



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 28, 2017 – 06:57 PM EST

PDB ID : 5X1B
Title : CO bound cytochrome c oxidase at 20 nsec after pump laser irradiation to release CO from O₂ reduction center
Authors : Shimada, A.; Kubo, M.; Baba, S.; Yamashita, K.; Hirata, K.; Ueno, G.; Nomura, T.; Kimura, T.; Shinzawa-Itoh, K.; Baba, J.; Hatano, K.; Eto, Y.; Miyamoto, A.; Murakami, H.; Kumasaka, T.; Owada, S.; Tono, K.; Yabashi, M.; Yamaguchi, Y.; Yanagisawa, S.; Sakaguchi, M.; Ogura, T.; Komiya, R.; Yan, J.; Yamashita, E.; Yamamoto, M.; Ago, H.; Yoshikawa, S.; Tsukihara, T.
Deposited on : unknown
Resolution : 2.40 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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030345
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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-20030345

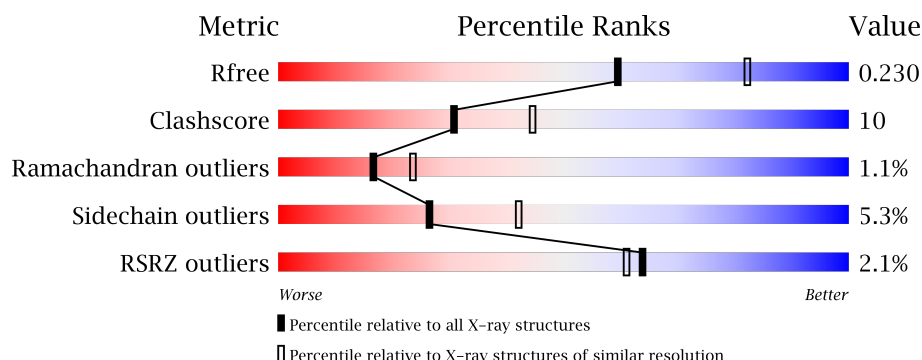
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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.

















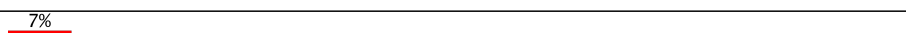
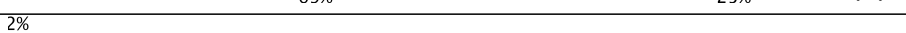





Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	3166 (2.40-2.40)
Clashscore	112137	3674 (2.40-2.40)
Ramachandran outliers	110173	3616 (2.40-2.40)
Sidechain outliers	110143	3617 (2.40-2.40)
RSRZ outliers	101464	3195 (2.40-2.40)

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>82%</div> <div>17%</div> <div>.</div> </div>
1	N	514	<div> <div>76%</div> <div>22%</div> <div>.</div> </div>
2	B	227	<div> <div>78%</div> <div>20%</div> <div>.</div> </div>
2	O	227	<div> <div>74%</div> <div>24%</div> <div>.</div> </div>
3	C	261	<div> <div>83%</div> <div>16%</div> <div>.</div> </div>

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

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	HEA	A	601	X	-	-	-
14	HEA	A	602	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	HEA	N	601	X	-	-	-
17	NA	A	605	-	-	-	X
18	CMO	N	606	-	-	-	X
19	TGL	A	607	-	-	-	X
19	TGL	D	201	-	-	-	X
19	TGL	L	101	-	-	-	X
19	TGL	N	609	-	-	-	X
19	TGL	N	610	-	-	-	X
19	TGL	N	611	-	-	-	X
20	PGV	A	609	-	-	-	X
20	PGV	N	607	-	-	-	X
21	EDO	A	612	-	-	-	X
21	EDO	A	613	-	-	-	X
21	EDO	A	614	-	-	X	X
21	EDO	B	305	-	-	-	X
21	EDO	F	102	-	-	-	X
21	EDO	G	104	-	-	-	X
21	EDO	T	104	-	-	-	X
23	CHD	J	101	-	-	-	X
23	CHD	W	101	-	-	-	X
24	PSC	B	303	-	-	-	X
24	PSC	R	201	-	-	-	X
26	CDL	C	303	-	-	-	X
26	CDL	C	307	-	-	-	X
26	CDL	P	304	-	-	-	X
26	CDL	T	103	-	-	-	X
27	PEK	G	102	-	-	-	X
27	PEK	T	101	-	-	-	X
27	PEK	T	102	-	-	-	X
29	DMU	Z	101	-	-	-	X

2 Entry composition

There are 30 unique types of molecules in this entry. The entry contains 31717 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	1	0
			4030	2694	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, mitochondrial.

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

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

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

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

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

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

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

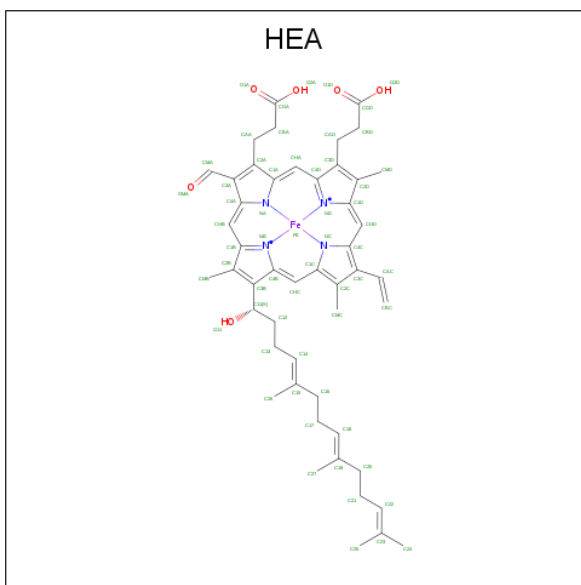
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

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 HEME-A (three-letter code: HEA) (formula: C₄₉H₅₆FeN₄O₆).



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

- 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

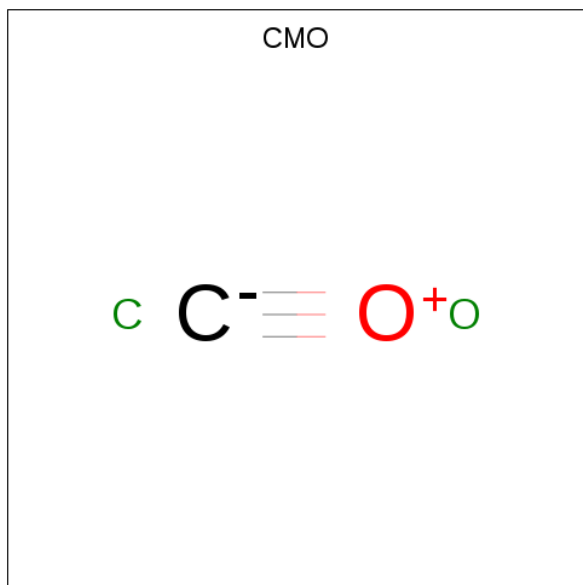
- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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).

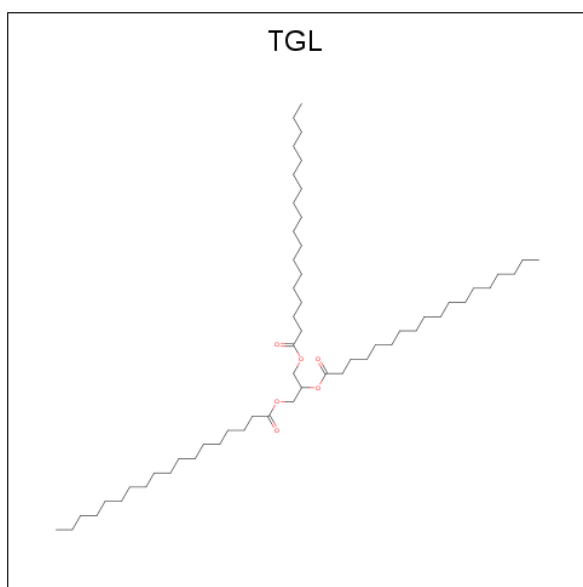
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	1	Total	Na	0	0
			1	1		
17	N	1	Total	Na	0	0
			1	1		

- Molecule 18 is CARBON MONOXIDE (three-letter code: CMO) (formula: CO).



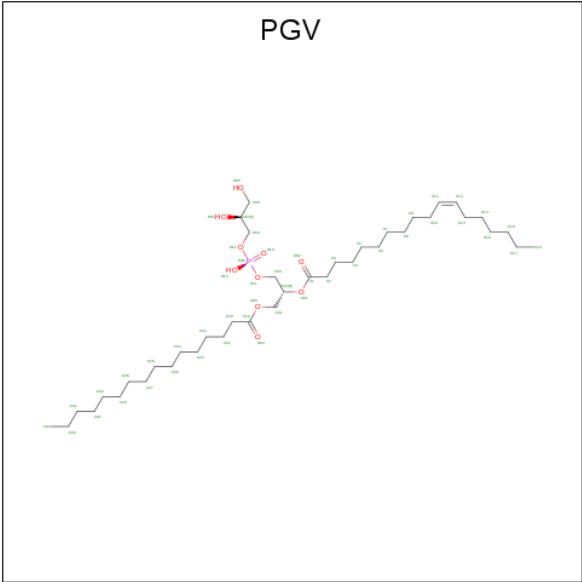
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
18	A	1	Total	C	O	0	0
			2	1	1		
18	N	1	Total	C	O	0	0
			2	1	1		

- Molecule 19 is TRISTEAROYLGLYCEROL (three-letter code: TGL) (formula: C₅₇H₁₁₀O₆).



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

- 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	G	1	Total	C	O	P	0	0
			51	40	10	1		
20	N	1	Total	C	O	P	0	0
			51	40	10	1		
20	N	1	Total	C	O	P	0	0
			51	40	10	1		
20	P	1	Total	C	O	P	0	0
			51	40	10	1		

- Molecule 21 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



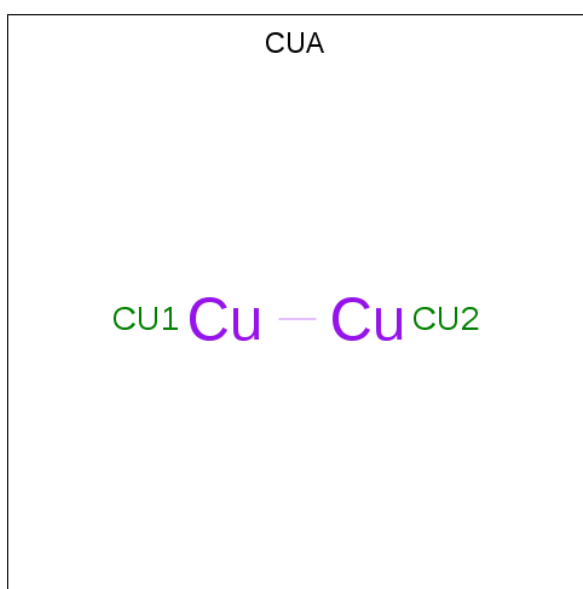
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	A	1	Total	C	O	0	0
			4	2	2		
21	A	1	Total	C	O	0	0
			4	2	2		
21	A	1	Total	C	O	0	0
			4	2	2		
21	A	1	Total	C	O	0	0
			4	2	2		
21	B	1	Total	C	O	0	0
			4	2	2		
21	B	1	Total	C	O	0	0
			4	2	2		
21	C	1	Total	C	O	0	0
			4	2	2		
21	C	1	Total	C	O	0	0
			4	2	2		
21	C	1	Total	C	O	0	0
			4	2	2		
21	F	1	Total	C	O	0	0
			4	2	2		
21	G	1	Total	C	O	0	0
			4	2	2		
21	K	1	Total	C	O	0	0
			4	2	2		
21	K	1	Total	C	O	0	0
			4	2	2		

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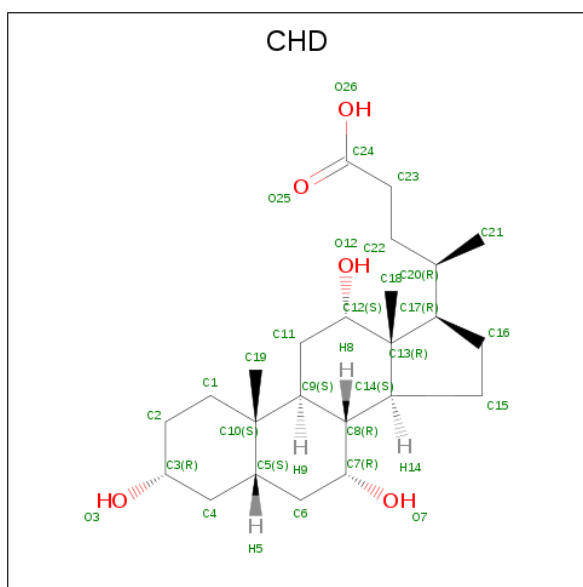
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	K	1	Total	C	O	0	0
			4	2	2		
21	L	1	Total	C	O	0	0
			4	2	2		
21	N	1	Total	C	O	0	0
			4	2	2		
21	T	1	Total	C	O	0	0
			4	2	2		

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



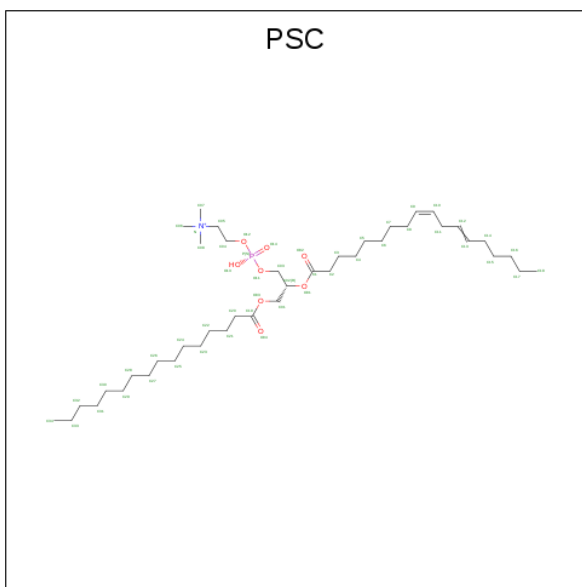
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	B	1	Total	Cu	0	0
			2	2		
22	O	1	Total	Cu	0	0
			2	2		

- Molecule 23 is CHOLIC ACID (three-letter code: CHD) (formula: C₂₄H₄₀O₅).



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

- Molecule 24 is (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).

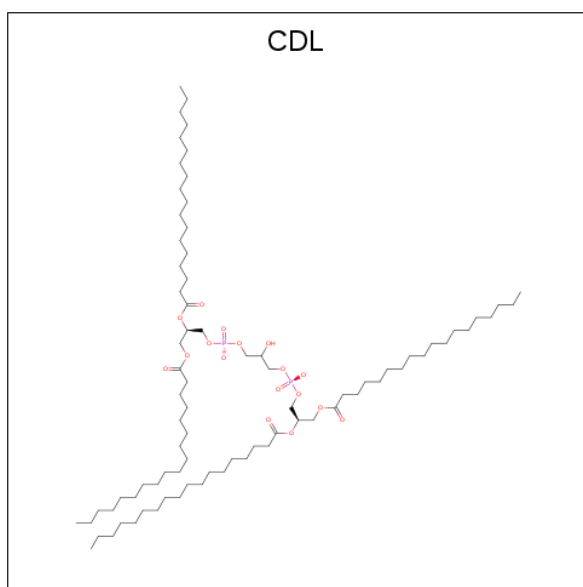


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
24	R	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

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

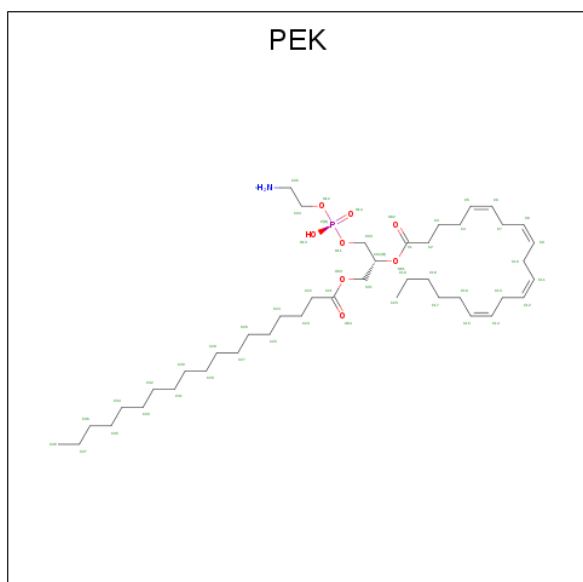
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	P	1	Total	X	0	0
			1	1		
25	C	1	Total	X	0	0
			1	1		

- 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	C	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 (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).

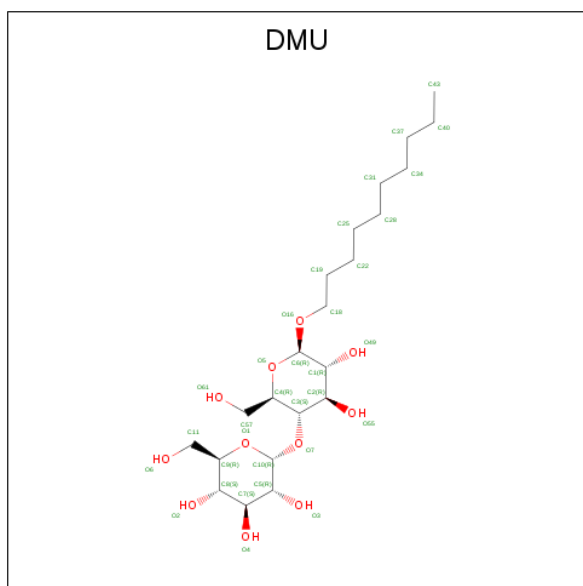


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
27	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
27	G	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
27	G	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
27	P	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
27	T	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
27	T	1	Total	C	N	O	P	0	0
			53	43	1	8	1		

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

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

- Molecule 29 is DECYL-BETA-D-MALTOPYRANOSIDE (three-letter code: DMU) (formula: C₂₂H₄₂O₁₁).



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

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

- Molecule 30 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	A	125	Total	O	0	0
			125	125		
30	B	77	Total	O	0	1
			78	78		
30	C	70	Total	O	0	0
			70	70		
30	D	41	Total	O	0	0
			41	41		
30	E	24	Total	O	0	0
			24	24		
30	F	36	Total	O	0	0
			36	36		
30	G	31	Total	O	0	0
			31	31		
30	H	33	Total	O	0	0
			33	33		
30	I	12	Total	O	0	0
			12	12		
30	J	19	Total	O	0	0
			19	19		
30	K	19	Total	O	0	0
			19	19		
30	L	14	Total	O	0	0
			14	14		
30	M	15	Total	O	0	0
			15	15		
30	N	117	Total	O	0	0
			117	117		
30	O	76	Total	O	0	1
			77	77		
30	P	54	Total	O	0	0
			54	54		
30	Q	29	Total	O	0	0
			29	29		
30	R	29	Total	O	0	0
			29	29		

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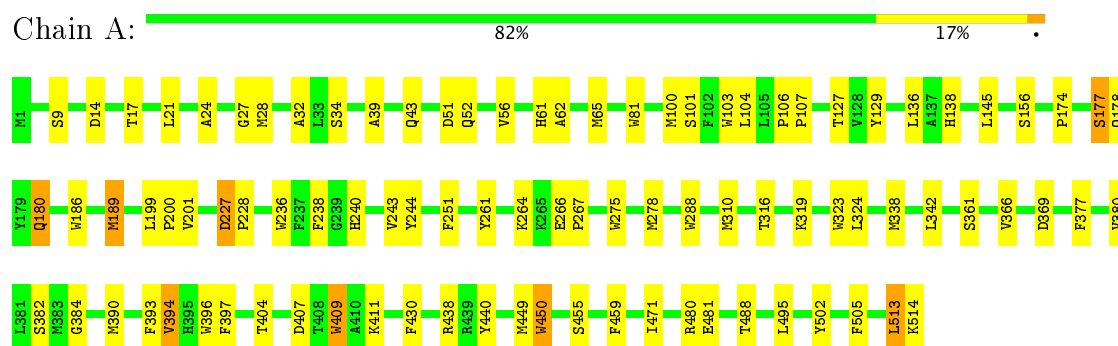
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	S	43	Total 43	O 43	0	0
30	T	20	Total 20	O 20	0	0
30	U	31	Total 31	O 31	0	0
30	V	19	Total 19	O 19	0	0
30	W	17	Total 17	O 17	0	0
30	X	9	Total 9	O 9	0	0
30	Y	6	Total 6	O 6	0	0
30	Z	4	Total 4	O 4	0	0

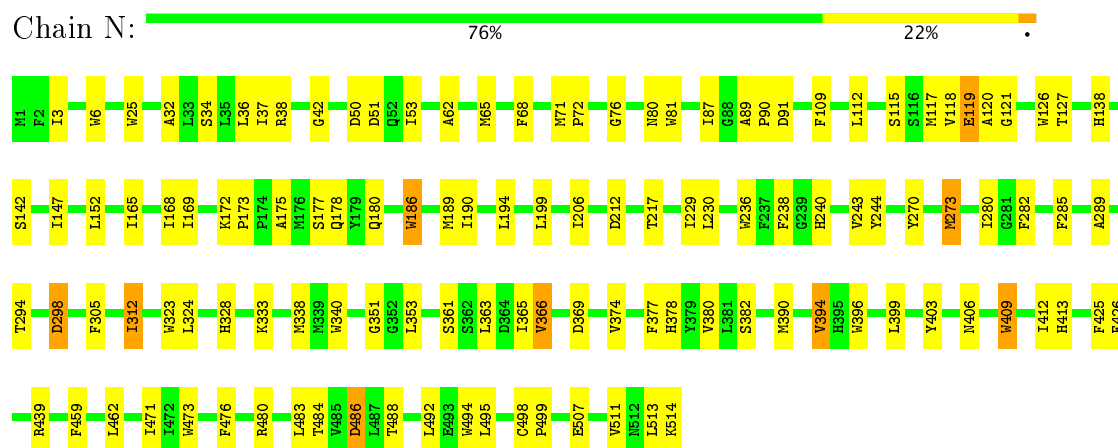
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

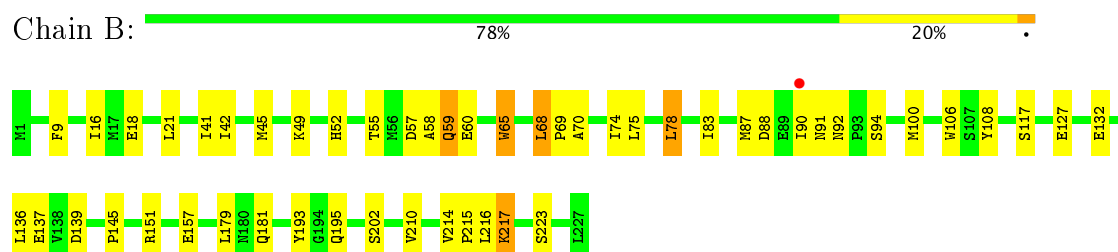
• Molecule 1: Cytochrome c oxidase subunit 1



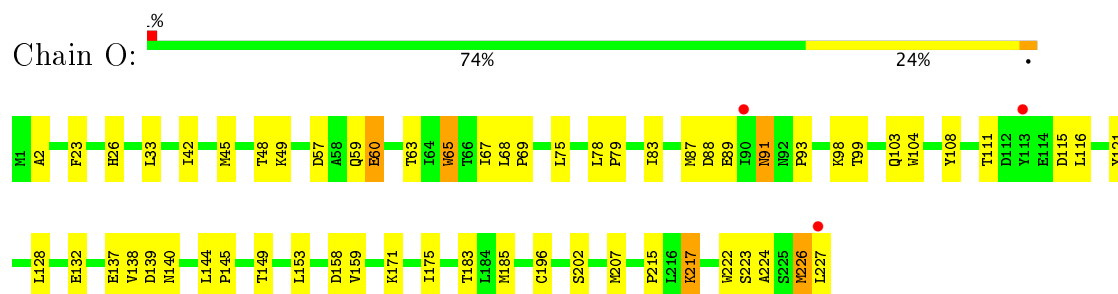
• Molecule 1: Cytochrome c oxidase subunit 1



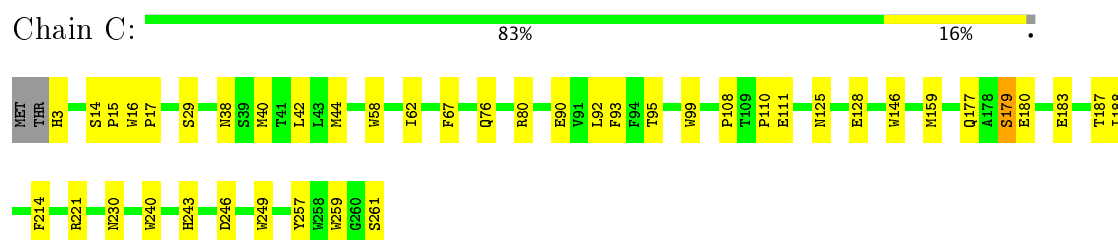
• Molecule 2: Cytochrome c oxidase subunit 2



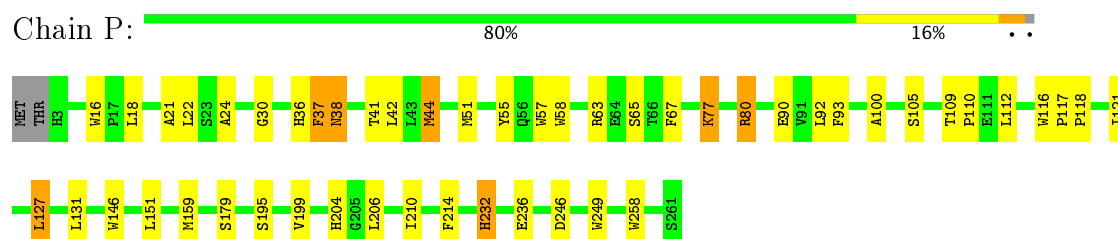
- Molecule 2: Cytochrome c oxidase subunit 2



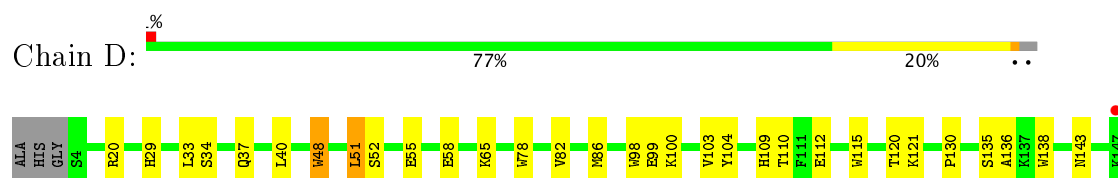
- Molecule 3: Cytochrome c oxidase subunit 3



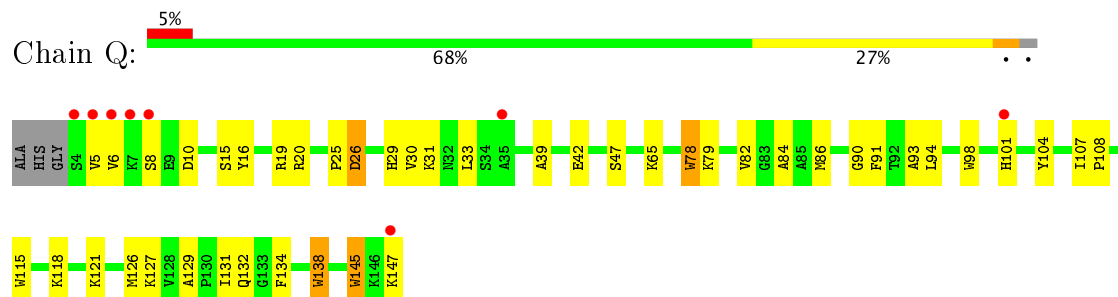
- Molecule 3: Cytochrome c oxidase subunit 3



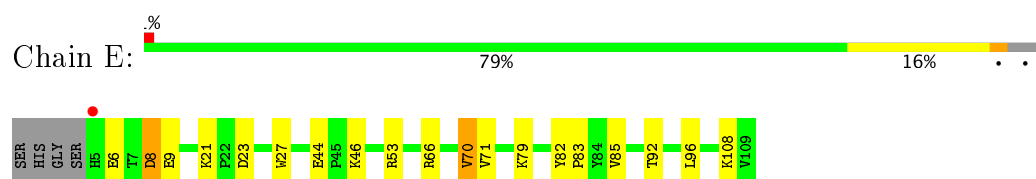
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial



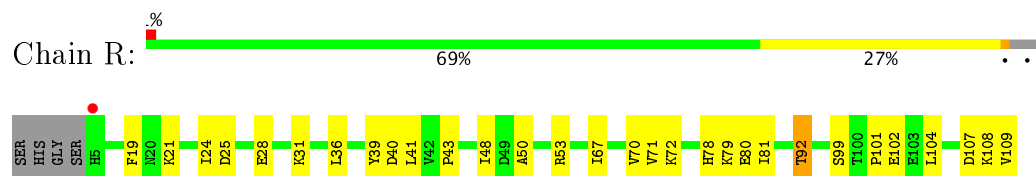
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial



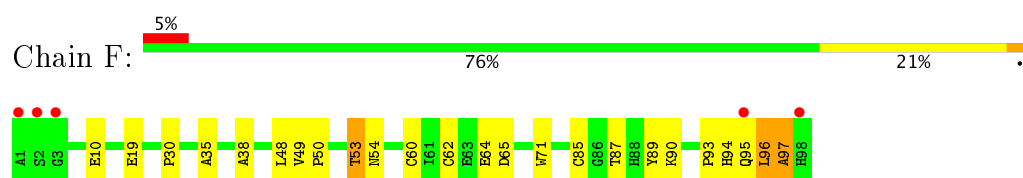
- Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial



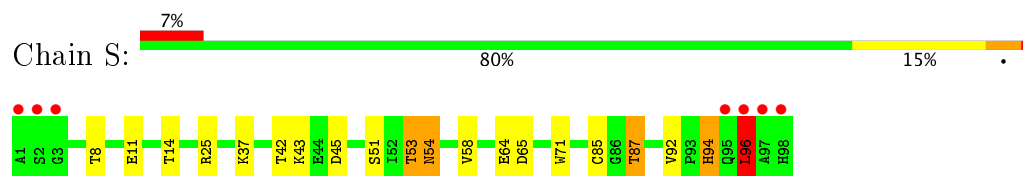
- Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial



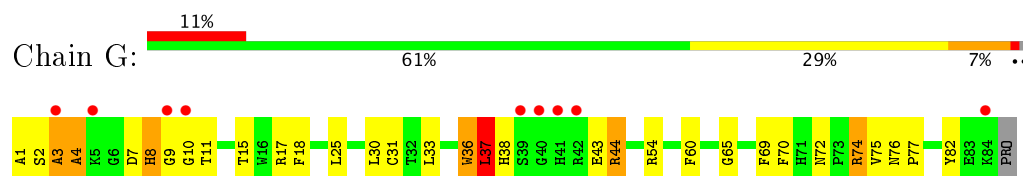
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



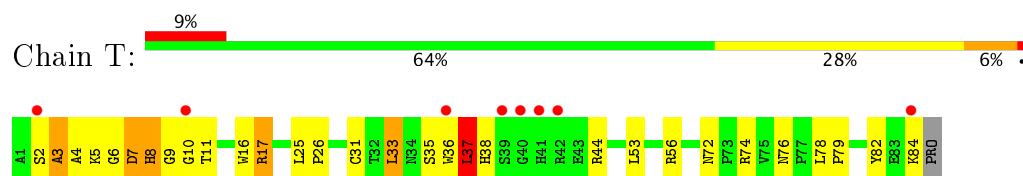
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



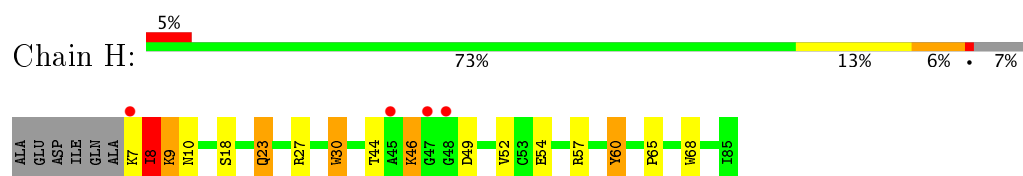
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



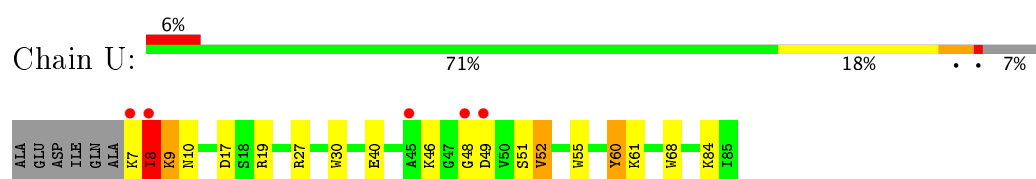
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



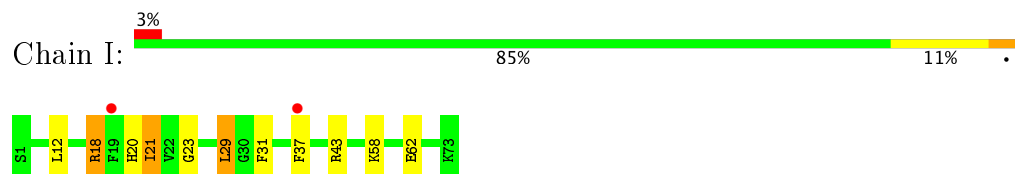
- Molecule 8: Cytochrome c oxidase subunit 6B1



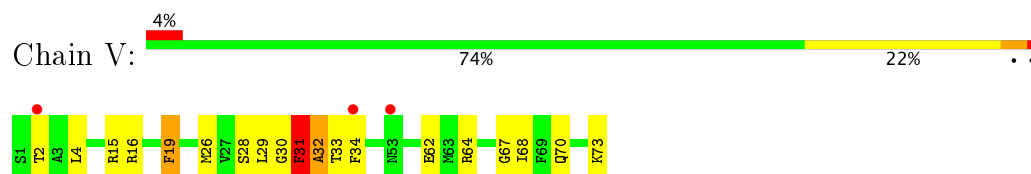
- Molecule 8: Cytochrome c oxidase subunit 6B1



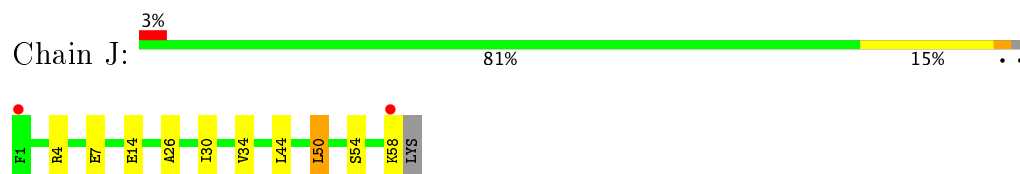
- Molecule 9: Cytochrome c oxidase subunit 6C



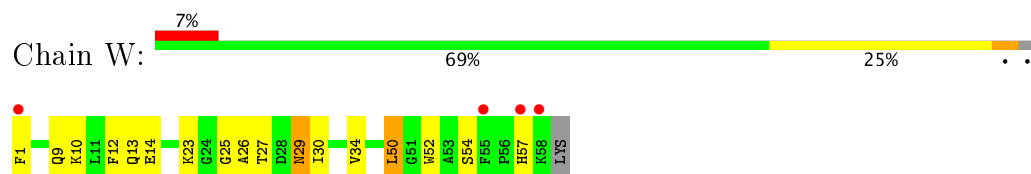
- Molecule 9: Cytochrome c oxidase subunit 6C



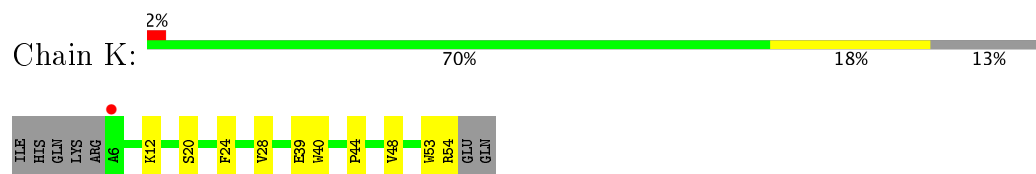
- Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial



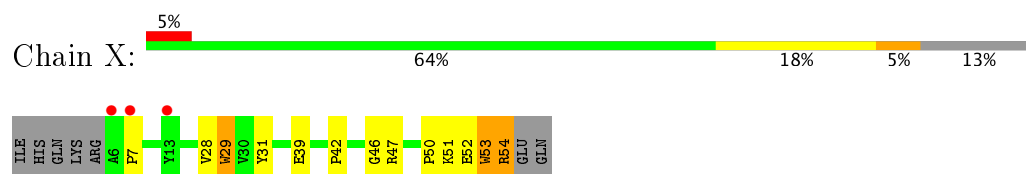
- Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial




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



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



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

Chain L:  2% 72% 23% ..



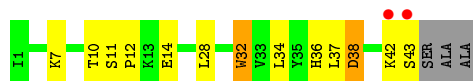
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial

Chain Y:  72% 23% ..



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

Chain M:  4% 65% 24% 7%



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

Chain Z:  4% 61% 24% 9% 7%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	185.85Å 209.49Å 179.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.40 14.99 – 2.40	Depositor EDS
% Data completeness (in resolution range)	97.7 (15.00-2.40) 98.2 (14.99-2.40)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.32 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0048	Depositor
R, R_{free}	0.182 , 0.230 0.182 , 0.230	Depositor DCC
R_{free} test set	13569 reflections (5.37%)	DCC
Wilson B-factor (Å ²)	56.1	Xtriage
Anisotropy	0.221	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 72.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	0.045 for l,-k,h	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	31717	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.52% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CMO, ZN, CHD, HEA, SAC, CDL, PSC, PEK, MG, TGL, EDO, 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	0.91	10/4164 (0.2%)	0.89	4/5689 (0.1%)
1	N	0.86	11/4156 (0.3%)	0.82	0/5678
2	B	0.81	2/1860 (0.1%)	0.90	1/2534 (0.0%)
2	O	0.73	2/1860 (0.1%)	0.83	0/2534
3	C	0.92	7/2197 (0.3%)	0.81	0/3005
3	P	0.89	4/2197 (0.2%)	0.80	0/3005
4	D	0.82	4/1229 (0.3%)	0.79	0/1658
4	Q	0.76	4/1229 (0.3%)	0.74	0/1658
5	E	0.67	1/871 (0.1%)	0.80	0/1182
5	R	0.65	0/871	0.74	0/1182
6	F	0.74	1/765 (0.1%)	0.86	2/1038 (0.2%)
6	S	0.72	0/765	0.82	1/1038 (0.1%)
7	G	0.86	1/690 (0.1%)	0.87	1/937 (0.1%)
7	T	0.80	1/690 (0.1%)	0.83	1/937 (0.1%)
8	H	0.85	2/682 (0.3%)	0.86	0/921
8	U	0.79	3/682 (0.4%)	0.79	0/921
9	I	0.69	0/605	0.83	0/802
9	V	0.60	0/605	0.80	1/802 (0.1%)
10	J	0.72	0/471	0.75	0/636
10	W	0.66	1/471 (0.2%)	0.77	0/636
11	K	0.81	1/398 (0.3%)	0.76	0/546
11	X	0.80	2/398 (0.5%)	0.75	0/546
12	L	0.80	0/393	0.76	0/526
12	Y	0.75	1/393 (0.3%)	0.75	0/526
13	M	0.81	1/345 (0.3%)	0.78	0/470
13	Z	0.68	0/345	0.75	0/470
All	All	0.82	59/29332 (0.2%)	0.82	11/39877 (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
7	G	0	1
7	T	0	2
All	All	0	3

The worst 5 of 59 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	58	TRP	CD2-CE2	7.46	1.50	1.41
1	N	126	TRP	CD2-CE2	7.33	1.50	1.41
1	A	396	TRP	CD2-CE2	6.55	1.49	1.41
2	B	106	TRP	CD2-CE2	6.42	1.49	1.41
1	N	340	TRP	CD2-CE2	6.38	1.49	1.41

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	227	ASP	CB-CG-OD1	7.54	125.08	118.30
1	A	438	ARG	NE-CZ-NH1	-6.50	117.05	120.30
6	S	96	LEU	CA-CB-CG	6.36	129.92	115.30
7	G	37	LEU	CA-CB-CG	6.03	129.17	115.30
6	F	48	LEU	CB-CG-CD2	-6.00	100.81	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	G	11	TPO	Peptide
7	T	10	GLY	Peptide
7	T	11	TPO	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	4030	0	4009	73	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	N	4027	0	4002	99	0
2	B	1824	0	1833	34	0
2	O	1824	0	1833	38	0
3	C	2110	0	2027	31	0
3	P	2110	0	2027	40	0
4	D	1195	0	1183	21	0
4	Q	1195	0	1183	31	0
5	E	852	0	845	8	0
5	R	852	0	845	21	0
6	F	748	0	728	13	0
6	S	748	0	728	18	0
7	G	675	0	643	29	0
7	T	675	0	643	23	0
8	H	662	0	623	13	0
8	U	662	0	623	9	0
9	I	601	0	613	8	0
9	V	601	0	613	23	0
10	J	460	0	459	8	0
10	W	460	0	459	11	0
11	K	384	0	366	6	0
11	X	384	0	366	12	0
12	L	380	0	380	12	0
12	Y	380	0	380	13	0
13	M	335	0	352	9	0
13	Z	335	0	352	15	0
14	A	120	0	108	12	0
14	N	120	0	108	13	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	N	1	0	0	0	0
18	A	2	0	0	1	0
18	N	2	0	0	0	0
19	A	63	0	110	3	0
19	D	63	0	110	1	0
19	L	63	0	110	4	0
19	N	189	0	330	11	0
20	A	102	0	152	3	0
20	C	102	0	152	0	0
20	G	51	0	76	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	N	102	0	152	8	0
20	P	51	0	76	3	0
21	A	20	0	30	9	0
21	B	8	0	12	1	0
21	C	12	0	18	0	0
21	F	4	0	6	0	0
21	G	4	0	6	0	0
21	K	12	0	18	0	0
21	L	4	0	6	0	0
21	N	4	0	6	1	0
21	T	4	0	6	1	0
22	B	2	0	0	0	0
22	O	2	0	0	0	0
23	B	29	0	39	1	0
23	C	58	0	78	3	0
23	J	29	0	39	1	0
23	O	29	0	39	1	0
23	P	58	0	78	2	0
23	W	29	0	38	1	0
24	B	52	0	80	12	0
24	R	52	0	80	6	0
25	C	1	0	0	0	0
25	P	1	0	0	0	0
26	C	200	0	312	15	0
26	P	100	0	156	7	0
26	T	100	0	156	13	0
27	C	53	0	77	3	0
27	G	106	0	154	10	0
27	P	53	0	77	4	0
27	T	106	0	154	4	0
28	F	1	0	0	0	0
28	S	1	0	0	0	0
29	M	33	0	42	1	0
29	Z	33	0	42	1	0
30	A	125	0	0	22	0
30	B	78	0	0	6	0
30	C	70	0	0	18	0
30	D	41	0	0	2	0
30	E	24	0	0	2	0
30	F	36	0	0	2	0
30	G	31	0	0	2	0
30	H	33	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	I	12	0	0	0	0
30	J	19	0	0	2	0
30	K	19	0	0	3	0
30	L	14	0	0	2	0
30	M	15	0	0	1	0
30	N	117	0	0	16	0
30	O	77	0	0	8	0
30	P	54	0	0	5	0
30	Q	29	0	0	7	0
30	R	29	0	0	3	0
30	S	43	0	0	4	0
30	T	20	0	0	6	0
30	U	31	0	0	3	0
30	V	19	0	0	4	0
30	W	17	0	0	1	0
30	X	9	0	0	4	0
30	Y	6	0	0	1	0
30	Z	4	0	0	0	0
All	All	31717	0	31348	645	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 10.

The worst 5 of 645 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)
1:N:240:HIS:NE2	1:N:244:TYR:CE2	1.73	1.45
1:A:240:HIS:NE2	1:A:244:TYR:HE2	1.01	1.42
1:A:240:HIS:NE2	1:A:244:TYR:CE2	1.78	1.30
1:A:240:HIS:CD2	1:A:244:TYR:HE2	1.49	1.29
1:N:240:HIS:NE2	1:N:244:TYR:HE2	0.80	1.28

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	513/514 (100%)	494 (96%)	19 (4%)	0	100	100
1	N	512/514 (100%)	488 (95%)	23 (4%)	1 (0%)	51	67
2	B	225/227 (99%)	213 (95%)	11 (5%)	1 (0%)	38	54
2	O	225/227 (99%)	211 (94%)	12 (5%)	2 (1%)	20	29
3	C	257/261 (98%)	250 (97%)	7 (3%)	0	100	100
3	P	257/261 (98%)	248 (96%)	6 (2%)	3 (1%)	15	21
4	D	142/147 (97%)	133 (94%)	9 (6%)	0	100	100
4	Q	142/147 (97%)	130 (92%)	9 (6%)	3 (2%)	8	9
5	E	103/109 (94%)	98 (95%)	4 (4%)	1 (1%)	18	26
5	R	103/109 (94%)	99 (96%)	3 (3%)	1 (1%)	18	26
6	F	96/98 (98%)	87 (91%)	7 (7%)	2 (2%)	8	9
6	S	96/98 (98%)	90 (94%)	5 (5%)	1 (1%)	18	26
7	G	81/85 (95%)	69 (85%)	8 (10%)	4 (5%)	2	1
7	T	81/85 (95%)	68 (84%)	5 (6%)	8 (10%)	1	0
8	H	77/85 (91%)	67 (87%)	9 (12%)	1 (1%)	14	19
8	U	77/85 (91%)	69 (90%)	4 (5%)	4 (5%)	2	1
9	I	71/73 (97%)	66 (93%)	5 (7%)	0	100	100
9	V	71/73 (97%)	64 (90%)	6 (8%)	1 (1%)	13	18
10	J	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
10	W	56/59 (95%)	53 (95%)	2 (4%)	1 (2%)	10	12
11	K	47/56 (84%)	47 (100%)	0	0	100	100
11	X	47/56 (84%)	41 (87%)	5 (11%)	1 (2%)	8	9
12	L	44/47 (94%)	43 (98%)	1 (2%)	0	100	100
12	Y	44/47 (94%)	40 (91%)	4 (9%)	0	100	100
13	M	41/46 (89%)	40 (98%)	0	1 (2%)	7	7
13	Z	41/46 (89%)	38 (93%)	2 (5%)	1 (2%)	7	7
All	All	3505/3614 (97%)	3301 (94%)	167 (5%)	37 (1%)	17	23

5 of 37 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	97	ALA
7	G	3	ALA
7	G	4	ALA
7	G	8	HIS
8	H	8	ILE

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	427/426 (100%)	411 (96%)	16 (4%)	39	59
1	N	426/426 (100%)	408 (96%)	18 (4%)	34	53
2	B	210/210 (100%)	198 (94%)	12 (6%)	24	38
2	O	210/210 (100%)	198 (94%)	12 (6%)	24	38
3	C	224/226 (99%)	220 (98%)	4 (2%)	64	81
3	P	224/226 (99%)	216 (96%)	8 (4%)	40	60
4	D	128/129 (99%)	125 (98%)	3 (2%)	56	75
4	Q	128/129 (99%)	121 (94%)	7 (6%)	25	40
5	E	92/95 (97%)	86 (94%)	6 (6%)	20	31
5	R	92/95 (97%)	87 (95%)	5 (5%)	26	41
6	F	81/81 (100%)	77 (95%)	4 (5%)	29	46
6	S	81/81 (100%)	74 (91%)	7 (9%)	12	18
7	G	67/68 (98%)	61 (91%)	6 (9%)	11	16
7	T	67/68 (98%)	63 (94%)	4 (6%)	22	35
8	H	71/75 (95%)	63 (89%)	8 (11%)	7	9
8	U	71/75 (95%)	65 (92%)	6 (8%)	12	19
9	I	57/57 (100%)	52 (91%)	5 (9%)	12	17
9	V	57/57 (100%)	51 (90%)	6 (10%)	8	11
10	J	49/50 (98%)	46 (94%)	3 (6%)	22	34
10	W	49/50 (98%)	43 (88%)	6 (12%)	6	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	K	39/46 (85%)	37 (95%)	2 (5%)	28	44
11	X	39/46 (85%)	37 (95%)	2 (5%)	28	44
12	L	39/40 (98%)	37 (95%)	2 (5%)	28	44
12	Y	39/40 (98%)	37 (95%)	2 (5%)	28	44
13	M	37/38 (97%)	35 (95%)	2 (5%)	26	41
13	Z	37/38 (97%)	32 (86%)	5 (14%)	4	5
All	All	3041/3082 (99%)	2880 (95%)	161 (5%)	26	42

5 of 161 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	M	38	ASP
1	N	486	ASP
10	W	14	GLU
1	N	91	ASP
1	N	273	MET

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

Mol	Chain	Res	Type
10	J	57	HIS
1	N	413	HIS
8	U	23	GLN
11	K	35	GLN
1	N	180	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	9,9,10	0.41	0	7,9,11	1.72	3 (42%)
2	FME	B	1	2	9,9,10	0.92	0	7,9,11	2.07	4 (57%)
7	TPO	G	11	7	9,10,11	1.48	2 (22%)	10,14,16	2.32	2 (20%)
9	SAC	I	1	9	8,8,9	1.23	1 (12%)	6,9,11	0.96	1 (16%)
1	FME	N	1	1	9,9,10	0.79	1 (11%)	7,9,11	1.44	1 (14%)
2	FME	O	1	2	9,9,10	0.95	0	7,9,11	1.65	1 (14%)
7	TPO	T	11	7	9,10,11	2.05	4 (44%)	10,14,16	1.86	2 (20%)
9	SAC	V	1	9	8,8,9	1.75	2 (25%)	6,9,11	1.23	1 (16%)

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	-	0/6/9/11	0/0/0/0
2	FME	B	1	2	-	0/6/9/11	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	-	0/6/9/11	0/0/0/0
2	FME	O	1	2	-	0/6/9/11	0/0/0/0
7	TPO	T	11	7	-	1/8/11/13	0/0/0/0
9	SAC	V	1	9	-	2/6/8/10	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)
1	N	1	FME	CA-C	2.02	1.52	1.50
7	G	11	TPO	CA-C	2.08	1.53	1.50
7	T	11	TPO	CB-CA	2.10	1.57	1.53
7	T	11	TPO	P-OG1	2.37	1.63	1.59
9	V	1	SAC	CA-C	2.38	1.53	1.50

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	FME	CB-CA-C	-3.75	105.48	111.65
1	N	1	FME	O-C-CA	-2.83	118.55	125.15
1	A	1	FME	O-C-CA	-2.56	119.19	125.15
2	B	1	FME	O-C-CA	-2.42	119.50	125.15
1	A	1	FME	CG-CB-CA	-2.39	106.06	112.97

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	V	1	SAC	C2A-C1A-N-CA
9	V	1	SAC	OAC-C1A-N-CA
7	G	11	TPO	OG1-CB-CA-N
7	T	11	TPO	OG1-CB-CA-N

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 72 ligands modelled in this entry, 2 are unknown and 8 are monoatomic - leaving 62 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
14	HEA	A	601	1	44,67,67	1.10	3 (6%)	37,103,103	1.81	8 (21%)
14	HEA	A	602	1	44,67,67	1.03	3 (6%)	37,103,103	1.70	7 (18%)
18	CMO	A	606	15	0,1,1	0.00	-	0,0,0	0.00	-
19	TGL	A	607	-	62,62,62	1.21	4 (6%)	65,65,65	1.45	11 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	PGV	A	608	-	50,50,50	0.78	2 (4%)	51,56,56	1.51	5 (9%)
20	PGV	A	609	-	50,50,50	1.09	2 (4%)	51,56,56	1.14	5 (9%)
21	EDO	A	610	-	3,3,3	0.51	0	2,2,2	0.59	0
21	EDO	A	611	-	3,3,3	0.36	0	2,2,2	0.64	0
21	EDO	A	612	-	3,3,3	0.51	0	2,2,2	0.11	0
21	EDO	A	613	-	3,3,3	0.53	0	2,2,2	0.27	0
21	EDO	A	614	-	3,3,3	0.58	0	2,2,2	0.09	0
22	CUA	B	301	2	0,1,1	0.00	-	0,0,0	0.00	-
23	CHD	B	302	-	29,32,32	0.77	0	47,51,51	1.25	4 (8%)
24	PSC	B	303	-	51,51,51	1.28	3 (5%)	56,59,59	1.15	4 (7%)
21	EDO	B	304	-	3,3,3	0.40	0	2,2,2	0.63	0
21	EDO	B	305	-	3,3,3	0.39	0	2,2,2	0.51	0
20	PGV	C	302	-	50,50,50	0.90	2 (4%)	51,56,56	0.97	4 (7%)
26	CDL	C	303	-	99,99,99	1.37	12 (12%)	101,111,111	1.26	8 (7%)
23	CHD	C	304	-	29,32,32	0.57	0	47,51,51	2.02	13 (27%)
23	CHD	C	305	-	29,32,32	0.92	1 (3%)	47,51,51	1.18	6 (12%)
27	PEK	C	306	-	52,52,52	1.02	2 (3%)	54,57,57	0.97	3 (5%)
26	CDL	C	307	-	99,99,99	1.41	13 (13%)	101,111,111	1.28	8 (7%)
20	PGV	C	308	-	50,50,50	1.19	2 (4%)	51,56,56	1.09	4 (7%)
21	EDO	C	309	-	3,3,3	0.37	0	2,2,2	0.70	0
21	EDO	C	310	-	3,3,3	0.52	0	2,2,2	0.35	0
21	EDO	C	311	-	3,3,3	0.53	0	2,2,2	0.32	0
19	TGL	D	201	-	62,62,62	1.12	3 (4%)	65,65,65	1.05	7 (10%)
21	EDO	F	102	-	3,3,3	0.56	0	2,2,2	0.05	0
27	PEK	G	101	-	52,52,52	0.93	2 (3%)	54,57,57	1.30	5 (9%)
27	PEK	G	102	-	52,52,52	1.20	3 (5%)	54,57,57	1.16	5 (9%)
20	PGV	G	103	-	50,50,50	1.05	2 (4%)	51,56,56	1.01	2 (3%)
21	EDO	G	104	-	3,3,3	0.40	0	2,2,2	0.59	0
23	CHD	J	101	-	29,32,32	0.60	0	47,51,51	1.54	9 (19%)
21	EDO	K	101	-	3,3,3	0.47	0	2,2,2	0.36	0
21	EDO	K	102	-	3,3,3	0.50	0	2,2,2	0.29	0
21	EDO	K	103	-	3,3,3	0.56	0	2,2,2	0.11	0
19	TGL	L	101	-	62,62,62	1.18	3 (4%)	65,65,65	1.30	6 (9%)
21	EDO	L	102	-	3,3,3	0.45	0	2,2,2	0.42	0
29	DMU	M	101	-	34,34,34	0.54	0	45,45,45	1.19	5 (11%)
14	HEA	N	601	1	44,67,67	1.05	4 (9%)	37,103,103	1.72	8 (21%)
14	HEA	N	602	1	44,67,67	1.12	2 (4%)	37,103,103	1.92	11 (29%)
18	CMO	N	606	-	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
20	PGV	N	607	-	50,50,50	1.08	2 (4%)	51,56,56	1.14	5 (9%)
20	PGV	N	608	-	50,50,50	0.89	3 (6%)	51,56,56	1.22	5 (9%)
19	TGL	N	609	-	62,62,62	1.11	3 (4%)	65,65,65	1.34	8 (12%)
19	TGL	N	610	-	62,62,62	1.12	3 (4%)	65,65,65	1.18	7 (10%)
19	TGL	N	611	-	62,62,62	1.17	3 (4%)	65,65,65	1.29	8 (12%)
21	EDO	N	612	-	3,3,3	0.56	0	2,2,2	0.14	0
22	CUA	O	301	2	0,1,1	0.00	-	0,0,0	0.00	-
23	CHD	O	302	-	29,32,32	0.97	1 (3%)	47,51,51	1.46	6 (12%)
27	PEK	P	302	-	52,52,52	0.86	2 (3%)	54,57,57	1.42	5 (9%)
20	PGV	P	303	-	50,50,50	0.92	2 (4%)	51,56,56	1.13	5 (9%)
26	CDL	P	304	-	99,99,99	1.37	12 (12%)	101,111,111	1.20	7 (6%)
23	CHD	P	305	-	29,32,32	0.49	0	47,51,51	1.84	13 (27%)
23	CHD	P	306	-	29,32,32	0.71	1 (3%)	47,51,51	1.52	11 (23%)
24	PSC	R	201	-	51,51,51	1.21	3 (5%)	56,59,59	1.06	5 (8%)
27	PEK	T	101	-	52,52,52	1.16	3 (5%)	54,57,57	1.14	5 (9%)
27	PEK	T	102	-	52,52,52	1.18	2 (3%)	54,57,57	1.19	4 (7%)
26	CDL	T	103	-	99,99,99	1.35	12 (12%)	101,111,111	1.36	12 (11%)
21	EDO	T	104	-	3,3,3	0.44	0	2,2,2	0.28	0
23	CHD	W	101	-	29,32,32	0.81	1 (3%)	47,51,51	2.09	15 (31%)
29	DMU	Z	101	-	34,34,34	0.53	0	45,45,45	1.18	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
14	HEA	A	601	1	3/3/7/16	0/24/76/76	0/0/8/8
14	HEA	A	602	1	1/1/7/16	0/24/76/76	0/0/8/8
18	CMO	A	606	15	-	0/0/0/0	0/0/0/0
19	TGL	A	607	-	-	0/65/65/65	0/0/0/0
20	PGV	A	608	-	-	0/55/55/55	0/0/0/0
20	PGV	A	609	-	-	0/55/55/55	0/0/0/0
21	EDO	A	610	-	-	0/1/1/1	0/0/0/0
21	EDO	A	611	-	-	0/1/1/1	0/0/0/0
21	EDO	A	612	-	-	0/1/1/1	0/0/0/0
21	EDO	A	613	-	-	0/1/1/1	0/0/0/0
21	EDO	A	614	-	-	0/1/1/1	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CUA	B	301	2	-	0/0/0/0	0/0/0/0
23	CHD	B	302	-	-	0/7/74/74	0/4/4/4
24	PSC	B	303	-	-	0/55/55/55	0/0/0/0
21	EDO	B	304	-	-	0/1/1/1	0/0/0/0
21	EDO	B	305	-	-	0/1/1/1	0/0/0/0
20	PGV	C	302	-	-	0/55/55/55	0/0/0/0
26	CDL	C	303	-	-	2/110/110/110	0/0/0/0
23	CHD	C	304	-	-	0/7/74/74	0/4/4/4
23	CHD	C	305	-	-	0/7/74/74	0/4/4/4
27	PEK	C	306	-	-	0/56/56/56	0/0/0/0
26	CDL	C	307	-	-	0/110/110/110	0/0/0/0
20	PGV	C	308	-	-	0/55/55/55	0/0/0/0
21	EDO	C	309	-	-	0/1/1/1	0/0/0/0
21	EDO	C	310	-	-	0/1/1/1	0/0/0/0
21	EDO	C	311	-	-	0/1/1/1	0/0/0/0
19	TGL	D	201	-	-	0/65/65/65	0/0/0/0
21	EDO	F	102	-	-	0/1/1/1	0/0/0/0
27	PEK	G	101	-	-	0/56/56/56	0/0/0/0
27	PEK	G	102	-	-	0/56/56/56	0/0/0/0
20	PGV	G	103	-	-	0/55/55/55	0/0/0/0
21	EDO	G	104	-	-	0/1/1/1	0/0/0/0
23	CHD	J	101	-	-	0/7/74/74	0/4/4/4
21	EDO	K	101	-	-	0/1/1/1	0/0/0/0
21	EDO	K	102	-	-	0/1/1/1	0/0/0/0
21	EDO	K	103	-	-	0/1/1/1	0/0/0/0
19	TGL	L	101	-	-	0/65/65/65	0/0/0/0
21	EDO	L	102	-	-	0/1/1/1	0/0/0/0
29	DMU	M	101	-	-	0/19/59/59	0/2/2/2
14	HEA	N	601	1	3/3/7/16	0/24/76/76	0/0/8/8
14	HEA	N	602	1	-	0/24/76/76	0/0/8/8
18	CMO	N	606	-	-	0/0/0/0	0/0/0/0
20	PGV	N	607	-	-	0/55/55/55	0/0/0/0
20	PGV	N	608	-	-	0/55/55/55	0/0/0/0
19	TGL	N	609	-	-	0/65/65/65	0/0/0/0
19	TGL	N	610	-	-	1/65/65/65	0/0/0/0
19	TGL	N	611	-	-	2/65/65/65	0/0/0/0
21	EDO	N	612	-	-	0/1/1/1	0/0/0/0
22	CUA	O	301	2	-	0/0/0/0	0/0/0/0
23	CHD	O	302	-	-	0/7/74/74	0/4/4/4
27	PEK	P	302	-	-	0/56/56/56	0/0/0/0
20	PGV	P	303	-	-	0/55/55/55	0/0/0/0
26	CDL	P	304	-	-	1/110/110/110	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CHD	P	305	-	-	0/7/74/74	0/4/4/4
23	CHD	P	306	-	-	0/7/74/74	0/4/4/4
24	PSC	R	201	-	-	0/55/55/55	0/0/0/0
27	PEK	T	101	-	-	0/56/56/56	0/0/0/0
27	PEK	T	102	-	-	0/56/56/56	0/0/0/0
26	CDL	T	103	-	-	0/110/110/110	0/0/0/0
21	EDO	T	104	-	-	0/1/1/1	0/0/0/0
23	CHD	W	101	-	-	0/7/74/74	0/4/4/4
29	DMU	Z	101	-	-	0/19/59/59	0/2/2/2

The worst 5 of 121 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	N	602	HEA	C4B-NB	-4.01	1.32	1.36
14	A	601	HEA	C1D-ND	-3.78	1.32	1.36
14	A	602	HEA	C4B-NB	-3.60	1.32	1.36
26	C	307	CDL	C19-C18	-3.12	1.33	1.51
26	T	103	CDL	C19-C18	-3.07	1.34	1.51

The worst 5 of 274 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	607	TGL	CG3-CG2-CG1	-5.40	99.69	111.86
14	A	602	HEA	CAD-CBD-CGD	-4.96	104.18	112.66
23	P	305	CHD	C6-C5-C4	-4.87	105.60	111.13
23	C	304	CHD	C23-C22-C20	-4.50	108.66	114.72
20	A	608	PGV	O03-C19-O04	-4.30	112.86	123.55

5 of 7 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
14	A	602	HEA	NB
14	A	601	HEA	ND
14	A	601	HEA	NA
14	A	601	HEA	NB
14	N	601	HEA	ND

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
26	P	304	CDL	CA4-OA6-CA5-C11
19	N	611	TGL	CG2-OG2-CB1-OB1

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Mol	Chain	Res	Type	Atoms
19	N	610	TGL	CG2-OG2-CB1-CB2
19	N	611	TGL	CG2-OG2-CB1-CB2
26	C	303	CDL	CA4-OA6-CA5-OA7

There are no ring outliers.

46 monomers are involved in 154 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	A	601	HEA	6	0
14	A	602	HEA	6	0
18	A	606	CMO	1	0
19	A	607	TGL	3	0
20	A	608	PGV	1	0
20	A	609	PGV	2	0
21	A	610	EDO	1	0
21	A	612	EDO	2	0
21	A	613	EDO	2	0
21	A	614	EDO	4	0
23	B	302	CHD	1	0
24	B	303	PSC	12	0
21	B	305	EDO	1	0
26	C	303	CDL	2	0
23	C	304	CHD	2	0
23	C	305	CHD	1	0
27	C	306	PEK	3	0
26	C	307	CDL	13	0
19	D	201	TGL	1	0
27	G	101	PEK	4	0
27	G	102	PEK	6	0
20	G	103	PGV	2	0
23	J	101	CHD	1	0
19	L	101	TGL	4	0
29	M	101	DMU	1	0
14	N	601	HEA	10	0
14	N	602	HEA	3	0
20	N	607	PGV	6	0
20	N	608	PGV	2	0
19	N	609	TGL	5	0
19	N	610	TGL	2	0
19	N	611	TGL	4	0
21	N	612	EDO	1	0
23	O	302	CHD	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	P	302	PEK	4	0
20	P	303	PGV	3	0
26	P	304	CDL	7	0
23	P	305	CHD	1	0
23	P	306	CHD	1	0
24	R	201	PSC	6	0
27	T	101	PEK	3	0
27	T	102	PEK	1	0
26	T	103	CDL	13	0
21	T	104	EDO	1	0
23	W	101	CHD	1	0
29	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%)	-1.13	0 100 100	41, 53, 66, 101	0
1	N	513/514 (99%)	-1.08	0 100 100	43, 60, 76, 104	0
2	B	226/227 (99%)	-0.98	1 (0%) 92 91	46, 59, 91, 128	0
2	O	226/227 (99%)	-0.81	3 (1%) 77 75	54, 69, 104, 151	0
3	C	259/261 (99%)	-0.90	0 100 100	46, 57, 75, 115	0
3	P	259/261 (99%)	-0.91	0 100 100	46, 62, 81, 121	0
4	D	144/147 (97%)	-0.68	1 (0%) 87 86	52, 66, 89, 117	0
4	Q	144/147 (97%)	-0.22	8 (5%) 25 24	64, 83, 125, 160	0
5	E	105/109 (96%)	-0.86	1 (0%) 82 80	50, 65, 92, 147	0
5	R	105/109 (96%)	-0.76	1 (0%) 82 80	62, 79, 105, 154	0
6	F	98/98 (100%)	-0.35	5 (5%) 29 27	52, 66, 134, 154	0
6	S	98/98 (100%)	-0.20	7 (7%) 17 15	58, 74, 145, 162	0
7	G	83/85 (97%)	-0.27	9 (10%) 6 6	55, 66, 143, 159	0
7	T	83/85 (97%)	-0.20	8 (9%) 9 8	53, 73, 147, 158	0
8	H	79/85 (92%)	-0.48	4 (5%) 29 27	54, 69, 141, 156	0
8	U	79/85 (92%)	-0.30	5 (6%) 21 19	61, 80, 139, 153	0
9	I	72/73 (98%)	-0.55	2 (2%) 53 51	58, 73, 101, 114	0
9	V	72/73 (98%)	-0.30	3 (4%) 37 35	59, 84, 114, 142	0
10	J	58/59 (98%)	-0.52	2 (3%) 46 44	57, 70, 111, 144	0
10	W	58/59 (98%)	-0.27	4 (6%) 18 16	66, 82, 123, 158	0
11	K	49/56 (87%)	-0.34	1 (2%) 65 63	59, 72, 93, 119	0
11	X	49/56 (87%)	-0.11	3 (6%) 22 20	70, 84, 119, 127	0
12	L	46/47 (97%)	-0.77	1 (2%) 62 59	49, 60, 80, 122	0
12	Y	46/47 (97%)	-0.63	0 100 100	60, 75, 102, 119	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	43/46 (93%)	-0.43	2 (4%) 32 30	50, 63, 99, 147	0
13	Z	43/46 (93%)	-0.01	2 (4%) 32 30	70, 79, 121, 164	0
All	All	3550/3614 (98%)	-0.75	73 (2%) 64 61	41, 64, 107, 164	0

The worst 5 of 73 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	Z	43	SER	10.8
2	O	90	ILE	9.4
6	F	1	ALA	9.2
7	G	40	GLY	6.8
6	S	2	SER	6.3

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	0.93	0.31	-	80,86,125,151	0
7	TPO	T	11	11/12	0.65	0.30	-	101,147,160,160	0
9	SAC	I	1	9/10	0.72	0.36	-	116,134,157,165	0
1	FME	A	1	10/11	0.94	0.29	-	74,86,128,147	0
2	FME	O	1	10/11	0.99	0.08	-	64,71,76,79	0
7	TPO	G	11	11/12	0.77	0.26	-	102,140,157,157	0
2	FME	B	1	10/11	0.98	0.07	-	58,65,72,72	0
9	SAC	V	1	9/10	0.43	0.50	-	138,151,167,167	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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
21	EDO	A	614	4/4	0.85	0.57	20.38	133,137,141,148	0
21	EDO	A	612	4/4	0.75	0.50	18.36	88,115,122,127	0
23	CHD	W	101	29/29	0.69	0.40	11.78	107,145,150,150	0
21	EDO	B	305	4/4	0.94	0.19	8.32	105,110,115,123	0
19	TGL	N	611	63/63	0.73	0.25	6.55	90,126,148,150	0
23	CHD	J	101	29/29	0.81	0.35	6.00	123,142,150,150	0
20	PGV	N	607	51/51	0.63	0.32	6.00	99,137,150,150	0
26	CDL	P	304	100/100	0.71	0.25	5.53	71,140,150,150	0
26	CDL	C	307	100/100	0.70	0.30	4.68	89,138,150,150	0
26	CDL	C	303	100/100	0.82	0.23	4.63	66,123,153,155	0
21	EDO	A	613	4/4	0.93	0.19	4.63	112,112,121,122	0
21	EDO	T	104	4/4	0.94	0.32	4.27	124,129,131,132	0
19	TGL	L	101	63/63	0.79	0.22	4.21	67,113,143,150	0
26	CDL	T	103	100/100	0.77	0.26	4.20	76,140,150,150	0
21	EDO	G	104	4/4	0.86	0.21	4.17	97,101,102,105	0
27	PEK	T	101	53/53	0.66	0.36	4.09	79,136,150,150	0
27	PEK	T	102	53/53	0.67	0.31	3.79	78,133,150,150	0
17	NA	A	605	1/1	0.99	0.16	3.69	59,59,59,59	0
19	TGL	N	609	63/63	0.85	0.18	3.60	60,120,149,150	0
18	CMO	N	606	2/2	0.99	0.14	3.50	77,77,77,80	0
21	EDO	F	102	4/4	0.87	0.27	3.45	80,88,96,96	0
24	PSC	B	303	52/52	0.53	0.35	3.15	75,147,150,150	0
20	PGV	A	609	51/51	0.65	0.26	3.09	69,115,159,161	0
19	TGL	N	610	63/63	0.64	0.29	2.98	90,134,149,150	0
19	TGL	A	607	63/63	0.84	0.18	2.76	54,97,122,132	0
24	PSC	R	201	52/52	0.67	0.29	2.61	76,137,150,150	0
19	TGL	D	201	63/63	0.75	0.24	2.51	87,126,147,150	0
29	DMU	Z	101	33/33	0.68	0.30	2.45	80,128,149,150	0
27	PEK	G	102	53/53	0.58	0.32	2.06	100,135,150,150	0
20	PGV	N	608	51/51	0.98	0.11	1.54	47,76,117,142	0
20	PGV	C	308	51/51	0.77	0.22	1.53	75,125,150,150	0
23	CHD	C	304	29/29	0.87	0.26	1.33	93,117,125,127	0
20	PGV	G	103	51/51	0.80	0.20	1.23	96,127,150,150	0
27	PEK	C	306	53/53	0.79	0.26	0.94	71,132,149,150	0
27	PEK	P	302	53/53	0.94	0.13	0.79	59,91,150,150	0
20	PGV	A	608	51/51	0.98	0.10	0.78	51,66,79,86	0
29	DMU	M	101	33/33	0.90	0.16	0.70	70,102,129,136	0
17	NA	N	605	1/1	0.98	0.11	0.60	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
27	PEK	G	101	53/53	0.94	0.12	0.56	57,72,126,136	0
20	PGV	P	303	51/51	0.98	0.10	0.48	51,72,132,148	0
23	CHD	P	305	29/29	0.91	0.19	0.40	120,135,145,147	0
21	EDO	B	304	4/4	0.98	0.09	0.28	71,75,75,75	0
21	EDO	N	612	4/4	0.95	0.10	0.16	79,80,82,84	0
21	EDO	A	610	4/4	0.97	0.10	-0.04	75,75,78,81	0
23	CHD	B	302	29/29	0.96	0.10	-0.06	48,64,74,77	0
23	CHD	O	302	29/29	0.97	0.09	-0.09	50,57,67,72	0
23	CHD	P	306	29/29	0.98	0.09	-0.10	57,65,72,73	0
14	HEA	N	601	60/60	0.99	0.09	-0.29	47,56,78,84	0
22	CUA	B	301	2/2	0.99	0.07	-0.41	54,54,54,58	0
23	CHD	C	305	29/29	0.96	0.09	-0.50	47,61,71,81	0
28	ZN	S	101	1/1	1.00	0.07	-0.52	70,70,70,70	0
14	HEA	N	602	60/60	0.99	0.08	-0.67	47,57,69,75	0
14	HEA	A	601	60/60	0.99	0.07	-0.74	34,46,65,70	0
20	PGV	C	302	51/51	0.98	0.08	-0.78	49,58,90,99	0
16	MG	A	604	1/1	0.99	0.06	-1.00	51,51,51,51	0
16	MG	N	604	1/1	0.98	0.07	-1.21	57,57,57,57	0
14	HEA	A	602	60/60	0.99	0.06	-1.34	45,51,60,62	0
28	ZN	F	101	1/1	1.00	0.04	-1.81	64,64,64,64	0
22	CUA	O	301	2/2	0.99	0.06	-2.07	66,66,66,67	0
25	UNX	C	301	1/1	0.94	0.37	-	26,26,26,26	1
18	CMO	A	606	2/2	1.00	0.06	-	55,55,55,55	0
21	EDO	K	103	4/4	0.85	0.23	-	90,92,99,101	0
25	UNX	P	301	1/1	0.84	0.40	-	15,15,15,15	1
21	EDO	L	102	4/4	0.97	0.06	-	83,84,84,90	0
21	EDO	K	101	4/4	0.76	0.18	-	86,107,118,131	0
15	CU	N	603	1/1	1.00	0.03	-	55,55,55,55	0
21	EDO	C	311	4/4	0.83	0.27	-	80,95,109,118	0
21	EDO	C	310	4/4	0.72	0.24	-	94,105,106,112	0
21	EDO	C	309	4/4	0.97	0.16	-	76,86,100,122	0
21	EDO	A	611	4/4	0.93	0.14	-	86,94,107,113	0
15	CU	A	603	1/1	1.00	0.01	-	55,55,55,55	0
21	EDO	K	102	4/4	0.88	0.21	-	101,108,112,116	0

6.5 Other polymers ⓘ

There are no such residues in this entry.