



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 01:50 AM GMT

PDB ID : 2DYR  
Title : Bovine heart cytochrome C oxidase at the fully oxidized state  
Authors : Shinzawa-Itoh, K.; Aoyama, H.; Muramoto, K.; Kurauchi, T.; Mizushima, T.; Yamashita, E.; Tsukihara, T.; Yoshikawa, S.  
Deposited on : 2006-09-16  
Resolution : 1.80 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

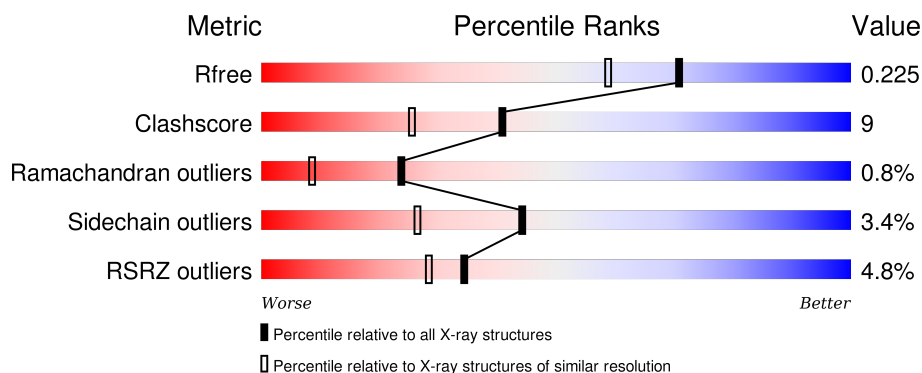
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 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.



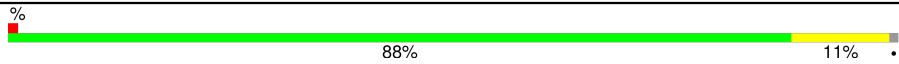
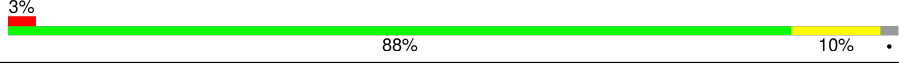
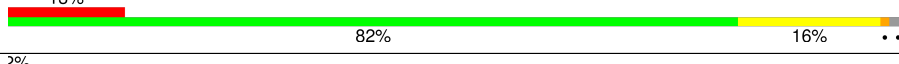


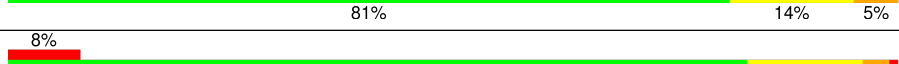
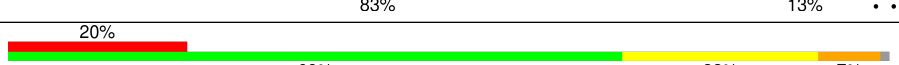
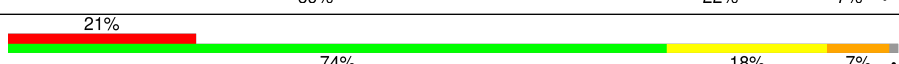
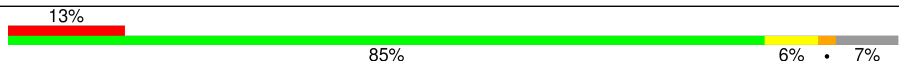
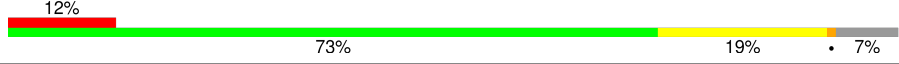

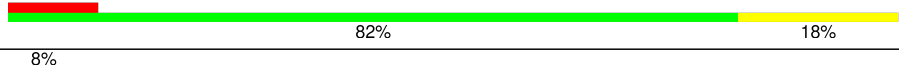
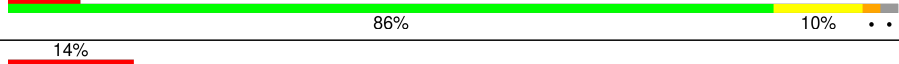
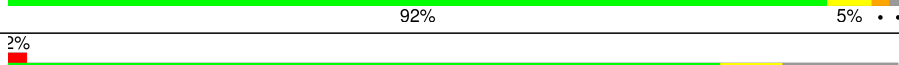
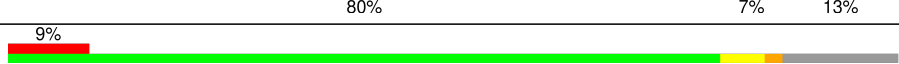





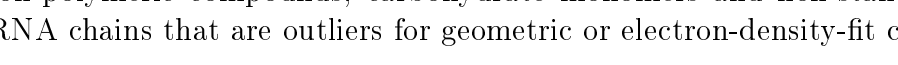
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (1.80-1.80)

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>87%</div> <div>13%</div> </div>
1	N	514	<div> <div>84%</div> <div>16%</div> </div>
2	B	227	<div> <div>2%</div> <div>81%</div> <div>17%</div> </div>
2	O	227	<div> <div>4%</div> <div>75%</div> <div>23%</div> </div>
3	C	261	<div> <div>90%</div> <div>10%</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
17	HEA	A	515	X	-	-	-
17	HEA	A	516	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	HEA	N	515	X	-	-	-
17	HEA	N	516	X	-	-	-
18	PGV	A	524	-	-	-	X
18	PGV	C	268	-	-	-	X
18	PGV	P	1268	-	-	-	X
18	PGV	Z	1524	-	-	-	X
20	TGL	B	521	-	-	-	X
20	TGL	D	523	-	-	-	X
20	TGL	L	522	-	-	X	X
20	TGL	N	1521	-	-	-	X
20	TGL	N	1522	-	-	-	X
20	TGL	Q	1523	-	-	-	X
21	PSC	B	230	-	-	-	X
21	PSC	O	1230	-	-	-	X
22	CHD	C	271	X	-	-	-
22	CHD	J	60	X	-	-	X
22	CHD	P	1271	X	-	-	-
22	CHD	W	1060	X	-	-	X
23	DMU	C	272	X	-	-	X
23	DMU	M	526	X	-	-	-
23	DMU	P	1272	X	-	-	X
23	DMU	Z	1526	X	-	-	X
26	CDL	C	270	-	-	-	X
26	CDL	G	269	-	-	X	X
26	CDL	P	1270	-	-	-	X
26	CDL	T	1269	-	-	X	X

## 2 Entry composition [i](#)

There are 28 unique types of molecules in this entry. The entry contains 32735 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 polypeptide Va.

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 polypeptide Vb.

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 polypeptide VIa-heart.

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	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 polypeptide VIc.

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 polypeptide VIIa-heart.

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 polypeptide VIIb.

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 polypeptide VIIc.

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 VIII-heart.

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		

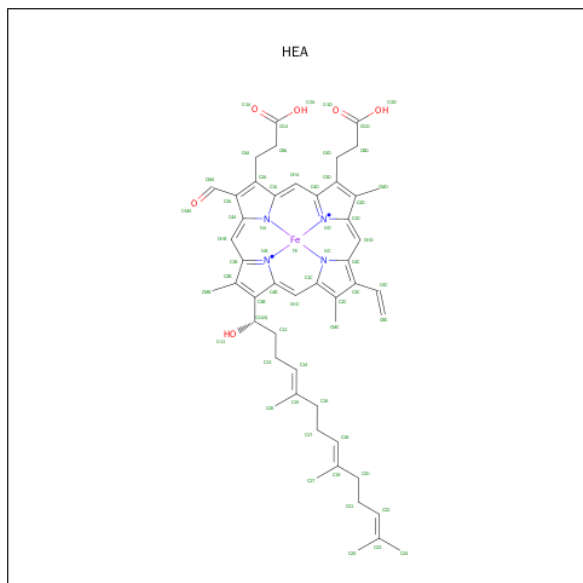
- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 16 is SODIUM ION (three-letter code: NA) (formula: Na).

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

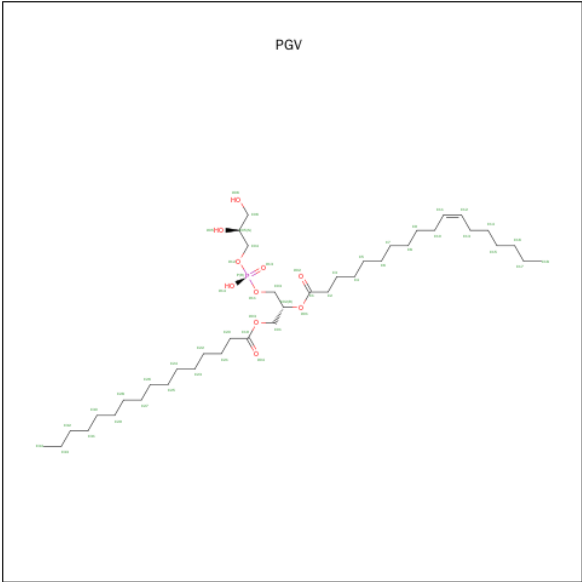
- Molecule 17 is HEME-A (three-letter code: HEA) (formula: C<sub>49</sub>H<sub>56</sub>FeN<sub>4</sub>O<sub>6</sub>).



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

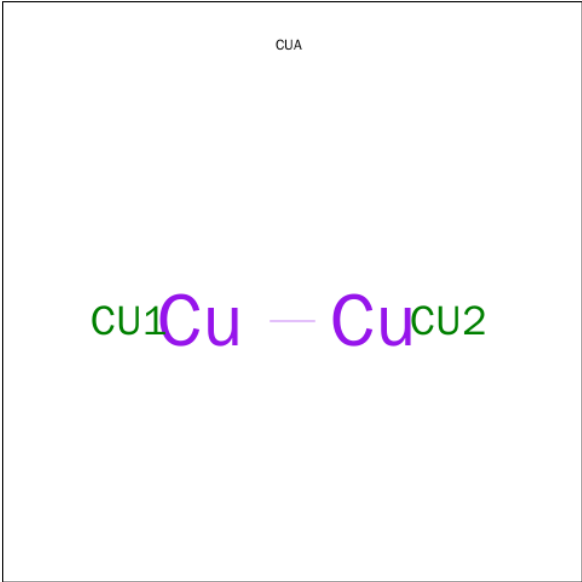
- Molecule 18 is (1R)-2-{{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (three-letter code: PGV) (formula: C<sub>40</sub>H<sub>77</sub>O<sub>10</sub>P).





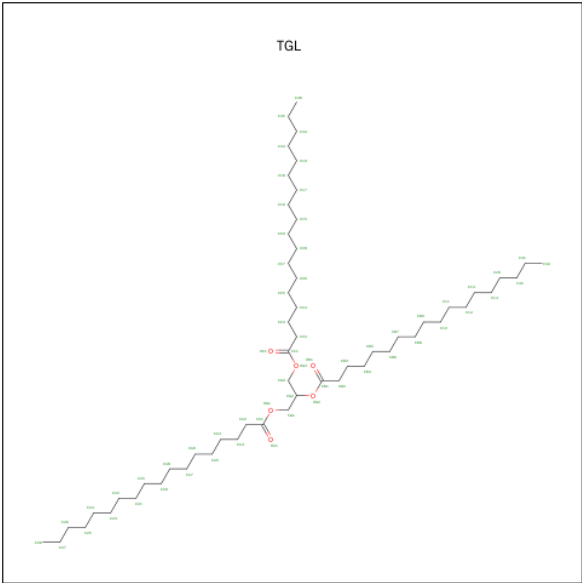
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
18	A	1	Total	C	O	P	0	0
			51	40	10	1		
18	A	1	Total	C	O	P	0	0
			51	40	10	1		
18	C	1	Total	C	O	P	0	0
			51	40	10	1		
18	C	1	Total	C	O	P	0	0
			51	40	10	1		
18	N	1	Total	C	O	P	0	0
			51	40	10	1		
18	P	1	Total	C	O	P	0	0
			51	40	10	1		
18	P	1	Total	C	O	P	0	0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

- Molecule 19 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu<sub>2</sub>).



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

- Molecule 20 is TRISTEAROYLGLYCEROL (three-letter code: TGL) (formula: C<sub>57</sub>H<sub>110</sub>O<sub>6</sub>).



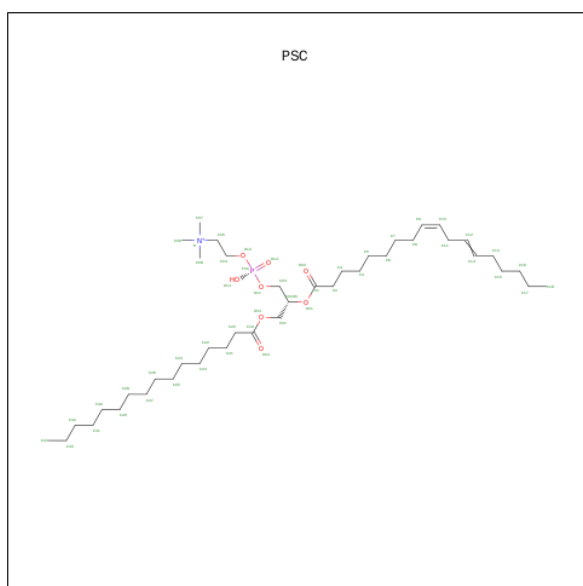
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
20	B	1	Total	C	O	0	0
			63	57	6		
20	D	1	Total	C	O	0	0
			63	57	6		

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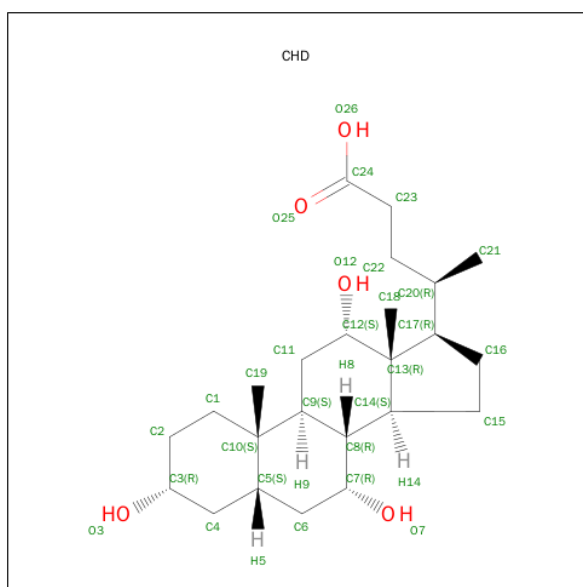
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
20	L	1	Total	C	O	0	0
			63	57	6		
20	N	1	Total	C	O	0	0
			63	57	6		
20	N	1	Total	C	O	0	0
			63	57	6		
20	Q	1	Total	C	O	0	0
			63	57	6		

- Molecule 21 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:  $C_{42}H_{81}NO_8P$ ).



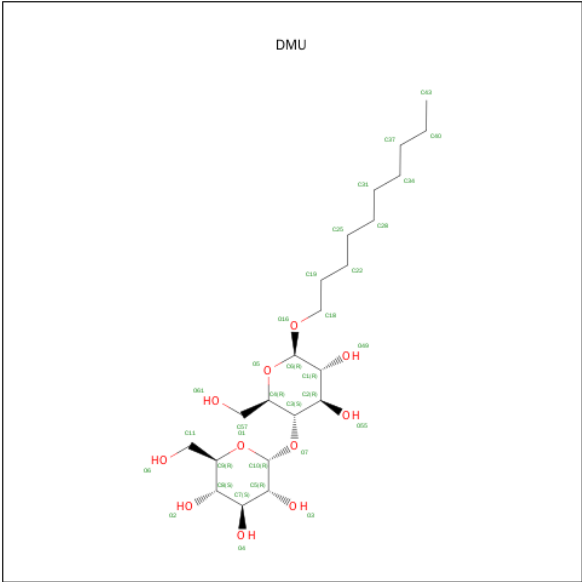
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
21	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
21	O	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

- 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
22	C	1	Total C O 29 24 5	0	0
22	J	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
22	W	1	Total C O 29 24 5	0	0

- Molecule 23 is SUGAR (DECYL-BETA-D-MALTOPYRANOSIDE) (three-letter code: DMU) (formula: C<sub>22</sub>H<sub>42</sub>O<sub>11</sub>).

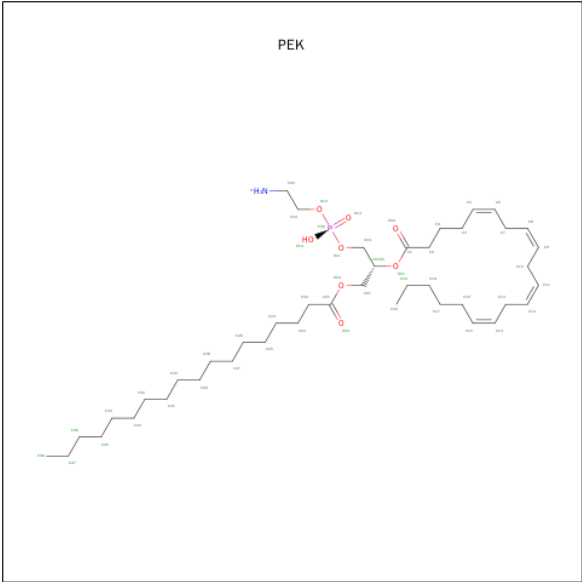


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	C	1	Total	C	O	0	0
			33	22	11		
23	M	1	Total	C	O	0	0
			33	22	11		
23	P	1	Total	C	O	0	0
			33	22	11		
23	Z	1	Total	C	O	0	0
			33	22	11		

- Molecule 24 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

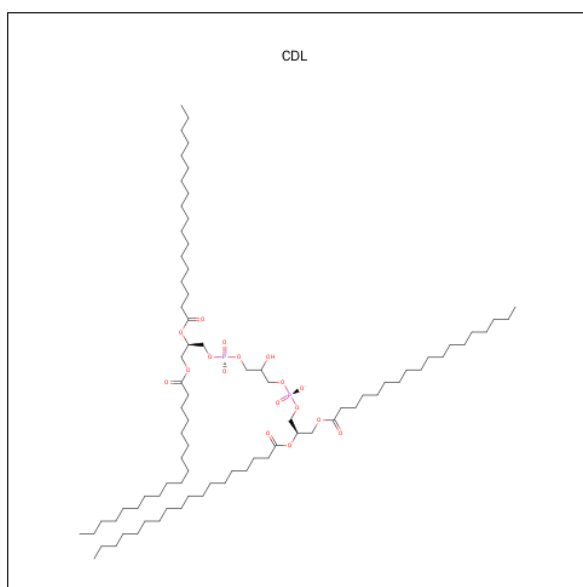
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
24	P	1	Total	X	0	0
			1	1		
24	C	1	Total	X	0	0
			1	1		

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
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	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 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
26	C	1	Total	C	O	P	0	0
			100	81	17	2		
26	G	1	Total	C	O	P	0	0
			100	81	17	2		
26	P	1	Total	C	O	P	0	0
			100	81	17	2		
26	T	1	Total	C	O	P	0	0
			100	81	17	2		

- 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 water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
28	A	243	Total	O	0	0
			243	243		
28	B	186	Total	O	0	0
			186	186		
28	C	127	Total	O	0	0
			127	127		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
28	D	109	Total 109	O 109	0	0
28	E	67	Total 67	O 67	0	0
28	F	85	Total 85	O 85	0	0
28	G	57	Total 57	O 57	0	0
28	H	66	Total 66	O 66	0	0
28	I	58	Total 58	O 58	0	0
28	J	21	Total 21	O 21	0	0
28	K	38	Total 38	O 38	0	0
28	L	22	Total 22	O 22	0	0
28	M	27	Total 27	O 27	0	0
28	N	212	Total 212	O 212	0	0
28	O	152	Total 152	O 152	0	0
28	P	120	Total 120	O 120	0	0
28	Q	75	Total 75	O 75	0	0
28	R	32	Total 32	O 32	0	0
28	S	53	Total 53	O 53	0	0
28	T	59	Total 59	O 59	0	0
28	U	62	Total 62	O 62	0	0
28	V	33	Total 33	O 33	0	0
28	W	18	Total 18	O 18	0	0
28	X	29	Total 29	O 29	0	0

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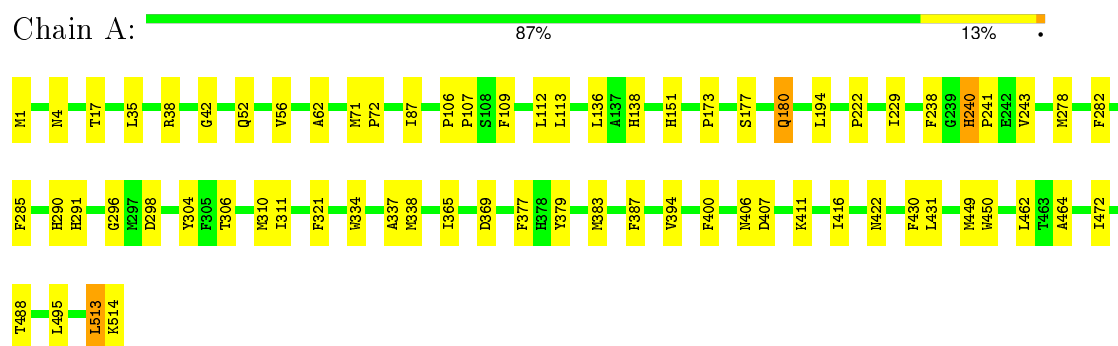
*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
28	Y	31	Total	O	0	0
			31	31		
28	Z	21	Total	O	0	0
			21	21		

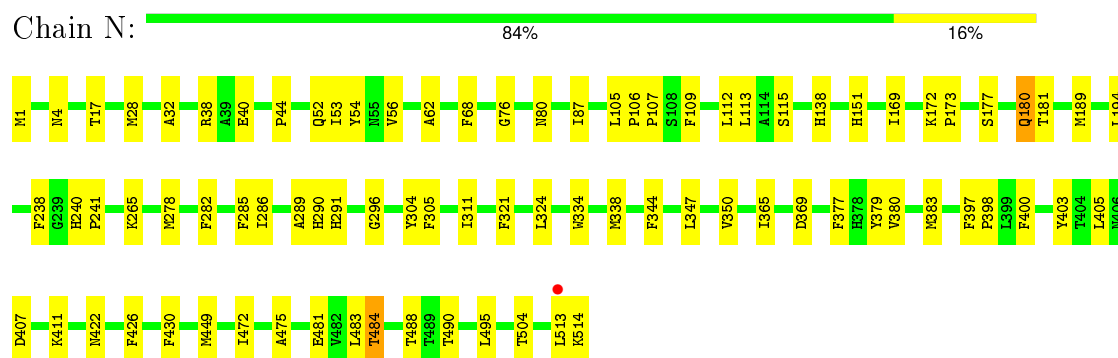
### 3 Residue-property plots

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 ( $\text{RSRZ} > 2$ ). 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.

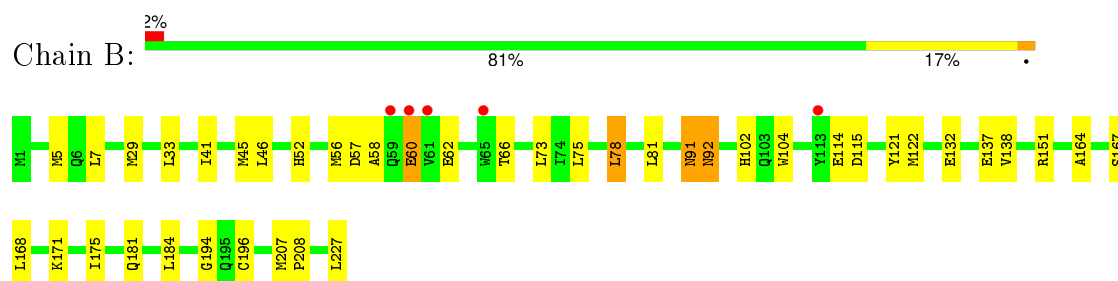
#### • Molecule 1: Cytochrome c oxidase subunit 1



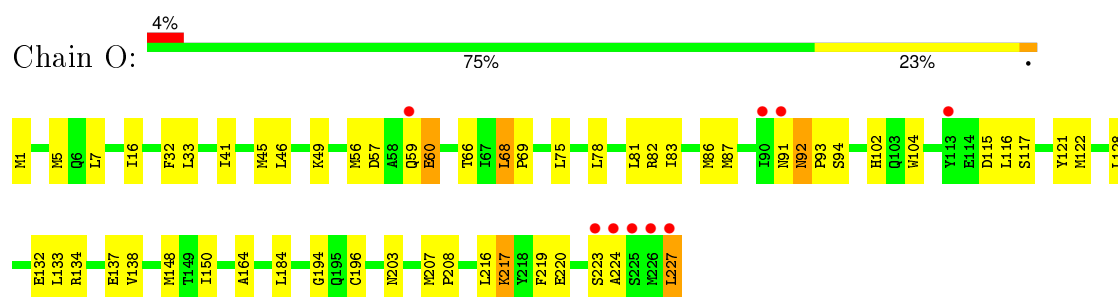
#### • Molecule 1: Cytochrome c oxidase subunit 1



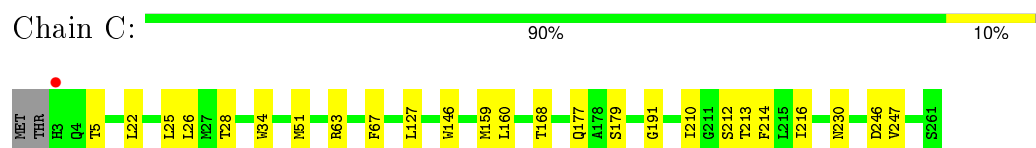
#### • Molecule 2: Cytochrome c oxidase subunit 2



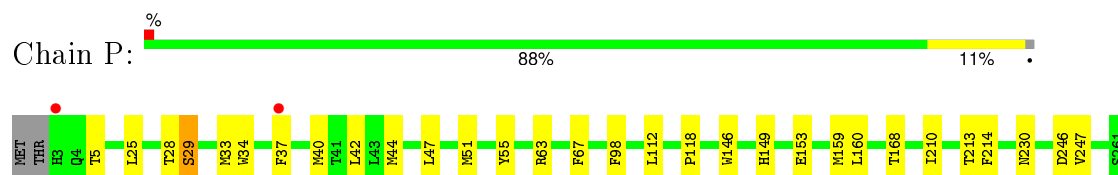
#### • Molecule 2: Cytochrome c oxidase subunit 2



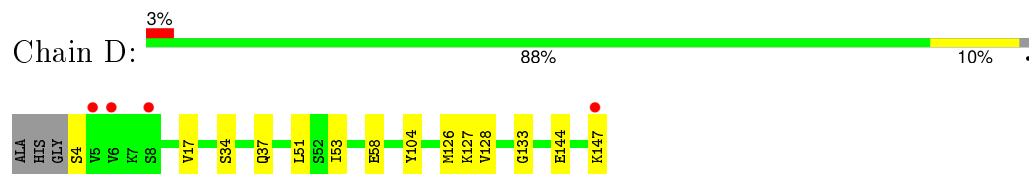
- Molecule 3: Cytochrome c oxidase subunit 3



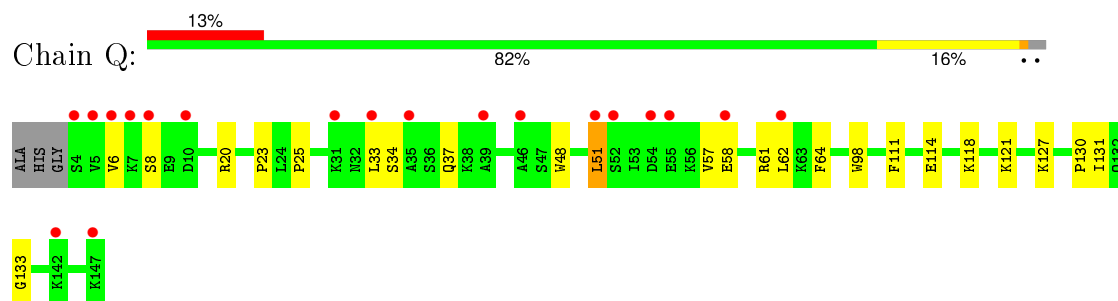
- Molecule 3: Cytochrome c oxidase subunit 3



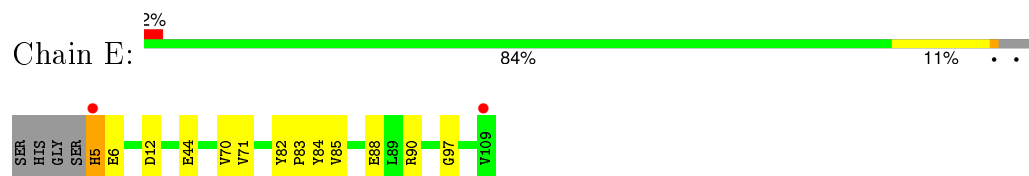
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1



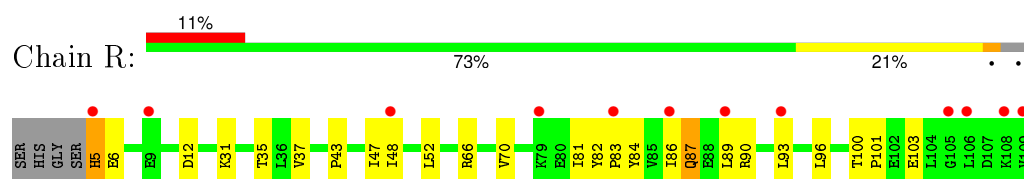
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1



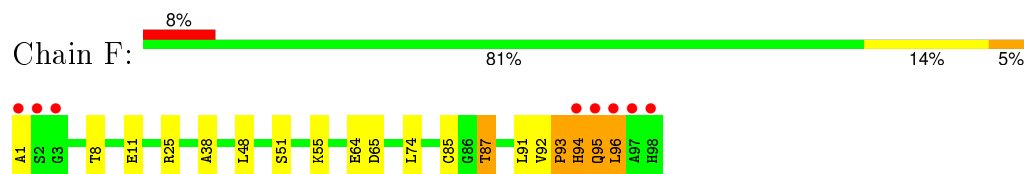
- Molecule 5: Cytochrome c oxidase polypeptide Va



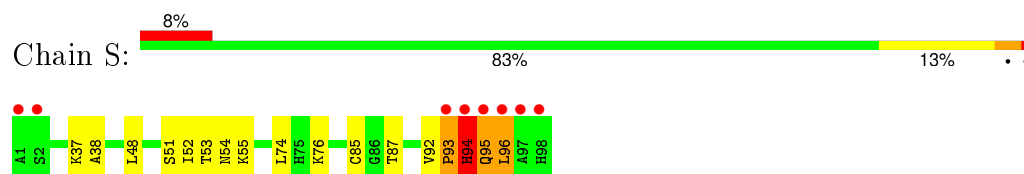
- Molecule 5: Cytochrome c oxidase polypeptide Va



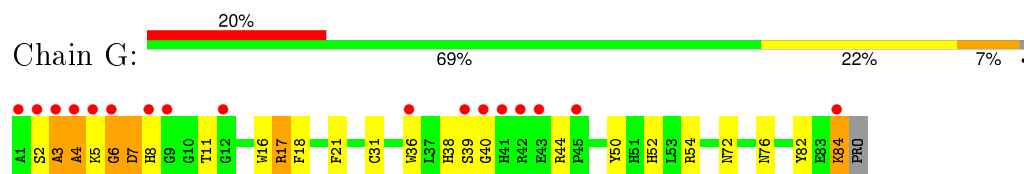
- Molecule 6: Cytochrome c oxidase polypeptide Vb



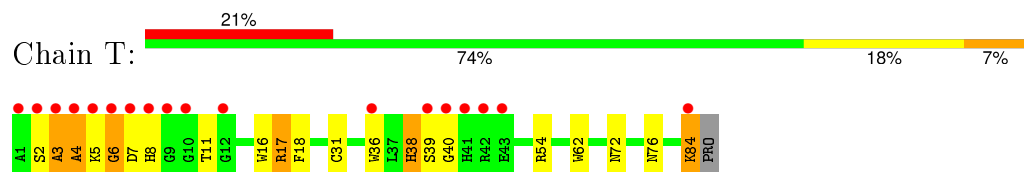
- Molecule 6: Cytochrome c oxidase polypeptide Vb



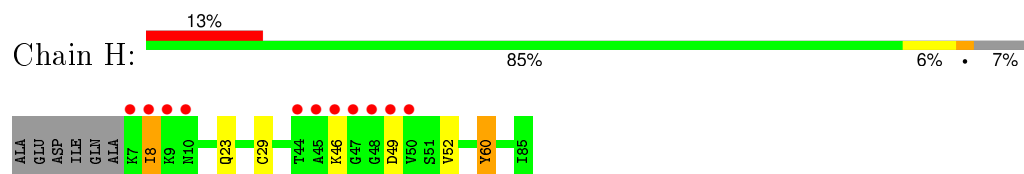
- Molecule 7: Cytochrome c oxidase polypeptide VIa-heart



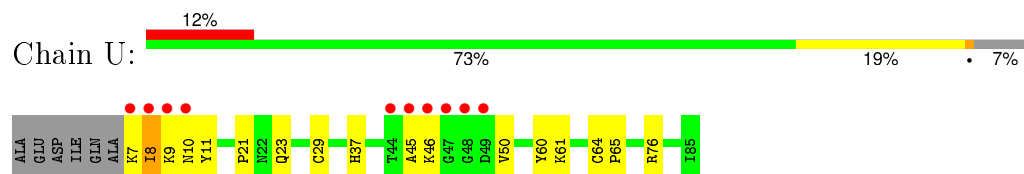
- Molecule 7: Cytochrome c oxidase polypeptide VIa-heart



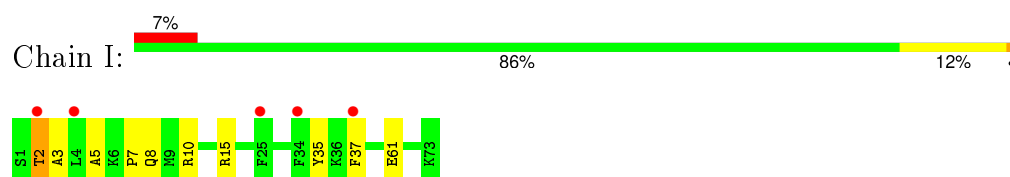
- Molecule 8: Cytochrome c oxidase subunit VIb isoform 1



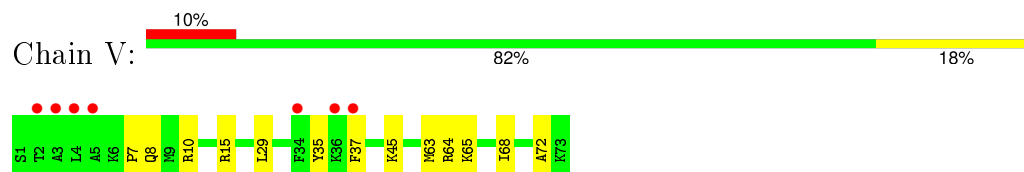
- Molecule 8: Cytochrome c oxidase subunit VIb isoform 1



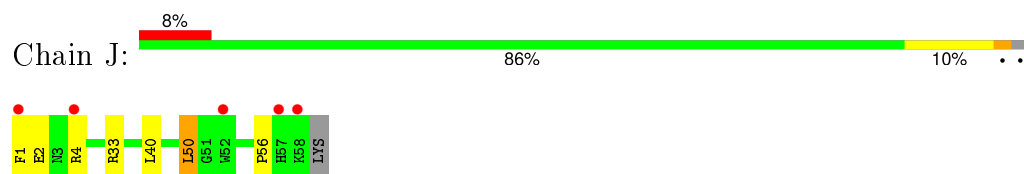
- Molecule 9: Cytochrome c oxidase polypeptide VIc



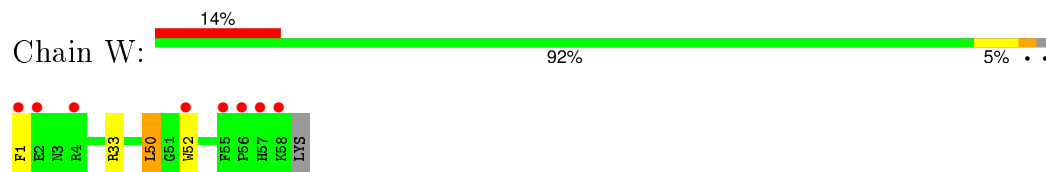
- Molecule 9: Cytochrome c oxidase polypeptide VIc



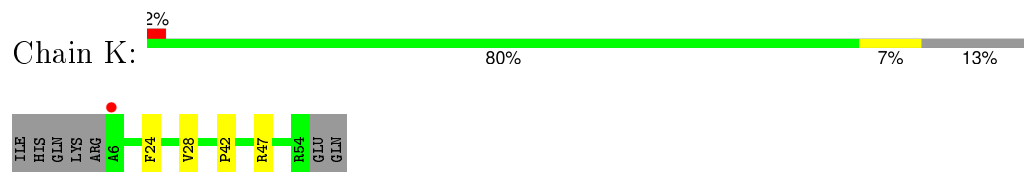
- Molecule 10: Cytochrome c oxidase polypeptide VIIa-heart



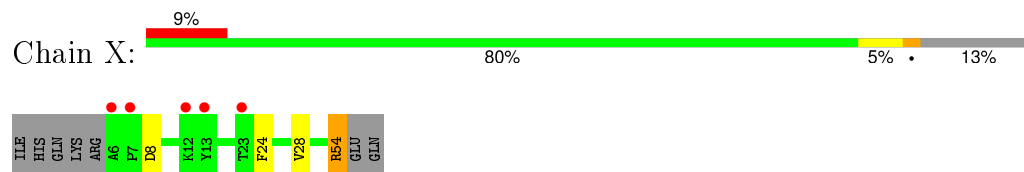
- Molecule 10: Cytochrome c oxidase polypeptide VIIa-heart



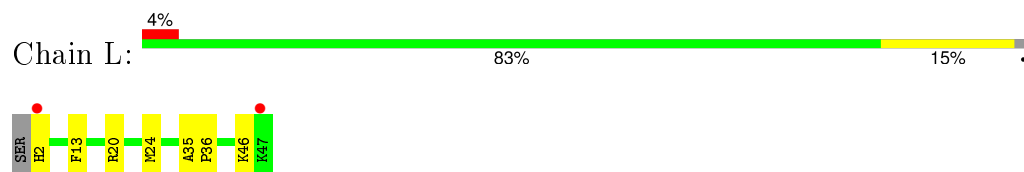
- Molecule 11: Cytochrome c oxidase polypeptide VIIb



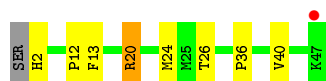
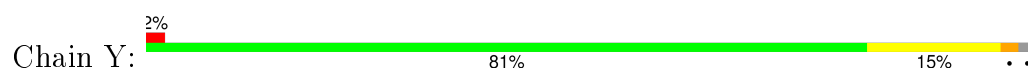
- Molecule 11: Cytochrome c oxidase polypeptide VIIb



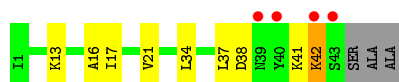
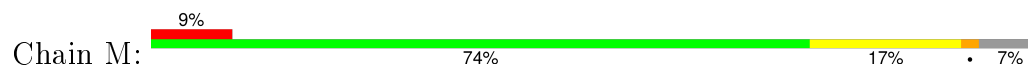
- Molecule 12: Cytochrome c oxidase polypeptide VIIc



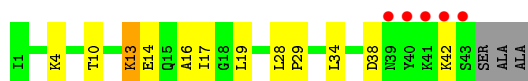
- Molecule 12: Cytochrome c oxidase polypeptide VIIc



- Molecule 13: Cytochrome c oxidase polypeptide VIII-heart



- Molecule 13: Cytochrome c oxidase polypeptide VIII-heart



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	182.59Å 205.14Å 178.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 1.80 68.19 – 1.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-1.80) 98.9 (68.19-1.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.09 (at 1.80Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, $R_{free}$	0.202 , 0.227 0.202 , 0.225	Depositor DCC
$R_{free}$ test set	22930 reflections (3.92%)	DCC
Wilson B-factor (Å <sup>2</sup> )	25.2	Xtriage
Anisotropy	0.024	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 64.0	EDS
Estimated twinning fraction	0.009 for l,-k,h	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	1 of 608996 reflections (0.000%)	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	32735	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.12% 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, CHD, HEA, SAC, CDL, PSC, PEK, MG, TGL, PGV, TPO, UNX, CUA, NA, FME, 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	0.49	0/4156	0.67	0/5678
1	N	0.48	0/4156	0.65	0/5678
2	B	0.48	0/1860	0.76	0/2534
2	O	0.50	0/1860	0.79	1/2534 (0.0%)
3	C	0.51	0/2197	0.58	0/3005
3	P	0.48	0/2197	0.61	0/3005
4	D	0.47	0/1229	0.66	1/1658 (0.1%)
4	Q	0.50	0/1229	0.65	1/1658 (0.1%)
5	E	0.50	0/871	0.66	0/1182
5	R	0.48	0/871	0.68	0/1182
6	F	0.47	0/765	0.83	3/1038 (0.3%)
6	S	0.47	0/765	0.87	3/1038 (0.3%)
7	G	0.51	0/690	0.70	1/937 (0.1%)
7	T	0.53	0/690	0.70	1/937 (0.1%)
8	H	0.47	0/682	0.68	0/921
8	U	0.48	0/682	0.67	0/921
9	I	0.52	0/605	0.59	0/802
9	V	0.51	0/605	0.62	0/802
10	J	0.45	0/471	0.60	0/636
10	W	0.46	0/471	0.63	0/636
11	K	0.48	0/398	0.66	0/546
11	X	0.47	0/398	0.65	0/546
12	L	0.48	0/393	0.55	0/526
12	Y	0.53	0/393	0.57	0/526
13	M	0.46	0/345	0.62	0/470
13	Z	0.45	0/345	0.62	0/470
All	All	0.49	0/29324	0.67	11/39866 (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
1	A	0	1
1	N	0	1
8	U	0	1
All	All	0	3

There are no bond length outliers.

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	S	94	HIS	N-CA-C	7.74	131.91	111.00
6	F	94	HIS	N-CA-C	7.14	130.29	111.00
4	D	133	GLY	N-CA-C	5.67	127.28	113.10
2	O	227	LEU	CA-CB-CG	5.64	128.28	115.30
4	Q	133	GLY	N-CA-C	5.61	127.12	113.10

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	240	HIS	Sidechain
1	N	240	HIS	Sidechain
8	U	11	TYR	Sidechain

## 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	63	0
1	N	4027	0	4001	74	0
2	B	1824	0	1833	28	0
2	O	1824	0	1833	39	0
3	C	2110	0	2027	24	0
3	P	2110	0	2027	29	0
4	D	1195	0	1183	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	Q	1195	0	1183	18	0
5	E	852	0	845	6	0
5	R	852	0	845	15	0
6	F	748	0	728	12	0
6	S	748	0	728	15	0
7	G	675	0	644	26	0
7	T	675	0	644	28	0
8	H	662	0	623	4	0
8	U	662	0	623	9	0
9	I	601	0	613	6	0
9	V	601	0	613	9	0
10	J	460	0	459	6	0
10	W	460	0	459	4	0
11	K	384	0	366	3	0
11	X	384	0	366	6	0
12	L	380	0	380	14	0
12	Y	380	0	380	9	0
13	M	335	0	352	6	0
13	Z	335	0	352	6	0
14	A	1	0	0	0	0
14	N	1	0	0	0	0
15	A	1	0	0	0	0
15	N	1	0	0	0	0
16	A	1	0	0	0	0
16	N	1	0	0	0	0
17	A	120	0	108	3	0
17	N	120	0	108	4	0
18	A	102	0	152	7	0
18	C	102	0	152	7	0
18	N	51	0	76	2	0
18	P	102	0	152	8	0
18	Z	51	0	76	4	0
19	B	2	0	0	0	0
19	O	2	0	0	0	0
20	B	63	0	110	10	0
20	D	63	0	110	5	0
20	L	63	0	110	23	0
20	N	126	0	220	30	0
20	Q	63	0	110	6	0
21	B	52	0	80	13	0
21	O	52	0	80	12	0
22	B	29	0	39	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	C	58	0	78	2	0
22	J	29	0	39	2	0
22	O	29	0	39	1	0
22	P	58	0	78	2	0
22	W	29	0	39	2	0
23	C	33	0	36	2	0
23	M	33	0	36	0	0
23	P	33	0	36	7	0
23	Z	33	0	36	1	0
24	C	1	0	0	0	0
24	P	1	0	0	0	0
25	C	106	0	154	11	0
25	G	53	0	77	7	0
25	P	106	0	154	12	0
25	T	53	0	77	8	0
26	C	100	0	156	16	0
26	G	100	0	156	21	0
26	P	100	0	156	13	0
26	T	100	0	156	21	0
27	F	1	0	0	0	0
27	S	1	0	0	0	0
28	A	243	0	0	4	0
28	B	186	0	0	4	0
28	C	127	0	0	2	0
28	D	109	0	0	4	0
28	E	67	0	0	0	0
28	F	85	0	0	1	0
28	G	57	0	0	2	0
28	H	66	0	0	1	0
28	I	58	0	0	3	0
28	J	21	0	0	1	0
28	K	38	0	0	0	0
28	L	22	0	0	2	0
28	M	27	0	0	2	0
28	N	212	0	0	3	0
28	O	152	0	0	2	0
28	P	120	0	0	3	0
28	Q	75	0	0	3	0
28	R	32	0	0	0	0
28	S	53	0	0	1	0
28	T	59	0	0	2	0
28	U	62	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	V	33	0	0	2	0
28	W	18	0	0	0	0
28	X	29	0	0	1	0
28	Y	31	0	0	2	0
28	Z	21	0	0	2	0
All	All	32735	0	31294	534	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 534 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)
7:G:84:LYS:HD2	7:G:84:LYS:H	1.17	1.05
7:T:84:LYS:H	7:T:84:LYS:HD2	1.19	1.02
3:C:63:ARG:HE	26:C:270:CDL:HA22	1.24	1.01
21:O:1230:PSC:H142	21:O:1230:PSC:H343	1.42	1.01
21:B:230:PSC:H343	21:B:230:PSC:H142	1.42	1.01

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%)	497 (97%)	15 (3%)	0	100	100
1	N	512/514 (100%)	497 (97%)	15 (3%)	0	100	100
2	B	225/227 (99%)	211 (94%)	12 (5%)	2 (1%)	21	7
2	O	225/227 (99%)	208 (92%)	15 (7%)	2 (1%)	21	7
3	C	257/261 (98%)	252 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	P	257/261 (98%)	251 (98%)	6 (2%)	0	100	100
4	D	142/147 (97%)	138 (97%)	4 (3%)	0	100	100
4	Q	142/147 (97%)	138 (97%)	4 (3%)	0	100	100
5	E	103/109 (94%)	103 (100%)	0	0	100	100
5	R	103/109 (94%)	102 (99%)	1 (1%)	0	100	100
6	F	96/98 (98%)	89 (93%)	5 (5%)	2 (2%)	9	1
6	S	96/98 (98%)	90 (94%)	3 (3%)	3 (3%)	5	0
7	G	81/85 (95%)	67 (83%)	7 (9%)	7 (9%)	1	0
7	T	81/85 (95%)	65 (80%)	9 (11%)	7 (9%)	1	0
8	H	77/85 (91%)	70 (91%)	5 (6%)	2 (3%)	7	1
8	U	77/85 (91%)	70 (91%)	5 (6%)	2 (3%)	7	1
9	I	71/73 (97%)	67 (94%)	4 (6%)	0	100	100
9	V	71/73 (97%)	66 (93%)	5 (7%)	0	100	100
10	J	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
10	W	56/59 (95%)	54 (96%)	2 (4%)	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%)	43 (98%)	1 (2%)	0	100	100
12	Y	44/47 (94%)	43 (98%)	1 (2%)	0	100	100
13	M	41/46 (89%)	41 (100%)	0	0	100	100
13	Z	41/46 (89%)	41 (100%)	0	0	100	100
All	All	3504/3614 (97%)	3350 (96%)	127 (4%)	27 (1%)	24	8

5 of 27 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	G	4	ALA
7	G	7	ASP
7	G	8	HIS
7	G	39	SER
6	S	94	HIS

### 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%)	417 (98%)	9 (2%)	61	47
1	N	426/426 (100%)	414 (97%)	12 (3%)	51	35
2	B	210/210 (100%)	201 (96%)	9 (4%)	35	17
2	O	210/210 (100%)	199 (95%)	11 (5%)	29	12
3	C	224/226 (99%)	220 (98%)	4 (2%)	66	54
3	P	224/226 (99%)	219 (98%)	5 (2%)	60	45
4	D	128/129 (99%)	126 (98%)	2 (2%)	70	59
4	Q	128/129 (99%)	125 (98%)	3 (2%)	58	42
5	E	92/95 (97%)	89 (97%)	3 (3%)	45	27
5	R	92/95 (97%)	89 (97%)	3 (3%)	45	27
6	F	81/81 (100%)	79 (98%)	2 (2%)	55	39
6	S	81/81 (100%)	78 (96%)	3 (4%)	41	23
7	G	67/68 (98%)	62 (92%)	5 (8%)	17	5
7	T	67/68 (98%)	61 (91%)	6 (9%)	12	3
8	H	71/75 (95%)	68 (96%)	3 (4%)	36	18
8	U	71/75 (95%)	68 (96%)	3 (4%)	36	18
9	I	57/57 (100%)	52 (91%)	5 (9%)	12	3
9	V	57/57 (100%)	55 (96%)	2 (4%)	43	25
10	J	49/50 (98%)	48 (98%)	1 (2%)	63	49
10	W	49/50 (98%)	48 (98%)	1 (2%)	63	49
11	K	39/46 (85%)	39 (100%)	0	100	100
11	X	39/46 (85%)	38 (97%)	1 (3%)	54	37
12	L	39/40 (98%)	38 (97%)	1 (3%)	54	37
12	Y	39/40 (98%)	37 (95%)	2 (5%)	29	12
13	M	37/38 (97%)	33 (89%)	4 (11%)	8	2
13	Z	37/38 (97%)	33 (89%)	4 (11%)	8	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3040/3082 (99%)	2936 (97%)	104 (3%)	44 26

5 of 104 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	M	42	LYS
1	N	504	THR
10	W	50	LEU
1	N	38	ARG
1	N	180	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
7	G	76	ASN
1	N	178	GLN
7	T	76	ASN
9	I	8	GLN
11	K	35	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	0.60	0	6,9,11	1.34	1 (16%)
2	FME	B	1	2	8,9,10	0.79	0	6,9,11	1.94	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	1.58	1 (12%)	7,14,16	1.04	0
9	SAC	I	1	9	7,8,9	2.50	2 (28%)	7,9,11	2.05	2 (28%)
1	FME	N	1	1	8,9,10	0.68	0	6,9,11	1.80	2 (33%)
2	FME	O	1	2	8,9,10	0.60	0	6,9,11	1.32	1 (16%)
7	TPO	T	11	7	8,10,11	1.33	1 (12%)	7,14,16	1.07	1 (14%)
9	SAC	V	1	9	7,8,9	2.69	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 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	T	11	TPO	CB-CA	2.94	1.59	1.54
7	G	11	TPO	CB-CA	3.51	1.60	1.54
9	I	1	SAC	CA-N	4.05	1.52	1.46
9	V	1	SAC	CA-N	4.49	1.52	1.46
9	I	1	SAC	OAC-C1A	5.01	1.34	1.23

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	-4.41	116.05	122.82
1	N	1	FME	CA-N-CN	-3.73	117.09	122.82
9	V	1	SAC	CA-N-C1A	-3.18	110.59	121.37
9	I	1	SAC	CA-N-C1A	-2.77	111.98	121.37
2	O	1	FME	CA-N-CN	-2.69	118.68	122.82

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
1	A	1	FME	O1-CN-N-CA
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 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1	FME	3	0
7	G	11	TPO	1	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 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	$\# Z  > 2$
17	HEA	A	515	1	40,67,67	1.19	3 (7%)	41,103,103	1.59	8 (19%)
17	HEA	A	516	1	40,67,67	1.53	6 (15%)	41,103,103	1.34	8 (19%)
18	PGV	A	524	-	50,50,50	1.06	3 (6%)	51,56,56	0.89	1 (1%)
18	PGV	A	525	-	50,50,50	0.89	2 (4%)	51,56,56	0.78	2 (3%)
22	CHD	B	1086	-	29,32,32	0.63	0	48,51,51	1.77	14 (29%)
19	CUA	B	228	2	0,1,1	0.00	-	0,0,0	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
21	PSC	B	230	-	51,51,51	1.18	3 (5%)	55,59,59	0.94	1 (1%)
20	TGL	B	521	-	62,62,62	0.67	0	65,65,65	1.49	11 (16%)
25	PEK	C	264	-	51,52,52	1.43	4 (7%)	52,57,57	1.08	3 (5%)
25	PEK	C	265	-	51,52,52	1.63	9 (17%)	52,57,57	1.11	5 (9%)
18	PGV	C	267	-	50,50,50	0.83	1 (2%)	51,56,56	0.86	2 (3%)
18	PGV	C	268	-	50,50,50	1.21	3 (6%)	51,56,56	0.78	1 (1%)
26	CDL	C	270	-	99,99,99	0.78	3 (3%)	101,111,111	0.94	5 (4%)
22	CHD	C	271	-	29,32,32	0.74	0	48,51,51	3.62	21 (43%)
23	DMU	C	272	-	34,34,34	2.96	8 (23%)	45,45,45	4.18	19 (42%)
22	CHD	C	525	-	29,32,32	0.76	1 (3%)	48,51,51	1.64	10 (20%)
20	TGL	D	523	-	62,62,62	0.76	1 (1%)	65,65,65	1.37	8 (12%)
25	PEK	G	1263	-	51,52,52	1.84	11 (21%)	52,57,57	1.15	3 (5%)
26	CDL	G	269	-	99,99,99	0.92	5 (5%)	101,111,111	0.94	6 (5%)
22	CHD	J	60	-	29,32,32	0.81	1 (3%)	48,51,51	3.21	25 (52%)
20	TGL	L	522	-	62,62,62	1.10	4 (6%)	65,65,65	1.69	13 (20%)
23	DMU	M	526	-	34,34,34	3.19	8 (23%)	45,45,45	4.31	19 (42%)
18	PGV	N	1266	-	50,50,50	0.93	2 (4%)	51,56,56	0.83	3 (5%)
20	TGL	N	1521	-	62,62,62	0.70	2 (3%)	65,65,65	1.47	10 (15%)
20	TGL	N	1522	-	62,62,62	1.13	5 (8%)	65,65,65	1.67	12 (18%)
17	HEA	N	515	1	40,67,67	1.26	6 (15%)	41,103,103	1.56	9 (21%)
17	HEA	N	516	1	40,67,67	1.37	6 (15%)	41,103,103	1.39	8 (19%)
21	PSC	O	1230	-	51,51,51	1.14	3 (5%)	55,59,59	0.94	1 (1%)
19	CUA	O	228	2	0,1,1	0.00	-	0,0,0	0.00	-
22	CHD	O	229	-	29,32,32	0.74	0	48,51,51	1.81	13 (27%)
25	PEK	P	1264	-	51,52,52	1.42	4 (7%)	52,57,57	1.12	3 (5%)
25	PEK	P	1265	-	51,52,52	1.66	11 (21%)	52,57,57	1.09	5 (9%)
18	PGV	P	1267	-	50,50,50	0.84	1 (2%)	51,56,56	0.86	1 (1%)
18	PGV	P	1268	-	50,50,50	1.24	3 (6%)	51,56,56	0.80	1 (1%)
26	CDL	P	1270	-	99,99,99	0.81	3 (3%)	101,111,111	0.92	5 (4%)
22	CHD	P	1271	-	29,32,32	0.72	0	48,51,51	3.56	21 (43%)
23	DMU	P	1272	-	34,34,34	2.97	8 (23%)	45,45,45	4.17	19 (42%)
22	CHD	P	1525	-	29,32,32	0.76	0	48,51,51	1.57	8 (16%)
20	TGL	Q	1523	-	62,62,62	0.79	2 (3%)	65,65,65	1.34	8 (12%)
26	CDL	T	1269	-	99,99,99	0.89	5 (5%)	101,111,111	0.95	6 (5%)
25	PEK	T	263	-	51,52,52	1.85	11 (21%)	52,57,57	1.15	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	CHD	W	1060	-	29,32,32	0.89	1 (3%)	48,51,51	3.19	25 (52%)
18	PGV	Z	1524	-	50,50,50	1.04	4 (8%)	51,56,56	0.86	2 (3%)
23	DMU	Z	1526	-	34,34,34	3.15	8 (23%)	45,45,45	4.25	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
17	HEA	A	515	1	3/3/7/16	0/24/76/76	0/0/8/8
17	HEA	A	516	1	3/3/7/16	0/24/76/76	0/0/8/8
18	PGV	A	524	-	-	2/55/55/55	0/0/0/0
18	PGV	A	525	-	-	0/55/55/55	0/0/0/0
22	CHD	B	1086	-	-	0/7/74/74	0/4/4/4
19	CUA	B	228	2	-	0/0/0/0	0/0/0/0
21	PSC	B	230	-	-	0/55/55/55	0/0/0/0
20	TGL	B	521	-	-	0/65/65/65	0/0/0/0
25	PEK	C	264	-	-	0/56/56/56	0/0/0/0
25	PEK	C	265	-	-	0/56/56/56	0/0/0/0
18	PGV	C	267	-	-	0/55/55/55	0/0/0/0
18	PGV	C	268	-	-	0/55/55/55	0/0/0/0
26	CDL	C	270	-	-	0/110/110/110	0/0/0/0
22	CHD	C	271	-	5/5/12/12	0/7/74/74	0/4/4/4
23	DMU	C	272	-	6/6/10/10	0/19/59/59	0/2/2/2
22	CHD	C	525	-	-	0/7/74/74	0/4/4/4
20	TGL	D	523	-	-	0/65/65/65	0/0/0/0
25	PEK	G	1263	-	-	0/56/56/56	0/0/0/0
26	CDL	G	269	-	-	0/110/110/110	0/0/0/0
22	CHD	J	60	-	5/5/12/12	0/7/74/74	0/4/4/4
20	TGL	L	522	-	-	0/65/65/65	0/0/0/0
23	DMU	M	526	-	5/5/10/10	0/19/59/59	0/2/2/2
18	PGV	N	1266	-	-	0/55/55/55	0/0/0/0
20	TGL	N	1521	-	-	0/65/65/65	0/0/0/0
20	TGL	N	1522	-	-	0/65/65/65	0/0/0/0
17	HEA	N	515	1	3/3/7/16	0/24/76/76	0/0/8/8
17	HEA	N	516	1	3/3/7/16	0/24/76/76	0/0/8/8
21	PSC	O	1230	-	-	0/55/55/55	0/0/0/0
19	CUA	O	228	2	-	0/0/0/0	0/0/0/0
22	CHD	O	229	-	-	0/7/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	PEK	P	1264	-	-	0/56/56/56	0/0/0/0
25	PEK	P	1265	-	-	0/56/56/56	0/0/0/0
18	PGV	P	1267	-	-	0/55/55/55	0/0/0/0
18	PGV	P	1268	-	-	0/55/55/55	0/0/0/0
26	CDL	P	1270	-	-	0/110/110/110	0/0/0/0
22	CHD	P	1271	-	5/5/12/12	0/7/74/74	0/4/4/4
23	DMU	P	1272	-	6/6/10/10	0/19/59/59	0/2/2/2
22	CHD	P	1525	-	-	0/7/74/74	0/4/4/4
20	TGL	Q	1523	-	-	0/65/65/65	0/0/0/0
26	CDL	T	1269	-	-	0/110/110/110	0/0/0/0
25	PEK	T	263	-	-	0/56/56/56	0/0/0/0
22	CHD	W	1060	-	5/5/12/12	0/7/74/74	0/4/4/4
18	PGV	Z	1524	-	-	2/55/55/55	0/0/0/0
23	DMU	Z	1526	-	5/5/10/10	0/19/59/59	0/2/2/2

The worst 5 of 161 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	Z	1526	DMU	O7-C3	-8.34	1.23	1.43
23	M	526	DMU	O7-C3	-8.28	1.23	1.43
23	M	526	DMU	O1-C9	-7.00	1.26	1.44
23	P	1272	DMU	O1-C9	-6.93	1.27	1.44
23	M	526	DMU	O16-C6	-6.92	1.27	1.40

The worst 5 of 367 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	P	1271	CHD	C17-C13-C12	-9.83	108.97	117.68
22	C	271	CHD	C17-C13-C12	-9.77	109.02	117.68
22	C	271	CHD	C19-C10-C9	-7.72	99.61	111.18
22	P	1271	CHD	C19-C10-C9	-7.14	100.48	111.18
23	M	526	DMU	C8-C7-C5	-6.67	98.34	110.79

5 of 54 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	M	526	DMU	C4
23	M	526	DMU	C5
23	M	526	DMU	C6
23	M	526	DMU	C2
23	M	526	DMU	C9

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	A	524	PGV	C02-O01-C1-C2
18	Z	1524	PGV	C02-O01-C1-C2
18	Z	1524	PGV	P-O11-C03-C02
18	A	524	PGV	P-O11-C03-C02

There are no ring outliers.

37 monomers are involved in 249 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	A	515	HEA	2	0
17	A	516	HEA	1	0
18	A	524	PGV	6	0
18	A	525	PGV	1	0
21	B	230	PSC	13	0
20	B	521	TGL	10	0
25	C	264	PEK	5	0
25	C	265	PEK	6	0
18	C	267	PGV	6	0
18	C	268	PGV	1	0
26	C	270	CDL	16	0
22	C	271	CHD	2	0
23	C	272	DMU	2	0
20	D	523	TGL	5	0
25	G	1263	PEK	7	0
26	G	269	CDL	21	0
22	J	60	CHD	2	0
20	L	522	TGL	23	0
18	N	1266	PGV	2	0
20	N	1521	TGL	14	0
20	N	1522	TGL	16	0
17	N	515	HEA	4	0
21	O	1230	PSC	12	0
22	O	229	CHD	1	0
25	P	1264	PEK	6	0
25	P	1265	PEK	6	0
18	P	1267	PGV	5	0
18	P	1268	PGV	3	0
26	P	1270	CDL	13	0
22	P	1271	CHD	2	0
23	P	1272	DMU	7	0
20	Q	1523	TGL	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	T	1269	CDL	21	0
25	T	263	PEK	8	0
22	W	1060	CHD	2	0
18	Z	1524	PGV	4	0
23	Z	1526	DMU	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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%)	-0.19	0 100 100	16, 22, 31, 72	0
1	N	513/514 (99%)	-0.24	1 (0%) 95 93	17, 24, 34, 66	0
2	B	226/227 (99%)	-0.47	5 (2%) 65 60	18, 29, 52, 90	0
2	O	226/227 (99%)	-0.18	9 (3%) 42 36	22, 32, 61, 84	0
3	C	259/261 (99%)	-0.50	1 (0%) 93 91	19, 25, 39, 70	0
3	P	259/261 (99%)	-0.44	2 (0%) 87 85	19, 26, 40, 74	0
4	D	144/147 (97%)	-0.30	4 (2%) 56 51	21, 31, 57, 86	0
4	Q	144/147 (97%)	1.04	19 (13%) 4 3	28, 42, 65, 100	0
5	E	105/109 (96%)	-0.01	2 (1%) 70 66	22, 31, 59, 101	0
5	R	105/109 (96%)	0.81	12 (11%) 7 5	25, 39, 71, 102	0
6	F	98/98 (100%)	0.26	8 (8%) 14 11	20, 32, 88, 110	0
6	S	98/98 (100%)	0.27	8 (8%) 14 11	20, 31, 93, 106	0
7	G	83/85 (97%)	0.83	17 (20%) 1 1	23, 34, 99, 107	0
7	T	83/85 (97%)	0.88	18 (21%) 1 1	23, 36, 102, 109	0
8	H	79/85 (92%)	0.25	11 (13%) 4 3	23, 35, 90, 108	0
8	U	79/85 (92%)	0.42	10 (12%) 5 4	27, 39, 91, 110	0
9	I	72/73 (98%)	0.35	5 (6%) 20 16	25, 44, 65, 85	0
9	V	72/73 (98%)	0.66	7 (9%) 10 7	24, 49, 68, 94	0
10	J	58/59 (98%)	0.38	5 (8%) 13 10	26, 36, 73, 99	0
10	W	58/59 (98%)	0.47	8 (13%) 4 3	26, 38, 75, 106	0
11	K	49/56 (87%)	-0.13	1 (2%) 68 64	27, 36, 50, 66	0
11	X	49/56 (87%)	0.84	5 (10%) 9 6	35, 41, 60, 76	0
12	L	46/47 (97%)	-0.36	2 (4%) 39 32	22, 28, 52, 87	0
12	Y	46/47 (97%)	-0.28	1 (2%) 65 60	26, 34, 65, 88	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	M	43/46 (93%)	-0.07	4 (9%) 11 8	23, 28, 75, 103	0
13	Z	43/46 (93%)	0.35	5 (11%) 6 5	31, 36, 80, 106	0
All	All	3550/3614 (98%)	-0.01	170 (4%) 34 28	16, 29, 64, 110	0

The worst 5 of 170 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	Q	5	VAL	26.1
4	Q	6	VAL	25.0
4	Q	4	SER	19.3
6	S	97	ALA	17.2
6	F	96	LEU	12.2

## 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
2	FME	O	1	10/11	0.93	0.15	-	37,38,47,53	0
7	TPO	T	11	11/12	0.53	0.31	-	76,84,110,112	0
2	FME	B	1	10/11	0.93	0.14	-	23,31,39,50	0
9	SAC	I	1	9/10	0.69	0.39	-	93,97,99,99	0
1	FME	N	1	10/11	0.90	0.16	-	39,43,65,69	0
9	SAC	V	1	9/10	0.51	0.49	-	99,100,104,104	0
1	FME	A	1	10/11	0.83	0.15	-	40,45,66,72	0
7	TPO	G	11	11/12	0.38	0.37	-	77,85,107,108	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
23	DMU	C	272	33/33	0.58	0.39	15.12	71,97,102,104	0
18	PGV	A	524	51/51	0.74	0.26	11.05	35,71,101,104	0
26	CDL	P	1270	100/100	0.67	0.37	9.51	42,88,101,105	0
20	TGL	L	522	63/63	0.71	0.30	9.41	34,65,79,81	0
20	TGL	N	1522	63/63	0.63	0.32	8.88	42,67,79,82	0
20	TGL	N	1521	63/63	0.78	0.24	8.00	49,67,84,86	0
26	CDL	C	270	100/100	0.73	0.38	7.76	44,87,100,106	0
22	CHD	W	1060	29/29	0.64	0.40	7.71	98,104,106,108	0
22	CHD	J	60	29/29	0.73	0.37	7.68	98,104,107,109	0
23	DMU	P	1272	33/33	0.56	0.39	7.25	73,96,104,105	0
20	TGL	B	521	63/63	0.80	0.23	7.23	49,64,85,90	0
18	PGV	Z	1524	51/51	0.78	0.27	6.79	38,71,101,104	0
20	TGL	D	523	63/63	0.74	0.23	5.39	47,65,79,82	0
20	TGL	Q	1523	63/63	0.67	0.23	3.64	45,70,80,84	0
26	CDL	G	269	100/100	0.59	0.32	3.59	61,83,101,105	0
18	PGV	C	268	51/51	0.62	0.39	2.85	65,84,103,106	0
21	PSC	B	230	52/52	0.61	0.35	2.80	48,84,113,116	0
26	CDL	T	1269	100/100	0.59	0.32	2.64	54,84,97,105	0
18	PGV	P	1268	51/51	0.69	0.37	2.30	65,84,104,106	0
23	DMU	Z	1526	33/33	0.89	0.19	2.15	40,49,61,64	0
21	PSC	O	1230	52/52	0.59	0.34	2.13	48,80,111,116	0
18	PGV	P	1267	51/51	0.96	0.12	1.91	23,34,59,61	0
22	CHD	P	1271	29/29	0.78	0.28	1.74	89,95,98,101	0
25	PEK	P	1264	53/53	0.95	0.13	1.65	25,44,68,72	0
25	PEK	G	1263	53/53	0.61	0.39	1.58	46,83,99,101	0
18	PGV	C	267	51/51	0.97	0.10	1.40	20,34,58,62	0
25	PEK	T	263	53/53	0.50	0.40	1.38	45,83,100,103	0
25	PEK	P	1265	53/53	0.52	0.33	1.37	46,89,107,109	0
22	CHD	C	271	29/29	0.76	0.26	1.32	87,95,96,97	0
15	MG	A	518	1/1	0.99	0.10	1.12	20,20,20,20	0
25	PEK	C	264	53/53	0.96	0.12	1.10	10,44,70,73	0
23	DMU	M	526	33/33	0.92	0.12	1.03	32,42,55,58	0
15	MG	N	1518	1/1	0.96	0.10	1.03	26,26,26,26	0
25	PEK	C	265	53/53	0.51	0.29	0.99	44,88,103,104	0
19	CUA	B	228	2/2	0.99	0.08	0.95	19,19,19,22	0
18	PGV	A	525	51/51	0.97	0.11	0.85	21,36,56,63	0
22	CHD	C	525	29/29	0.97	0.12	0.81	21,27,30,33	0
18	PGV	N	1266	51/51	0.97	0.11	0.74	20,38,55,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
17	HEA	N	515	60/60	0.98	0.11	0.49	18,24,41,43	0
17	HEA	A	515	60/60	0.99	0.11	0.44	12,20,44,45	0
22	CHD	P	1525	29/29	0.96	0.10	0.24	20,27,31,34	0
17	HEA	N	516	60/60	0.99	0.10	-0.18	17,20,29,31	0
17	HEA	A	516	60/60	0.99	0.10	-0.25	15,18,29,29	0
19	CUA	O	228	2/2	0.98	0.08	-0.44	26,26,26,27	0
22	CHD	O	229	29/29	0.98	0.07	-0.46	19,22,28,32	0
22	CHD	B	1086	29/29	0.97	0.07	-0.48	20,24,30,37	0
27	ZN	S	99	1/1	0.99	0.06	-0.69	27,27,27,27	0
16	NA	N	1519	1/1	0.93	0.07	-0.71	30,30,30,30	0
27	ZN	F	99	1/1	0.99	0.06	-1.06	25,25,25,25	0
16	NA	A	519	1/1	0.96	0.06	-1.33	27,27,27,27	0
24	UNX	C	262	1/1	0.86	0.27	-	47,47,47,47	0
14	CU	A	517	1/1	1.00	0.09	-	20,20,20,20	0
24	UNX	P	1262	1/1	0.90	0.44	-	43,43,43,43	0
14	CU	N	517	1/1	1.00	0.09	-	21,21,21,21	0

## 6.5 Other polymers

There are no such residues in this entry.