



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 07:25 AM GMT

PDB ID : 3AG4
Title : Bovine Heart Cytochrome c Oxidase in the Cyanide Ion-bound Fully Reduced State at 100 K
Authors : Muramoto, K.; Ohta, K.; Shinzawa-Itoh, K.; Kanda, K.; Taniguchi, M.; Nabekura, H.; Yamashita, E.; Tsukihara, T.; Yoshikawa, S.
Deposited on : 2010-03-19
Resolution : 2.05 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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

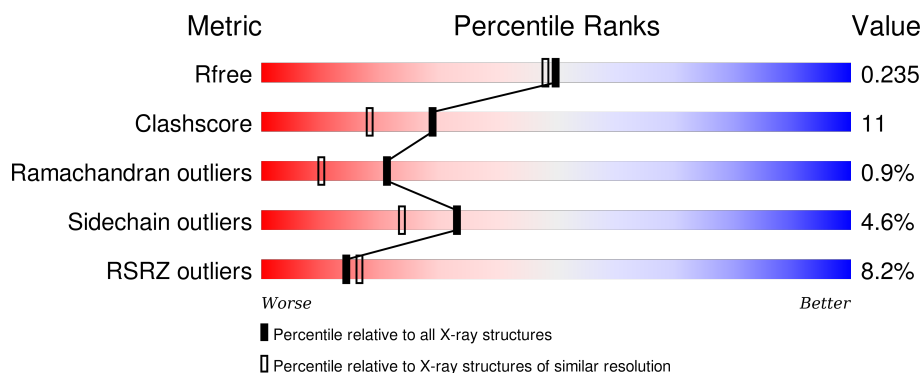
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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.



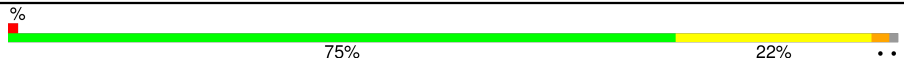

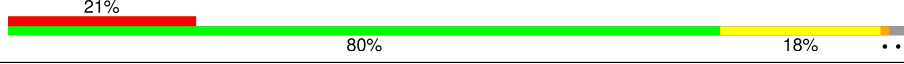
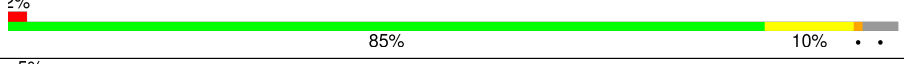

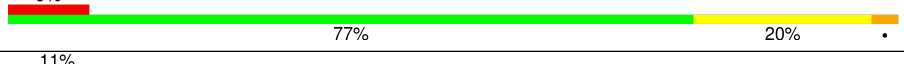


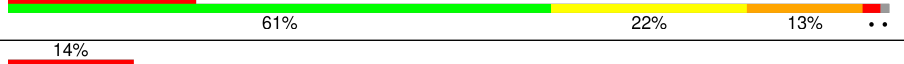


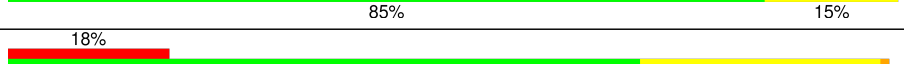

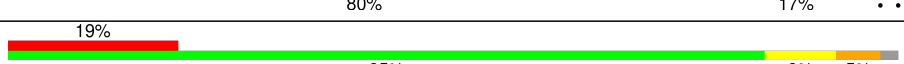
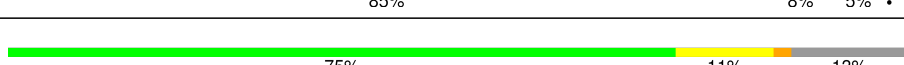
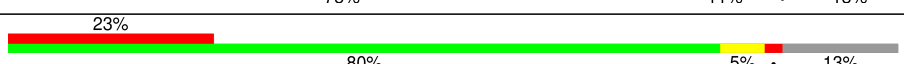
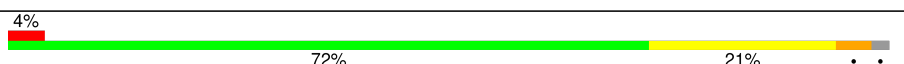
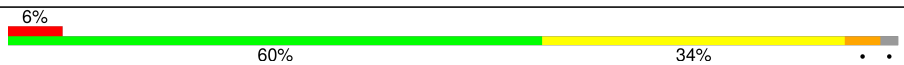
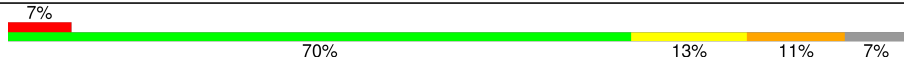

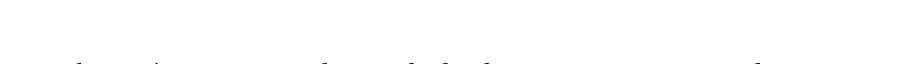
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1192 (2.04-2.04)
Clashscore	102246	1269 (2.04-2.04)
Ramachandran outliers	100387	1258 (2.04-2.04)
Sidechain outliers	100360	1258 (2.04-2.04)
RSRZ outliers	91569	1194 (2.04-2.04)

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>11%</div> <div> <div></div> <div>76%</div> <div>20%</div> <div>.</div> </div> </div>
1	N	514	<div> <div>6%</div> <div> <div></div> <div>77%</div> <div>20%</div> <div>.</div> </div> </div>
2	B	227	<div> <div>2%</div> <div> <div></div> <div>74%</div> <div>22%</div> <div>..</div> </div> </div>
2	O	227	<div> <div>3%</div> <div> <div></div> <div>71%</div> <div>26%</div> <div>.</div> </div> </div>
3	C	261	<div> <div></div> <div> <div></div> <div>80%</div> <div>16%</div> <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	515	X	-	-	-
14	HEA	A	516	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	HEA	N	515	X	-	-	-
14	HEA	N	516	X	-	-	-
15	CYN	N	520	-	-	X	-
19	TGL	A	521	-	-	-	X
19	TGL	D	523	-	-	-	X
19	TGL	L	522	-	-	-	X
19	TGL	N	1521	-	-	-	X
19	TGL	N	1522	-	-	-	X
20	PGV	A	524	-	-	-	X
20	PGV	N	1524	-	-	-	X
20	PGV	P	1268	-	-	-	X
22	CHD	C	271	X	-	-	-
22	CHD	J	60	X	-	-	X
22	CHD	P	1271	X	-	-	-
22	CHD	W	1059	X	-	-	X
25	CDL	C	270	-	-	X	X
25	CDL	G	269	-	-	X	X
25	CDL	P	1270	-	-	-	X
25	CDL	T	1269	-	-	X	X
26	PSC	E	229	-	-	-	X
26	PSC	R	1229	-	-	-	X
28	DMU	G	272	X	-	-	X
28	DMU	M	526	X	-	-	-
28	DMU	P	1272	X	-	-	X
28	DMU	Z	1526	X	-	-	-

2 Entry composition

There are 29 unique types of molecules in this entry. The entry contains 32324 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	514	Total	C	N	O	S	0	0	0
			4027	2691	623	678	35			
1	N	514	Total	C	N	O	S	0	0	0
			4027	2691	623	678	35			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	259	Total	C	N	O	S	0	0	0
			2110	1412	336	350	12			
3	P	259	Total	C	N	O	S	0	0	0
			2110	1412	336	350	12			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	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.

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.

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 polypeptide 7A1.

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.

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

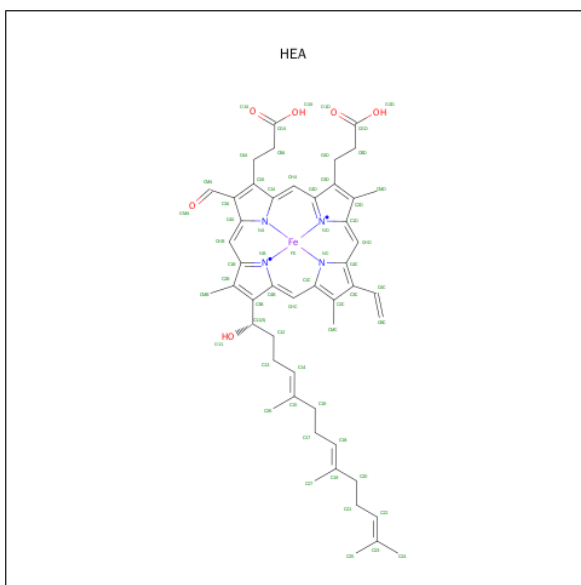
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C.

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

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

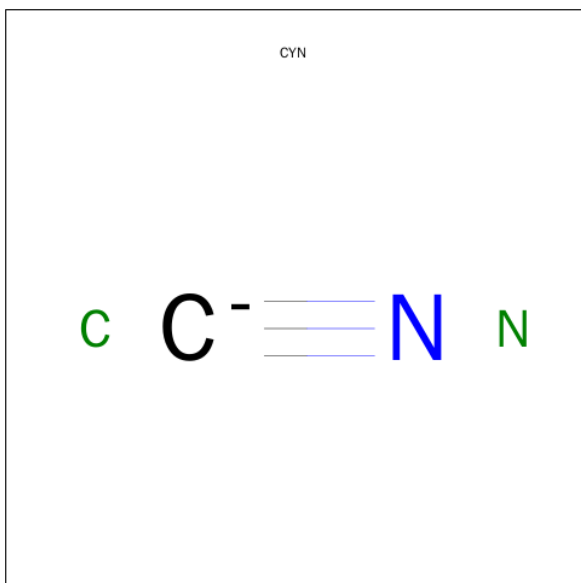
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	M	43	Total	C	N	O	0	0	0
			335	223	53	59			
13	Z	43	Total	C	N	O	0	0	0
			335	223	53	59			

- 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	0	0
			60	49	1	4	6		
14	A	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
14	N	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
14	N	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		

- Molecule 15 is CYANIDE ION (three-letter code: CYN) (formula: CN).



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

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

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

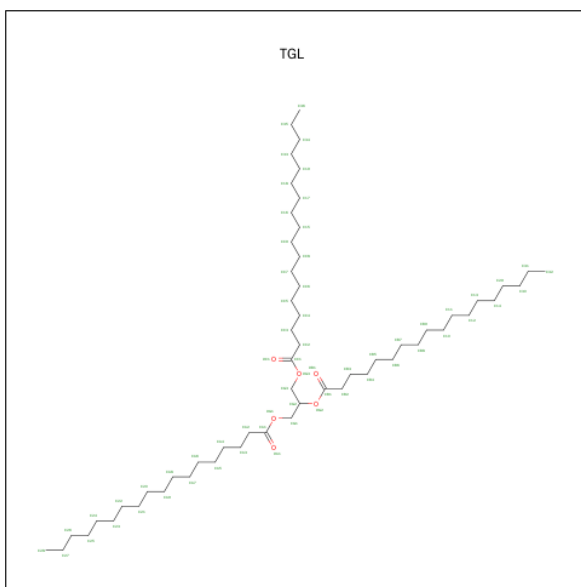
- Molecule 17 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

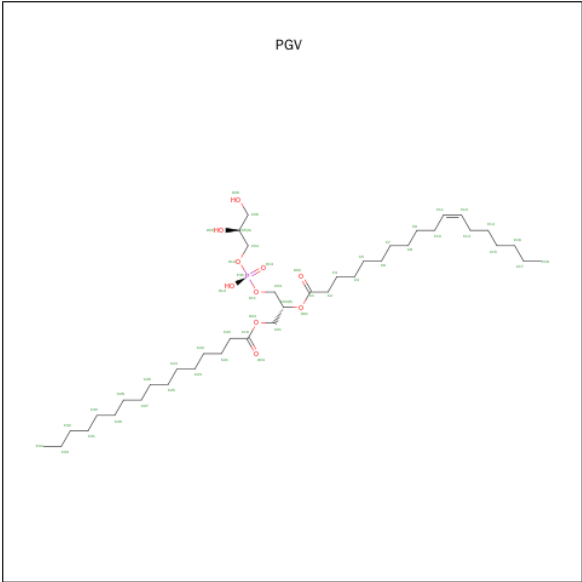
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	A	1	Total Na 1 1	0	0
18	N	1	Total Na 1 1	0	0

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



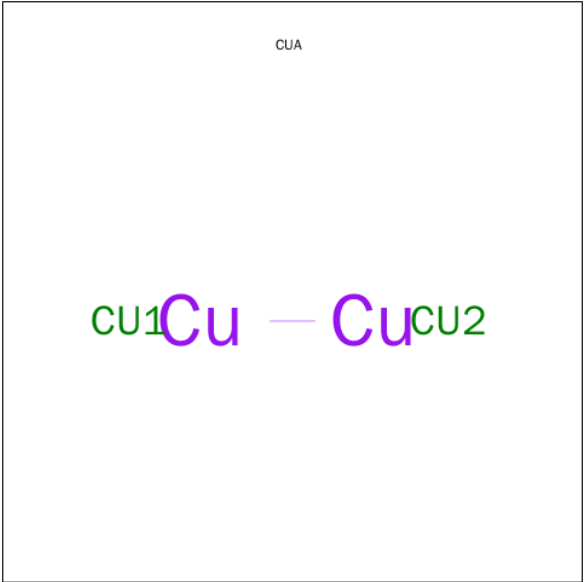
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	A	1	Total	C	O	0	0
			63	57	6		
19	D	1	Total	C	O	0	0
			63	57	6		
19	L	1	Total	C	O	0	0
			63	57	6		
19	N	1	Total	C	O	0	0
			63	57	6		
19	N	1	Total	C	O	0	0
			63	57	6		
19	Q	1	Total	C	O	0	0
			63	57	6		

- 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).



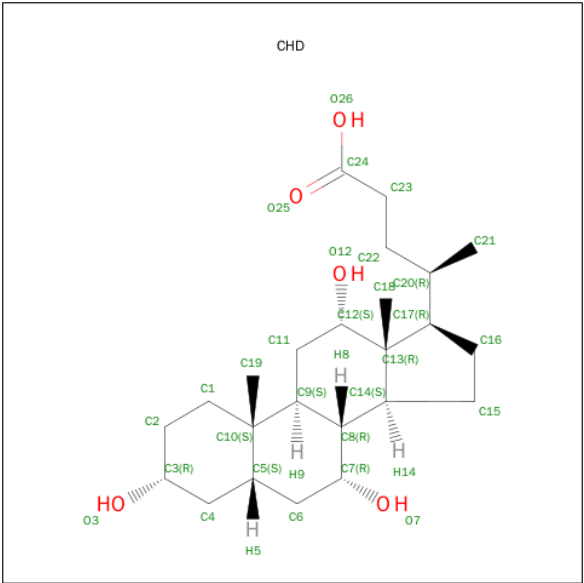
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
20	A	1	Total	C	O	P	0	0
			51	40	10	1		
20	A	1	Total	C	O	P	0	0
			51	40	10	1		
20	C	1	Total	C	O	P	0	0
			51	40	10	1		
20	C	1	Total	C	O	P	0	0
			51	40	10	1		
20	N	1	Total	C	O	P	0	0
			51	40	10	1		
20	N	1	Total	C	O	P	0	0
			51	40	10	1		
20	P	1	Total	C	O	P	0	0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

- Molecule 21 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu₂).



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

- Molecule 22 is CHOLIC ACID (three-letter code: CHD) (formula: C₂₄H₄₀O₅).



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

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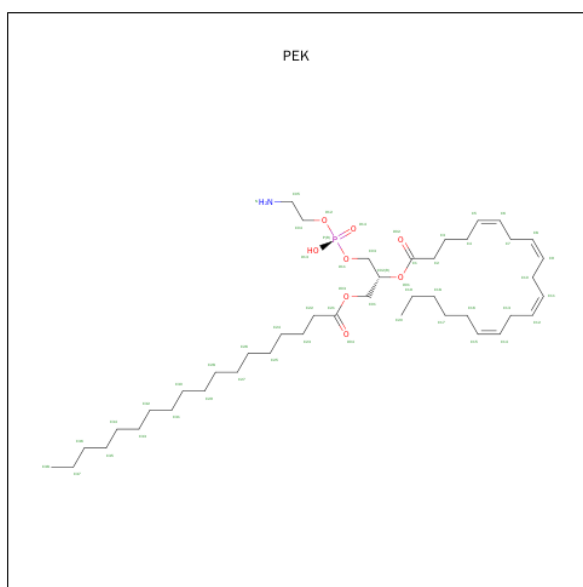
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	C	1	Total C O 29 24 5	0	0
22	J	1	Total C O 29 24 5	0	0
22	O	1	Total C O 29 24 5	0	0
22	P	1	Total C O 29 24 5	0	0
22	P	1	Total C O 29 24 5	0	0
22	W	1	Total C O 29 24 5	0	0

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

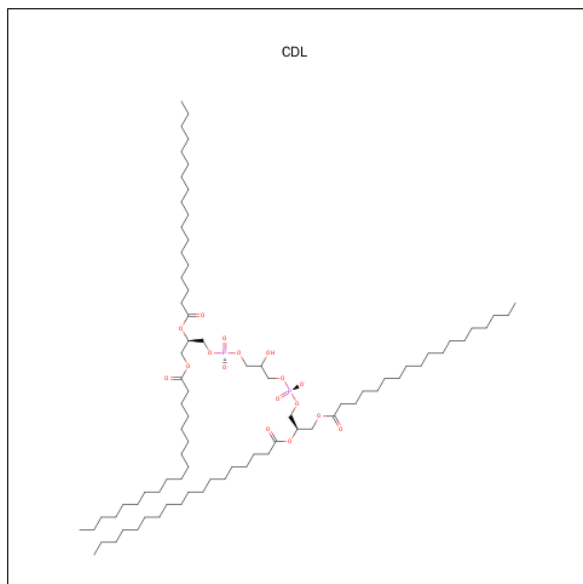
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	P	1	Total X 1 1	0	0
23	C	1	Total X 1 1	0	0

- Molecule 24 is (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).



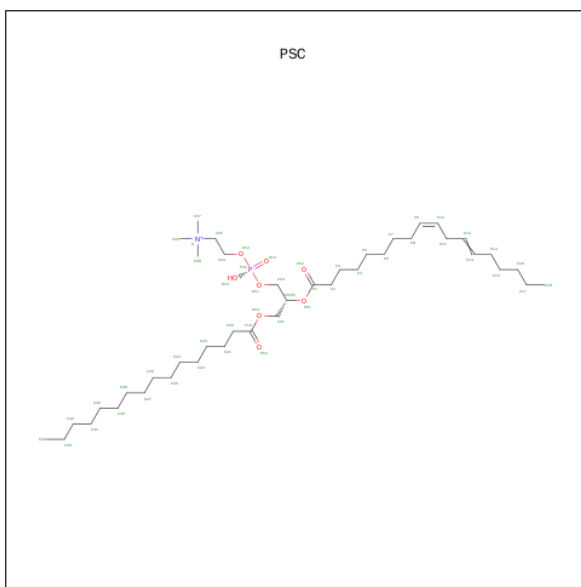
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
24	G	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
24	G	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
24	S	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
24	T	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
24	T	1	Total	C	N	O	P	0	0
			53	43	1	8	1		

- Molecule 25 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



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

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

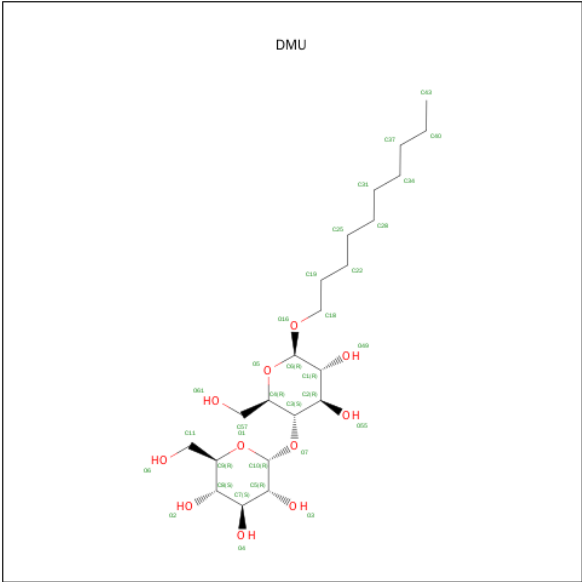


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
26	E	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
26	R	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

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

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

- Molecule 28 is SUGAR (DECYL-BETA-D-MALTOPYRANOSIDE) (three-letter code: DMU) (formula: C₂₂H₄₂O₁₁).



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

- Molecule 29 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	A	225	Total	O	0	0
			225	225		
29	B	125	Total	O	0	0
			125	125		
29	C	106	Total	O	0	0
			106	106		
29	D	91	Total	O	0	0
			91	91		
29	E	62	Total	O	0	0
			62	62		
29	F	75	Total	O	0	0
			75	75		
29	G	41	Total	O	0	0
			41	41		
29	H	47	Total	O	0	0
			47	47		

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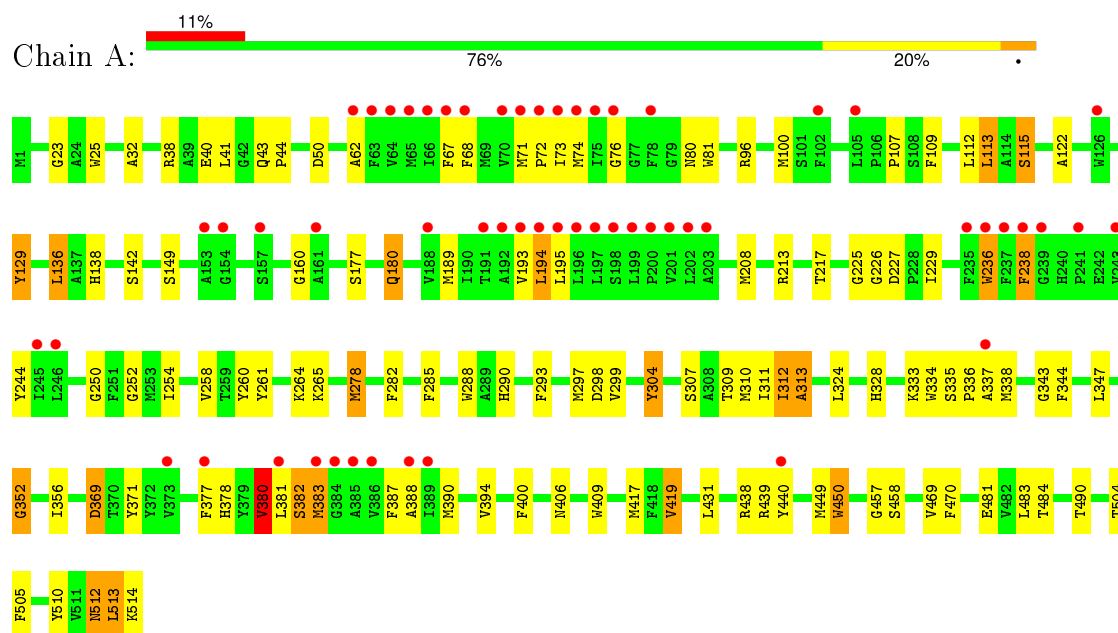
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	I	38	Total 38	O 38	0	0
29	J	20	Total 20	O 20	0	0
29	K	20	Total 20	O 20	0	0
29	L	22	Total 22	O 22	0	0
29	M	15	Total 15	O 15	0	0
29	N	199	Total 199	O 199	0	0
29	O	107	Total 107	O 107	0	0
29	P	100	Total 100	O 100	0	0
29	Q	55	Total 55	O 55	0	0
29	R	40	Total 40	O 40	0	0
29	S	56	Total 56	O 56	0	0
29	T	36	Total 36	O 36	0	0
29	U	41	Total 41	O 41	0	0
29	V	18	Total 18	O 18	0	0
29	W	12	Total 12	O 12	0	0
29	X	14	Total 14	O 14	0	0
29	Y	12	Total 12	O 12	0	0
29	Z	11	Total 11	O 11	0	0

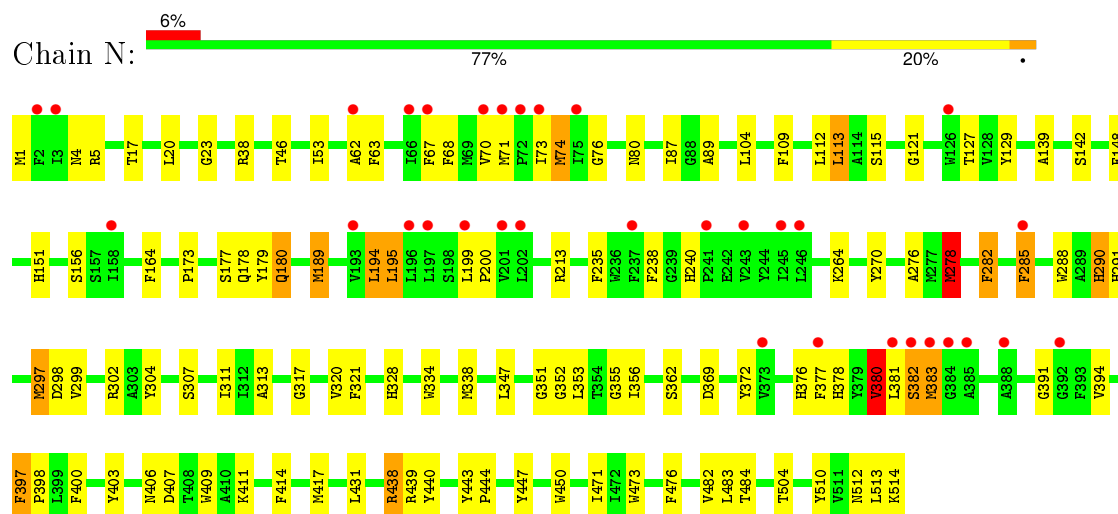
3 Residue-property plots

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 ($\text{RSRZ} > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

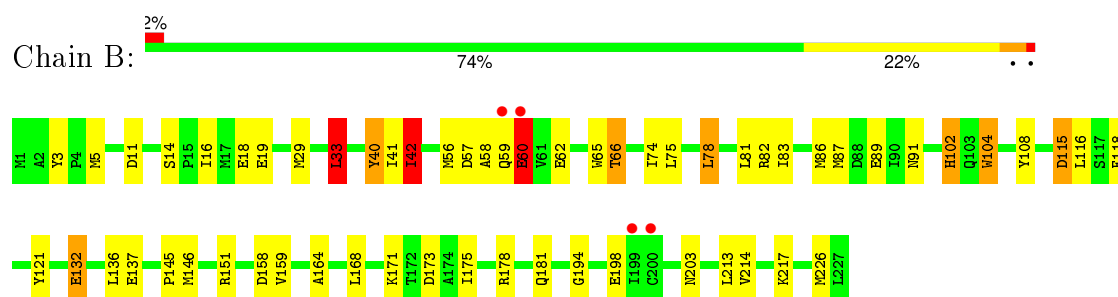
• Molecule 1: Cytochrome c oxidase subunit 1



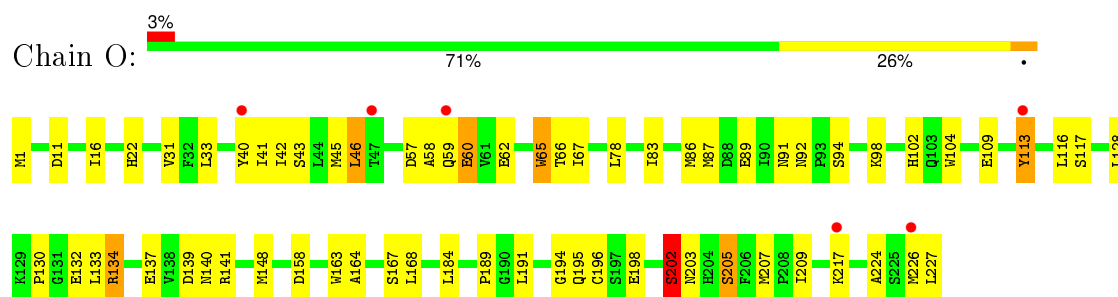
• Molecule 1: Cytochrome c oxidase subunit 1



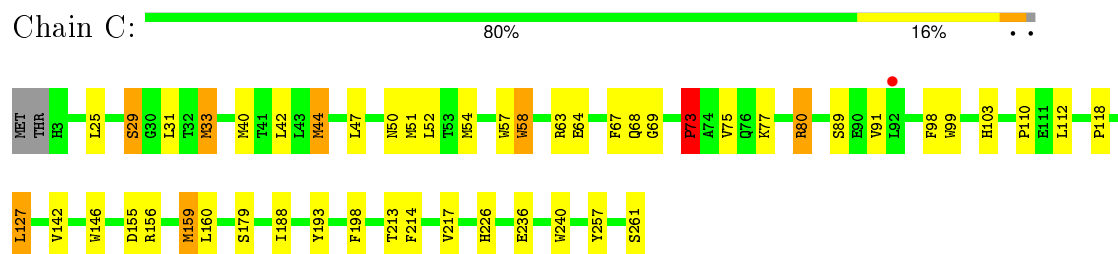
• Molecule 2: Cytochrome c oxidase subunit 2



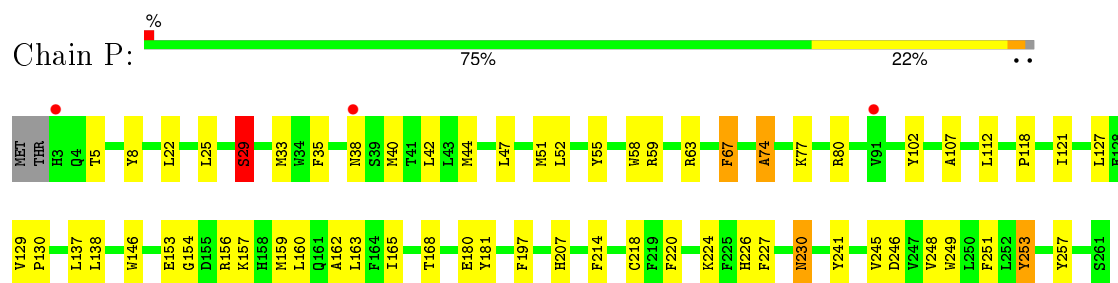
• Molecule 2: Cytochrome c oxidase subunit 2



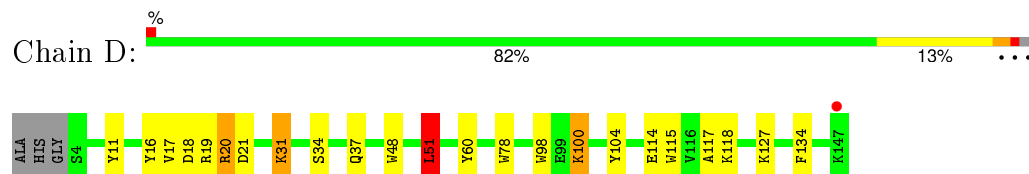
• Molecule 3: Cytochrome c oxidase subunit 3



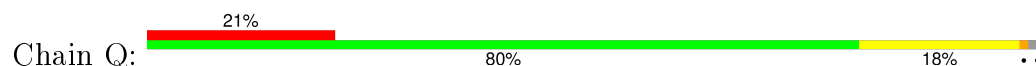
• Molecule 3: Cytochrome c oxidase subunit 3

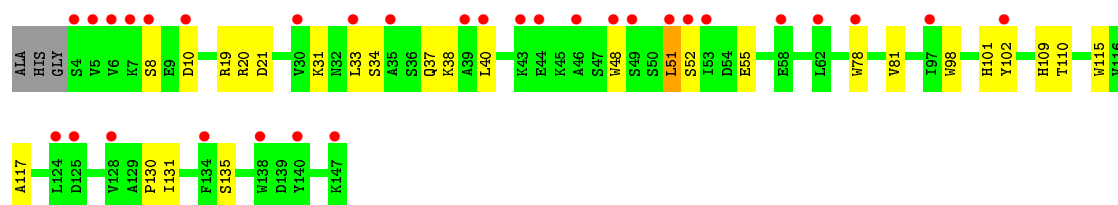


• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1

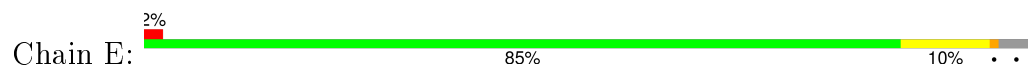


• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1

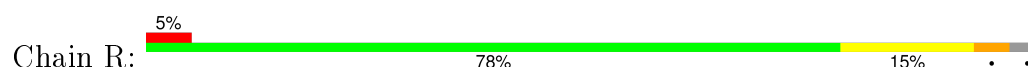




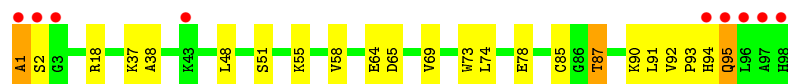
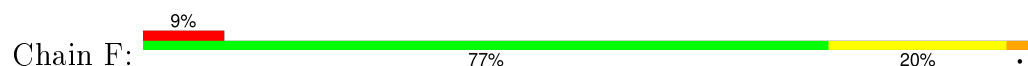
• Molecule 5: Cytochrome c oxidase subunit 5A



• Molecule 5: Cytochrome c oxidase subunit 5A



• Molecule 6: Cytochrome c oxidase subunit 5B



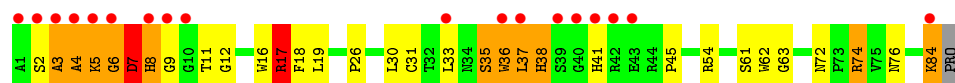
• Molecule 6: Cytochrome c oxidase subunit 5B



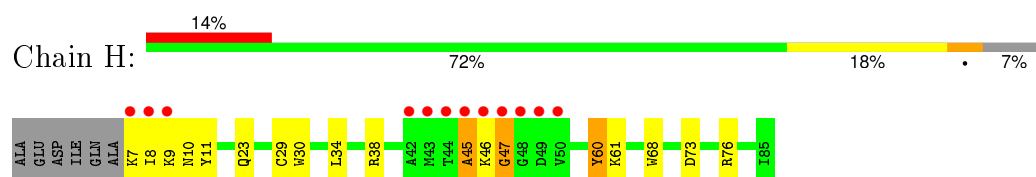
• Molecule 7: Cytochrome c oxidase subunit 6A2



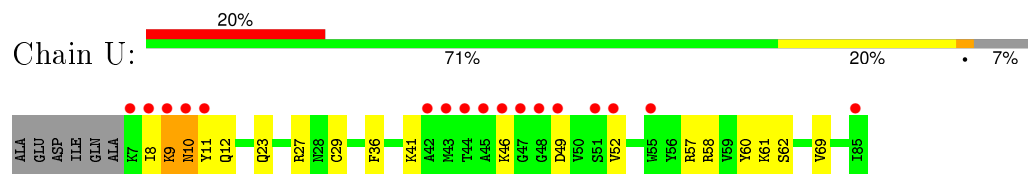
• Molecule 7: Cytochrome c oxidase subunit 6A2



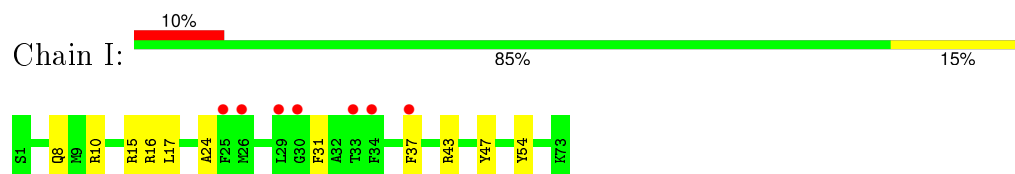
• Molecule 8: Cytochrome c oxidase subunit 6B1



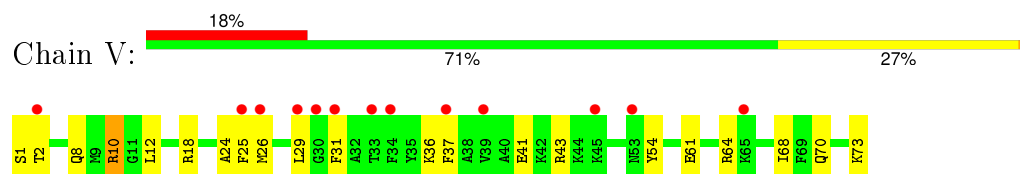
- Molecule 8: Cytochrome c oxidase subunit 6B1



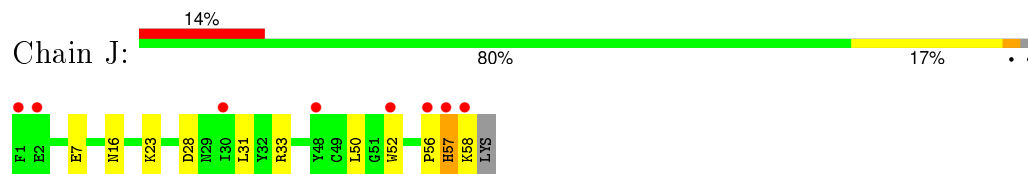
- Molecule 9: Cytochrome c oxidase subunit 6C



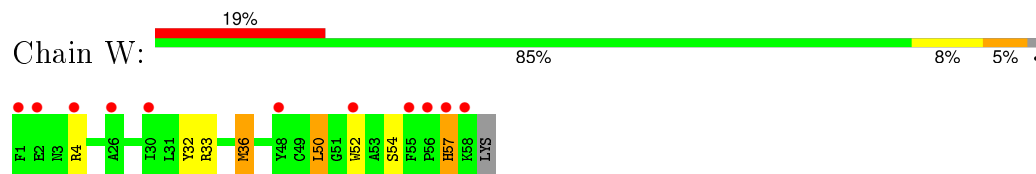
- Molecule 9: Cytochrome c oxidase subunit 6C



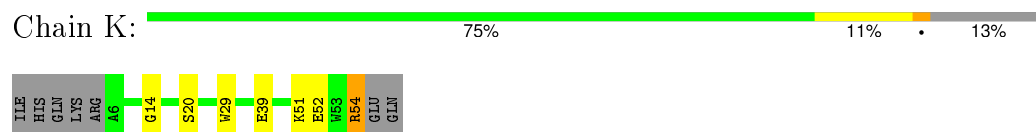
- Molecule 10: Cytochrome c oxidase polypeptide 7A1



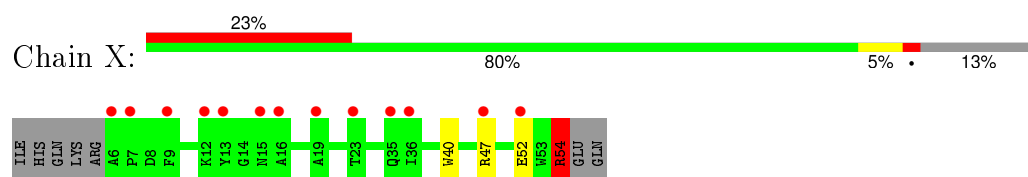
- Molecule 10: Cytochrome c oxidase polypeptide 7A1



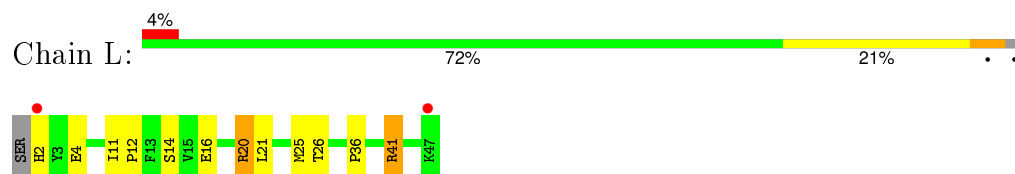
- Molecule 11: Cytochrome c oxidase subunit 7B



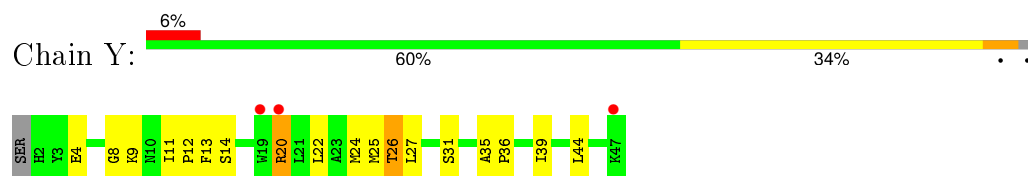
- Molecule 11: Cytochrome c oxidase subunit 7B



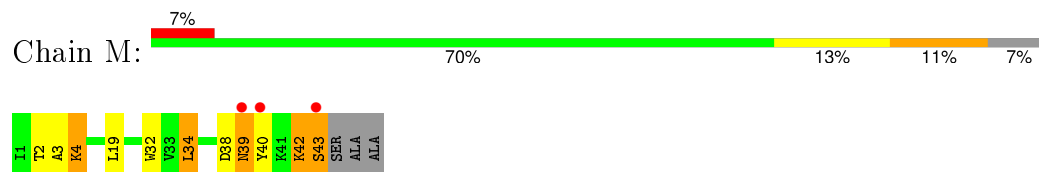
- Molecule 12: Cytochrome c oxidase subunit 7C



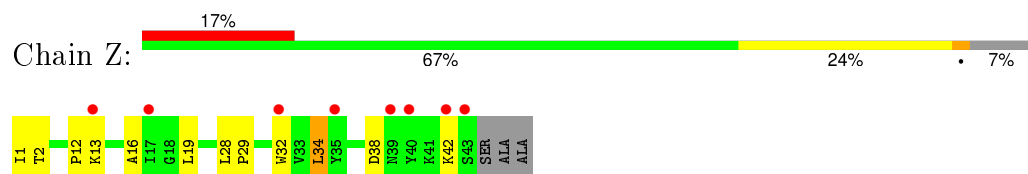
- Molecule 12: Cytochrome c oxidase subunit 7C



- Molecule 13: Cytochrome c oxidase subunit 8B



- Molecule 13: Cytochrome c oxidase subunit 8B



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	183.36Å 206.65Å 178.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.05 52.61 – 2.05	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-2.05) 99.8 (52.61-2.05)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.60 (at 2.05Å)	Xtriage
Refinement program	REFMAC 5.3	Depositor
R, R_{free}	0.186 , 0.219 0.204 , 0.235	Depositor DCC
R_{free} test set	21000 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	34.5	Xtriage
Anisotropy	0.525	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 63.1	EDS
Estimated twinning fraction	0.006 for l,-k,h	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	2 of 419430 reflections (0.000%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	32324	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.85% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, CHD, HEA, SAC, CDL, PSC, PEK, MG, TGL, PGV, TPO, UNX, CUA, NA, FME, CYN, CU, DMU

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.69	52/4156 (1.3%)	1.27	32/5678 (0.6%)
1	N	1.51	31/4156 (0.7%)	1.11	14/5678 (0.2%)
2	B	1.53	13/1860 (0.7%)	1.21	11/2534 (0.4%)
2	O	1.24	3/1860 (0.2%)	1.08	5/2534 (0.2%)
3	C	1.52	14/2197 (0.6%)	1.07	6/3005 (0.2%)
3	P	1.51	16/2197 (0.7%)	1.05	3/3005 (0.1%)
4	D	1.55	12/1229 (1.0%)	1.22	7/1658 (0.4%)
4	Q	1.12	2/1229 (0.2%)	0.95	3/1658 (0.2%)
5	E	1.45	1/871 (0.1%)	1.04	2/1182 (0.2%)
5	R	1.20	2/871 (0.2%)	0.96	1/1182 (0.1%)
6	F	1.46	4/765 (0.5%)	1.17	2/1038 (0.2%)
6	S	1.28	1/765 (0.1%)	1.16	4/1038 (0.4%)
7	G	1.35	1/690 (0.1%)	1.10	5/937 (0.5%)
7	T	1.36	3/690 (0.4%)	1.23	5/937 (0.5%)
8	H	1.35	1/682 (0.1%)	1.12	5/921 (0.5%)
8	U	1.13	1/682 (0.1%)	0.95	0/921
9	I	1.34	3/605 (0.5%)	1.03	0/802
9	V	1.18	0/605	0.95	1/802 (0.1%)
10	J	1.25	0/471	1.04	1/636 (0.2%)
10	W	1.16	0/471	1.00	0/636
11	K	1.44	3/398 (0.8%)	1.08	1/546 (0.2%)
11	X	1.18	2/398 (0.5%)	0.96	2/546 (0.4%)
12	L	1.64	4/393 (1.0%)	1.11	2/526 (0.4%)
12	Y	1.42	0/393	1.04	0/526
13	M	1.49	1/345 (0.3%)	1.18	1/470 (0.2%)
13	Z	1.22	0/345	0.97	1/470 (0.2%)
All	All	1.45	170/29324 (0.6%)	1.12	114/39866 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is

detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
6	F	0	1
6	S	0	1
10	J	0	1
10	W	0	1
12	L	0	1
All	All	0	5

The worst 5 of 170 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	181	TYR	CD1-CE1	9.79	1.54	1.39
1	A	438	ARG	CB-CG	-9.36	1.27	1.52
1	A	388	ALA	CA-CB	8.80	1.71	1.52
3	P	29	SER	CB-OG	-8.78	1.30	1.42
1	N	139	ALA	CA-CB	8.50	1.70	1.52

The worst 5 of 114 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	20	ARG	NE-CZ-NH2	-16.98	111.81	120.30
1	A	310	MET	CG-SD-CE	-14.80	76.53	100.20
1	A	278	MET	CG-SD-CE	-14.00	77.80	100.20
1	N	278	MET	CG-SD-CE	-12.95	79.47	100.20
4	D	20	ARG	NE-CZ-NH1	12.84	126.72	120.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	F	93	PRO	Peptide
10	J	57	HIS	Peptide
12	L	2	HIS	Peptide
6	S	93	PRO	Peptide
10	W	57	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	4027	0	4001	74	0
1	N	4027	0	4001	84	0
2	B	1824	0	1833	34	0
2	O	1824	0	1833	58	0
3	C	2110	0	2027	36	0
3	P	2110	0	2027	46	0
4	D	1195	0	1183	17	0
4	Q	1195	0	1183	21	0
5	E	852	0	845	5	0
5	R	852	0	845	11	0
6	F	748	0	728	16	0
6	S	748	0	728	25	0
7	G	675	0	643	37	0
7	T	675	0	643	49	0
8	H	662	0	623	6	0
8	U	662	0	623	11	0
9	I	601	0	613	9	0
9	V	601	0	613	17	0
10	J	460	0	459	7	0
10	W	460	0	459	9	0
11	K	384	0	366	2	0
11	X	384	0	366	4	0
12	L	380	0	380	11	0
12	Y	380	0	380	15	0
13	M	335	0	352	9	0
13	Z	335	0	352	8	0
14	A	120	0	108	13	0
14	N	120	0	108	13	0
15	A	2	0	0	0	0
15	N	2	0	0	2	0
16	A	1	0	0	0	0
16	N	1	0	0	0	0
17	A	1	0	0	0	0
17	N	1	0	0	0	0
18	A	1	0	0	0	0
18	N	1	0	0	0	0
19	A	63	0	110	7	0
19	D	63	0	110	13	0
19	L	63	0	110	15	0
19	N	126	0	220	22	0
19	Q	63	0	110	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	A	102	0	152	10	0
20	C	102	0	152	6	0
20	N	102	0	152	7	0
20	P	102	0	152	5	0
21	B	2	0	0	0	0
21	O	2	0	0	0	0
22	B	29	0	36	3	0
22	C	58	0	70	4	0
22	J	29	0	36	2	0
22	O	29	0	36	1	0
22	P	58	0	73	5	0
22	W	29	0	35	6	0
23	C	1	0	0	0	0
23	P	1	0	0	0	0
24	C	53	0	77	3	0
24	G	106	0	154	24	0
24	S	53	0	77	16	0
24	T	106	0	154	28	0
25	C	100	0	156	21	0
25	G	100	0	156	28	0
25	P	100	0	156	19	0
25	T	100	0	156	34	0
26	E	52	0	80	16	0
26	R	52	0	80	14	0
27	F	1	0	0	0	0
27	S	1	0	0	0	0
28	G	33	0	38	3	0
28	M	33	0	38	1	0
28	P	33	0	38	5	0
28	Z	33	0	39	2	0
29	A	225	0	0	8	0
29	B	125	0	0	4	0
29	C	106	0	0	2	0
29	D	91	0	0	1	0
29	E	62	0	0	0	0
29	F	75	0	0	2	0
29	G	41	0	0	3	0
29	H	47	0	0	2	0
29	I	38	0	0	1	0
29	J	20	0	0	1	0
29	K	20	0	0	1	0
29	L	22	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	M	15	0	0	1	0
29	N	199	0	0	4	0
29	O	107	0	0	4	0
29	P	100	0	0	3	0
29	Q	55	0	0	2	0
29	R	40	0	0	1	0
29	S	56	0	0	5	0
29	T	36	0	0	4	0
29	U	41	0	0	4	0
29	V	18	0	0	1	0
29	W	12	0	0	0	0
29	X	14	0	0	0	0
29	Y	12	0	0	1	0
29	Z	11	0	0	0	0
All	All	32324	0	31275	705	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 11.

The worst 5 of 705 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:74:MET:CB	1:N:74:MET:CG	1.76	1.56
1:A:312:ILE:CG1	1:A:312:ILE:CD1	1.78	1.54
4:D:100:LYS:CE	4:D:100:LYS:NZ	1.69	1.51
3:C:73:PRO:CB	3:C:73:PRO:CG	1.75	1.48
14:A:516:HEA:O11	14:A:516:HEA:C11	1.64	1.45

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	512/514 (100%)	495 (97%)	17 (3%)	0	100	100
1	N	512/514 (100%)	495 (97%)	16 (3%)	1 (0%)	52	43
2	B	225/227 (99%)	212 (94%)	11 (5%)	2 (1%)	21	10
2	O	225/227 (99%)	211 (94%)	12 (5%)	2 (1%)	21	10
3	C	257/261 (98%)	251 (98%)	6 (2%)	0	100	100
3	P	257/261 (98%)	251 (98%)	5 (2%)	1 (0%)	39	28
4	D	142/147 (97%)	137 (96%)	5 (4%)	0	100	100
4	Q	142/147 (97%)	137 (96%)	5 (4%)	0	100	100
5	E	103/109 (94%)	97 (94%)	6 (6%)	0	100	100
5	R	103/109 (94%)	102 (99%)	1 (1%)	0	100	100
6	F	96/98 (98%)	91 (95%)	3 (3%)	2 (2%)	9	2
6	S	96/98 (98%)	89 (93%)	4 (4%)	3 (3%)	5	0
7	G	81/85 (95%)	66 (82%)	7 (9%)	8 (10%)	1	0
7	T	81/85 (95%)	67 (83%)	9 (11%)	5 (6%)	2	0
8	H	77/85 (91%)	67 (87%)	4 (5%)	6 (8%)	1	0
8	U	77/85 (91%)	70 (91%)	5 (6%)	2 (3%)	7	1
9	I	71/73 (97%)	69 (97%)	2 (3%)	0	100	100
9	V	71/73 (97%)	66 (93%)	5 (7%)	0	100	100
10	J	56/59 (95%)	54 (96%)	2 (4%)	0	100	100
10	W	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
11	K	47/56 (84%)	46 (98%)	0	1 (2%)	9	2
11	X	47/56 (84%)	44 (94%)	3 (6%)	0	100	100
12	L	44/47 (94%)	43 (98%)	1 (2%)	0	100	100
12	Y	44/47 (94%)	42 (96%)	2 (4%)	0	100	100
13	M	41/46 (89%)	41 (100%)	0	0	100	100
13	Z	41/46 (89%)	38 (93%)	3 (7%)	0	100	100
All	All	3504/3614 (97%)	3336 (95%)	135 (4%)	33 (1%)	21	10

5 of 33 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	60	GLU
6	F	95	GLN
7	G	4	ALA

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Mol	Chain	Res	Type
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	426/426 (100%)	414 (97%)	12 (3%)	51	44
1	N	426/426 (100%)	414 (97%)	12 (3%)	51	44
2	B	210/210 (100%)	200 (95%)	10 (5%)	31	22
2	O	210/210 (100%)	197 (94%)	13 (6%)	23	13
3	C	224/226 (99%)	217 (97%)	7 (3%)	47	39
3	P	224/226 (99%)	218 (97%)	6 (3%)	52	45
4	D	128/129 (99%)	126 (98%)	2 (2%)	70	67
4	Q	128/129 (99%)	125 (98%)	3 (2%)	58	51
5	E	92/95 (97%)	91 (99%)	1 (1%)	80	79
5	R	92/95 (97%)	86 (94%)	6 (6%)	21	11
6	F	81/81 (100%)	76 (94%)	5 (6%)	23	13
6	S	81/81 (100%)	73 (90%)	8 (10%)	10	3
7	G	67/68 (98%)	59 (88%)	8 (12%)	6	2
7	T	67/68 (98%)	57 (85%)	10 (15%)	4	1
8	H	71/75 (95%)	67 (94%)	4 (6%)	26	16
8	U	71/75 (95%)	66 (93%)	5 (7%)	19	10
9	I	57/57 (100%)	53 (93%)	4 (7%)	19	10
9	V	57/57 (100%)	53 (93%)	4 (7%)	19	10
10	J	49/50 (98%)	48 (98%)	1 (2%)	63	58
10	W	49/50 (98%)	46 (94%)	3 (6%)	23	13
11	K	39/46 (85%)	38 (97%)	1 (3%)	54	47
11	X	39/46 (85%)	37 (95%)	2 (5%)	29	19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	L	39/40 (98%)	38 (97%)	1 (3%)	54	47
12	Y	39/40 (98%)	37 (95%)	2 (5%)	29	19
13	M	37/38 (97%)	31 (84%)	6 (16%)	3	0
13	Z	37/38 (97%)	33 (89%)	4 (11%)	8	2
All	All	3040/3082 (99%)	2900 (95%)	140 (5%)	33	24

5 of 140 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	N	109	PHE
2	O	78	LEU
10	W	4	ARG
1	N	238	PHE
1	N	369	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 52 such sidechains are listed below:

Mol	Chain	Res	Type
1	N	178	GLN
2	O	52	HIS
9	V	8	GLN
1	N	180	GLN
1	N	512	ASN

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	1.01	1 (12%)	6,9,11	6.38	4 (66%)
2	FME	B	1	2	8,9,10	1.97	2 (25%)	6,9,11	7.04	4 (66%)
7	TPO	G	11	7	8,10,11	2.04	4 (50%)	7,14,16	1.84	2 (28%)
9	SAC	I	1	9	7,8,9	2.32	2 (28%)	7,9,11	1.11	1 (14%)
1	FME	N	1	1	8,9,10	1.33	1 (12%)	6,9,11	6.11	4 (66%)
2	FME	O	1	2	8,9,10	1.09	1 (12%)	6,9,11	6.52	2 (33%)
7	TPO	T	11	7	8,10,11	2.07	4 (50%)	7,14,16	2.43	2 (28%)
9	SAC	V	1	9	7,8,9	3.08	2 (28%)	7,9,11	1.71	3 (42%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	FME	A	1	1	-	1/6/9/11	0/0/0/0
2	FME	B	1	2	-	1/6/9/11	0/0/0/0
7	TPO	G	11	7	-	0/8/11/13	0/0/0/0
9	SAC	I	1	9	-	0/6/8/10	0/0/0/0
1	FME	N	1	1	-	1/6/9/11	0/0/0/0
2	FME	O	1	2	-	1/6/9/11	0/0/0/0
7	TPO	T	11	7	-	0/8/11/13	0/0/0/0
9	SAC	V	1	9	-	0/6/8/10	0/0/0/0

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	FME	O1-CN	-4.18	1.09	1.22
2	O	1	FME	O1-CN	-2.48	1.15	1.22
1	A	1	FME	O1-CN	-2.39	1.15	1.22
2	B	1	FME	CB-CA	-2.01	1.49	1.53
7	T	11	TPO	CB-CA	2.14	1.57	1.54

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	FME	CA-N-CN	-16.27	97.80	122.82
2	O	1	FME	CA-N-CN	-15.72	98.64	122.82
1	A	1	FME	CA-N-CN	-14.12	101.11	122.82
1	N	1	FME	CA-N-CN	-13.38	102.24	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	FME	CG-CB-CA	-4.47	99.92	113.06

There are no chirality outliers.

All (4) torsion outliers are listed below:

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

There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	G	11	TPO	1	0
1	N	1	FME	1	0
2	O	1	FME	1	0
7	T	11	TPO	1	0
9	V	1	SAC	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 56 ligands modelled in this entry, 2 are unknown and 8 are monoatomic - leaving 46 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
14	HEA	A	515	1	40,67,67	1.48	9 (22%)	41,103,103	2.58	17 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	HEA	A	516	1,15	40,67,67	2.21	10 (25%)	41,103,103	3.37	23 (56%)
15	CYN	A	520	14,16	0,1,1	0.00	-	0,0,0	0.00	-
19	TGL	A	521	-	62,62,62	1.41	7 (11%)	65,65,65	2.41	16 (24%)
20	PGV	A	522	-	50,50,50	0.97	2 (4%)	51,56,56	1.30	5 (9%)
20	PGV	A	524	-	50,50,50	1.15	2 (4%)	51,56,56	1.39	7 (13%)
22	CHD	B	1085	-	29,32,32	1.50	5 (17%)	48,51,51	5.70	35 (72%)
21	CUA	B	228	2	0,1,1	0.00	-	0,0,0	0.00	-
24	PEK	C	264	-	51,52,52	0.89	2 (3%)	52,57,57	1.80	12 (23%)
20	PGV	C	267	-	50,50,50	0.87	3 (6%)	51,56,56	1.42	6 (11%)
20	PGV	C	268	-	50,50,50	1.25	2 (4%)	51,56,56	1.51	7 (13%)
25	CDL	C	270	-	99,99,99	1.33	12 (12%)	101,111,111	1.44	15 (14%)
22	CHD	C	271	-	29,32,32	0.82	1 (3%)	48,51,51	5.09	34 (70%)
22	CHD	C	525	-	29,32,32	1.80	6 (20%)	48,51,51	5.50	34 (70%)
19	TGL	D	523	-	62,62,62	1.57	7 (11%)	65,65,65	1.56	11 (16%)
26	PSC	E	229	-	51,51,51	1.25	3 (5%)	55,59,59	1.39	6 (10%)
24	PEK	G	1263	-	51,52,52	1.15	3 (5%)	52,57,57	1.22	6 (11%)
24	PEK	G	265	-	51,52,52	1.18	3 (5%)	52,57,57	1.26	3 (5%)
25	CDL	G	269	-	99,99,99	1.45	14 (14%)	101,111,111	1.54	17 (16%)
28	DMU	G	272	-	34,34,34	1.24	4 (11%)	45,45,45	3.36	23 (51%)
22	CHD	J	60	-	29,32,32	0.69	0	48,51,51	4.93	40 (83%)
19	TGL	L	522	-	62,62,62	1.53	8 (12%)	65,65,65	1.84	17 (26%)
28	DMU	M	526	-	34,34,34	0.83	1 (2%)	45,45,45	3.46	26 (57%)
20	PGV	N	1266	-	50,50,50	0.92	1 (2%)	51,56,56	1.37	6 (11%)
19	TGL	N	1521	-	62,62,62	1.30	6 (9%)	65,65,65	1.55	11 (16%)
19	TGL	N	1522	-	62,62,62	1.54	7 (11%)	65,65,65	1.65	15 (23%)
20	PGV	N	1524	-	50,50,50	1.18	2 (4%)	51,56,56	1.35	6 (11%)
14	HEA	N	515	1	40,67,67	1.08	3 (7%)	41,103,103	2.41	9 (21%)
14	HEA	N	516	1,15	40,67,67	1.74	7 (17%)	41,103,103	3.28	19 (46%)
15	CYN	N	520	14,16	0,1,1	0.00	-	0,0,0	0.00	-
21	CUA	O	228	2	0,1,1	0.00	-	0,0,0	0.00	-
22	CHD	O	229	-	29,32,32	1.26	3 (10%)	48,51,51	5.62	33 (68%)
20	PGV	P	1267	-	50,50,50	0.84	2 (4%)	51,56,56	1.46	7 (13%)
20	PGV	P	1268	-	50,50,50	1.22	2 (4%)	51,56,56	1.54	7 (13%)
25	CDL	P	1270	-	99,99,99	1.33	12 (12%)	101,111,111	1.40	13 (12%)
22	CHD	P	1271	-	29,32,32	0.72	0	48,51,51	4.91	37 (77%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	DMU	P	1272	-	34,34,34	1.20	1 (2%)	45,45,45	3.30	24 (53%)
22	CHD	P	1525	-	29,32,32	1.39	4 (13%)	48,51,51	5.20	38 (79%)
19	TGL	Q	1523	-	62,62,62	1.32	6 (9%)	65,65,65	1.29	10 (15%)
26	PSC	R	1229	-	51,51,51	1.20	3 (5%)	55,59,59	1.05	4 (7%)
24	PEK	S	1265	-	51,52,52	1.32	4 (7%)	52,57,57	1.32	4 (7%)
24	PEK	T	1264	-	51,52,52	0.93	2 (3%)	52,57,57	1.91	8 (15%)
25	CDL	T	1269	-	99,99,99	1.34	12 (12%)	101,111,111	1.45	17 (16%)
24	PEK	T	263	-	51,52,52	1.19	2 (3%)	52,57,57	1.22	5 (9%)
22	CHD	W	1059	-	29,32,32	1.07	2 (6%)	48,51,51	5.17	33 (68%)
28	DMU	Z	1526	-	34,34,34	0.94	2 (5%)	45,45,45	3.23	21 (46%)

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	515	1	3/3/7/16	0/24/76/76	0/0/8/8
14	HEA	A	516	1,15	3/3/7/16	0/24/76/76	0/0/8/8
15	CYN	A	520	14,16	-	0/0/0/0	0/0/0/0
19	TGL	A	521	-	-	0/65/65/65	0/0/0/0
20	PGV	A	522	-	-	0/55/55/55	0/0/0/0
20	PGV	A	524	-	-	1/55/55/55	0/0/0/0
22	CHD	B	1085	-	-	0/7/74/74	0/4/4/4
21	CUA	B	228	2	-	0/0/0/0	0/0/0/0
24	PEK	C	264	-	-	0/56/56/56	0/0/0/0
20	PGV	C	267	-	-	0/55/55/55	0/0/0/0
20	PGV	C	268	-	-	0/55/55/55	0/0/0/0
25	CDL	C	270	-	-	0/110/110/110	0/0/0/0
22	CHD	C	271	-	1/1/12/12	0/7/74/74	0/4/4/4
22	CHD	C	525	-	-	0/7/74/74	0/4/4/4
19	TGL	D	523	-	-	0/65/65/65	0/0/0/0
26	PSC	E	229	-	-	0/55/55/55	0/0/0/0
24	PEK	G	1263	-	-	0/56/56/56	0/0/0/0
24	PEK	G	265	-	-	0/56/56/56	0/0/0/0
25	CDL	G	269	-	-	0/110/110/110	0/0/0/0
28	DMU	G	272	-	6/6/10/10	0/19/59/59	0/2/2/2
22	CHD	J	60	-	2/2/12/12	0/7/74/74	0/4/4/4
19	TGL	L	522	-	-	0/65/65/65	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	DMU	M	526	-	4/4/10/10	0/19/59/59	0/2/2/2
20	PGV	N	1266	-	-	0/55/55/55	0/0/0/0
19	TGL	N	1521	-	-	0/65/65/65	0/0/0/0
19	TGL	N	1522	-	-	0/65/65/65	0/0/0/0
20	PGV	N	1524	-	-	3/55/55/55	0/0/0/0
14	HEA	N	515	1	3/3/7/16	0/24/76/76	0/0/8/8
14	HEA	N	516	1,15	3/3/7/16	0/24/76/76	0/0/8/8
15	CYN	N	520	14,16	-	0/0/0/0	0/0/0/0
21	CUA	O	228	2	-	0/0/0/0	0/0/0/0
22	CHD	O	229	-	-	0/7/74/74	0/4/4/4
20	PGV	P	1267	-	-	0/55/55/55	0/0/0/0
20	PGV	P	1268	-	-	0/55/55/55	0/0/0/0
25	CDL	P	1270	-	-	0/110/110/110	0/0/0/0
22	CHD	P	1271	-	1/1/12/12	0/7/74/74	0/4/4/4
28	DMU	P	1272	-	6/6/10/10	0/19/59/59	0/2/2/2
22	CHD	P	1525	-	-	0/7/74/74	0/4/4/4
19	TGL	Q	1523	-	-	0/65/65/65	0/0/0/0
26	PSC	R	1229	-	-	0/55/55/55	0/0/0/0
24	PEK	S	1265	-	-	0/56/56/56	0/0/0/0
24	PEK	T	1264	-	-	0/56/56/56	0/0/0/0
25	CDL	T	1269	-	-	0/110/110/110	0/0/0/0
24	PEK	T	263	-	-	0/56/56/56	0/0/0/0
22	CHD	W	1059	-	2/2/12/12	0/7/74/74	0/4/4/4
28	DMU	Z	1526	-	5/5/10/10	0/19/59/59	0/2/2/2

The worst 5 of 187 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	516	HEA	C3C-C2C	-5.25	1.33	1.40
22	C	525	CHD	C13-C12	-4.86	1.46	1.54
22	C	525	CHD	C1-C10	-4.41	1.45	1.54
14	N	516	HEA	C3C-C2C	-3.62	1.35	1.40
19	A	521	TGL	OC1-CC1	-3.61	1.11	1.22

The worst 5 of 687 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	1085	CHD	C18-C13-C12	-17.19	92.32	109.09
22	O	229	CHD	C18-C13-C12	-12.62	96.78	109.09
22	C	525	CHD	C19-C10-C9	-9.83	96.45	111.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	P	1525	CHD	C18-C13-C12	-8.93	100.38	109.09
22	C	271	CHD	C18-C13-C12	-8.70	100.61	109.09

5 of 39 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
28	P	1272	DMU	C5
28	P	1272	DMU	C6
28	P	1272	DMU	C9
28	P	1272	DMU	C4
28	P	1272	DMU	C2

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
20	A	524	PGV	C02-O01-C1-C2
20	N	1524	PGV	C02-O01-C1-O02
20	N	1524	PGV	P-O11-C03-C02
20	N	1524	PGV	C02-O01-C1-C2

There are no ring outliers.

42 monomers are involved in 341 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	A	515	HEA	5	0
14	A	516	HEA	8	0
19	A	521	TGL	7	0
20	A	522	PGV	2	0
20	A	524	PGV	8	0
22	B	1085	CHD	3	0
24	C	264	PEK	3	0
20	C	267	PGV	3	0
20	C	268	PGV	3	0
25	C	270	CDL	21	0
22	C	271	CHD	3	0
22	C	525	CHD	1	0
19	D	523	TGL	13	0
26	E	229	PSC	16	0
24	G	1263	PEK	11	0
24	G	265	PEK	13	0
25	G	269	CDL	28	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	G	272	DMU	3	0
22	J	60	CHD	2	0
19	L	522	TGL	15	0
28	M	526	DMU	1	0
19	N	1521	TGL	7	0
19	N	1522	TGL	15	0
20	N	1524	PGV	7	0
14	N	515	HEA	3	0
14	N	516	HEA	10	0
15	N	520	CYN	2	0
22	O	229	CHD	1	0
20	P	1267	PGV	3	0
20	P	1268	PGV	2	0
25	P	1270	CDL	19	0
22	P	1271	CHD	4	0
28	P	1272	DMU	5	0
22	P	1525	CHD	1	0
19	Q	1523	TGL	10	0
26	R	1229	PSC	14	0
24	S	1265	PEK	16	0
24	T	1264	PEK	9	0
25	T	1269	CDL	34	0
24	T	263	PEK	19	0
22	W	1059	CHD	6	0
28	Z	1526	DMU	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	0.58	56 (10%) 7 8	23, 29, 40, 63	0
1	N	513/514 (99%)	0.35	33 (6%) 23 26	30, 36, 47, 68	0
2	B	226/227 (99%)	-0.29	4 (1%) 71 76	24, 35, 59, 78	0
2	O	226/227 (99%)	-0.01	6 (2%) 58 64	33, 45, 70, 88	0
3	C	259/261 (99%)	-0.39	1 (0%) 93 94	26, 32, 43, 62	0
3	P	259/261 (99%)	-0.40	3 (1%) 81 84	29, 36, 47, 67	0
4	D	144/147 (97%)	-0.40	1 (0%) 89 91	30, 37, 56, 70	0
4	Q	144/147 (97%)	1.33	31 (21%) 1 1	39, 52, 76, 118	0
5	E	105/109 (96%)	0.03	2 (1%) 70 75	31, 38, 63, 99	0
5	R	105/109 (96%)	0.29	5 (4%) 34 40	36, 43, 68, 103	0
6	F	98/98 (100%)	0.40	9 (9%) 11 12	29, 39, 80, 127	0
6	S	98/98 (100%)	0.57	11 (11%) 7 7	34, 43, 86, 123	0
7	G	83/85 (97%)	0.78	15 (18%) 2 2	29, 39, 110, 113	0
7	T	83/85 (97%)	0.76	18 (21%) 1 1	29, 42, 102, 110	0
8	H	79/85 (92%)	0.38	12 (15%) 3 3	30, 41, 90, 112	0
8	U	79/85 (92%)	0.95	17 (21%) 1 1	37, 48, 94, 113	0
9	I	72/73 (98%)	0.27	7 (9%) 10 11	34, 46, 80, 83	0
9	V	72/73 (98%)	0.85	13 (18%) 2 2	39, 55, 82, 85	0
10	J	58/59 (98%)	0.27	8 (13%) 4 4	31, 41, 65, 96	0
10	W	58/59 (98%)	0.61	11 (18%) 2 1	34, 45, 69, 107	0
11	K	49/56 (87%)	-0.33	0 100 100	33, 41, 52, 62	0
11	X	49/56 (87%)	1.23	13 (26%) 1 0	44, 51, 64, 76	0
12	L	46/47 (97%)	-0.40	2 (4%) 39 44	29, 34, 50, 79	0
12	Y	46/47 (97%)	0.10	3 (6%) 22 25	34, 45, 61, 81	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	43/46 (93%)	-0.18	3 (6%) 19 22	30, 34, 71, 101	0
13	Z	43/46 (93%)	0.52	8 (18%) 2 1	41, 46, 90, 112	0
All	All	3550/3614 (98%)	0.25	292 (8%) 14 16	23, 38, 69, 127	0

The worst 5 of 292 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	Q	6	VAL	32.3
4	Q	5	VAL	14.3
6	S	97	ALA	14.2
4	Q	4	SER	13.0
6	F	96	LEU	11.3

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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
7	TPO	G	11	11/12	0.45	0.32	-	74,82,105,105	0
1	FME	A	1	10/11	0.92	0.14	-	46,51,63,76	0
2	FME	O	1	10/11	0.95	0.14	-	41,42,49,55	0
7	TPO	T	11	11/12	0.53	0.26	-	75,82,101,102	0
9	SAC	V	1	9/10	0.15	0.56	-	88,90,92,93	0
9	SAC	I	1	9/10	0.80	0.28	-	77,82,84,85	0
1	FME	N	1	10/11	0.87	0.23	-	50,54,74,77	0
2	FME	B	1	10/11	0.96	0.13	-	31,33,40,56	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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
28	DMU	G	272	33/33	0.54	0.31	9.31	85,116,119,121	0
20	PGV	A	524	51/51	0.75	0.28	8.83	45,75,117,118	0
25	CDL	P	1270	100/100	0.68	0.37	6.51	46,100,119,122	0
20	PGV	N	1524	51/51	0.68	0.33	5.06	54,81,117,119	0
22	CHD	W	1059	29/29	0.67	0.47	4.99	107,115,119,120	0
22	CHD	J	60	29/29	0.72	0.28	4.67	105,109,113,114	0
25	CDL	C	270	100/100	0.75	0.31	4.63	49,96,120,122	0
19	TGL	N	1522	63/63	0.55	0.33	4.08	54,76,92,95	0
28	DMU	P	1272	33/33	0.56	0.35	3.96	104,118,124,125	0
19	TGL	D	523	63/63	0.77	0.22	3.79	48,70,93,94	0
19	TGL	L	522	63/63	0.69	0.27	3.32	43,68,84,87	0
25	CDL	T	1269	100/100	0.65	0.32	2.86	66,96,122,126	0
25	CDL	G	269	100/100	0.64	0.34	2.76	72,99,122,124	0
19	TGL	N	1521	63/63	0.76	0.23	2.67	71,92,105,109	0
19	TGL	A	521	63/63	0.81	0.21	2.53	49,82,106,110	0
26	PSC	R	1229	52/52	0.67	0.32	2.52	53,109,133,136	0
26	PSC	E	229	52/52	0.72	0.33	2.40	53,106,131,133	0
20	PGV	P	1268	51/51	0.66	0.31	2.23	64,100,119,121	0
22	CHD	P	1271	29/29	0.91	0.22	1.75	68,86,90,91	0
22	CHD	C	271	29/29	0.85	0.31	1.73	72,84,87,90	0
24	PEK	T	263	53/53	0.54	0.38	1.69	54,103,127,128	0
19	TGL	Q	1523	63/63	0.72	0.22	1.61	67,83,98,100	0
28	DMU	Z	1526	33/33	0.78	0.26	1.55	44,59,75,75	0
20	PGV	P	1267	51/51	0.97	0.13	1.51	29,40,77,85	0
28	DMU	M	526	33/33	0.89	0.16	1.34	36,51,69,71	0
24	PEK	S	1265	53/53	0.58	0.30	1.08	50,87,111,114	0
20	PGV	C	268	51/51	0.69	0.29	1.04	60,91,117,117	0
24	PEK	T	1264	53/53	0.94	0.15	1.04	30,54,83,85	0
20	PGV	C	267	51/51	0.96	0.13	0.93	23,36,72,75	0
24	PEK	G	1263	53/53	0.66	0.37	0.87	59,107,131,132	0
14	HEA	N	515	60/60	0.97	0.20	0.72	30,36,50,52	0
24	PEK	C	264	53/53	0.95	0.13	0.71	27,50,76,79	0
24	PEK	G	265	53/53	0.55	0.27	0.70	51,91,109,114	0
20	PGV	A	522	51/51	0.97	0.17	0.57	25,36,68,72	0
14	HEA	N	516	60/60	0.96	0.19	0.50	32,40,54,57	0
17	MG	A	518	1/1	0.98	0.17	0.44	25,25,25,25	0
20	PGV	N	1266	51/51	0.97	0.15	0.42	28,43,70,75	0
14	HEA	A	515	60/60	0.98	0.20	0.25	18,27,40,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
14	HEA	A	516	60/60	0.97	0.17	0.01	23,35,51,52	0
22	CHD	B	1085	29/29	0.95	0.09	-0.40	29,34,40,50	0
27	ZN	F	99	1/1	0.99	0.07	-0.40	35,35,35,35	0
22	CHD	C	525	29/29	0.96	0.11	-0.41	25,35,39,46	0
22	CHD	O	229	29/29	0.95	0.08	-0.42	27,34,42,45	0
17	MG	N	518	1/1	0.92	0.12	-0.44	33,33,33,33	0
27	ZN	S	99	1/1	0.99	0.07	-0.45	38,38,38,38	0
22	CHD	P	1525	29/29	0.94	0.11	-0.57	28,38,43,51	0
21	CUA	B	228	2/2	0.99	0.13	-0.74	28,28,28,28	0
18	NA	A	519	1/1	0.97	0.09	-1.08	30,30,30,30	0
21	CUA	O	228	2/2	0.98	0.09	-1.31	36,36,36,37	0
15	CYN	A	520	2/2	0.98	0.13	-1.45	31,31,31,31	0
18	NA	N	519	1/1	0.92	0.06	-1.73	40,40,40,40	0
15	CYN	N	520	2/2	0.88	0.15	-1.84	42,42,42,43	0
16	CU	N	517	1/1	0.99	0.16	-	37,37,37,37	0
23	UNX	C	262	1/1	0.64	0.58	-	49,49,49,49	0
16	CU	A	517	1/1	1.00	0.17	-	31,31,31,31	0
23	UNX	P	262	1/1	0.80	0.60	-	49,49,49,49	0

6.5 Other polymers [i](#)

There are no such residues in this entry.