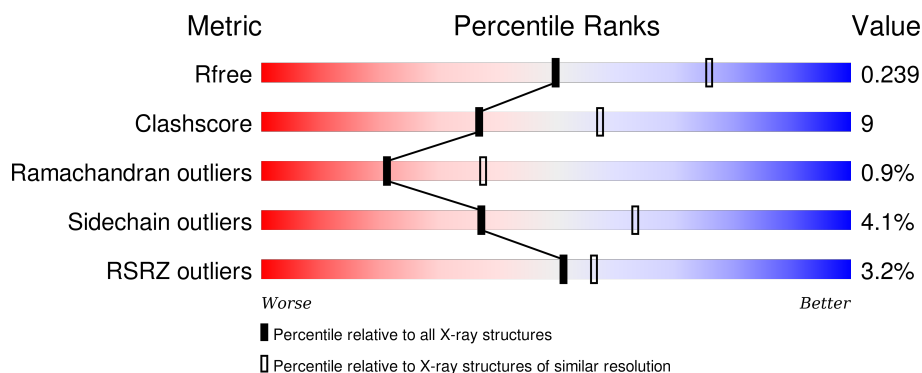
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.













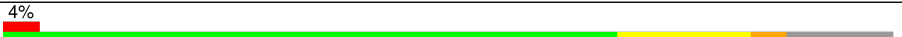

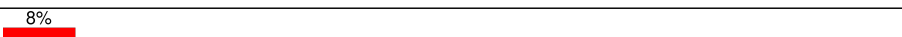
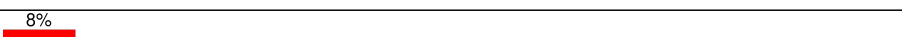
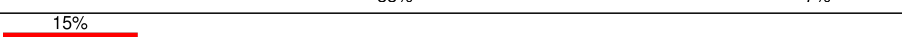
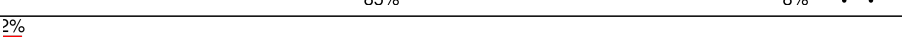

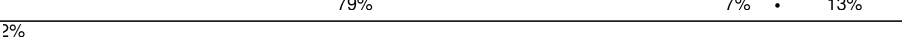

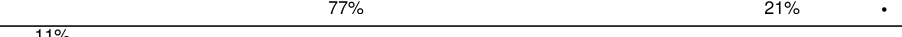
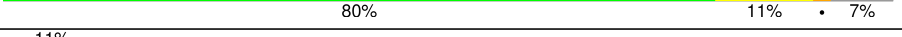
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	514	<div> <div>82%</div> <div>17%</div> <div>.</div> </div>
1	N	514	<div> <div>82%</div> <div>17%</div> </div>
2	B	227	<div> <div>78%</div> <div>19%</div> <div>.</div> </div>
2	O	227	<div> <div>2%</div> <div>73%</div> <div>24%</div> <div>.</div> </div>
3	C	261	<div> <div>84%</div> <div>15%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
3	P	261	
4	D	147	
4	Q	147	
5	E	109	
5	R	109	
6	F	98	
6	S	98	
7	G	85	
7	T	85	
8	H	85	
8	U	85	
9	I	73	
9	V	73	
10	J	59	
10	W	59	
11	K	56	
11	X	56	
12	L	47	
12	Y	47	
13	M	46	
13	Z	46	

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	PER	A	520	-	-	-	X
15	PER	N	520	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	HEA	A	515	X	-	-	-
18	HEA	A	516	X	-	-	-
18	HEA	N	515	X	-	-	-
18	HEA	N	516	X	-	-	-
19	PGV	A	521	-	-	-	X
19	PGV	A	524	-	-	-	X
19	PGV	C	267	-	-	-	X
19	PGV	N	1266	-	-	-	X
19	PGV	N	1268	-	-	-	X
19	PGV	N	1524	-	-	-	X
19	PGV	P	1267	-	-	-	X
21	TGL	B	521	-	-	-	X
21	TGL	D	523	-	-	-	X
21	TGL	L	522	-	-	-	X
21	TGL	N	1521	-	-	-	X
21	TGL	N	1522	-	-	-	X
21	TGL	O	1523	-	-	-	X
22	PSC	B	230	-	-	-	X
22	PSC	O	1230	-	-	-	X
23	CHD	B	1086	X	-	-	-
23	CHD	C	271	X	-	-	X
23	CHD	C	525	X	-	-	-
23	CHD	G	86	X	-	-	-
23	CHD	J	60	X	-	-	X
23	CHD	P	1271	X	-	-	-
23	CHD	P	1525	X	-	-	-
23	CHD	W	1060	X	-	-	X
24	DMU	C	272	X	-	-	X
24	DMU	M	526	X	-	-	-
24	DMU	P	1272	X	-	-	X
24	DMU	Z	1526	X	-	-	-
26	PEK	G	264	-	-	-	X
26	PEK	P	1264	-	-	-	X
27	CDL	C	270	-	-	-	X
27	CDL	G	269	-	-	-	X
27	CDL	P	1270	-	-	-	X
27	CDL	T	1269	-	-	-	X

## 2 Entry composition [i](#)

There are 29 unique types of molecules in this entry. The entry contains 31827 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	0	0
			4027	2691	623	678	35			
1	N	514	Total	C	N	O	S	0	0	0
			4027	2691	623	678	35			

- 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	0	0
			2110	1412	336	350	12			
3	P	259	Total	C	N	O	S	0	0	0
			2110	1412	336	350	12			

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

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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	104	Total	C	N	O	S	0	0	0
			842	538	141	161	2			
5	R	104	Total	C	N	O	S	0	0	0
			842	538	141	161	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	93	Total	C	N	O	S	0	0	0
			717	447	127	138	5			
6	S	93	Total	C	N	O	S	0	0	0
			717	447	127	138	5			

- Molecule 7 is a protein called Cytochrome c oxidase polypeptide 6A2.

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

- Molecule 8 is a protein called Cytochrome c oxidase subunit VIb isoform 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	75	Total	C	N	O	S	0	0	0
			628	395	114	114	5			
8	U	75	Total	C	N	O	S	0	0	0
			628	395	114	114	5			

- Molecule 9 is a protein called Cytochrome c oxidase polypeptide VIc.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	71	Total	C	N	O	S	0	0	0
			585	381	105	95	4			
9	V	71	Total	C	N	O	S	0	0	0
			585	381	105	95	4			

- Molecule 10 is a protein called Cytochrome c oxidase polypeptide 7A1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	57	Total	C	N	O	S	0	0	0
			451	291	76	81	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	W	57	Total	C	N	O	S	0	0	0
			451	291	76	81	3			

- Molecule 11 is a protein called Cytochrome c oxidase polypeptide 7B.

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.

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			

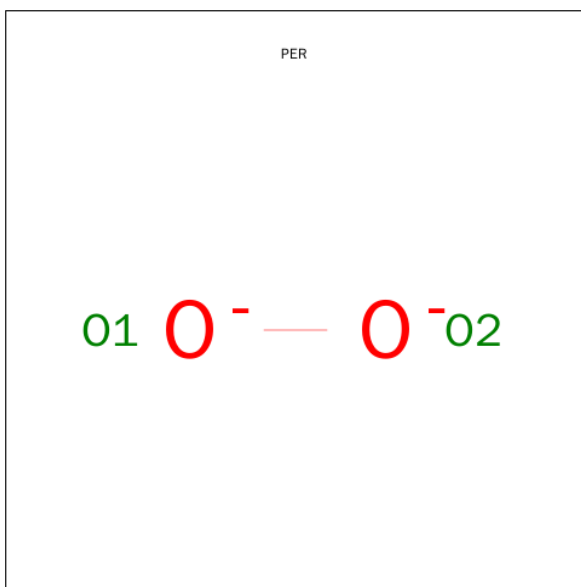
- Molecule 13 is a protein called Cytochrome c oxidase polypeptide 8H.

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

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

- Molecule 15 is PEROXIDE ION (three-letter code: PER) (formula: O<sub>2</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	A	1	Total O 2 2	0	0
15	N	1	Total O 2 2	0	0

- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 17 is SODIUM ION (three-letter code: NA) (formula: Na).

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

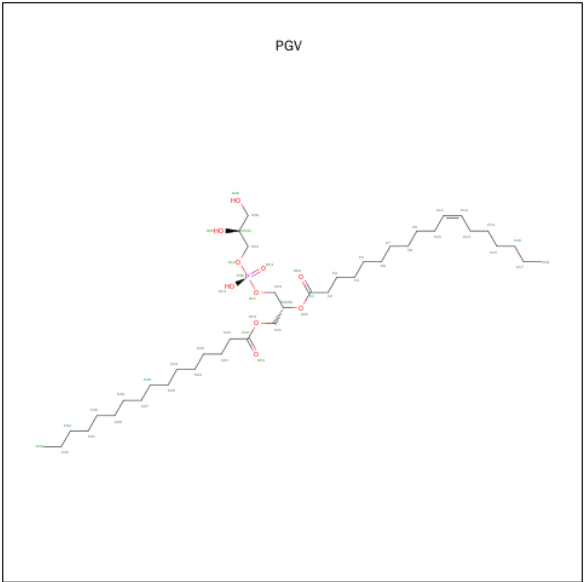
- Molecule 18 is HEME-A (three-letter code: HEA) (formula: C<sub>49</sub>H<sub>56</sub>FeN<sub>4</sub>O<sub>6</sub>).





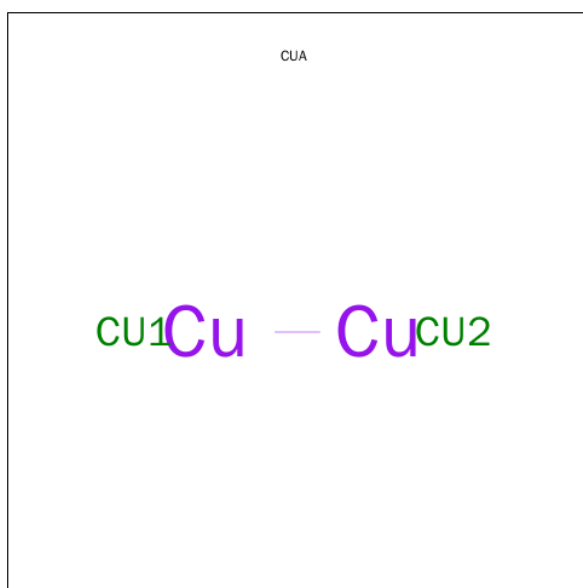
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	A	1	Total 60	C 49	Fe 1	N 4	O 6	0	0
18	A	1	Total 60	C 49	Fe 1	N 4	O 6	0	0
18	N	1	Total 60	C 49	Fe 1	N 4	O 6	0	0
18	N	1	Total 60	C 49	Fe 1	N 4	O 6	0	0

- Molecule 19 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<sub>40</sub>H<sub>77</sub>O<sub>10</sub>P).



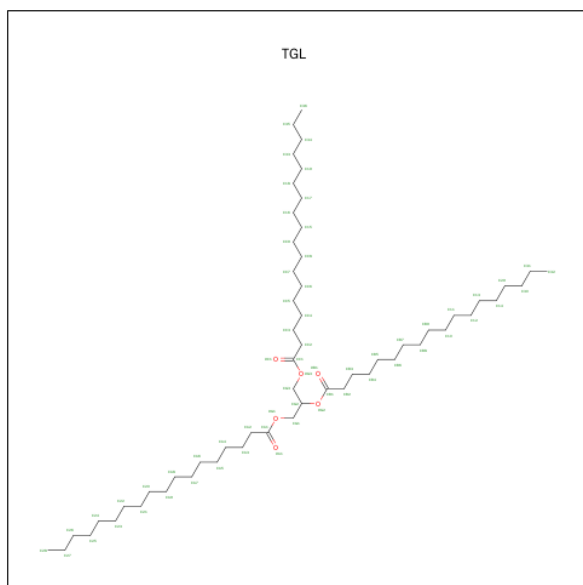
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
19	A	1	Total	C	O	P	0	0
			51	40	10	1		
19	A	1	Total	C	O	P	0	0
			51	40	10	1		
19	C	1	Total	C	O	P	0	0
			51	40	10	1		
19	C	1	Total	C	O	P	0	0
			51	40	10	1		
19	N	1	Total	C	O	P	0	0
			51	40	10	1		
19	N	1	Total	C	O	P	0	0
			51	40	10	1		
19	N	1	Total	C	O	P	0	0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

- Molecule 20 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu<sub>2</sub>).



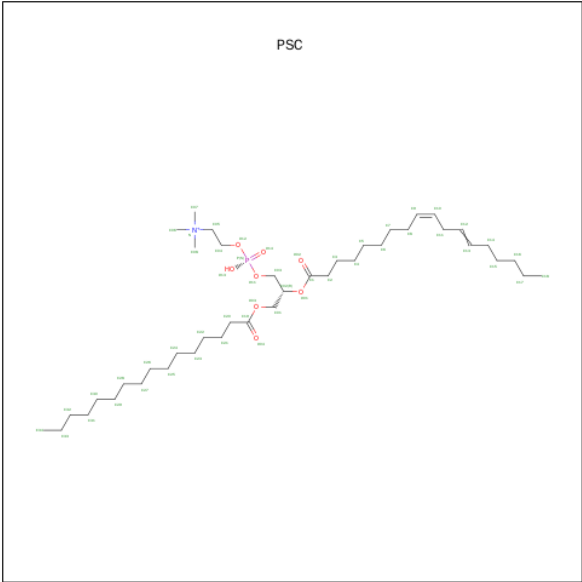
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
20	B	1	Total	Cu	0	0
			2	2		
20	O	1	Total	Cu	0	0
			2	2		

- Molecule 21 is TRISTEAROYLGLYCEROL (three-letter code: TGL) (formula: C<sub>57</sub>H<sub>110</sub>O<sub>6</sub>).



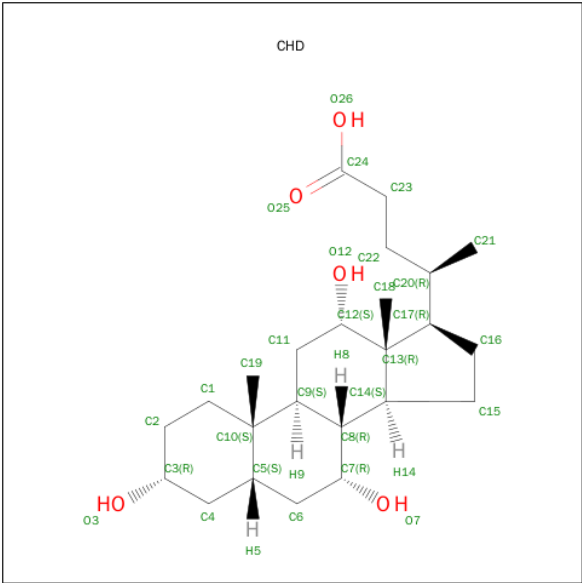
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	B	1	Total	C	O	0	0
			63	57	6		
21	D	1	Total	C	O	0	0
			63	57	6		
21	L	1	Total	C	O	0	0
			63	57	6		
21	N	1	Total	C	O	0	0
			63	57	6		
21	N	1	Total	C	O	0	0
			63	57	6		
21	O	1	Total	C	O	0	0
			63	57	6		

- Molecule 22 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<sub>42</sub>H<sub>81</sub>NO<sub>8</sub>P).



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

- Molecule 23 is CHOLIC ACID (three-letter code: CHD) (formula: C<sub>24</sub>H<sub>40</sub>O<sub>5</sub>).



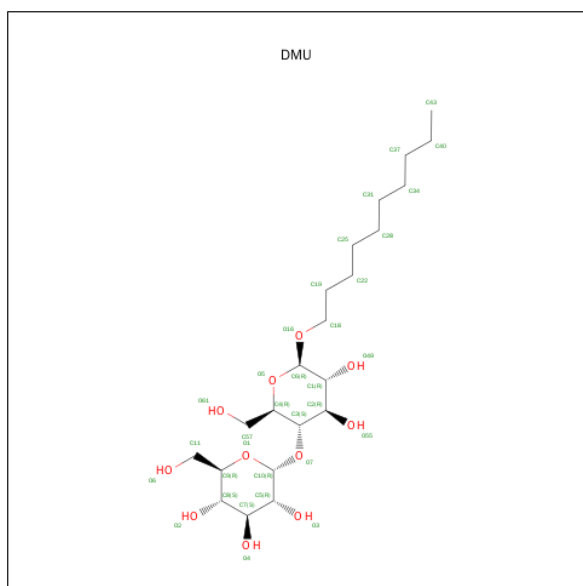
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	B	1	Total	C	O	0	0
			29	24	5		
23	C	1	Total	C	O	0	0
			29	24	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	C	1	Total	C	O	0	0
			29	24	5		
23	G	1	Total	C	O	0	0
			29	24	5		
23	J	1	Total	C	O	0	0
			29	24	5		
23	P	1	Total	C	O	0	0
			29	24	5		
23	P	1	Total	C	O	0	0
			29	24	5		
23	W	1	Total	C	O	0	0
			29	24	5		

- Molecule 24 is SUGAR (DECYL-BETA-D-MALTOPYRANOSIDE) (three-letter code: DMU) (formula: C<sub>22</sub>H<sub>42</sub>O<sub>11</sub>).

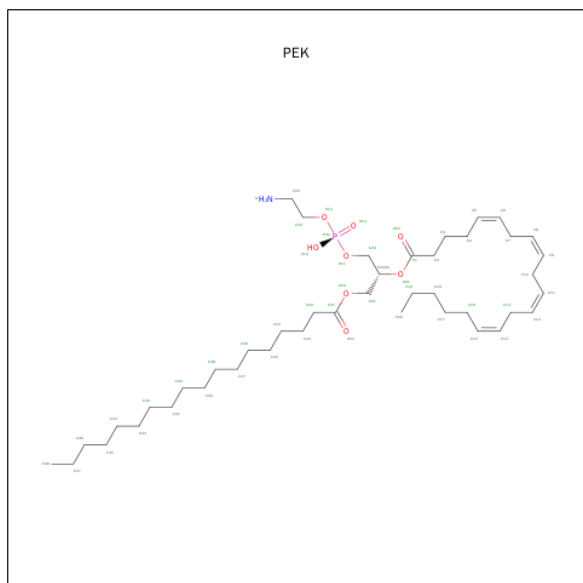


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
24	C	1	Total	C	O	0	0
			33	22	11		
24	M	1	Total	C	O	0	0
			33	22	11		
24	P	1	Total	C	O	0	0
			33	22	11		
24	Z	1	Total	C	O	0	0
			33	22	11		

- Molecule 25 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

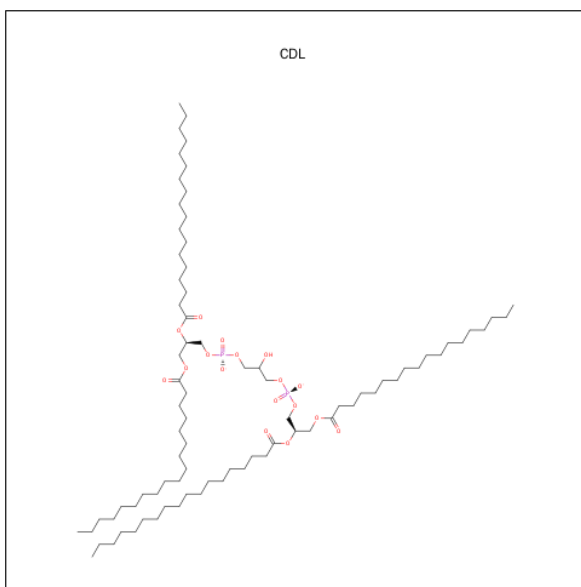
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	P	1	Total X 1 1	0	0
25	C	1	Total X 1 1	0	0

- Molecule 26 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<sub>43</sub>H<sub>78</sub>NO<sub>8</sub>P).



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

- Molecule 27 is CARDIOLIPIN (three-letter code: CDL) (formula: C<sub>81</sub>H<sub>156</sub>O<sub>17</sub>P<sub>2</sub>).



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

- Molecule 28 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 29 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	A	186	Total	O	0	0
			186	186		
29	B	97	Total	O	0	0
			97	97		
29	C	86	Total	O	0	0
			86	86		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	D	66	Total 66	O 66	0	0
29	E	43	Total 43	O 43	0	0
29	F	61	Total 61	O 61	0	0
29	G	42	Total 42	O 42	0	0
29	H	27	Total 27	O 27	0	0
29	I	23	Total 23	O 23	0	0
29	J	12	Total 12	O 12	0	0
29	K	14	Total 14	O 14	0	0
29	L	17	Total 17	O 17	0	0
29	M	13	Total 13	O 13	0	0
29	N	171	Total 171	O 171	0	0
29	O	90	Total 90	O 90	0	0
29	P	80	Total 80	O 80	0	0
29	Q	43	Total 43	O 43	0	0
29	R	37	Total 37	O 37	0	0
29	S	50	Total 50	O 50	0	0
29	T	37	Total 37	O 37	0	0
29	U	31	Total 31	O 31	0	0
29	V	20	Total 20	O 20	0	0
29	W	9	Total 9	O 9	0	0
29	X	11	Total 11	O 11	0	0

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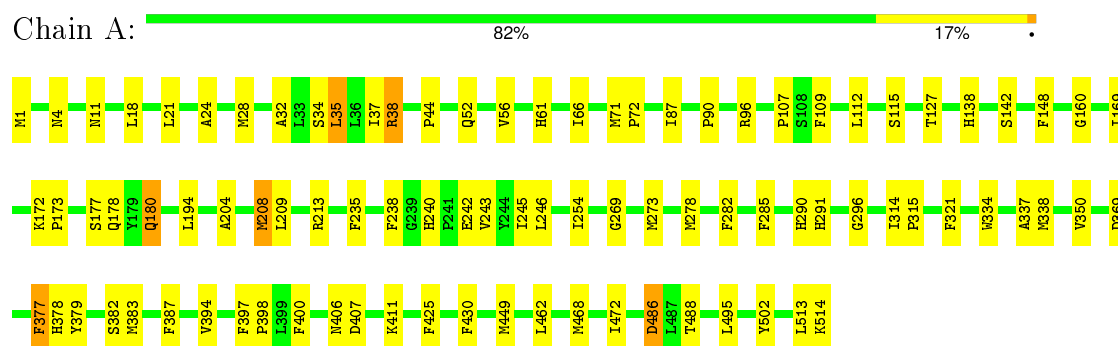
*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	Y	17	Total 17	O 17	0	0
29	Z	8	Total 8	O 8	0	0

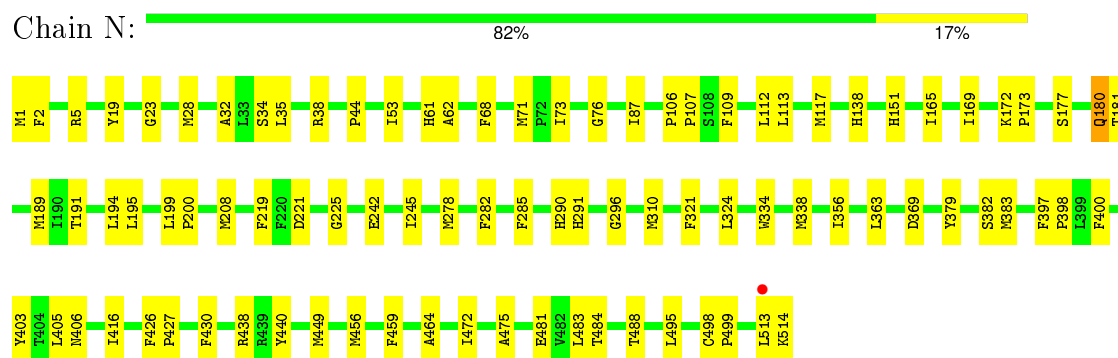
### 3 Residue-property plots

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.

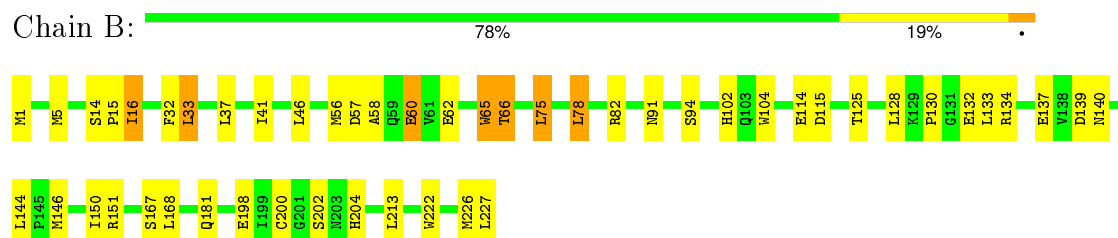
#### • Molecule 1: Cytochrome c oxidase subunit 1



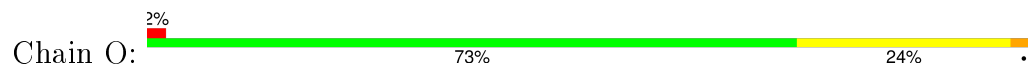
#### • Molecule 1: Cytochrome c oxidase subunit 1

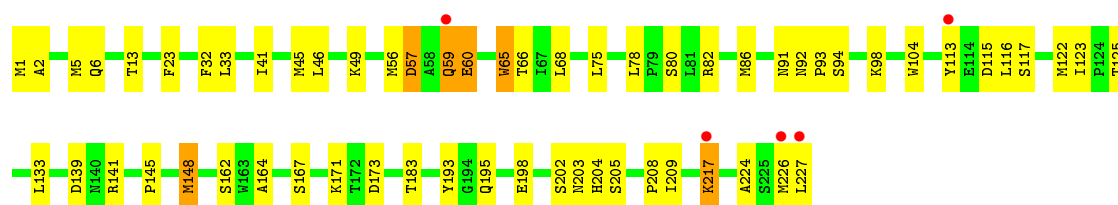


#### • Molecule 2: Cytochrome c oxidase subunit 2



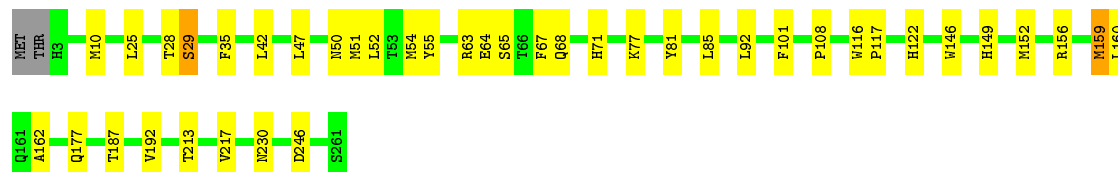
#### • Molecule 2: Cytochrome c oxidase subunit 2





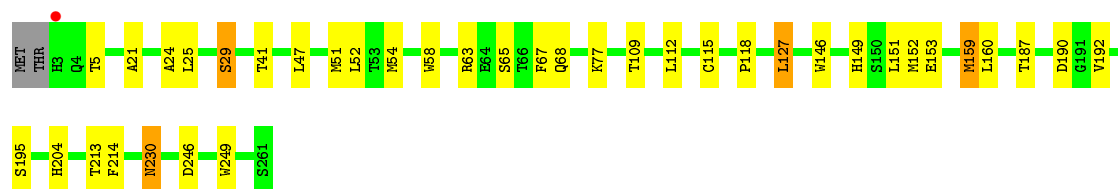
• Molecule 3: Cytochrome c oxidase subunit 3

Chain C: 84% 15% ..



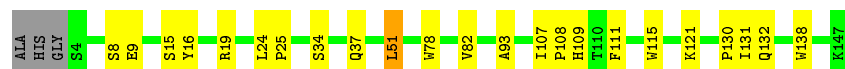
• Molecule 3: Cytochrome c oxidase subunit 3

Chain P: 85% 13% ..



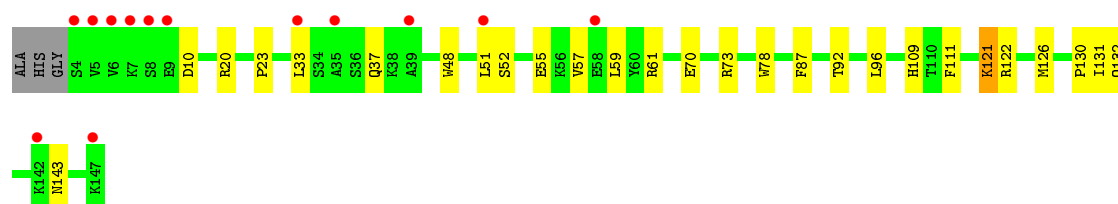
• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1

Chain D: 82% 15% ..



• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1

Chain Q: 9% 80% 18% ..

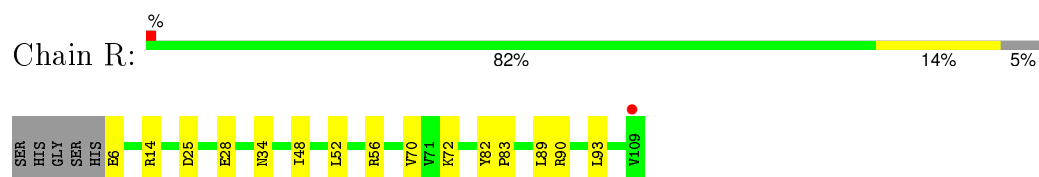


• Molecule 5: Cytochrome c oxidase subunit 5A

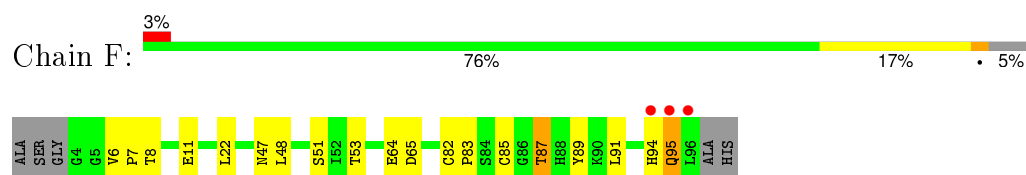
Chain E: 3% 81% 15% 5%



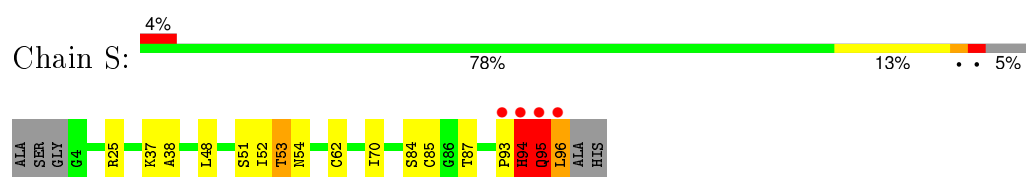
- Molecule 5: Cytochrome c oxidase subunit 5A



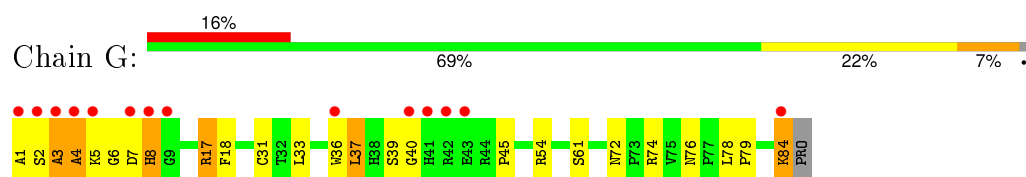
- Molecule 6: Cytochrome c oxidase subunit 5B



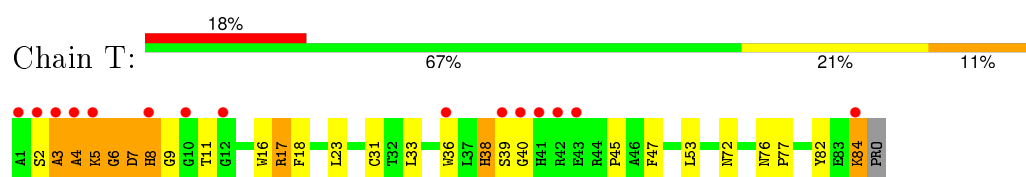
- Molecule 6: Cytochrome c oxidase subunit 5B



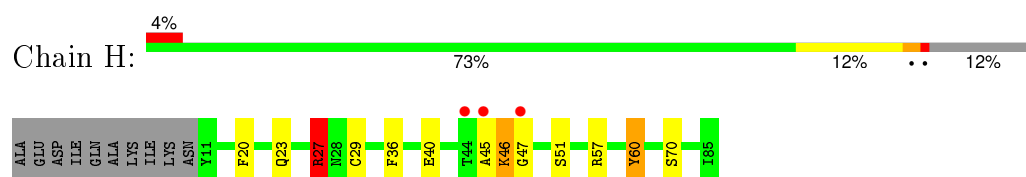
- Molecule 7: Cytochrome c oxidase polypeptide 6A2



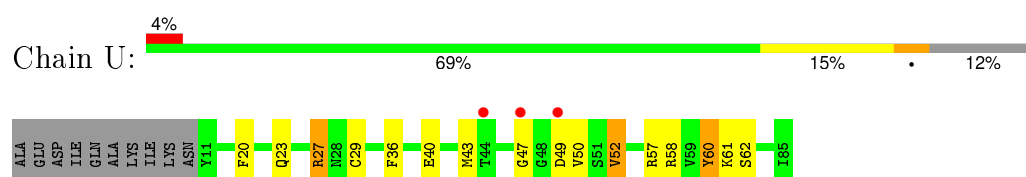
- Molecule 7: Cytochrome c oxidase polypeptide 6A2



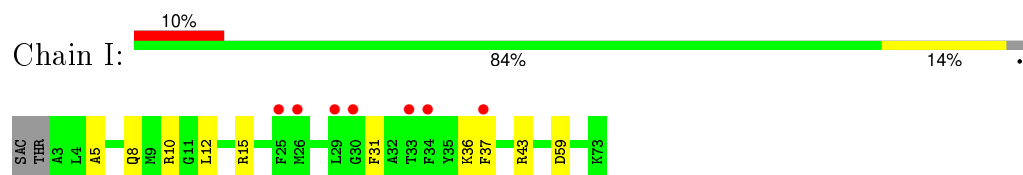
- Molecule 8: Cytochrome c oxidase subunit VIb isoform 1



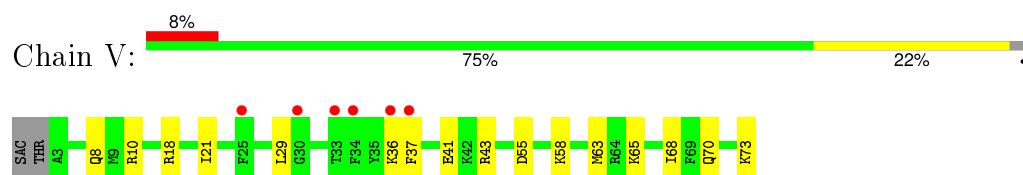
- Molecule 8: Cytochrome c oxidase subunit VIb isoform 1



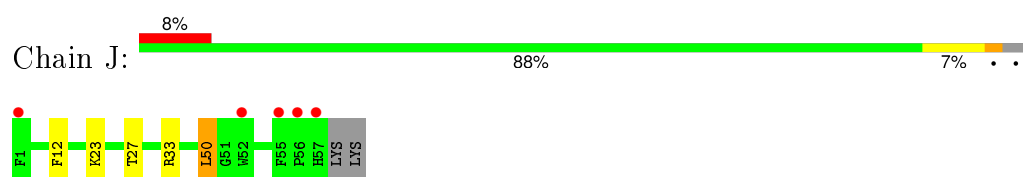
- Molecule 9: Cytochrome c oxidase polypeptide VIc



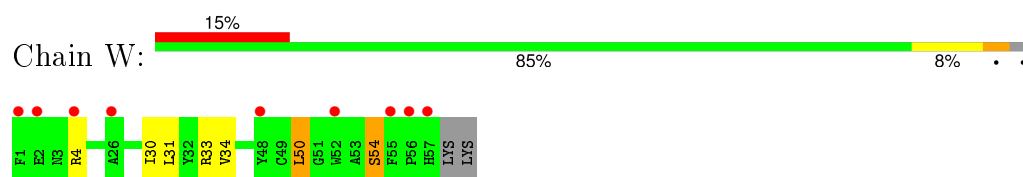
- Molecule 9: Cytochrome c oxidase polypeptide VIc



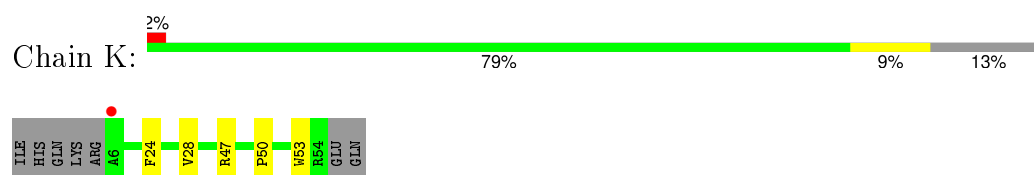
- Molecule 10: Cytochrome c oxidase polypeptide 7A1



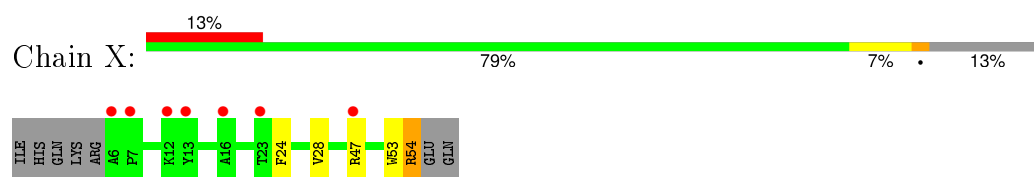
- Molecule 10: Cytochrome c oxidase polypeptide 7A1



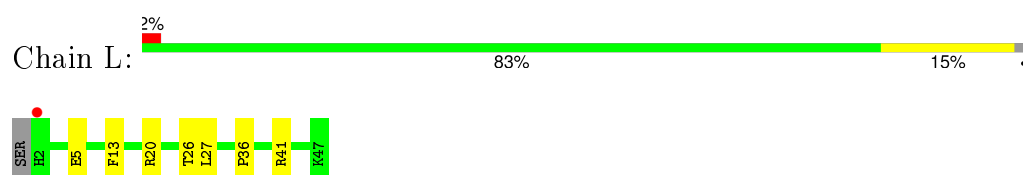
- Molecule 11: Cytochrome c oxidase polypeptide 7B



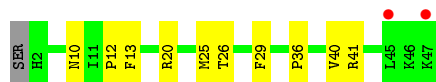
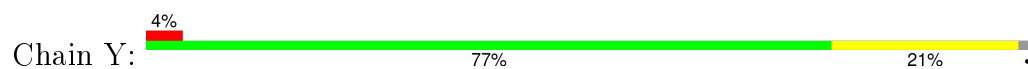
- Molecule 11: Cytochrome c oxidase polypeptide 7B



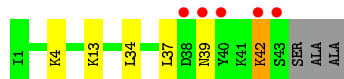
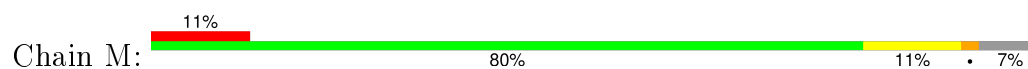
- Molecule 12: Cytochrome c oxidase subunit 7C



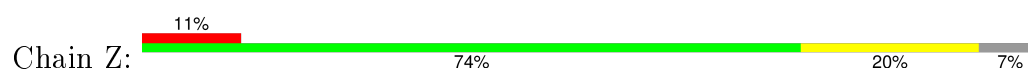
- Molecule 12: Cytochrome c oxidase subunit 7C



- Molecule 13: Cytochrome c oxidase polypeptide 8H



- Molecule 13: Cytochrome c oxidase polypeptide 8H



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	184.16Å 207.62Å 178.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.50 38.33 – 2.49	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-2.50) 91.1 (38.33-2.49)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.76 (at 2.48Å)	Xtriage
Refinement program	REFMAC 5.2	Depositor
R, $R_{free}$	0.185 , 0.233 0.192 , 0.239	Depositor DCC
$R_{free}$ test set	9990 reflections (4.88%)	DCC
Wilson B-factor (Å <sup>2</sup> )	27.8	Xtriage
Anisotropy	0.449	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 52.3	EDS
Estimated twinning fraction	0.004 for l,-k,h	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 215713 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	31827	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.21% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: ZN, TPO, CHD, TGL, CDL, PSC, PEK, MG, PER, PGV, UNX, DMU, CUA, NA, FME, CU, HEA

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	1.01	0/4156	0.85	5/5678 (0.1%)
1	N	0.96	0/4156	0.81	3/5678 (0.1%)
2	B	0.97	1/1860 (0.1%)	0.91	2/2534 (0.1%)
2	O	0.91	1/1860 (0.1%)	0.90	0/2534
3	C	0.98	1/2197 (0.0%)	0.77	0/3005
3	P	0.93	1/2197 (0.0%)	0.81	1/3005 (0.0%)
4	D	0.99	0/1229	0.82	1/1658 (0.1%)
4	Q	0.84	0/1229	0.76	0/1658
5	E	0.94	0/860	0.87	1/1167 (0.1%)
5	R	0.85	0/860	0.78	0/1167
6	F	0.89	0/733	0.94	0/996
6	S	0.83	0/733	0.93	1/996 (0.1%)
7	G	0.98	1/690 (0.1%)	0.88	0/937
7	T	0.94	2/690 (0.3%)	0.88	2/937 (0.2%)
8	H	0.96	0/648	0.82	1/877 (0.1%)
8	U	0.82	0/648	0.73	0/877
9	I	1.00	0/598	0.89	1/792 (0.1%)
9	V	0.93	0/598	0.79	0/792
10	J	0.87	0/462	0.76	0/625
10	W	0.80	0/462	0.82	0/625
11	K	0.97	0/398	0.85	0/546
11	X	0.81	0/398	0.76	0/546
12	L	0.96	0/393	0.85	1/526 (0.2%)
12	Y	0.81	0/393	0.78	0/526
13	M	0.96	0/345	0.80	0/470
13	Z	0.75	0/345	0.69	0/470
All	All	0.94	7/29138 (0.0%)	0.83	19/39622 (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
6	S	0	1

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	36	TRP	CB-CG	7.94	1.64	1.50
2	B	198	GLU	C-O	6.96	1.36	1.23
7	T	36	TRP	CB-CG	6.95	1.62	1.50
2	O	198	GLU	C-O	6.42	1.35	1.23
7	T	5	LYS	CB-CG	5.51	1.67	1.52

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	208	MET	CG-SD-CE	7.33	111.93	100.20
1	A	35	LEU	CB-CG-CD1	-6.52	99.91	111.00
3	P	152	MET	CG-SD-CE	6.22	110.15	100.20
6	S	94	HIS	N-CA-C	6.16	127.62	111.00
1	A	96	ARG	NE-CZ-NH2	-6.13	117.23	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	S	93	PRO	Peptide

## 5.2 Too-close contacts

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	4027	0	4001	69	0
1	N	4027	0	4001	78	0
2	B	1824	0	1833	35	0
2	O	1824	0	1833	40	0
3	C	2110	0	2027	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	P	2110	0	2027	31	0
4	D	1195	0	1183	23	0
4	Q	1195	0	1183	22	0
5	E	842	0	838	9	0
5	R	842	0	838	8	0
6	F	717	0	700	11	0
6	S	717	0	700	12	0
7	G	675	0	644	24	0
7	T	675	0	644	37	0
8	H	628	0	580	7	0
8	U	628	0	580	12	0
9	I	585	0	597	9	0
9	V	585	0	597	9	0
10	J	451	0	446	3	0
10	W	451	0	446	5	0
11	K	384	0	366	5	0
11	X	384	0	366	7	0
12	L	380	0	380	11	0
12	Y	380	0	380	9	0
13	M	335	0	352	3	0
13	Z	335	0	352	6	0
14	A	1	0	0	0	0
14	N	1	0	0	0	0
15	A	2	0	0	1	0
15	N	2	0	0	1	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	120	0	108	12	0
18	N	120	0	108	8	0
19	A	102	0	152	5	0
19	C	102	0	152	5	0
19	N	153	0	228	12	0
19	P	51	0	76	5	0
20	B	2	0	0	0	0
20	O	2	0	0	0	0
21	B	63	0	110	10	0
21	D	63	0	110	5	0
21	L	63	0	110	13	0
21	N	126	0	220	26	0
21	O	63	0	110	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	B	52	0	80	13	0
22	O	52	0	80	12	0
23	B	29	0	37	0	0
23	C	58	0	73	4	0
23	G	29	0	36	2	0
23	J	29	0	35	2	0
23	P	58	0	73	5	0
23	W	29	0	35	1	0
24	C	33	0	37	2	0
24	M	33	0	38	0	0
24	P	33	0	37	3	0
24	Z	33	0	38	2	0
25	C	1	0	0	0	0
25	P	1	0	0	0	0
26	C	53	0	77	4	0
26	G	106	0	154	16	0
26	P	106	0	154	13	0
26	T	53	0	77	14	0
27	C	100	0	156	13	0
27	G	100	0	156	17	0
27	P	100	0	156	9	0
27	T	100	0	156	17	0
28	F	1	0	0	0	0
28	S	1	0	0	0	0
29	A	186	0	0	2	0
29	B	97	0	0	2	0
29	C	86	0	0	5	0
29	D	66	0	0	0	0
29	E	43	0	0	1	0
29	F	61	0	0	2	0
29	G	42	0	0	4	0
29	H	27	0	0	1	0
29	I	23	0	0	6	0
29	J	12	0	0	0	0
29	K	14	0	0	0	0
29	L	17	0	0	2	0
29	M	13	0	0	1	0
29	N	171	0	0	2	0
29	O	90	0	0	2	0
29	P	80	0	0	2	0
29	Q	43	0	0	1	0
29	R	37	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	S	50	0	0	4	0
29	T	37	0	0	2	0
29	U	31	0	0	0	0
29	V	20	0	0	0	0
29	W	9	0	0	0	0
29	X	11	0	0	0	0
29	Y	17	0	0	0	0
29	Z	8	0	0	1	0
All	All	31827	0	31063	578	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 578 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)
26:P:1265:PEK:C7	26:P:1265:PEK:C6	1.88	1.48
26:P:1265:PEK:H383	27:T:1269:CDL:H272	1.33	1.08
15:A:520:PER:O1	15:A:520:PER:O2	1.70	1.08
15:N:520:PER:O2	15:N:520:PER:O1	1.70	1.08
6:S:52:ILE:O	6:S:94:HIS:CE1	2.09	1.05

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	512/514 (100%)	494 (96%)	18 (4%)	0	100	100
1	N	512/514 (100%)	492 (96%)	20 (4%)	0	100	100
2	B	225/227 (99%)	209 (93%)	13 (6%)	3 (1%)	15	26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	O	225/227 (99%)	210 (93%)	12 (5%)	3 (1%)	15	26
3	C	257/261 (98%)	252 (98%)	5 (2%)	0	100	100
3	P	257/261 (98%)	251 (98%)	6 (2%)	0	100	100
4	D	142/147 (97%)	135 (95%)	7 (5%)	0	100	100
4	Q	142/147 (97%)	136 (96%)	6 (4%)	0	100	100
5	E	102/109 (94%)	100 (98%)	1 (1%)	1 (1%)	19	34
5	R	102/109 (94%)	101 (99%)	1 (1%)	0	100	100
6	F	91/98 (93%)	85 (93%)	5 (6%)	1 (1%)	17	31
6	S	91/98 (93%)	84 (92%)	5 (6%)	2 (2%)	8	13
7	G	81/85 (95%)	66 (82%)	7 (9%)	8 (10%)	1	0
7	T	81/85 (95%)	66 (82%)	8 (10%)	7 (9%)	1	1
8	H	73/85 (86%)	69 (94%)	1 (1%)	3 (4%)	3	4
8	U	73/85 (86%)	68 (93%)	4 (6%)	1 (1%)	14	24
9	I	69/73 (94%)	64 (93%)	4 (6%)	1 (1%)	14	24
9	V	69/73 (94%)	66 (96%)	2 (3%)	1 (1%)	14	24
10	J	55/59 (93%)	54 (98%)	1 (2%)	0	100	100
10	W	55/59 (93%)	55 (100%)	0	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%)	44 (100%)	0	0	100	100
12	Y	44/47 (94%)	43 (98%)	1 (2%)	0	100	100
13	M	41/46 (89%)	40 (98%)	1 (2%)	0	100	100
13	Z	41/46 (89%)	39 (95%)	2 (5%)	0	100	100
All	All	3478/3614 (96%)	3315 (95%)	132 (4%)	31 (1%)	21	37

5 of 31 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	95	GLN
7	G	4	ALA
7	G	7	ASP
7	G	39	SER
6	S	95	GLN

### 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	426/426 (100%)	416 (98%)	10 (2%)	58	83
1	N	426/426 (100%)	416 (98%)	10 (2%)	58	83
2	B	210/210 (100%)	199 (95%)	11 (5%)	29	51
2	O	210/210 (100%)	192 (91%)	18 (9%)	13	24
3	C	224/226 (99%)	218 (97%)	6 (3%)	52	79
3	P	224/226 (99%)	219 (98%)	5 (2%)	60	84
4	D	128/129 (99%)	126 (98%)	2 (2%)	70	90
4	Q	128/129 (99%)	125 (98%)	3 (2%)	58	83
5	E	91/95 (96%)	89 (98%)	2 (2%)	60	84
5	R	91/95 (96%)	89 (98%)	2 (2%)	60	84
6	F	79/81 (98%)	76 (96%)	3 (4%)	40	67
6	S	79/81 (98%)	73 (92%)	6 (8%)	16	30
7	G	67/68 (98%)	60 (90%)	7 (10%)	9	16
7	T	67/68 (98%)	63 (94%)	4 (6%)	24	43
8	H	67/75 (89%)	61 (91%)	6 (9%)	12	22
8	U	67/75 (89%)	62 (92%)	5 (8%)	17	31
9	I	56/57 (98%)	53 (95%)	3 (5%)	27	49
9	V	56/57 (98%)	52 (93%)	4 (7%)	18	34
10	J	48/50 (96%)	46 (96%)	2 (4%)	36	62
10	W	48/50 (96%)	45 (94%)	3 (6%)	22	40
11	K	39/46 (85%)	38 (97%)	1 (3%)	54	81
11	X	39/46 (85%)	37 (95%)	2 (5%)	29	52
12	L	39/40 (98%)	38 (97%)	1 (3%)	54	81
12	Y	39/40 (98%)	38 (97%)	1 (3%)	54	81
13	M	37/38 (97%)	33 (89%)	4 (11%)	8	15
13	Z	37/38 (97%)	34 (92%)	3 (8%)	15	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3022/3082 (98%)	2898 (96%)	124 (4%)	37 63

5 of 124 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	M	39	ASN
2	O	33	LEU
9	V	29	LEU
13	M	42	LYS
1	N	338	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 42 such sidechains are listed below:

Mol	Chain	Res	Type
10	J	29	ASN
1	N	512	ASN
7	T	66	ASN
11	K	35	GLN
1	N	178	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 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	0.64	0	6,9,11	3.06	3 (50%)
2	FME	B	1	2	8,9,10	0.83	0	6,9,11	3.34	1 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	TPO	G	11	7	8,10,11	1.72	2 (25%)	7,14,16	1.30	1 (14%)
1	FME	N	1	1	8,9,10	0.54	0	6,9,11	3.55	3 (50%)
2	FME	O	1	2	8,9,10	0.63	0	6,9,11	2.70	2 (33%)
7	TPO	T	11	7	8,10,11	1.60	1 (12%)	7,14,16	1.87	2 (28%)

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
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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	11	TPO	P-O2P	2.11	1.62	1.54
7	G	11	TPO	P-O1P	2.58	1.59	1.51
7	T	11	TPO	P-O1P	2.98	1.61	1.51

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	FME	CA-N-CN	-7.29	111.62	122.82
1	N	1	FME	CA-N-CN	-7.22	111.72	122.82
2	O	1	FME	CA-N-CN	-5.38	114.54	122.82
1	A	1	FME	O1-CN-N	-4.24	118.66	124.76
1	A	1	FME	CA-N-CN	-4.21	116.34	122.82

There are no chirality outliers.

All (4) torsion outliers are listed below:

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

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

There are no ring outliers.

5 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1	FME	3	0
2	B	1	FME	3	0
1	N	1	FME	1	0
2	O	1	FME	3	0
7	T	11	TPO	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 56 ligands modelled in this entry, 2 are unknown and 8 are monoatomic - leaving 46 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	$\# Z  > 2$
18	HEA	A	515	1	40,67,67	1.06	2 (5%)	41,103,103	2.73	18 (43%)
18	HEA	A	516	1,15	40,67,67	2.19	14 (35%)	41,103,103	4.60	23 (56%)
15	PER	A	520	18,14	0,1,1	0.00	-	0,0,0	0.00	-
19	PGV	A	521	-	50,50,50	1.06	2 (4%)	51,56,56	1.28	5 (9%)
19	PGV	A	524	-	50,50,50	1.15	2 (4%)	51,56,56	1.25	5 (9%)
23	CHD	B	1086	-	29,32,32	1.19	3 (10%)	48,51,51	5.34	32 (66%)
20	CUA	B	228	2	0,1,1	0.00	-	0,0,0	0.00	-
22	PSC	B	230	-	51,51,51	1.26	3 (5%)	55,59,59	1.24	5 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
21	TGL	B	521	-	62,62,62	1.25	6 (9%)	65,65,65	1.73	10 (15%)
26	PEK	C	265	-	51,52,52	1.31	4 (7%)	52,57,57	1.29	4 (7%)
19	PGV	C	267	-	50,50,50	0.84	2 (4%)	51,56,56	1.21	5 (9%)
19	PGV	C	268	-	50,50,50	1.15	2 (4%)	51,56,56	1.34	4 (7%)
27	CDL	C	270	-	99,99,99	1.31	13 (13%)	101,111,111	1.34	11 (10%)
23	CHD	C	271	-	29,32,32	0.75	0	48,51,51	4.76	32 (66%)
24	DMU	C	272	-	34,34,34	1.16	2 (5%)	45,45,45	3.43	23 (51%)
23	CHD	C	525	-	29,32,32	1.19	2 (6%)	48,51,51	4.92	35 (72%)
21	TGL	D	523	-	62,62,62	1.42	6 (9%)	65,65,65	1.52	12 (18%)
26	PEK	G	1263	-	51,52,52	1.27	4 (7%)	52,57,57	1.27	4 (7%)
26	PEK	G	264	-	51,52,52	0.97	3 (5%)	52,57,57	1.28	4 (7%)
27	CDL	G	269	-	99,99,99	1.35	11 (11%)	101,111,111	1.28	10 (9%)
23	CHD	G	86	-	29,32,32	1.05	2 (6%)	48,51,51	5.05	33 (68%)
23	CHD	J	60	-	29,32,32	0.89	1 (3%)	48,51,51	4.90	33 (68%)
21	TGL	L	522	-	62,62,62	1.33	5 (8%)	65,65,65	1.49	8 (12%)
24	DMU	M	526	-	34,34,34	0.78	2 (5%)	45,45,45	3.18	23 (51%)
19	PGV	N	1266	-	50,50,50	0.93	3 (6%)	51,56,56	1.41	6 (11%)
19	PGV	N	1268	-	50,50,50	1.15	2 (4%)	51,56,56	1.39	5 (9%)
21	TGL	N	1521	-	62,62,62	1.43	7 (11%)	65,65,65	1.68	13 (20%)
21	TGL	N	1522	-	62,62,62	1.47	7 (11%)	65,65,65	1.40	10 (15%)
19	PGV	N	1524	-	50,50,50	1.09	2 (4%)	51,56,56	1.27	5 (9%)
18	HEA	N	515	1	40,67,67	0.86	0	41,103,103	2.60	16 (39%)
18	HEA	N	516	1,15	40,67,67	1.28	6 (15%)	41,103,103	2.08	11 (26%)
15	PER	N	520	18,14	0,1,1	0.00	-	0,0,0	0.00	-
22	PSC	O	1230	-	51,51,51	1.20	3 (5%)	55,59,59	1.09	3 (5%)
21	TGL	O	1523	-	62,62,62	1.37	6 (9%)	65,65,65	1.24	9 (13%)
20	CUA	O	228	2	0,1,1	0.00	-	0,0,0	0.00	-
26	PEK	P	1264	-	51,52,52	0.99	4 (7%)	52,57,57	1.53	7 (13%)
26	PEK	P	1265	-	51,52,52	1.65	5 (9%)	52,57,57	1.40	7 (13%)
19	PGV	P	1267	-	50,50,50	0.87	2 (4%)	51,56,56	1.03	4 (7%)
27	CDL	P	1270	-	99,99,99	1.31	10 (10%)	101,111,111	1.30	12 (11%)
23	CHD	P	1271	-	29,32,32	0.75	0	48,51,51	4.90	30 (62%)
24	DMU	P	1272	-	34,34,34	1.17	2 (5%)	45,45,45	3.34	24 (53%)
23	CHD	P	1525	-	29,32,32	0.89	1 (3%)	48,51,51	5.18	37 (77%)
27	CDL	T	1269	-	99,99,99	1.29	12 (12%)	101,111,111	1.44	12 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
26	PEK	T	263	-	51,52,52	1.43	5 (9%)	52,57,57	1.43	5 (9%)
23	CHD	W	1060	-	29,32,32	1.06	2 (6%)	48,51,51	5.12	34 (70%)
24	DMU	Z	1526	-	34,34,34	0.94	2 (5%)	45,45,45	3.22	19 (42%)

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
18	HEA	A	515	1	3/3/7/16	0/24/76/76	0/0/8/8
18	HEA	A	516	1,15	3/3/7/16	0/24/76/76	0/0/8/8
15	PER	A	520	18,14	-	0/0/0/0	0/0/0/0
19	PGV	A	521	-	-	0/55/55/55	0/0/0/0
19	PGV	A	524	-	-	1/55/55/55	0/0/0/0
23	CHD	B	1086	-	1/1/12/12	0/7/74/74	0/4/4/4
20	CUA	B	228	2	-	0/0/0/0	0/0/0/0
22	PSC	B	230	-	-	0/55/55/55	0/0/0/0
21	TGL	B	521	-	-	0/65/65/65	0/0/0/0
26	PEK	C	265	-	-	0/56/56/56	0/0/0/0
19	PGV	C	267	-	-	0/55/55/55	0/0/0/0
19	PGV	C	268	-	-	0/55/55/55	0/0/0/0
27	CDL	C	270	-	-	0/110/110/110	0/0/0/0
23	CHD	C	271	-	2/2/12/12	0/7/74/74	0/4/4/4
24	DMU	C	272	-	5/5/10/10	0/19/59/59	0/2/2/2
23	CHD	C	525	-	1/1/12/12	0/7/74/74	0/4/4/4
21	TGL	D	523	-	-	0/65/65/65	0/0/0/0
26	PEK	G	1263	-	-	0/56/56/56	0/0/0/0
26	PEK	G	264	-	-	0/56/56/56	0/0/0/0
27	CDL	G	269	-	-	1/110/110/110	0/0/0/0
23	CHD	G	86	-	1/1/12/12	0/7/74/74	0/4/4/4
23	CHD	J	60	-	1/1/12/12	0/7/74/74	0/4/4/4
21	TGL	L	522	-	-	0/65/65/65	0/0/0/0
24	DMU	M	526	-	5/5/10/10	0/19/59/59	0/2/2/2
19	PGV	N	1266	-	-	0/55/55/55	0/0/0/0
19	PGV	N	1268	-	-	0/55/55/55	0/0/0/0
21	TGL	N	1521	-	-	0/65/65/65	0/0/0/0
21	TGL	N	1522	-	-	0/65/65/65	0/0/0/0
19	PGV	N	1524	-	-	1/55/55/55	0/0/0/0
18	HEA	N	515	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
18	HEA	N	516	1,15	3/3/7/16	0/24/76/76	0/0/8/8
15	PER	N	520	18,14	-	0/0/0/0	0/0/0/0
22	PSC	O	1230	-	-	0/55/55/55	0/0/0/0
21	TGL	O	1523	-	-	0/65/65/65	0/0/0/0
20	CUA	O	228	2	-	0/0/0/0	0/0/0/0
26	PEK	P	1264	-	-	0/56/56/56	0/0/0/0
26	PEK	P	1265	-	-	0/56/56/56	0/0/0/0
19	PGV	P	1267	-	-	0/55/55/55	0/0/0/0
27	CDL	P	1270	-	-	0/110/110/110	0/0/0/0
23	CHD	P	1271	-	2/2/12/12	0/7/74/74	0/4/4/4
24	DMU	P	1272	-	5/5/10/10	0/19/59/59	0/2/2/2
23	CHD	P	1525	-	1/1/12/12	0/7/74/74	0/4/4/4
27	CDL	T	1269	-	-	0/110/110/110	0/0/0/0
26	PEK	T	263	-	-	0/56/56/56	0/0/0/0
23	CHD	W	1060	-	1/1/12/12	0/7/74/74	0/4/4/4
24	DMU	Z	1526	-	5/5/10/10	0/19/59/59	0/2/2/2

The worst 5 of 172 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	516	HEA	C4B-NB	-4.39	1.30	1.36
18	A	516	HEA	C4A-NA	-4.30	1.30	1.36
23	B	1086	CHD	C13-C14	-3.22	1.49	1.55
26	P	1264	PEK	O03-C01	-3.13	1.38	1.45
27	C	270	CDL	C59-C58	-3.11	1.33	1.51

The worst 5 of 608 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	1086	CHD	C18-C13-C12	-14.56	94.89	109.09
18	A	516	HEA	CAD-C3D-C4D	-13.81	112.02	127.01
23	G	86	CHD	C18-C13-C12	-10.07	99.27	109.09
23	W	1060	CHD	C6-C5-C4	-8.49	101.57	111.05
23	B	1086	CHD	C19-C10-C9	-8.01	99.18	111.18

5 of 42 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
24	M	526	DMU	C2
24	M	526	DMU	C4
24	M	526	DMU	C9

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Mol	Chain	Res	Type	Atom
24	M	526	DMU	C6
24	M	526	DMU	C5

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	A	524	PGV	C02-O01-C1-C2
19	N	1524	PGV	C02-O01-C1-C2
27	G	269	CDL	PB2-OB2-CB2-C1

There are no ring outliers.

40 monomers are involved in 244 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	A	515	HEA	7	0
18	A	516	HEA	5	0
15	A	520	PER	1	0
19	A	524	PGV	5	0
22	B	230	PSC	13	0
21	B	521	TGL	10	0
26	C	265	PEK	4	0
19	C	267	PGV	3	0
19	C	268	PGV	2	0
27	C	270	CDL	13	0
23	C	271	CHD	4	0
24	C	272	DMU	2	0
21	D	523	TGL	5	0
26	G	1263	PEK	12	0
26	G	264	PEK	4	0
27	G	269	CDL	17	0
23	G	86	CHD	2	0
23	J	60	CHD	2	0
21	L	522	TGL	13	0
19	N	1266	PGV	1	0
19	N	1268	PGV	2	0
21	N	1521	TGL	7	0
21	N	1522	TGL	19	0
19	N	1524	PGV	9	0
18	N	515	HEA	7	0
18	N	516	HEA	1	0
15	N	520	PER	1	0
22	O	1230	PSC	12	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	O	1523	TGL	6	0
26	P	1264	PEK	5	0
26	P	1265	PEK	8	0
19	P	1267	PGV	5	0
27	P	1270	CDL	9	0
23	P	1271	CHD	3	0
24	P	1272	DMU	3	0
23	P	1525	CHD	2	0
27	T	1269	CDL	17	0
26	T	263	PEK	14	0
23	W	1060	CHD	1	0
24	Z	1526	DMU	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	513/514 (99%)	-0.61	0 100 100	11, 17, 25, 51	0
1	N	513/514 (99%)	-0.63	1 (0%) 95 96	15, 23, 33, 56	0
2	B	226/227 (99%)	-0.75	0 100 100	12, 23, 49, 86	0
2	O	226/227 (99%)	-0.50	5 (2%) 65 69	20, 30, 60, 84	0
3	C	259/261 (99%)	-0.88	0 100 100	13, 21, 34, 58	0
3	P	259/261 (99%)	-0.81	1 (0%) 93 93	16, 24, 40, 64	0
4	D	144/147 (97%)	-0.61	0 100 100	14, 26, 48, 70	0
4	Q	144/147 (97%)	0.39	13 (9%) 12 12	27, 41, 63, 105	0
5	E	104/109 (95%)	-0.67	3 (2%) 55 60	18, 27, 54, 75	0
5	R	104/109 (95%)	-0.29	1 (0%) 84 86	23, 35, 57, 77	0
6	F	93/98 (94%)	-0.20	3 (3%) 51 56	15, 27, 49, 94	0
6	S	93/98 (94%)	0.09	4 (4%) 39 44	20, 33, 55, 102	0
7	G	83/85 (97%)	0.22	14 (16%) 2 2	15, 28, 99, 105	0
7	T	83/85 (97%)	0.41	15 (18%) 2 2	17, 33, 98, 102	0
8	H	75/85 (88%)	-0.14	3 (4%) 42 47	18, 29, 70, 78	0
8	U	75/85 (88%)	-0.00	3 (4%) 42 47	24, 34, 72, 79	0
9	I	71/73 (97%)	0.15	7 (9%) 9 10	21, 34, 60, 65	0
9	V	71/73 (97%)	0.36	6 (8%) 13 14	23, 45, 60, 70	0
10	J	57/59 (96%)	-0.24	5 (8%) 12 13	19, 32, 59, 82	0
10	W	57/59 (96%)	0.27	9 (15%) 3 2	25, 37, 68, 92	0
11	K	49/56 (87%)	-0.30	1 (2%) 68 72	19, 31, 43, 50	0
11	X	49/56 (87%)	0.92	7 (14%) 4 3	33, 42, 59, 71	0
12	L	46/47 (97%)	-0.58	1 (2%) 65 69	17, 26, 48, 74	0
12	Y	46/47 (97%)	-0.23	2 (4%) 39 44	26, 35, 60, 82	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	M	43/46 (93%)	-0.24	5 (11%) 6 6	15, 24, 72, 97	0
13	Z	43/46 (93%)	0.32	5 (11%) 6 6	28, 36, 89, 106	0
All	All	3526/3614 (97%)	-0.40	114 (3%) 51 56	11, 26, 57, 106	0

The worst 5 of 114 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	Q	5	VAL	18.4
4	Q	6	VAL	10.5
4	Q	4	SER	10.2
4	Q	8	SER	9.8
13	Z	43	SER	8.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
7	TPO	G	11	11/12	0.51	0.33	-	74,81,102,102	0
1	FME	A	1	10/11	0.92	0.19	-	44,46,62,65	0
7	TPO	T	11	11/12	0.59	0.36	-	74,80,100,101	0
1	FME	N	1	10/11	0.92	0.19	-	48,50,63,64	0
2	FME	O	1	10/11	0.96	0.12	-	30,31,37,38	0
2	FME	B	1	10/11	0.98	0.13	-	19,21,26,33	0

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
19	PGV	A	524	51/51	0.81	0.26	8.79	30,65,100,103	0
27	CDL	C	270	100/100	0.80	0.30	7.49	40,86,103,105	0
27	CDL	P	1270	100/100	0.71	0.34	6.80	44,89,104,105	0
23	CHD	W	1060	29/29	0.72	0.50	6.72	97,100,102,103	0
23	CHD	J	60	29/29	0.68	0.48	5.68	95,98,101,103	0
21	TGL	B	521	63/63	0.84	0.24	5.62	31,58,87,89	0
24	DMU	C	272	33/33	0.62	0.35	5.55	64,101,103,105	0
21	TGL	N	1522	63/63	0.66	0.34	5.31	25,66,80,81	0
24	DMU	P	1272	33/33	0.57	0.40	5.03	74,102,105,106	0
21	TGL	L	522	63/63	0.79	0.28	4.44	25,61,74,78	0
21	TGL	N	1521	63/63	0.82	0.23	3.97	43,63,85,90	0
19	PGV	N	1266	51/51	0.98	0.20	3.85	15,28,50,52	0
19	PGV	C	267	51/51	0.96	0.18	3.65	13,24,55,58	0
26	PEK	G	264	53/53	0.96	0.18	3.52	15,31,57,58	0
19	PGV	N	1524	51/51	0.81	0.29	3.38	36,68,102,102	0
21	TGL	D	523	63/63	0.81	0.23	3.26	38,57,83,86	0
22	PSC	O	1230	52/52	0.74	0.29	3.08	38,82,113,115	0
19	PGV	N	1268	51/51	0.76	0.29	2.92	62,89,99,101	0
19	PGV	P	1267	51/51	0.96	0.18	2.83	16,28,59,60	0
15	PER	N	520	2/2	0.98	0.13	2.82	13,13,13,13	0
23	CHD	C	271	29/29	0.86	0.31	2.80	71,83,86,86	0
19	PGV	A	521	51/51	0.98	0.18	2.79	12,24,48,57	0
22	PSC	B	230	52/52	0.79	0.31	2.62	31,86,112,114	0
27	CDL	G	269	100/100	0.73	0.31	2.57	42,77,109,113	0
21	TGL	O	1523	63/63	0.77	0.23	2.57	34,64,86,90	0
26	PEK	P	1264	53/53	0.94	0.20	2.46	20,37,65,65	0
27	CDL	T	1269	100/100	0.72	0.27	2.32	43,76,109,113	0
15	PER	A	520	2/2	0.99	0.18	2.17	8,8,8,10	0
26	PEK	C	265	53/53	0.59	0.33	1.81	39,87,101,104	0
24	DMU	Z	1526	33/33	0.82	0.23	1.76	32,50,66,68	0
26	PEK	P	1265	53/53	0.72	0.30	1.76	32,83,103,103	0
26	PEK	T	263	53/53	0.64	0.38	1.44	35,81,112,112	0
19	PGV	C	268	51/51	0.77	0.26	1.40	53,87,97,98	0
23	CHD	P	1271	29/29	0.82	0.27	1.36	74,82,84,84	0
26	PEK	G	1263	53/53	0.67	0.37	1.33	46,88,115,116	0
18	HEA	N	515	60/60	0.98	0.16	1.04	14,25,37,39	0
24	DMU	M	526	33/33	0.91	0.16	0.85	15,38,57,59	0
18	HEA	A	515	60/60	0.99	0.16	0.43	8,17,40,45	0
23	CHD	C	525	29/29	0.96	0.10	0.40	14,24,31,33	0
16	MG	N	1518	1/1	0.85	0.13	0.11	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
18	HEA	N	516	60/60	0.98	0.12	-0.09	9,20,26,28	0
23	CHD	P	1525	29/29	0.95	0.10	-0.13	17,27,31,35	0
23	CHD	B	1086	29/29	0.97	0.10	-0.27	11,20,27,33	0
20	CUA	B	228	2/2	0.99	0.09	-0.28	17,17,17,18	0
18	HEA	A	516	60/60	0.99	0.12	-0.35	9,16,24,27	0
23	CHD	G	86	29/29	0.98	0.08	-0.39	17,21,25,26	0
17	NA	A	519	1/1	0.96	0.07	-1.36	16,16,16,16	0
28	ZN	F	99	1/1	1.00	0.07	-1.48	26,26,26,26	0
28	ZN	S	99	1/1	0.99	0.05	-1.60	28,28,28,28	0
16	MG	A	518	1/1	0.96	0.08	-2.27	21,21,21,21	0
20	CUA	O	228	2/2	0.98	0.07	-2.29	25,25,25,26	0
17	NA	N	1519	1/1	0.97	0.04	-2.85	24,24,24,24	0
14	CU	A	517	1/1	1.00	0.09	-	17,17,17,17	0
25	UNX	C	262	1/1	0.82	0.21	-	26,26,26,26	0
14	CU	N	517	1/1	1.00	0.10	-	18,18,18,18	0
25	UNX	P	1262	1/1	0.74	0.30	-	29,29,29,29	0

## 6.5 Other polymers

There are no such residues in this entry.