



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 6, 2017 – 06:27 PM EST

PDB ID : 5IY5
Title : Electron transfer complex of cytochrome c and cytochrome c oxidase at 2.0 angstrom resolution
Authors : Shimada, S.; Baba, J.; Aoe, S.; Shimada, A.; Yamashita, E.; Tsukihara, T.
Deposited on : 2016-03-24
Resolution : 2.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20028442
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20028442

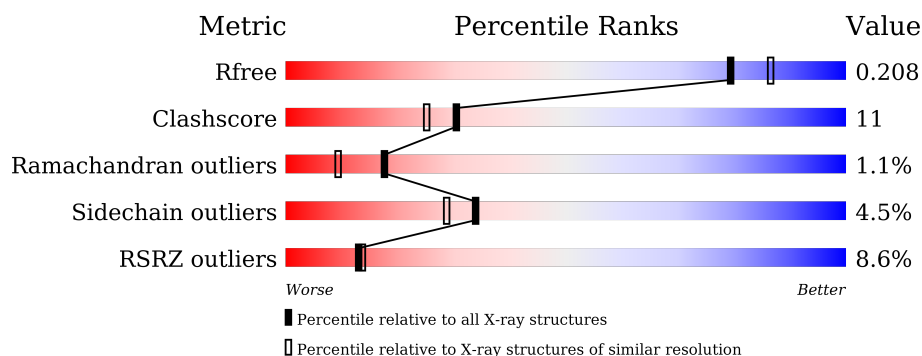
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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>4%</div> <div> <div></div> <div>85%</div> <div>14%</div> <div>.</div> </div> </div>
1	N	514	<div> <div>5%</div> <div> <div></div> <div>88%</div> <div>11%</div> <div>.</div> </div> </div>
2	B	227	<div> <div>%</div> <div> <div></div> <div>75%</div> <div>21%</div> <div>.</div> </div> </div>
2	O	227	<div> <div>%</div> <div> <div></div> <div>80%</div> <div>16%</div> <div>.</div> </div> </div>
3	C	259	<div> <div>%</div> <div> <div></div> <div>86%</div> <div>13%</div> <div>.</div> </div> </div>
3	P	259	<div> <div>2%</div> <div> <div></div> <div>86%</div> <div>14%</div> <div>.</div> </div> </div>

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Mol	Chain	Length	Quality of chain
4	D	144	
4	Q	144	
5	E	105	
5	R	105	
6	F	98	
6	S	98	
7	G	84	
7	T	84	
8	H	79	
8	U	79	
9	I	73	
9	V	73	
10	J	58	
10	W	58	
11	K	49	
11	X	49	
12	L	46	
12	Y	46	
13	M	43	
13	Z	43	
14	1	105	
14	2	105	

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
16	MG	A	602	-	-	-	X
16	MG	N	603	-	-	-	X
18	HEA	A	605	X	-	-	-
18	HEA	N	606	X	-	-	-
20	PGV	A	607	-	-	-	X
20	PGV	C	305	-	-	-	X
20	PGV	P	305	-	-	-	X
21	TGL	B	301	-	-	-	X
21	TGL	D	201	-	-	-	X
21	TGL	L	101	-	-	-	X
21	TGL	N	608	-	-	-	X
21	TGL	Q	201	-	-	-	X
23	EDO	N	613	-	-	-	X
24	CHD	J	101	-	-	-	X
24	CHD	P	307	-	-	-	X
24	CHD	W	101	-	-	-	X
26	CDL	C	306	-	-	-	X
26	CDL	G	101	-	-	X	X
26	CDL	P	306	-	-	-	X
26	CDL	T	101	-	-	X	X
27	UNL	C	308	-	-	-	X
27	UNL	C	310	-	-	X	X
27	UNL	J	102	-	-	-	X
27	UNL	L	102	-	-	-	X
27	UNL	N	601	-	-	X	X
27	UNL	N	609	-	-	-	X
27	UNL	N	610	-	-	-	X
27	UNL	P	308	-	-	X	X
27	UNL	P	310	-	-	X	X
27	UNL	Y	101	-	-	-	X
28	PSC	V	101	-	-	X	-
29	ZN	S	101	-	-	X	-
30	DMU	Z	101	-	-	-	X

2 Entry composition [i](#)

There are 32 unique types of molecules in this entry. The entry contains 34765 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	11	0
			4084	2731	628	685	40			
1	N	514	Total	C	N	O	S	0	8	0
			4065	2717	627	683	38			

- 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	2	0
			1836	1192	283	343	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	6	0
			2149	1437	343	355	14			
3	P	259	Total	C	N	O	S	0	5	0
			2143	1433	342	354	14			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	144	Total	C	N	O	S	0	0	0
			1195	777	196	218	4			
4	Q	144	Total	C	N	O	S	0	1	0
			1203	782	199	218	4			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	84	Total	C	N	O	P	S	0	0
			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 6B1.

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 14 is a protein called Cytochrome c.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	1	105	Total	C	N	O	S	0	0	0
			826	526	144	152	4			
14	2	105	Total	C	N	O	S	0	0	0
			826	526	144	152	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	0	ACE	-	acetylation	UNP P00004
2	0	ACE	-	acetylation	UNP P00004

- Molecule 15 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

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

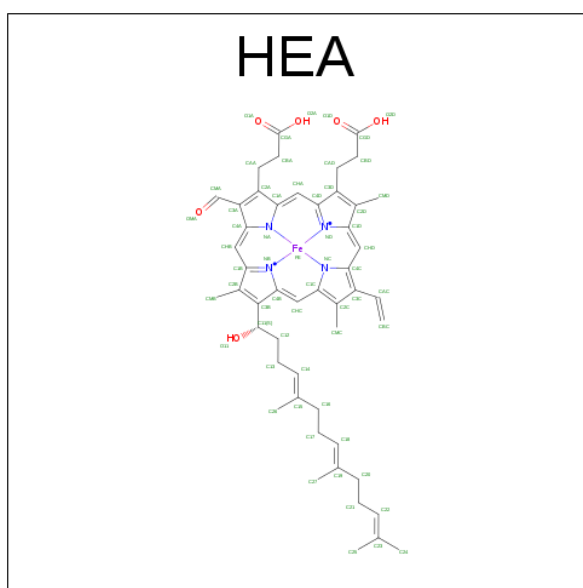
- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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).

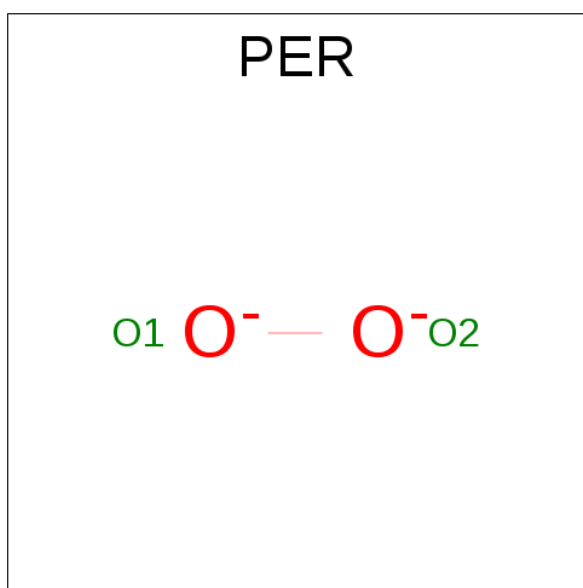
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	P	1	Total Na 1 1	0	0
17	A	1	Total Na 1 1	0	0
17	C	1	Total Na 1 1	0	0
17	N	1	Total Na 1 1	0	0

- Molecule 18 is HEME-A (three-letter code: HEA) (formula: $C_{49}H_{56}FeN_4O_6$).



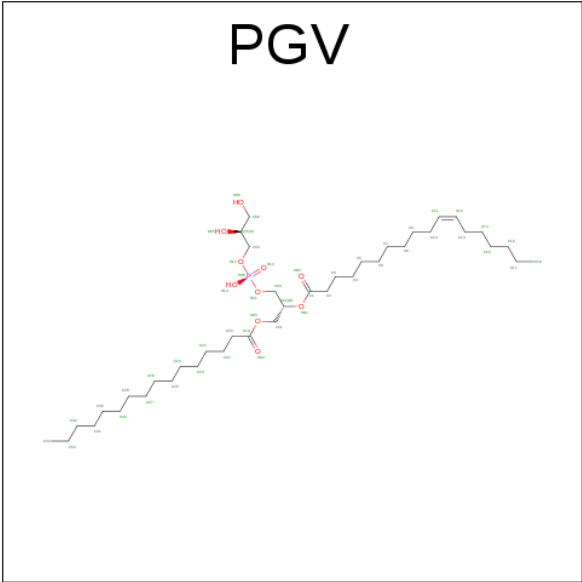
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	A	1	Total	C	Fe	N	O	0	1
			69	58	1	4	6		
18	A	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
18	N	1	Total	C	Fe	N	O	0	1
			69	58	1	4	6		
18	N	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		

- Molecule 19 is PEROXIDE ION (three-letter code: PER) (formula: O₂).



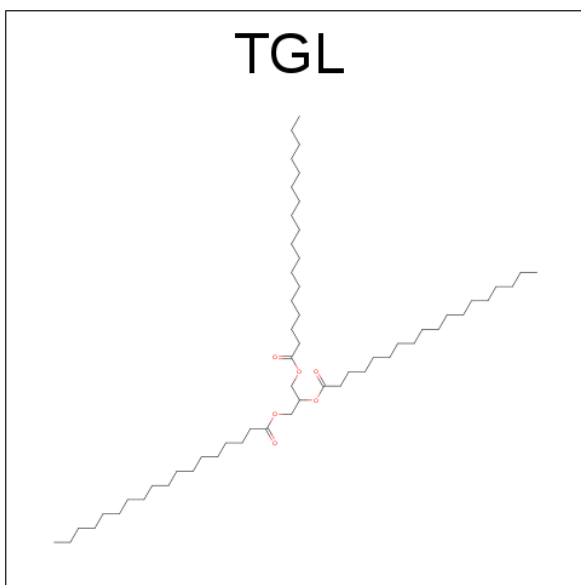
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	A	1	Total	O	0	0
			2	2		
19	N	1	Total	O	0	0
			2	2		

- Molecule 20 is (1R)-2-{{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (three-letter code: PGV) (formula: C₄₀H₇₇O₁₀P).



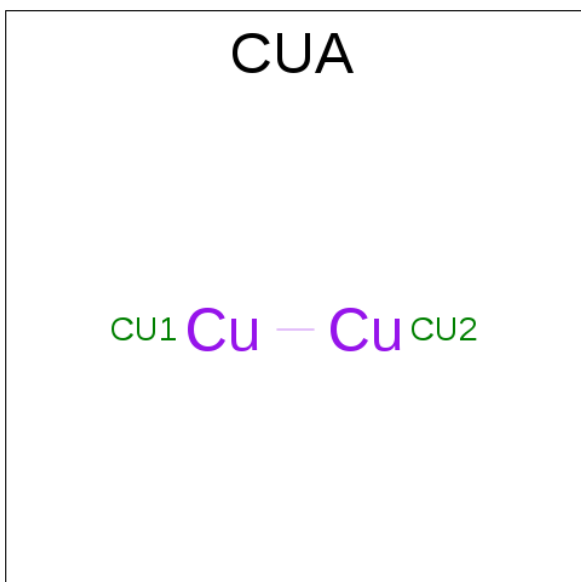
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
20	A	1	Total	C	O	P	0	0
			51	40	10	1		
20	A	1	Total	C	O	P	0	0
			51	40	10	1		
20	C	1	Total	C	O	P	0	0
			51	40	10	1		
20	C	1	Total	C	O	P	0	0
			51	40	10	1		
20	N	1	Total	C	O	P	0	0
			51	40	10	1		
20	P	1	Total	C	O	P	0	0
			51	40	10	1		
20	P	1	Total	C	O	P	0	0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

- Molecule 21 is TRISTEAROYLGLYCEROL (three-letter code: TGL) (formula: C₅₇H₁₁₀O₆).



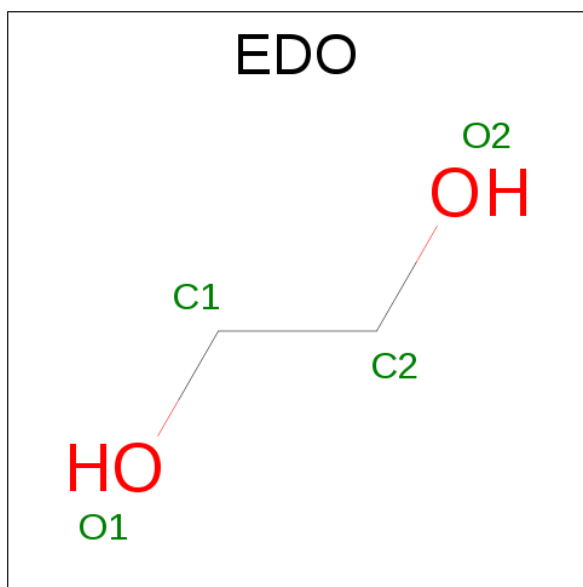
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	B	1	Total	C	O	0	0
			63	57	6		
21	D	1	Total	C	O	0	0
			63	57	6		
21	L	1	Total	C	O	0	0
			63	57	6		
21	N	1	Total	C	O	0	0
			63	57	6		
21	Q	1	Total	C	O	0	0
			63	57	6		

- Molecule 22 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu₂).



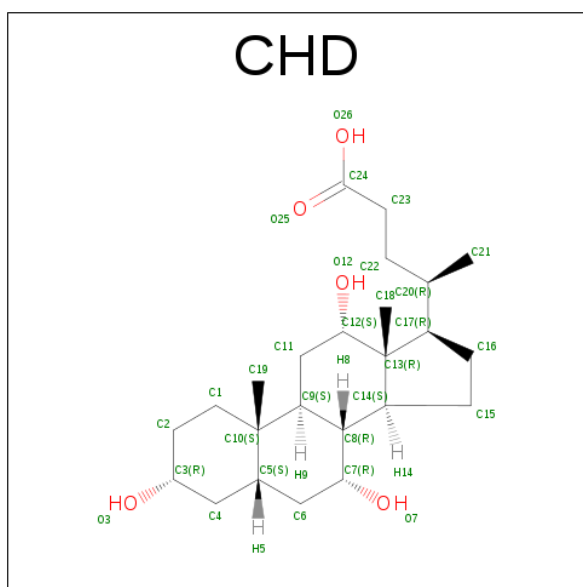
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	B	1	Total Cu 2 2	0	0
22	O	1	Total Cu 2 2	0	0

- Molecule 23 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



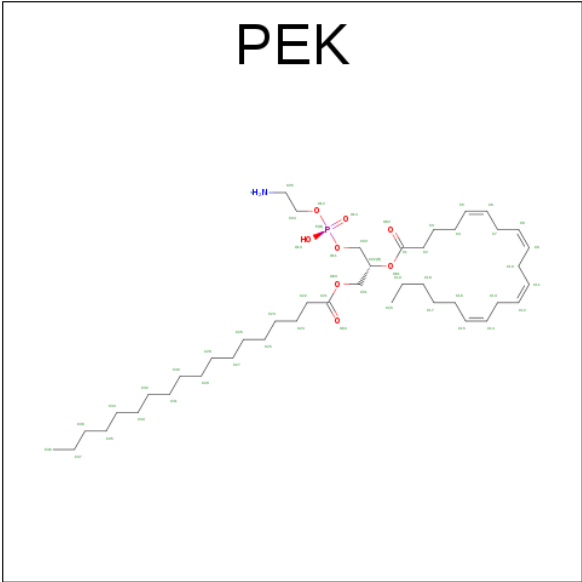
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	B	1	Total C O 4 2 2	0	0
23	C	1	Total C O 4 2 2	0	0
23	E	1	Total C O 4 2 2	0	0
23	F	1	Total C O 4 2 2	0	0
23	G	1	Total C O 4 2 2	0	0
23	I	1	Total C O 4 2 2	0	0
23	N	1	Total C O 4 2 2	0	0
23	N	1	Total C O 4 2 2	0	0
23	S	1	Total C O 4 2 2	0	0

- Molecule 24 is CHOLIC ACID (three-letter code: CHD) (formula: C₂₄H₄₀O₅).



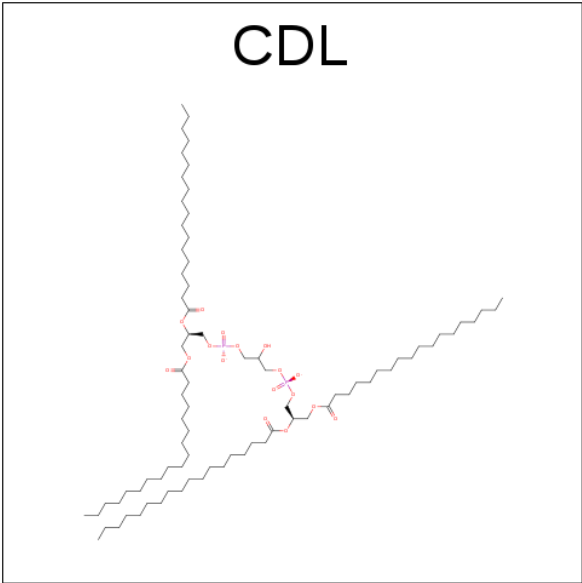
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
24	C	1	Total	C	O	0	0
			29	24	5		
24	C	1	Total	C	O	0	0
			29	24	5		
24	G	1	Total	C	O	0	0
			29	24	5		
24	J	1	Total	C	O	0	0
			29	24	5		
24	P	1	Total	C	O	0	0
			29	24	5		
24	P	1	Total	C	O	0	0
			29	24	5		
24	T	1	Total	C	O	0	0
			29	24	5		
24	W	1	Total	C	O	0	0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

- 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: C₄₃H₇₈NO₈P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	C	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		

- Molecule 26 is CARDIOLIPIN (three-letter code: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).



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		

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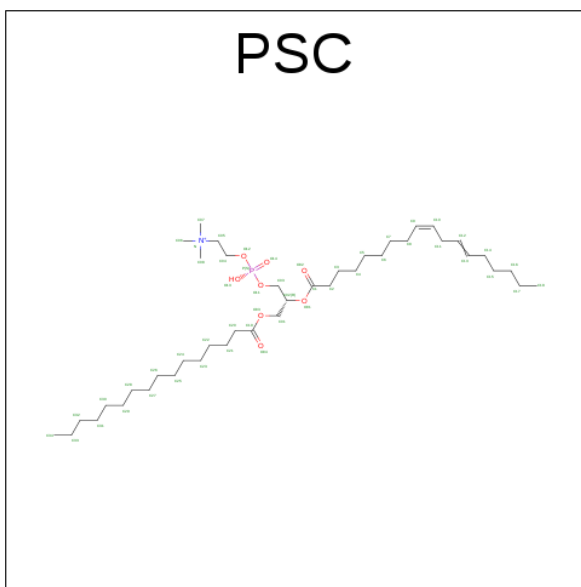
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	P	1	Total	C	O	P	0	0
			100	81	17	2		
26	T	1	Total	C	O	P	0	0
			100	81	17	2		

- Molecule 27 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
27	P	3	Total	C	0	0
			43	43		
27	J	1	Total	C	0	0
			10	10		
27	C	3	Total	C	0	0
			42	42		
27	W	1	Total	C	0	0
			9	9		
27	T	1	Total	C	0	0
			18	18		
27	N	4	Total	C	0	0
			63	63		
27	Y	1	Total	C	0	0
			10	10		
27	L	1	Total	C	0	0
			10	10		

- Molecule 28 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: C₄₂H₈₁NO₈P).



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

- Molecule 29 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 30 is DECYL-BETA-D-MALTOPYRANOSIDE (three-letter code: DMU) (formula: C₂₂H₄₂O₁₁).



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

- Molecule 31 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $\text{C}_{34}\text{H}_{32}\text{FeN}_4\text{O}_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
31	1	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
31	2	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 32 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	A	252	Total	O	0	0
			252	252		
32	B	193	Total	O	0	0
			193	193		
32	C	137	Total	O	0	0
			137	137		
32	D	122	Total	O	0	0
			122	122		
32	E	119	Total	O	0	0
			119	119		
32	F	97	Total	O	0	0
			97	97		
32	G	60	Total	O	0	0
			60	60		
32	H	76	Total	O	0	0
			76	76		
32	I	49	Total	O	0	0
			49	49		
32	J	30	Total	O	0	0
			30	30		
32	K	29	Total	O	0	0
			29	29		
32	L	33	Total	O	0	0
			33	33		
32	M	26	Total	O	0	0
			26	26		
32	N	229	Total	O	0	0
			229	229		
32	O	141	Total	O	0	0
			141	141		
32	P	110	Total	O	0	0
			110	110		
32	Q	99	Total	O	0	0
			99	99		
32	R	83	Total	O	0	0
			83	83		

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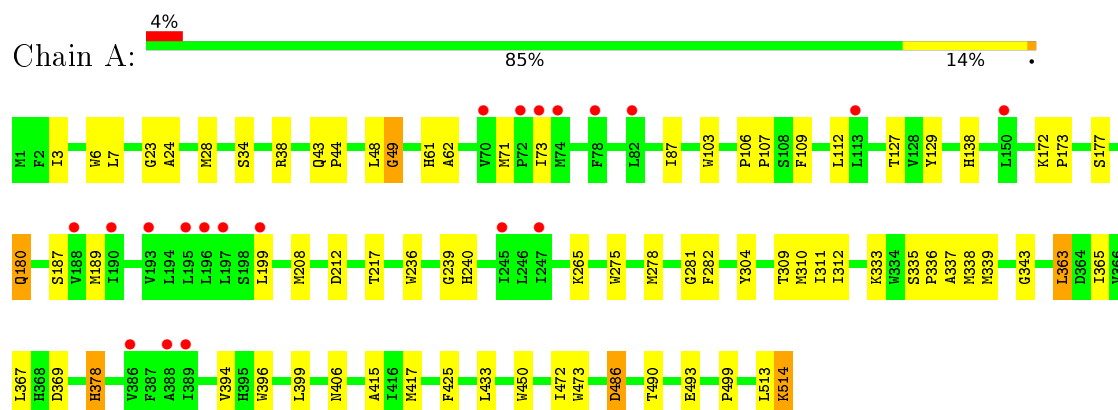
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	S	95	Total 95	O 95	0	0
32	T	41	Total 41	O 41	0	0
32	U	54	Total 54	O 54	0	0
32	V	17	Total 17	O 17	0	0
32	W	10	Total 10	O 10	0	0
32	X	17	Total 17	O 17	0	0
32	Y	21	Total 21	O 21	0	0
32	Z	16	Total 16	O 16	0	0
32	1	53	Total 53	O 53	0	0
32	2	28	Total 28	O 28	0	0

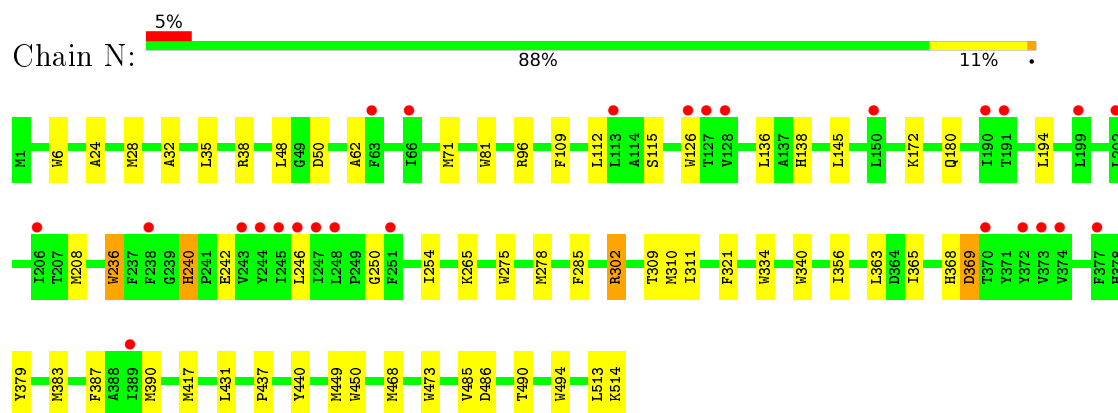
3 Residue-property plots

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.

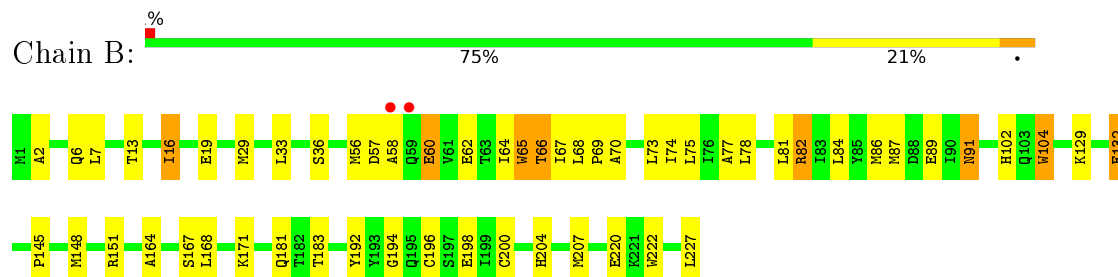
• Molecule 1: Cytochrome c oxidase subunit 1



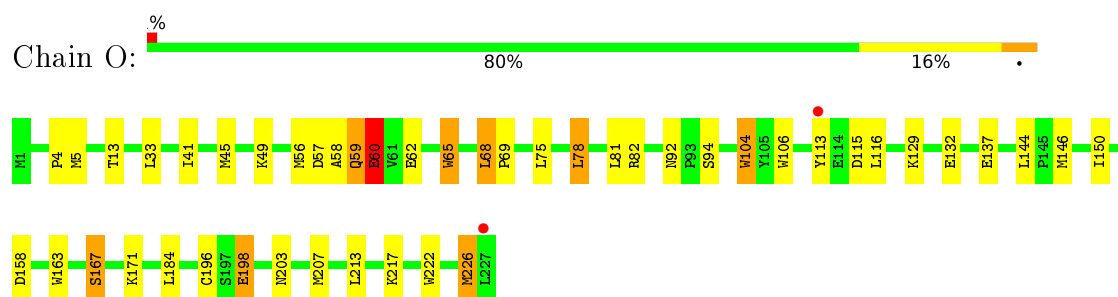
• Molecule 1: Cytochrome c oxidase subunit 1



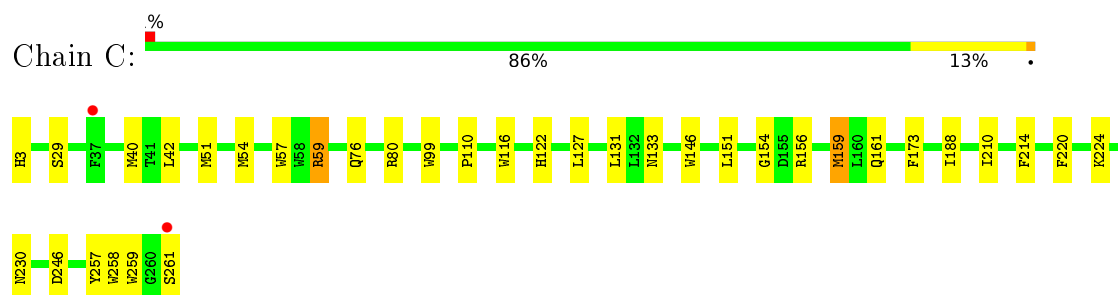
• Molecule 2: Cytochrome c oxidase subunit 2



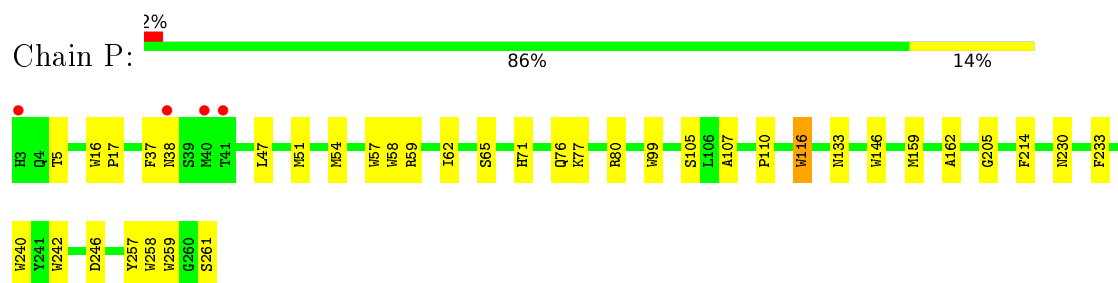
• Molecule 2: Cytochrome c oxidase subunit 2



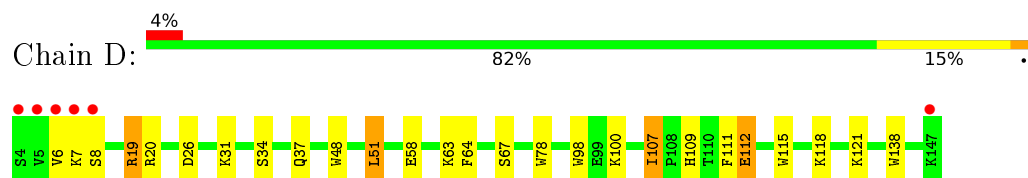
• Molecule 3: Cytochrome c oxidase subunit 3



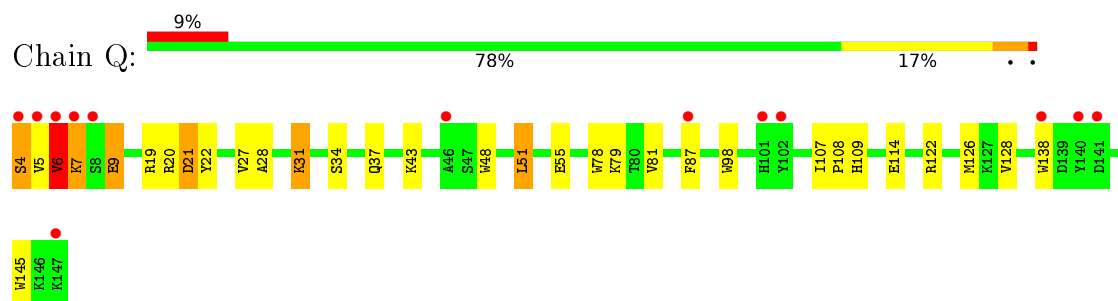
• Molecule 3: Cytochrome c oxidase subunit 3



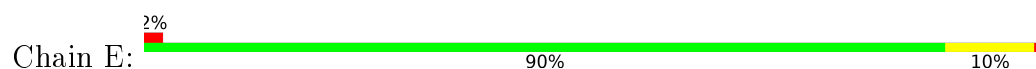
• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

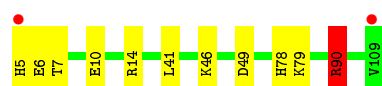


• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial



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

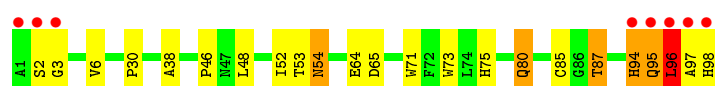




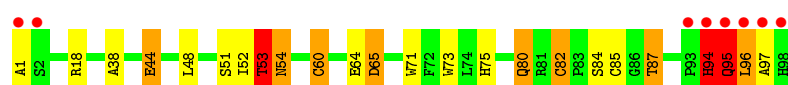
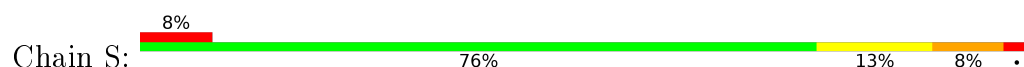
- Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial



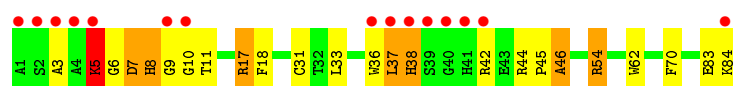
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



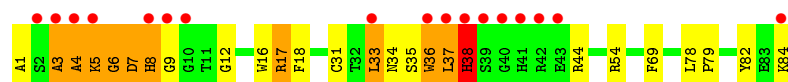
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



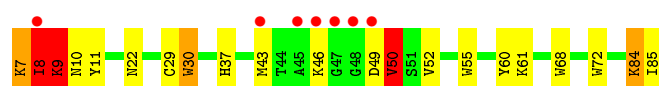
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



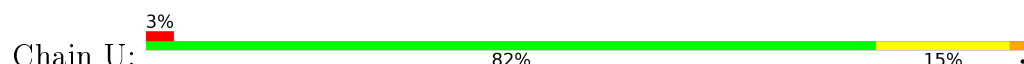
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial

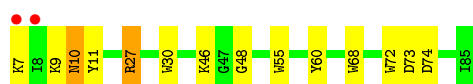


- Molecule 8: Cytochrome c oxidase subunit 6B1

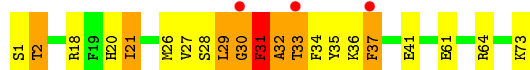


- Molecule 8: Cytochrome c oxidase subunit 6B1

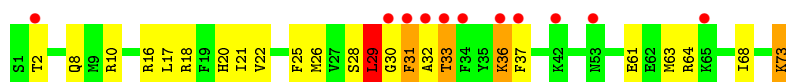




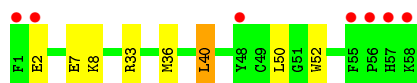
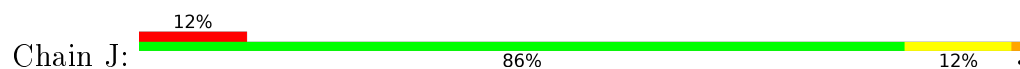
- Molecule 9: Cytochrome c oxidase subunit 6C



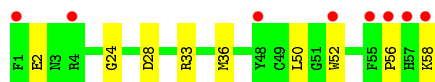
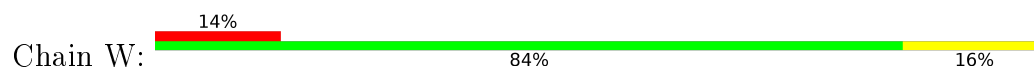
- Molecule 9: Cytochrome c oxidase subunit 6C



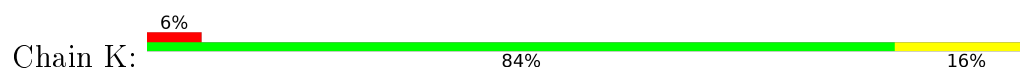
- Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial



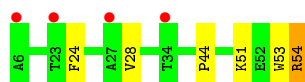
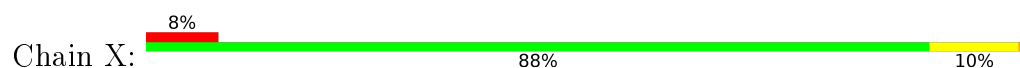
- Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial



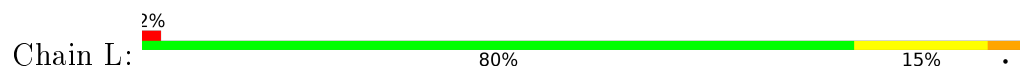
- Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial



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

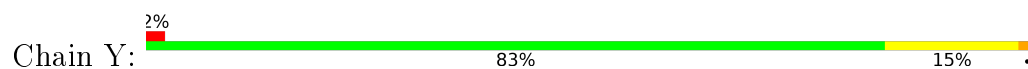


- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial

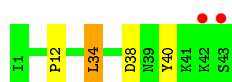




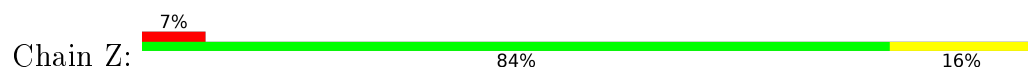
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial



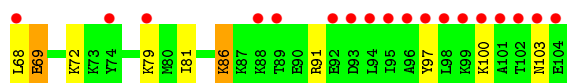
- Molecule 13: Cytochrome c oxidase subunit 8B, mitochondrial



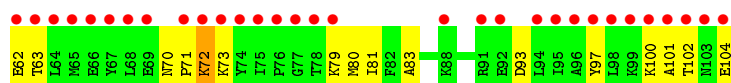
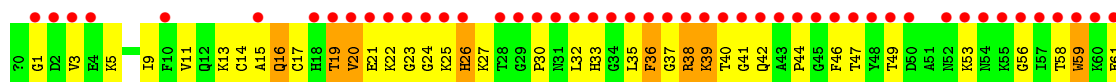
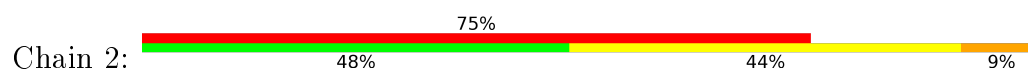
- Molecule 13: Cytochrome c oxidase subunit 8B, mitochondrial



- Molecule 14: Cytochrome c



- Molecule 14: Cytochrome c



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	113.29Å 183.87Å 148.93Å 90.00° 102.12° 90.00°	Depositor
Resolution (Å)	40.00 – 2.00 49.35 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.4 (40.00-2.00) 99.4 (49.35-2.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.74 (at 2.00Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.167 , 0.207 0.168 , 0.208	Depositor DCC
R_{free} test set	19990 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	33.5	Xtriage
Anisotropy	0.586	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 72.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	34765	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.47% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: CDL, ZN, CHD, ACE, PSC, SAC, NA, MG, PER, EDO, PGV, TPO, CU, DMU, CUA, PEK, HEM, FME, UNL, TGL, 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	1.31	11/4244 (0.3%)	1.04	9/5793 (0.2%)
1	N	1.20	9/4214 (0.2%)	0.94	5/5754 (0.1%)
2	B	1.26	6/1878 (0.3%)	1.09	4/2558 (0.2%)
2	O	0.99	6/1860 (0.3%)	0.96	1/2534 (0.0%)
3	C	1.20	5/2247 (0.2%)	0.87	1/3070 (0.0%)
3	P	1.15	7/2238 (0.3%)	0.86	0/3058
4	D	1.21	7/1229 (0.6%)	1.13	8/1658 (0.5%)
4	Q	1.09	5/1240 (0.4%)	0.97	2/1672 (0.1%)
5	E	1.04	0/871	0.99	5/1182 (0.4%)
5	R	1.01	1/871 (0.1%)	0.89	0/1182
6	F	1.17	3/765 (0.4%)	1.04	2/1038 (0.2%)
6	S	1.15	4/765 (0.5%)	1.15	5/1038 (0.5%)
7	G	1.17	2/690 (0.3%)	1.01	3/937 (0.3%)
7	T	1.20	1/690 (0.1%)	1.09	5/937 (0.5%)
8	H	1.25	7/682 (1.0%)	1.19	4/921 (0.4%)
8	U	1.05	4/682 (0.6%)	0.99	4/921 (0.4%)
9	I	1.09	0/605	1.09	2/802 (0.2%)
9	V	0.86	0/605	0.96	1/802 (0.1%)
10	J	0.96	1/471 (0.2%)	0.88	1/636 (0.2%)
10	W	0.87	1/471 (0.2%)	0.86	0/636
11	K	1.13	1/398 (0.3%)	0.96	0/546
11	X	0.94	1/398 (0.3%)	0.86	0/546
12	L	1.15	0/393	0.90	0/526
12	Y	1.05	0/393	0.95	1/526 (0.2%)
13	M	1.05	0/345	1.01	1/470 (0.2%)
13	Z	1.01	1/345 (0.3%)	1.01	2/470 (0.4%)
14	1	0.73	1/840 (0.1%)	0.78	0/1120
14	2	0.68	1/840 (0.1%)	0.74	0/1120
All	All	1.14	85/31270 (0.3%)	0.98	66/42453 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	N	0	1
6	S	0	2
8	H	0	2
9	V	0	2
All	All	0	8

The worst 5 of 85 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	116	TRP	CD2-CE2	8.38	1.51	1.41
2	B	132	GLU	CD-OE2	8.22	1.34	1.25
6	S	60	CYS	CB-SG	8.20	1.96	1.82
2	B	167	SER	CB-OG	-8.05	1.31	1.42
1	N	236	TRP	CD2-CE2	7.79	1.50	1.41

The worst 5 of 66 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	20	ARG	NE-CZ-NH2	-11.62	114.49	120.30
2	B	82	ARG	NE-CZ-NH2	11.54	126.07	120.30
1	A	71	MET	CG-SD-CE	-11.09	82.46	100.20
1	A	486	ASP	CB-CG-OD1	10.23	127.51	118.30
5	E	90	ARG	NE-CZ-NH1	9.99	125.29	120.30

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	240	HIS	Sidechain
8	H	8	ILE	Peptide
8	H	9	LYS	Peptide
1	N	240	HIS	Sidechain
6	S	94	HIS	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	4084	0	4069	63	0
1	N	4065	0	4046	44	0
2	B	1836	0	1843	43	0
2	O	1824	0	1833	40	0
3	C	2149	0	2075	24	0
3	P	2143	0	2067	29	0
4	D	1195	0	1183	16	0
4	Q	1203	0	1196	30	0
5	E	852	0	845	8	0
5	R	852	0	845	5	0
6	F	748	0	728	25	0
6	S	748	0	729	25	0
7	G	675	0	643	20	0
7	T	675	0	644	26	0
8	H	662	0	623	36	0
8	U	662	0	623	7	0
9	I	601	0	613	39	0
9	V	601	0	613	19	0
10	J	460	0	459	7	0
10	W	460	0	459	12	0
11	K	384	0	366	5	0
11	X	384	0	366	8	0
12	L	380	0	380	12	0
12	Y	380	0	380	6	0
13	M	335	0	352	1	0
13	Z	335	0	352	4	0
14	1	826	0	849	27	0
14	2	826	0	848	40	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	1	0	0	0	0
17	C	1	0	0	0	0
17	N	1	0	0	0	0
17	P	1	0	0	0	0
18	A	129	0	88	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	N	129	0	88	10	0
19	A	2	0	0	0	0
19	N	2	0	0	1	0
20	A	102	0	152	9	0
20	C	102	0	152	14	0
20	N	51	0	76	1	0
20	P	102	0	152	10	0
21	B	63	0	110	6	0
21	D	63	0	110	12	0
21	L	63	0	110	20	0
21	N	63	0	110	2	0
21	Q	63	0	110	10	0
22	B	2	0	0	0	0
22	O	2	0	0	0	0
23	B	4	0	6	0	0
23	C	4	0	6	0	0
23	E	4	0	6	1	0
23	F	4	0	6	0	0
23	G	4	0	6	0	0
23	I	4	0	6	0	0
23	N	8	0	12	0	0
23	S	4	0	6	0	0
24	C	58	0	78	4	0
24	G	29	0	39	0	0
24	J	29	0	38	5	0
24	P	58	0	78	2	0
24	T	29	0	39	1	0
24	W	29	0	37	5	0
25	C	53	0	77	7	0
25	P	53	0	77	3	0
26	C	100	0	156	15	0
26	G	100	0	156	23	0
26	P	100	0	156	12	0
26	T	100	0	156	24	0
27	C	42	0	0	4	0
27	J	10	0	0	1	0
27	L	10	0	0	1	0
27	N	63	0	0	2	0
27	P	43	0	0	6	0
27	T	18	0	0	1	0
27	W	9	0	0	1	0
27	Y	10	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	E	52	0	80	19	0
28	V	52	0	80	21	0
29	F	1	0	0	0	0
29	S	1	0	0	2	0
30	M	33	0	42	1	0
30	Z	33	0	42	1	0
31	1	43	0	30	5	0
31	2	43	0	30	3	0
32	1	53	0	0	6	0
32	2	28	0	0	7	0
32	A	252	0	0	19	0
32	B	193	0	0	6	0
32	C	137	0	0	7	0
32	D	122	0	0	7	0
32	E	119	0	0	6	0
32	F	97	0	0	2	2
32	G	60	0	0	11	0
32	H	76	0	0	7	0
32	I	49	0	0	5	0
32	J	30	0	0	3	0
32	K	29	0	0	1	0
32	L	33	0	0	1	0
32	M	26	0	0	2	0
32	N	229	0	0	6	0
32	O	141	0	0	3	0
32	P	110	0	0	9	0
32	Q	99	0	0	7	0
32	R	83	0	0	1	0
32	S	95	0	0	5	0
32	T	41	0	0	3	0
32	U	54	0	0	4	2
32	V	17	0	0	2	0
32	W	10	0	0	0	0
32	X	17	0	0	3	0
32	Y	21	0	0	0	0
32	Z	16	0	0	0	0
All	All	34765	0	32732	716	2

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 11.

The worst 5 of 716 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)
14:1:17:CYS:SG	31:1:201:HEM:CAC	2.06	1.41
27:C:310:UNL:C4	27:C:310:UNL:C6	1.76	1.36
32:A:927:HOH:O	26:T:101:CDL:H412	1.17	1.28
5:E:79:LYS:HE3	32:E:387:HOH:O	1.31	1.24
27:W:102:UNL:C5	27:W:102:UNL:C4	2.17	1.23

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:F:266:HOH:O	32:U:148:HOH:O[1_455]	2.11	0.09
32:F:276:HOH:O	32:U:141:HOH:O[1_455]	2.14	0.06

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	524/514 (102%)	510 (97%)	14 (3%)	0	100	100
1	N	520/514 (101%)	504 (97%)	16 (3%)	0	100	100
2	B	227/227 (100%)	217 (96%)	9 (4%)	1 (0%)	39	33
2	O	225/227 (99%)	216 (96%)	8 (4%)	1 (0%)	39	33
3	C	263/259 (102%)	259 (98%)	4 (2%)	0	100	100
3	P	262/259 (101%)	256 (98%)	5 (2%)	1 (0%)	39	33
4	D	142/144 (99%)	135 (95%)	7 (5%)	0	100	100
4	Q	143/144 (99%)	136 (95%)	5 (4%)	2 (1%)	14	6
5	E	103/105 (98%)	102 (99%)	1 (1%)	0	100	100
5	R	103/105 (98%)	102 (99%)	1 (1%)	0	100	100
6	F	96/98 (98%)	90 (94%)	4 (4%)	2 (2%)	9	3
6	S	96/98 (98%)	90 (94%)	3 (3%)	3 (3%)	5	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	G	81/84 (96%)	65 (80%)	10 (12%)	6 (7%)	1	0
7	T	81/84 (96%)	64 (79%)	10 (12%)	7 (9%)	1	0
8	H	77/79 (98%)	70 (91%)	4 (5%)	3 (4%)	4	1
8	U	77/79 (98%)	73 (95%)	3 (4%)	1 (1%)	15	7
9	I	71/73 (97%)	67 (94%)	1 (1%)	3 (4%)	3	1
9	V	71/73 (97%)	65 (92%)	4 (6%)	2 (3%)	6	2
10	J	56/58 (97%)	56 (100%)	0	0	100	100
10	W	56/58 (97%)	55 (98%)	0	1 (2%)	11	4
11	K	47/49 (96%)	47 (100%)	0	0	100	100
11	X	47/49 (96%)	44 (94%)	3 (6%)	0	100	100
12	L	44/46 (96%)	42 (96%)	2 (4%)	0	100	100
12	Y	44/46 (96%)	42 (96%)	2 (4%)	0	100	100
13	M	41/43 (95%)	38 (93%)	3 (7%)	0	100	100
13	Z	41/43 (95%)	41 (100%)	0	0	100	100
14	1	103/105 (98%)	90 (87%)	11 (11%)	2 (2%)	10	4
14	2	103/105 (98%)	81 (79%)	15 (15%)	7 (7%)	1	0
All	All	3744/3768 (99%)	3557 (95%)	145 (4%)	42 (1%)	17	9

5 of 42 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	2	SER
6	F	96	LEU
7	G	3	ALA
7	G	7	ASP
7	G	8	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	437/426 (103%)	429 (98%)	8 (2%)	66	69
1	N	433/426 (102%)	425 (98%)	8 (2%)	66	69
2	B	212/210 (101%)	204 (96%)	8 (4%)	40	36
2	O	210/210 (100%)	196 (93%)	14 (7%)	20	14
3	C	230/224 (103%)	225 (98%)	5 (2%)	60	62
3	P	229/224 (102%)	225 (98%)	4 (2%)	68	71
4	D	128/128 (100%)	123 (96%)	5 (4%)	39	35
4	Q	129/128 (101%)	123 (95%)	6 (5%)	32	27
5	E	92/92 (100%)	90 (98%)	2 (2%)	60	62
5	R	92/92 (100%)	90 (98%)	2 (2%)	60	62
6	F	81/81 (100%)	77 (95%)	4 (5%)	31	25
6	S	81/81 (100%)	75 (93%)	6 (7%)	17	11
7	G	67/67 (100%)	60 (90%)	7 (10%)	9	4
7	T	67/67 (100%)	60 (90%)	7 (10%)	9	4
8	H	71/71 (100%)	63 (89%)	8 (11%)	7	4
8	U	71/71 (100%)	69 (97%)	2 (3%)	51	50
9	I	57/57 (100%)	50 (88%)	7 (12%)	6	3
9	V	57/57 (100%)	51 (90%)	6 (10%)	8	4
10	J	49/49 (100%)	48 (98%)	1 (2%)	63	65
10	W	49/49 (100%)	47 (96%)	2 (4%)	37	32
11	K	39/39 (100%)	37 (95%)	2 (5%)	29	23
11	X	39/39 (100%)	38 (97%)	1 (3%)	54	54
12	L	39/39 (100%)	36 (92%)	3 (8%)	16	10
12	Y	39/39 (100%)	36 (92%)	3 (8%)	16	10
13	M	37/37 (100%)	34 (92%)	3 (8%)	15	9
13	Z	37/37 (100%)	35 (95%)	2 (5%)	27	21
14	1	86/86 (100%)	78 (91%)	8 (9%)	11	6
14	2	86/86 (100%)	75 (87%)	11 (13%)	5	3
All	All	3244/3212 (101%)	3099 (96%)	145 (4%)	34	29

5 of 145 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	N	109	PHE
2	O	167	SER
14	2	14	CYS
1	N	138	HIS
2	O	65	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 54 such sidechains are listed below:

Mol	Chain	Res	Type
1	N	4	ASN
1	N	512	ASN
9	V	20	HIS
1	N	80	ASN
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 ⓘ

8 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	FME	A	1	1	8,9,10	1.47	1 (12%)	5,9,11	2.73	4 (80%)
2	FME	B	1	2	8,9,10	2.54	3 (37%)	5,9,11	4.86	2 (40%)
7	TPO	G	11	7	7,10,11	1.58	1 (14%)	10,14,16	1.62	2 (20%)
9	SAC	I	1	9	7,8,9	2.19	2 (28%)	7,9,11	2.08	2 (28%)
1	FME	N	1	1	8,9,10	0.80	0	5,9,11	3.22	3 (60%)
2	FME	O	1	2	8,9,10	0.77	0	5,9,11	1.13	1 (20%)
7	TPO	T	11	7	7,10,11	1.97	1 (14%)	10,14,16	1.62	4 (40%)
9	SAC	V	1	9	7,8,9	2.46	2 (28%)	7,9,11	1.52	1 (14%)

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	-	1/8/11/13	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	-	0/6/9/11	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 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	FME	O1-CN	-3.62	1.10	1.22
2	B	1	FME	CB-CA	2.51	1.58	1.53
7	G	11	TPO	P-O1P	3.11	1.60	1.50
9	I	1	SAC	CA-N	3.28	1.50	1.46
7	T	11	TPO	P-O1P	3.57	1.62	1.50

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	FME	O-C-CA	-2.40	119.13	125.69
1	A	1	FME	CG-CB-CA	-2.40	105.87	113.07
1	N	1	FME	CG-CB-CA	-2.28	106.21	113.07
1	A	1	FME	O-C-CA	-2.26	119.51	125.69
2	O	1	FME	O-C-CA	-2.08	120.01	125.69

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	G	11	TPO	OG1-CB-CA-N
1	N	1	FME	O1-CN-N-CA
2	B	1	FME	O1-CN-N-CA
1	A	1	FME	O1-CN-N-CA

There are no ring outliers.

2 monomers are involved in 3 short contacts:

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 76 ligands modelled in this entry, 15 are unknown and 10 are monoatomic - leaving 51 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	$\# Z > 2$
31	HEM	1	201	14	24,50,50	0.66	0	16,82,82	1.94	5 (31%)
31	HEM	2	201	14	24,50,50	0.80	1 (4%)	16,82,82	1.44	2 (12%)
18	HEA	A	604[A]	-	40,67,67	1.18	3 (7%)	36,103,103	2.34	12 (33%)
18	HEA	A	604[B]	-	40,67,67	1.17	2 (5%)	36,103,103	2.22	11 (30%)
18	HEA	A	605	1,19	40,67,67	1.43	7 (17%)	36,103,103	2.13	9 (25%)
19	PER	A	606	18,15	0,1,1	0.00	-	0,0,0	0.00	-
20	PGV	A	607	-	50,50,50	1.09	2 (4%)	51,56,56	1.09	5 (9%)
20	PGV	A	608	-	50,50,50	1.05	5 (10%)	51,56,56	1.27	6 (11%)
21	TGL	B	301	-	62,62,62	1.43	8 (12%)	65,65,65	1.95	10 (15%)
22	CUA	B	302	2	0,1,1	0.00	-	0,0,0	0.00	-
23	EDO	B	303	-	3,3,3	0.75	0	2,2,2	0.46	0
24	CHD	C	301	-	29,32,32	1.29	4 (13%)	48,51,51	1.82	12 (25%)
25	PEK	C	303	-	51,52,52	0.95	2 (3%)	52,57,57	1.29	5 (9%)
20	PGV	C	304	-	50,50,50	0.79	2 (4%)	51,56,56	1.31	6 (11%)
20	PGV	C	305	-	50,50,50	1.38	3 (6%)	51,56,56	1.50	6 (11%)
26	CDL	C	306	-	99,99,99	1.35	12 (12%)	101,111,111	1.44	10 (9%)
24	CHD	C	307	-	29,32,32	0.87	0	48,51,51	3.57	25 (52%)
23	EDO	C	311	-	3,3,3	0.59	0	2,2,2	0.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	TGL	D	201	-	62,62,62	1.37	6 (9%)	65,65,65	1.53	8 (12%)
28	PSC	E	201	-	51,51,51	1.29	3 (5%)	55,59,59	1.56	9 (16%)
23	EDO	E	202	-	3,3,3	0.49	0	2,2,2	0.80	0
23	EDO	F	102	-	3,3,3	0.43	0	2,2,2	0.62	0
26	CDL	G	101	-	99,99,99	1.41	12 (12%)	101,111,111	1.39	13 (12%)
24	CHD	G	102	-	29,32,32	1.12	2 (6%)	48,51,51	2.06	13 (27%)
23	EDO	G	103	-	3,3,3	0.80	0	2,2,2	0.74	0
23	EDO	I	101	-	3,3,3	0.61	0	2,2,2	0.34	0
24	CHD	J	101	-	29,32,32	0.83	0	48,51,51	2.20	15 (31%)
21	TGL	L	101	-	62,62,62	1.53	7 (11%)	65,65,65	1.62	13 (20%)
30	DMU	M	101	-	34,34,34	0.73	0	45,45,45	1.77	10 (22%)
18	HEA	N	605[A]	-	40,67,67	1.10	4 (10%)	36,103,103	2.34	14 (38%)
18	HEA	N	605[B]	-	40,67,67	1.09	4 (10%)	36,103,103	2.33	15 (41%)
18	HEA	N	606	1,19	40,67,67	1.40	8 (20%)	36,103,103	1.71	7 (19%)
19	PER	N	607	18,15	0,1,1	0.00	-	0,0,0	0.00	-
21	TGL	N	608	-	62,62,62	1.45	7 (11%)	65,65,65	2.14	14 (21%)
20	PGV	N	612	-	50,50,50	0.84	1 (2%)	51,56,56	1.20	4 (7%)
23	EDO	N	613	-	3,3,3	0.56	0	2,2,2	0.36	0
23	EDO	N	614	-	3,3,3	0.40	0	2,2,2	0.54	0
22	CUA	O	301	2	0,1,1	0.00	-	0,0,0	0.00	-
24	CHD	P	301	-	29,32,32	1.05	2 (6%)	48,51,51	1.87	13 (27%)
25	PEK	P	303	-	51,52,52	0.97	3 (5%)	52,57,57	1.00	3 (5%)
20	PGV	P	304	-	50,50,50	0.81	2 (4%)	51,56,56	1.17	6 (11%)
20	PGV	P	305	-	50,50,50	1.26	2 (4%)	51,56,56	1.42	5 (9%)
26	CDL	P	306	-	99,99,99	1.38	12 (12%)	101,111,111	1.25	11 (10%)
24	CHD	P	307	-	29,32,32	0.57	0	48,51,51	2.43	18 (37%)
21	TGL	Q	201	-	62,62,62	1.38	6 (9%)	65,65,65	1.29	8 (12%)
23	EDO	S	102	-	3,3,3	0.61	0	2,2,2	0.88	0
26	CDL	T	101	-	99,99,99	1.40	12 (12%)	101,111,111	1.51	12 (11%)
24	CHD	T	103	-	29,32,32	1.06	2 (6%)	48,51,51	2.02	16 (33%)
28	PSC	V	101	-	51,51,51	1.19	3 (5%)	55,59,59	1.33	5 (9%)
24	CHD	W	101	-	29,32,32	0.85	1 (3%)	48,51,51	3.28	22 (45%)
30	DMU	Z	101	-	34,34,34	0.73	1 (2%)	45,45,45	1.08	5 (11%)

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
31	HEM	1	201	14	-	0/6/54/54	0/0/8/8
31	HEM	2	201	14	-	0/6/54/54	0/0/8/8
18	HEA	A	604[A]	-	-	0/24/76/76	0/0/8/8
18	HEA	A	604[B]	-	-	0/24/76/76	0/0/8/8
18	HEA	A	605	1,19	2/2/7/16	0/24/76/76	0/0/8/8
19	PER	A	606	18,15	-	0/0/0/0	0/0/0/0
20	PGV	A	607	-	-	0/55/55/55	0/0/0/0
20	PGV	A	608	-	-	0/55/55/55	0/0/0/0
21	TGL	B	301	-	-	0/65/65/65	0/0/0/0
22	CUA	B	302	2	-	0/0/0/0	0/0/0/0
23	EDO	B	303	-	-	0/1/1/1	0/0/0/0
24	CHD	C	301	-	-	0/7/74/74	0/4/4/4
25	PEK	C	303	-	-	0/56/56/56	0/0/0/0
20	PGV	C	304	-	-	0/55/55/55	0/0/0/0
20	PGV	C	305	-	-	0/55/55/55	0/0/0/0
26	CDL	C	306	-	-	0/110/110/110	0/0/0/0
24	CHD	C	307	-	-	0/7/74/74	0/4/4/4
23	EDO	C	311	-	-	0/1/1/1	0/0/0/0
21	TGL	D	201	-	-	0/65/65/65	0/0/0/0
28	PSC	E	201	-	-	0/55/55/55	0/0/0/0
23	EDO	E	202	-	-	0/1/1/1	0/0/0/0
23	EDO	F	102	-	-	0/1/1/1	0/0/0/0
26	CDL	G	101	-	-	0/110/110/110	0/0/0/0
24	CHD	G	102	-	-	0/7/74/74	0/4/4/4
23	EDO	G	103	-	-	0/1/1/1	0/0/0/0
23	EDO	I	101	-	-	0/1/1/1	0/0/0/0
24	CHD	J	101	-	-	0/7/74/74	0/4/4/4
21	TGL	L	101	-	-	0/65/65/65	0/0/0/0
30	DMU	M	101	-	-	0/19/59/59	0/2/2/2
18	HEA	N	605[A]	-	-	0/24/76/76	0/0/8/8
18	HEA	N	605[B]	-	-	0/24/76/76	0/0/8/8
18	HEA	N	606	1,19	2/2/7/16	0/24/76/76	0/0/8/8
19	PER	N	607	18,15	-	0/0/0/0	0/0/0/0
21	TGL	N	608	-	-	0/65/65/65	0/0/0/0
20	PGV	N	612	-	-	0/55/55/55	0/0/0/0
23	EDO	N	613	-	-	0/1/1/1	0/0/0/0
23	EDO	N	614	-	-	0/1/1/1	0/0/0/0
22	CUA	O	301	2	-	0/0/0/0	0/0/0/0
24	CHD	P	301	-	-	0/7/74/74	0/4/4/4
25	PEK	P	303	-	-	0/56/56/56	0/0/0/0
20	PGV	P	304	-	-	0/55/55/55	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	PGV	P	305	-	-	0/55/55/55	0/0/0/0
26	CDL	P	306	-	-	0/110/110/110	0/0/0/0
24	CHD	P	307	-	-	0/7/74/74	0/4/4/4
21	TGL	Q	201	-	-	1/65/65/65	0/0/0/0
23	EDO	S	102	-	-	0/1/1/1	0/0/0/0
26	CDL	T	101	-	-	0/110/110/110	0/0/0/0
24	CHD	T	103	-	-	0/7/74/74	0/4/4/4
28	PSC	V	101	-	-	0/55/55/55	0/0/0/0
24	CHD	W	101	-	-	0/7/74/74	0/4/4/4
30	DMU	Z	101	-	-	0/19/59/59	0/2/2/2

The worst 5 of 151 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	605	HEA	C4A-NA	-4.15	1.31	1.36
21	B	301	TGL	OC1-CC1	-3.93	1.11	1.22
26	P	306	CDL	C59-C58	-3.37	1.32	1.51
21	L	101	TGL	C20-CA9	-3.23	1.33	1.51
26	C	306	CDL	C59-C58	-3.16	1.33	1.51

The worst 5 of 383 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	307	CHD	C6-C5-C4	-7.94	102.55	111.07
18	N	605[A]	HEA	C13-C12-C11	-7.39	106.05	114.74
18	N	605[B]	HEA	C13-C12-C11	-7.39	106.05	114.74
18	A	604[B]	HEA	C13-C12-C11	-6.92	106.60	114.74
18	A	604[A]	HEA	C13-C12-C11	-6.92	106.60	114.74

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
18	N	606	HEA	ND
18	N	606	HEA	NB
18	A	605	HEA	ND
18	A	605	HEA	NB

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
21	Q	201	TGL	CG2-OG2-CB1-CB2

There are no ring outliers.

38 monomers are involved in 249 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	1	201	HEM	5	0
31	2	201	HEM	3	0
18	A	604[B]	HEA	6	0
18	A	605	HEA	3	0
20	A	607	PGV	5	0
20	A	608	PGV	4	0
21	B	301	TGL	6	0
24	C	301	CHD	1	0
25	C	303	PEK	7	0
20	C	304	PGV	5	0
20	C	305	PGV	9	0
26	C	306	CDL	15	0
24	C	307	CHD	3	0
21	D	201	TGL	12	0
28	E	201	PSC	19	0
23	E	202	EDO	1	0
26	G	101	CDL	23	0
24	J	101	CHD	5	0
21	L	101	TGL	20	0
30	M	101	DMU	1	0
18	N	605[A]	HEA	1	0
18	N	605[B]	HEA	6	0
18	N	606	HEA	3	0
19	N	607	PER	1	0
21	N	608	TGL	2	0
20	N	612	PGV	1	0
24	P	301	CHD	1	0
25	P	303	PEK	3	0
20	P	304	PGV	6	0
20	P	305	PGV	4	0
26	P	306	CDL	12	0
24	P	307	CHD	1	0
21	Q	201	TGL	10	0
26	T	101	CDL	24	0
24	T	103	CHD	1	0
28	V	101	PSC	21	0
24	W	101	CHD	5	0
30	Z	101	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	513/514 (99%)	0.21	20 (3%) 43 45	22, 30, 39, 74	0
1	N	513/514 (99%)	0.22	26 (5%) 32 33	27, 36, 48, 71	0
2	B	226/227 (99%)	-0.34	2 (0%) 85 86	26, 35, 59, 109	0
2	O	226/227 (99%)	-0.15	2 (0%) 85 86	34, 49, 78, 98	0
3	C	259/259 (100%)	-0.54	2 (0%) 87 88	26, 35, 48, 83	0
3	P	259/259 (100%)	-0.55	4 (1%) 76 77	28, 38, 52, 87	0
4	D	144/144 (100%)	-0.54	6 (4%) 40 41	30, 38, 63, 144	0
4	Q	144/144 (100%)	0.16	13 (9%) 12 12	32, 50, 81, 139	0
5	E	105/105 (100%)	-0.41	2 (1%) 70 70	30, 38, 62, 134	0
5	R	105/105 (100%)	-0.61	1 (0%) 84 84	33, 41, 62, 123	0
6	F	98/98 (100%)	-0.05	8 (8%) 14 15	30, 40, 95, 141	0
6	S	98/98 (100%)	0.25	8 (8%) 14 15	32, 45, 106, 141	0
7	G	83/84 (98%)	0.56	15 (18%) 2 2	34, 44, 116, 138	0
7	T	83/84 (98%)	0.80	17 (20%) 1 1	31, 47, 111, 136	0
8	H	79/79 (100%)	-0.11	7 (8%) 12 13	33, 43, 90, 106	0
8	U	79/79 (100%)	-0.17	2 (2%) 61 61	38, 49, 69, 137	0
9	I	72/73 (98%)	-0.15	3 (4%) 40 41	33, 46, 66, 79	0
9	V	72/73 (98%)	0.99	11 (15%) 3 3	36, 63, 85, 111	0
10	J	58/58 (100%)	0.36	7 (12%) 6 6	36, 46, 75, 135	0
10	W	58/58 (100%)	0.72	8 (13%) 4 4	39, 53, 84, 144	0
11	K	49/49 (100%)	-0.15	3 (6%) 25 26	35, 42, 58, 70	0
11	X	49/49 (100%)	0.61	4 (8%) 14 15	47, 58, 77, 78	0
12	L	46/46 (100%)	-0.53	1 (2%) 65 66	30, 38, 59, 104	0
12	Y	46/46 (100%)	-0.51	1 (2%) 65 66	36, 46, 69, 111	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	43/43 (100%)	-0.21	2 (4%) 35 37	32, 40, 79, 127	0
13	Z	43/43 (100%)	-0.05	3 (6%) 19 21	36, 50, 81, 108	0
14	1	104/105 (99%)	2.81	65 (62%) 0 1	45, 90, 118, 125	0
14	2	104/105 (99%)	4.61	79 (75%) 0 1	67, 115, 139, 147	0
All	All	3758/3768 (99%)	0.17	322 (8%) 13 14	22, 40, 98, 147	0

The worst 5 of 322 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	Q	5	VAL	13.6
4	Q	7	LYS	13.4
6	S	1	ALA	13.2
10	W	57	HIS	12.5
14	2	57	ILE	12.1

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
1	FME	N	1	10/11	0.96	0.17	-	43,61,73,95	0
7	TPO	T	11	11/12	0.45	0.34	-	85,109,117,125	0
7	TPO	G	11	11/12	0.50	0.33	-	81,97,160,160	0
1	FME	A	1	10/11	0.95	0.13	-	40,52,71,88	0
9	SAC	I	1	9/10	0.75	0.39	-	98,106,110,119	0
2	FME	O	1	10/11	0.98	0.14	-	49,56,65,78	0
9	SAC	V	1	9/10	0.31	0.91	-	131,137,150,153	0
2	FME	B	1	10/11	0.98	0.10	-	30,35,39,51	0

6.3 Carbohydrates [i](#)

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
27	UNL	Y	101	10/-	0.78	0.39	8.44	69,76,86,94	0
24	CHD	J	101	29/29	0.84	0.33	7.80	61,75,106,109	0
27	UNL	J	102	10/-	0.73	0.29	7.36	61,65,77,92	0
26	CDL	P	306	100/100	0.79	0.27	6.77	49,97,149,159	0
24	CHD	W	101	29/29	0.70	0.43	6.71	73,114,126,130	0
27	UNL	L	102	10/-	0.80	0.27	6.68	61,75,82,86	0
20	PGV	A	607	51/51	0.77	0.30	6.28	44,84,151,159	0
27	UNL	P	310	7/-	0.84	0.27	6.24	53,60,76,88	0
26	CDL	C	306	100/100	0.83	0.23	5.11	51,86,124,152	0
27	UNL	C	310	7/-	0.79	0.34	5.11	41,64,76,83	0
21	TGL	Q	201	63/63	0.74	0.21	4.63	52,82,104,109	0
16	MG	A	602	1/1	0.95	0.21	3.83	36,36,36,36	0
27	UNL	C	308	18/-	0.85	0.20	3.81	55,66,77,81	0
27	UNL	N	609	16/-	0.77	0.32	3.80	54,59,79,85	0
20	PGV	C	305	51/51	0.74	0.25	3.41	55,80,122,138	0
21	TGL	D	201	63/63	0.76	0.22	3.36	47,70,101,105	0
26	CDL	T	101	100/100	0.73	0.25	3.21	61,95,153,161	0
27	UNL	P	308	20/-	0.86	0.20	3.03	58,64,72,73	0
21	TGL	B	301	63/63	0.90	0.18	2.54	33,68,103,114	0
30	DMU	Z	101	33/33	0.77	0.30	2.54	55,76,107,113	0
21	TGL	L	101	63/63	0.78	0.26	2.48	45,70,98,107	0
26	CDL	G	101	100/100	0.66	0.30	2.47	58,103,158,163	0
27	UNL	N	610	18/-	0.85	0.19	2.43	51,59,69,70	0
23	EDO	N	613	4/4	0.98	0.16	2.42	38,38,39,41	0
16	MG	N	603	1/1	0.96	0.25	2.38	42,42,42,42	0
21	TGL	N	608	63/63	0.83	0.19	2.28	51,73,104,115	0
27	UNL	N	601	17/-	0.76	0.18	2.23	52,60,83,85	0
20	PGV	P	305	51/51	0.73	0.23	2.21	54,86,135,150	0
24	CHD	P	307	29/29	0.89	0.29	2.08	71,80,88,95	0
27	UNL	P	309	16/-	0.68	0.17	1.99	70,79,89,95	0
23	EDO	F	102	4/4	0.97	0.14	1.93	45,47,49,49	0
27	UNL	W	102	9/-	0.78	0.24	1.79	59,62,79,82	0
23	EDO	N	614	4/4	0.94	0.16	1.78	56,59,63,85	0
20	PGV	P	304	51/51	0.95	0.13	1.78	30,46,73,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
29	ZN	F	101	1/1	1.00	0.10	1.71	36,36,36,36	0
27	UNL	C	309	17/-	0.77	0.16	1.68	60,71,87,90	0
24	CHD	C	307	29/29	0.82	0.26	1.47	73,85,93,99	0
28	PSC	V	101	52/52	0.82	0.23	1.44	49,77,145,166	0
30	DMU	M	101	33/33	0.92	0.14	1.41	40,46,62,65	0
28	PSC	E	201	52/52	0.76	0.26	1.29	50,79,162,163	0
27	UNL	N	611	12/-	0.84	0.15	1.24	48,56,68,69	0
20	PGV	C	304	51/51	0.96	0.12	1.23	31,38,95,103	0
23	EDO	B	303	4/4	0.98	0.13	1.19	30,31,33,36	0
25	PEK	C	303	53/53	0.93	0.16	1.04	34,48,88,97	0
20	PGV	N	612	51/51	0.97	0.15	0.99	33,43,70,80	0
23	EDO	I	101	4/4	0.83	0.14	0.79	55,59,63,72	0
20	PGV	A	608	51/51	0.97	0.15	0.70	29,41,68,74	0
27	UNL	T	102	18/-	0.76	0.18	0.54	47,66,85,92	0
24	CHD	P	301	29/29	0.91	0.12	0.31	40,45,52,55	0
18	HEA	N	606	60/60	0.99	0.19	0.29	27,33,41,47	0
18	HEA	N	605[A]	60/60	0.98	0.18	0.28	32,38,47,50	9
25	PEK	P	303	53/53	0.95	0.13	0.28	39,53,94,101	0
18	HEA	N	605[B]	60/60	0.98	0.18	0.28	32,38,44,47	9
23	EDO	S	102	4/4	0.97	0.08	0.26	44,45,46,53	0
18	HEA	A	605	60/60	0.99	0.14	0.07	22,26,33,39	0
23	EDO	G	103	4/4	0.97	0.09	-0.36	37,39,49,51	0
24	CHD	G	102	29/29	0.96	0.08	-0.37	35,38,43,52	0
24	CHD	T	103	29/29	0.96	0.08	-0.42	30,36,42,53	0
18	HEA	A	604[B]	60/60	0.99	0.15	-0.56	23,28,35,40	9
31	HEM	1	201	43/43	0.95	0.19	-0.65	57,81,94,99	0
31	HEM	2	201	43/43	0.94	0.27	-0.70	79,101,135,149	0
17	NA	N	604	1/1	0.97	0.09	-0.74	45,45,45,45	0
23	EDO	C	311	4/4	0.97	0.08	-0.74	48,51,51,52	0
18	HEA	A	604[A]	60/60	0.99	0.15	-0.82	23,28,38,40	9
24	CHD	C	301	29/29	0.96	0.08	-1.16	34,40,48,53	0
22	CUA	B	302	2/2	1.00	0.11	-1.63	27,27,27,29	0
22	CUA	O	301	2/2	0.99	0.09	-2.24	42,42,42,43	0
17	NA	A	603	1/1	1.00	0.05	-2.65	31,31,31,31	0
29	ZN	S	101	1/1	0.99	0.05	-2.66	37,37,37,37	0
19	PER	A	606	2/2	0.99	0.10	-3.27	40,40,40,54	0
19	PER	N	607	2/2	0.98	0.10	-4.93	36,36,36,48	0
23	EDO	E	202	4/4	0.85	0.33	-	57,61,68,79	0
17	NA	C	302	1/1	0.58	0.58	-	59,59,59,59	0
15	CU	N	602	1/1	1.00	0.14	-	35,35,35,35	0
15	CU	A	601	1/1	1.00	0.13	-	29,29,29,29	0
17	NA	P	302	1/1	0.55	0.51	-	57,57,57,57	0

6.5 Other polymers [i](#)

There are no such residues in this entry.