wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 07:30 AM GMT

PDB ID	:	3ASN
Title	:	Bovine heart cytochrome C oxidase in the fully oxidized state measured at 1.7470 angstrom wavelength
Authors	:	Suga, M.; Yano, N.; Muramoto, K.; Shinzawa-Itoh, K.; Maeda, T.; Yamashita, E.; Tsukihara, T.; Yoshikawa, S.
Deposited on	:	2010-12-17
Resolution	:	3.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

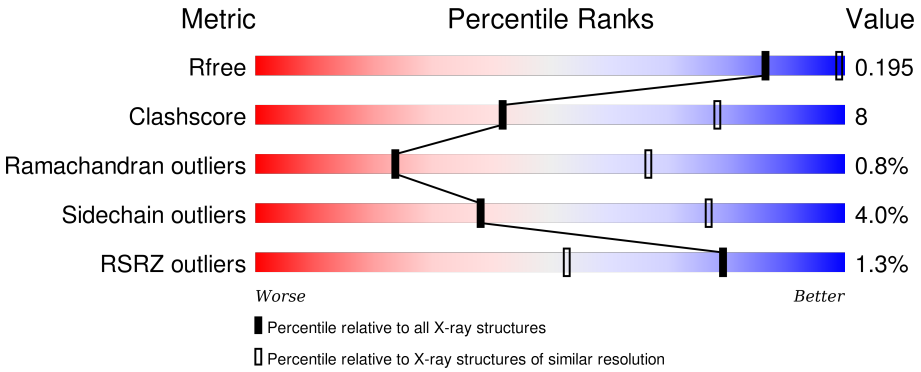
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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



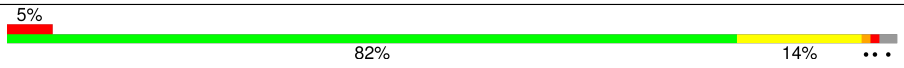
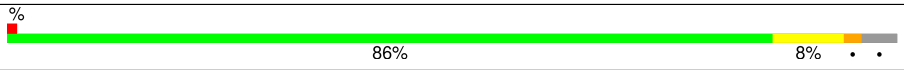
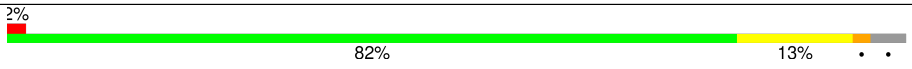
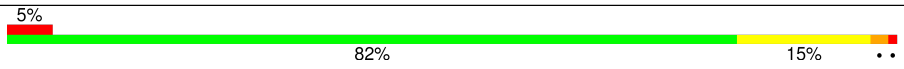
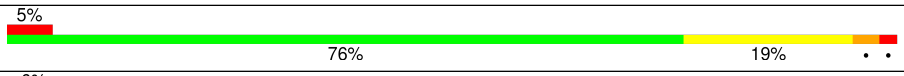
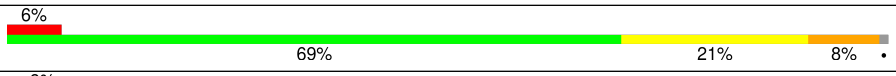
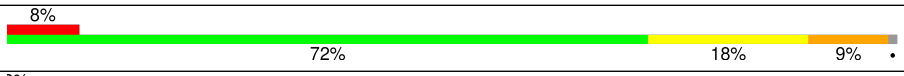
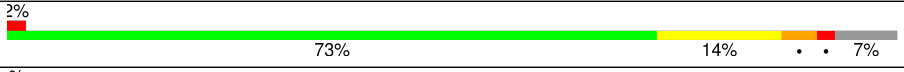
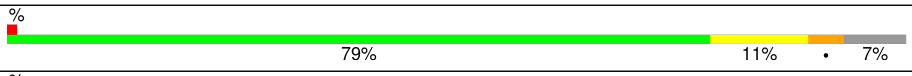
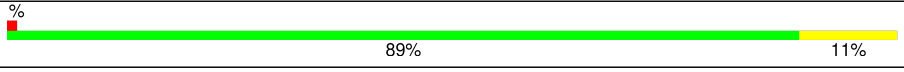
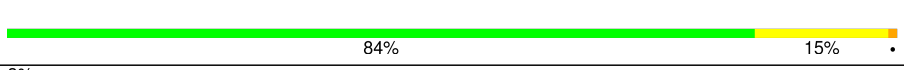
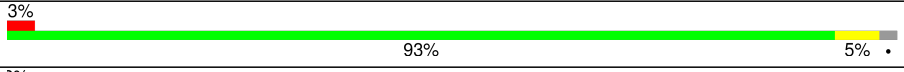
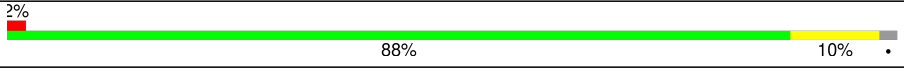
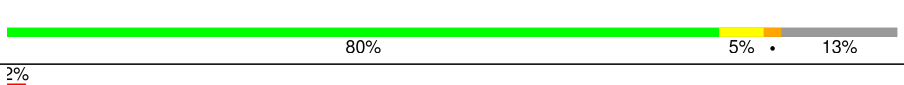
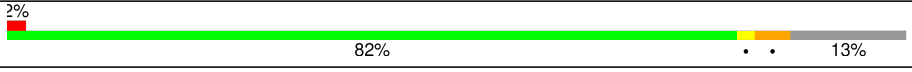
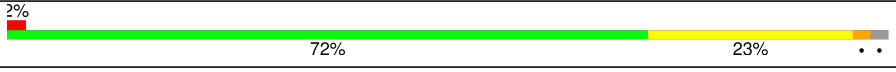
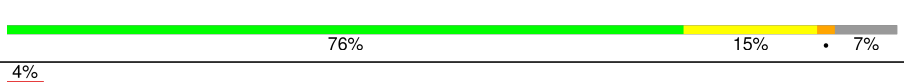
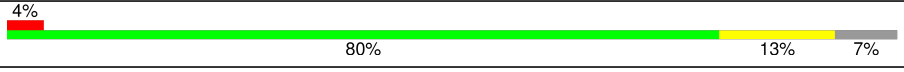
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	86% 13%
1	N	514	87% 13%
2	B	227	81% 19%
2	O	227	% 76% 22%
3	C	261	86% 13%

Continued on next page...

Continued from previous page...

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	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	HEA	N	515	X	-	-	-
14	HEA	N	516	X	-	-	-
18	TGL	A	521	-	-	-	X
18	TGL	D	523	-	-	-	X
18	TGL	L	522	-	-	-	X
18	TGL	N	1521	-	-	-	X
18	TGL	N	1522	-	-	-	X
18	TGL	N	1523	-	-	-	X
19	PGV	A	522	-	-	-	X
19	PGV	A	524	-	-	-	X
19	PGV	C	267	-	-	-	X
19	PGV	C	268	-	-	-	X
19	PGV	N	1266	-	-	-	X
19	PGV	N	1524	-	-	-	X
19	PGV	P	1267	-	-	-	X
19	PGV	P	1268	-	-	-	X
21	PSC	B	229	-	-	-	X
21	PSC	O	1229	-	-	-	X
22	CHD	J	60	-	-	-	X
22	CHD	P	1271	-	-	-	X
22	CHD	W	1059	-	-	-	X
24	PEK	C	264	-	-	-	X
24	PEK	G	1263	-	-	-	X
24	PEK	P	1265	-	-	-	X
24	PEK	T	263	-	-	-	X
25	CDL	C	270	-	-	-	X
25	CDL	G	269	-	-	-	X
25	CDL	P	1270	-	-	-	X
25	CDL	T	1269	-	-	X	X
27	DMU	M	526	X	-	-	-
27	DMU	Z	1526	X	-	-	X

2 Entry composition

There are 28 unique types of molecules in this entry. The entry contains 32377 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	0
			675	431	129	113	1	1			
7	T	84	Total	C	N	O	P	S	0	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.

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

Continued on next page...

Continued from previous page...

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			

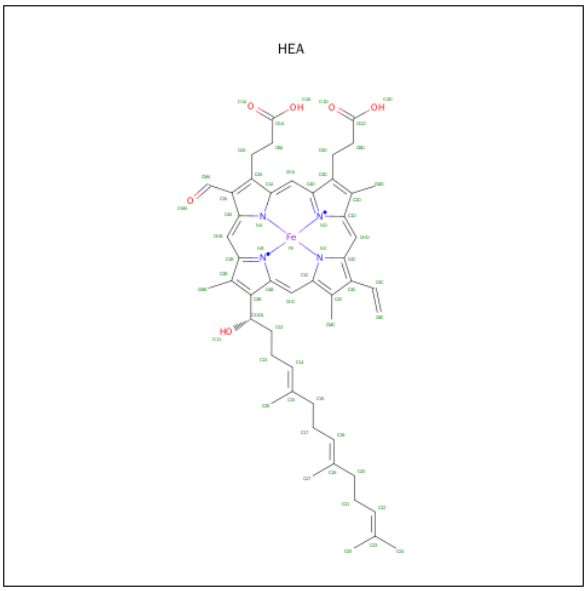
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C.

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: $C_{49}H_{56}FeN_4O_6$).



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

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

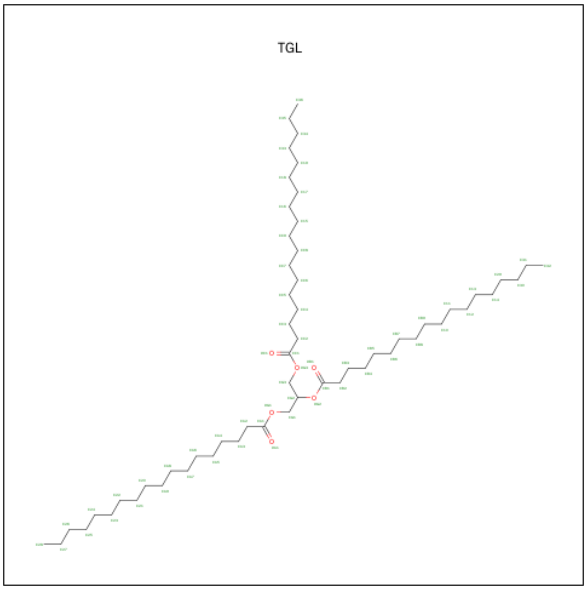
- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

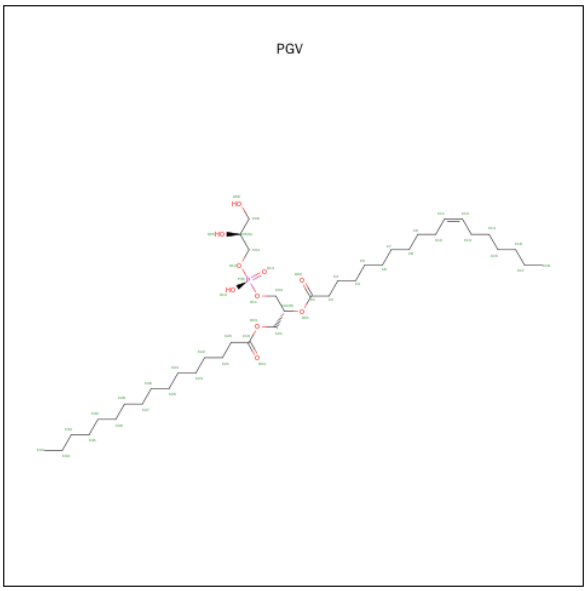
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	A	1	Total Na 1 1	0	0
17	N	1	Total Na 1 1	0	0

- Molecule 18 is TRISTEAROYLGLYCEROL (three-letter code: TGL) (formula: $C_{57}H_{110}O_6$).



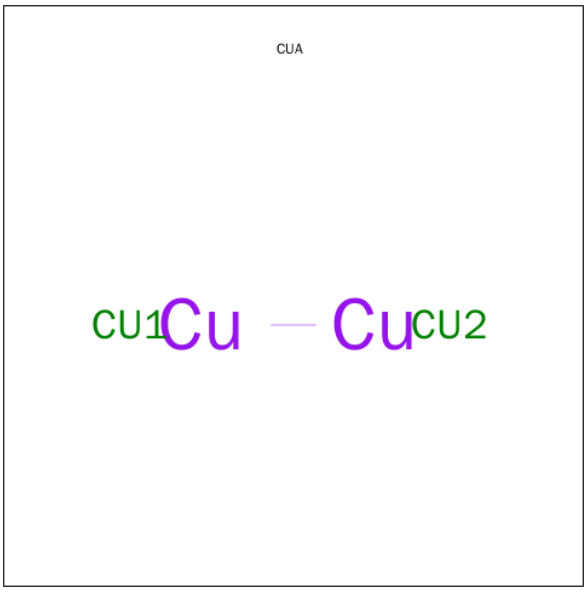
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	A	1	Total C O 63 57 6	0	0
18	D	1	Total C O 63 57 6	0	0
18	L	1	Total C O 63 57 6	0	0
18	N	1	Total C O 63 57 6	0	0
18	N	1	Total C O 63 57 6	0	0
18	N	1	Total C O 63 57 6	0	0

- Molecule 19 is (1R)-2-{[{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (three-letter code: PGV) (formula: $C_{40}H_{77}O_{10}P$).



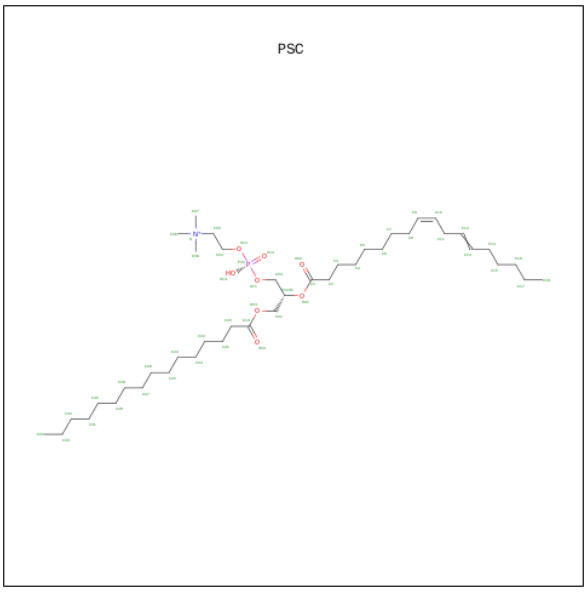
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
19	A	1	Total	C	O	P	0	0
			51	40	10	1		
19	A	1	Total	C	O	P	0	0
			51	40	10	1		
19	C	1	Total	C	O	P	0	0
			51	40	10	1		
19	C	1	Total	C	O	P	0	0
			51	40	10	1		
19	N	1	Total	C	O	P	0	0
			51	40	10	1		
19	N	1	Total	C	O	P	0	0
			51	40	10	1		
19	P	1	Total	C	O	P	0	0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

- Molecule 20 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu_2).



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

- Molecule 21 is (7R,17E,20E)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSA-17,20-DIEN-1-AMINIUM 4-OXIDE (three-letter code: PSC) (formula: $C_{42}H_{81}NO_8P$).



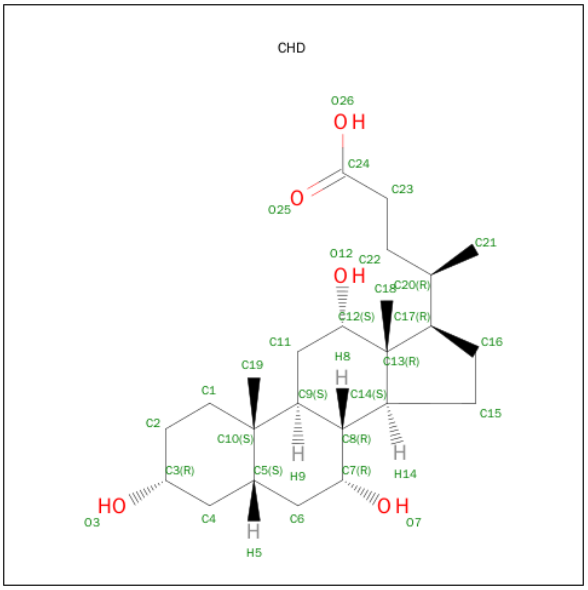
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	B	1	Total C N O P 52 42 1 8 1	0	0

Continued on next page...

Continued from previous page...

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

- Molecule 22 is CHOLIC ACID (three-letter code: CHD) (formula: $C_{24}H_{40}O_5$).

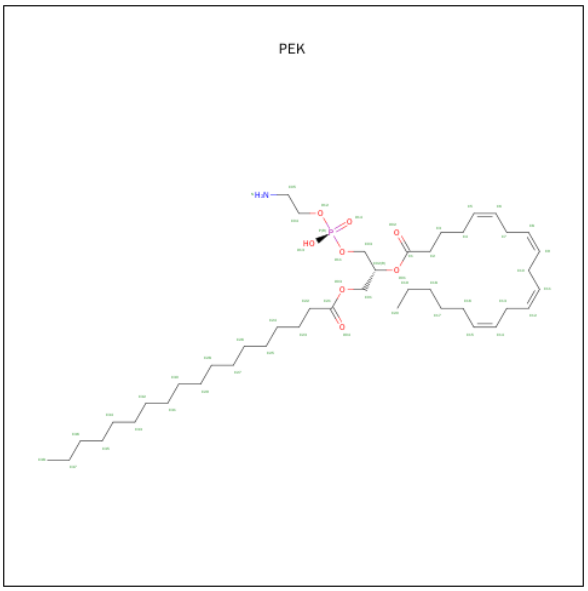


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	B	1	Total	C	O	0	0
			29	24	5		
22	C	1	Total	C	O	0	0
			29	24	5		
22	C	1	Total	C	O	0	0
			29	24	5		
22	G	1	Total	C	O	0	0
			29	24	5		
22	J	1	Total	C	O	0	0
			29	24	5		
22	P	1	Total	C	O	0	0
			29	24	5		
22	P	1	Total	C	O	0	0
			29	24	5		
22	W	1	Total	C	O	0	0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

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

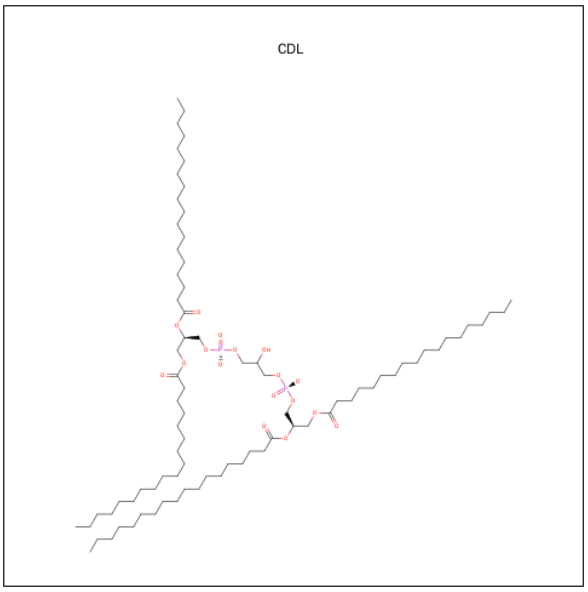
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	P	1	Total X 1 1	0	0
23	C	1	Total X 1 1	0	0

- 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: $C_{43}H_{78}NO_8P$).



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

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

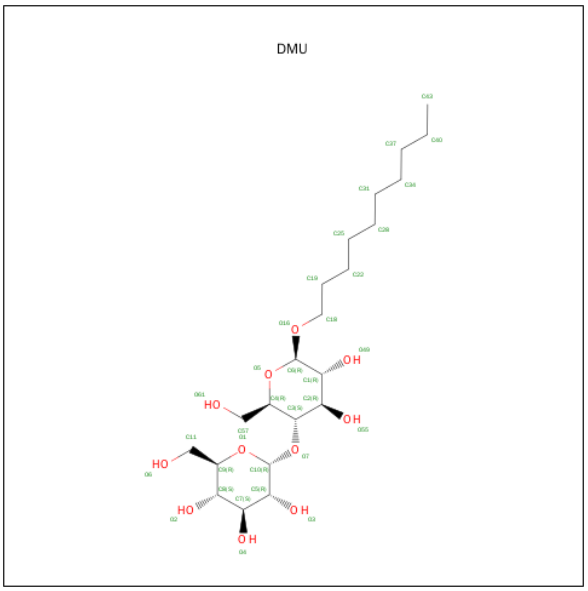


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
25	C	1	Total	C	O	P	0	0
			100	81	17	2		
25	G	1	Total	C	O	P	0	0
			100	81	17	2		
25	P	1	Total	C	O	P	0	0
			100	81	17	2		
25	T	1	Total	C	O	P	0	0
			100	81	17	2		

- Molecule 26 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 27 is SUGAR (DECYL-BETA-D-MALTOPYRANOSIDE) (three-letter code: DMU) (formula: $C_{22}H_{42}O_{11}$).



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

- Molecule 28 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	A	212	Total O 212 212	0	0
28	B	127	Total O 127 127	0	0
28	C	110	Total O 110 110	0	0
28	D	104	Total O 104 104	0	0
28	E	66	Total O 66 66	0	0
28	F	81	Total O 81 81	0	0
28	G	52	Total O 52 52	0	0
28	H	47	Total O 47 47	0	0
28	I	32	Total O 32 32	0	0
28	J	18	Total O 18 18	0	0

Continued on next page...

Continued from previous page...

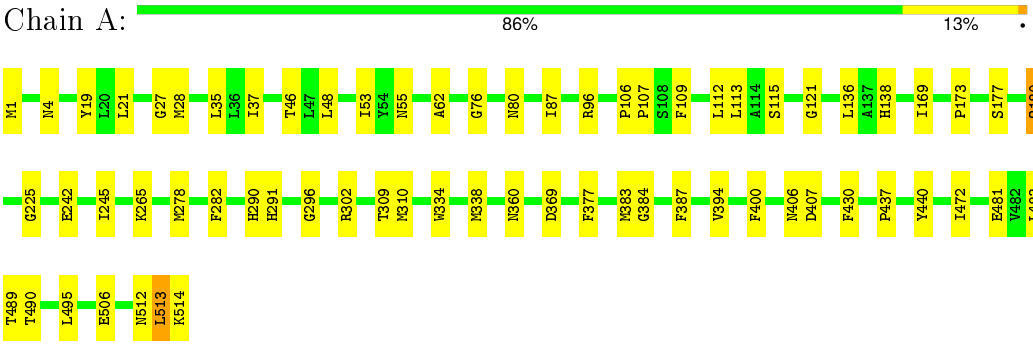
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	K	20	Total O 20 20	0	0
28	L	27	Total O 27 27	0	0
28	M	20	Total O 20 20	0	0
28	N	210	Total O 210 210	0	0
28	O	115	Total O 115 115	0	0
28	P	109	Total O 109 109	0	0
28	Q	60	Total O 60 60	0	0
28	R	45	Total O 45 45	0	0
28	S	79	Total O 79 79	0	0
28	T	42	Total O 42 42	0	0
28	U	47	Total O 47 47	0	0
28	V	24	Total O 24 24	0	0
28	W	17	Total O 17 17	0	0
28	X	18	Total O 18 18	0	0
28	Y	17	Total O 17 17	0	0
28	Z	12	Total O 12 12	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 errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

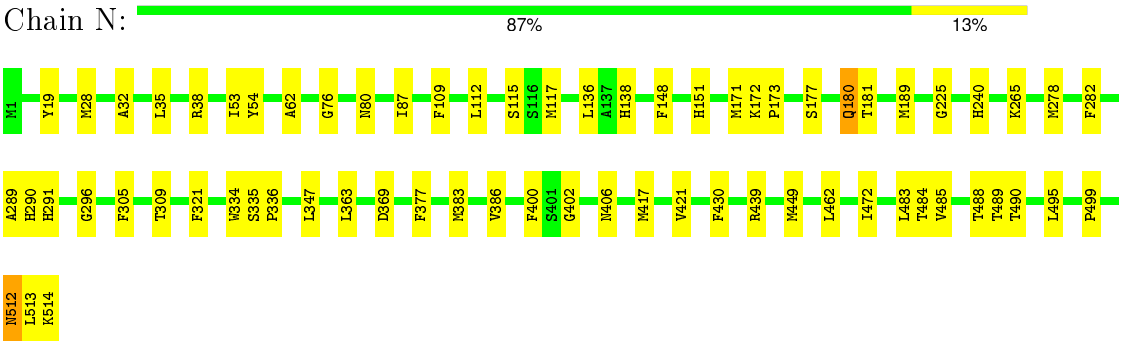
- Molecule 1: Cytochrome c oxidase subunit 1

Chain A:



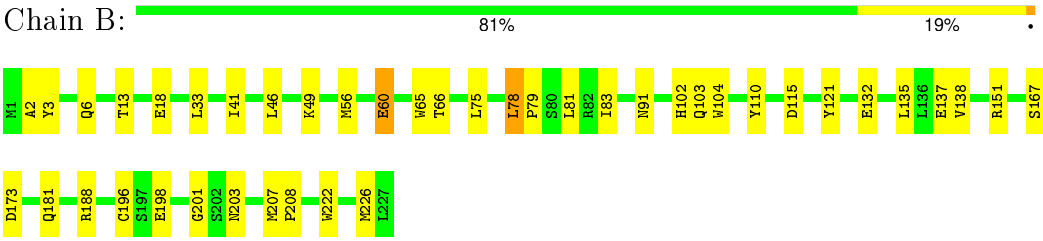
- Molecule 1: Cytochrome c oxidase subunit 1

Chain N:



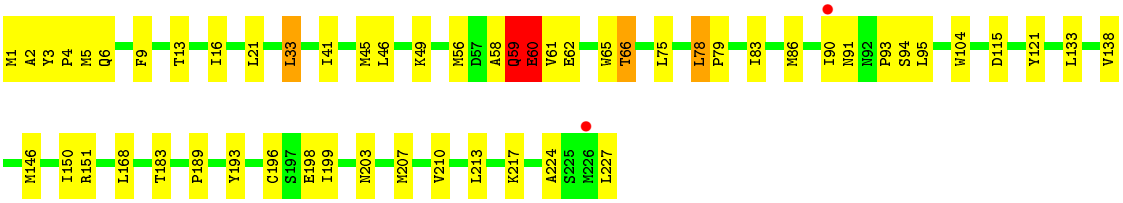
- Molecule 2: Cytochrome c oxidase subunit 2

Chain B:

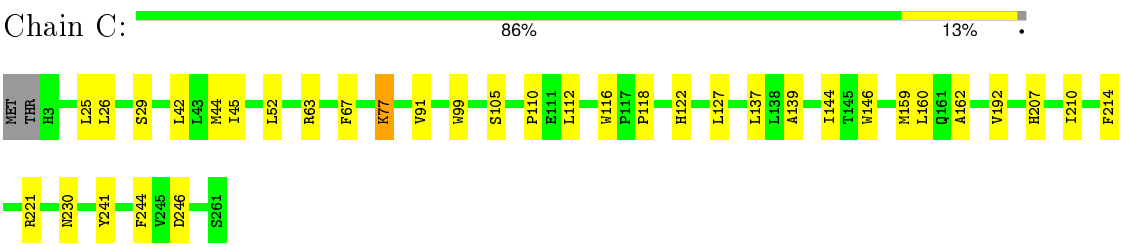


- Molecule 2: Cytochrome c oxidase subunit 2

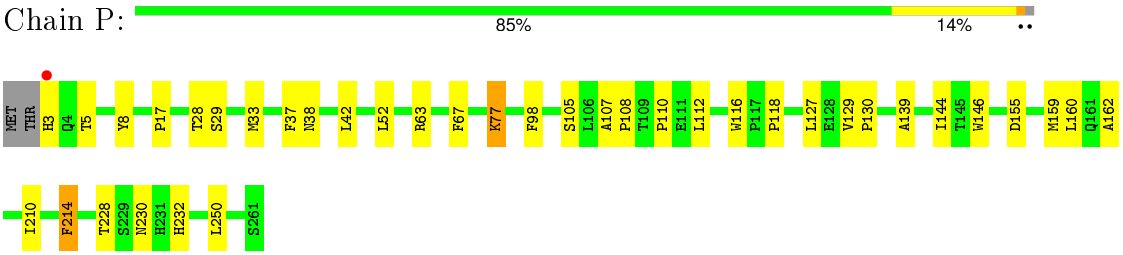
Chain O:



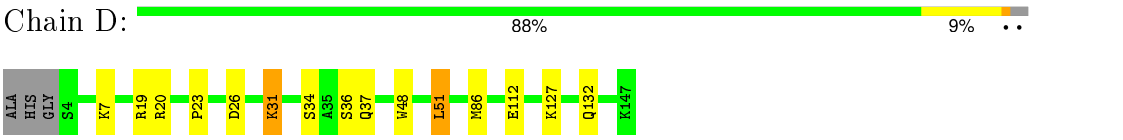
• Molecule 3: Cytochrome c oxidase subunit 3



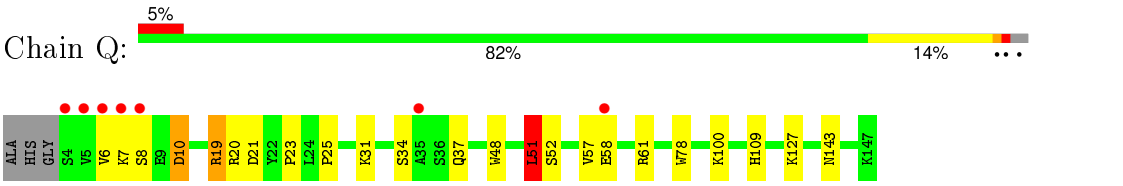
• Molecule 3: Cytochrome c oxidase subunit 3



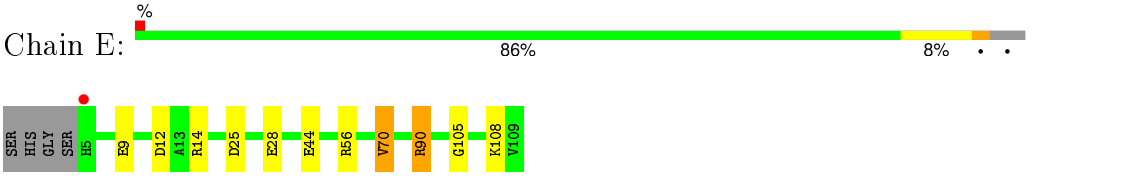
• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1



• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1

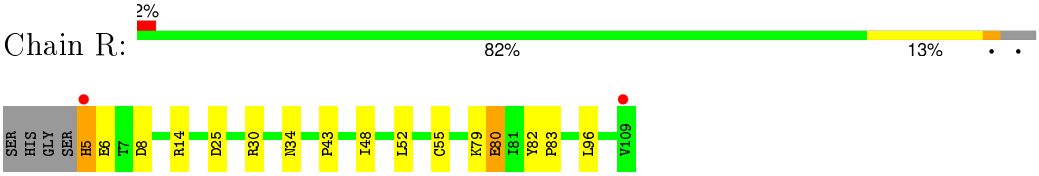


• Molecule 5: Cytochrome c oxidase subunit 5A



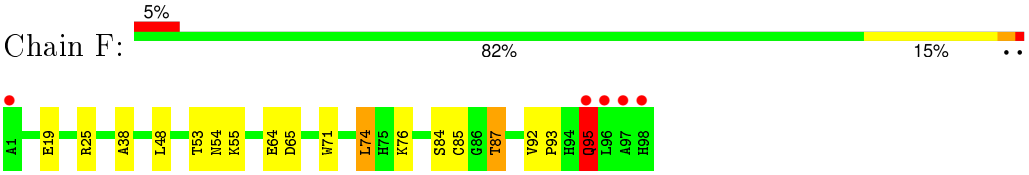
• Molecule 5: Cytochrome c oxidase subunit 5A

Chain R:



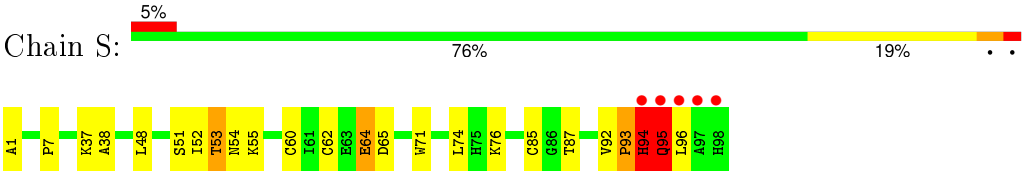
• Molecule 6: Cytochrome c oxidase subunit 5B

Chain F:



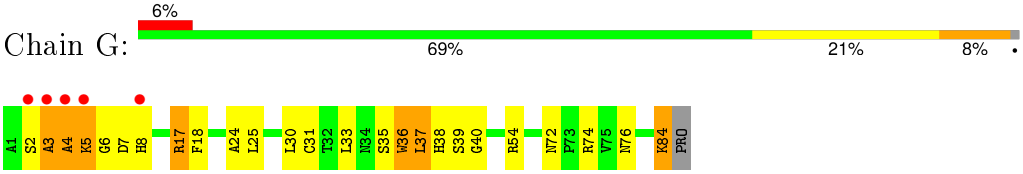
• Molecule 6: Cytochrome c oxidase subunit 5B

Chain S:



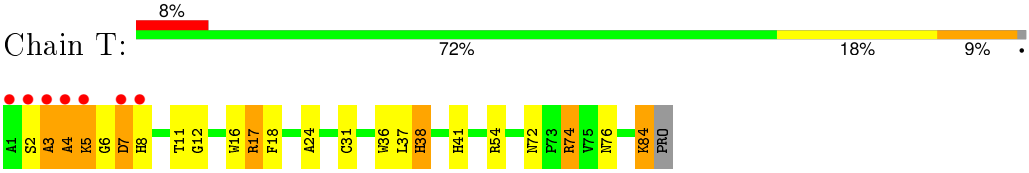
• Molecule 7: Cytochrome c oxidase subunit 6A2

Chain G:



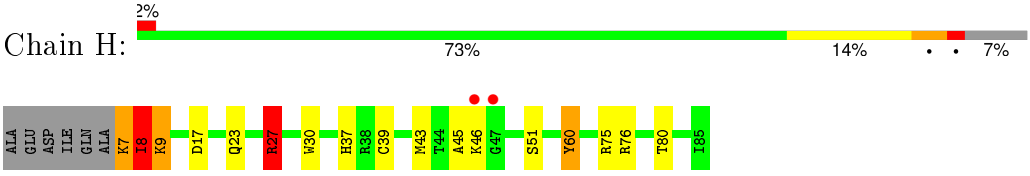
• Molecule 7: Cytochrome c oxidase subunit 6A2

Chain T:



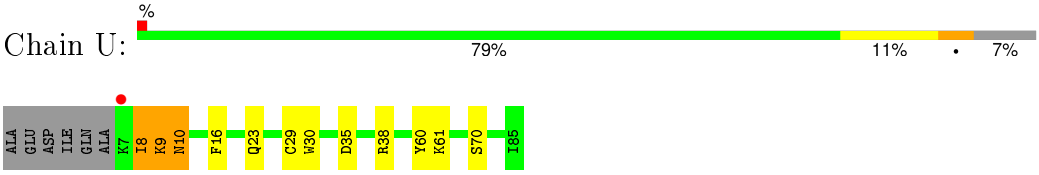
• Molecule 8: Cytochrome c oxidase subunit 6B1

Chain H:



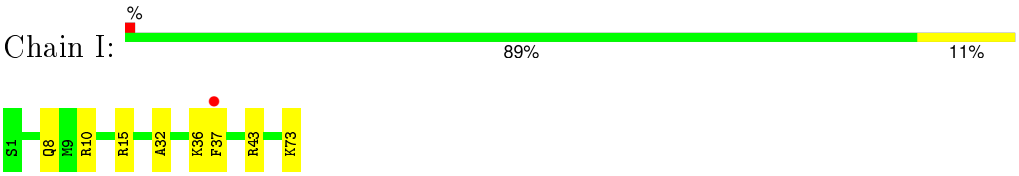
• Molecule 8: Cytochrome c oxidase subunit 6B1

Chain U:



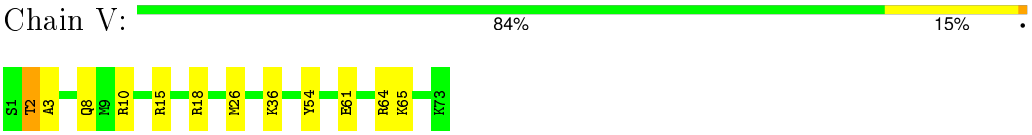
• Molecule 9: Cytochrome c oxidase subunit 6C

Chain I:



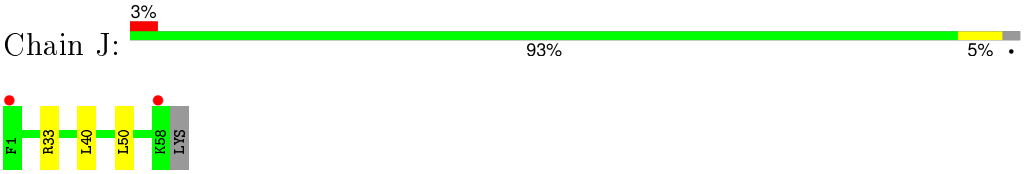
- Molecule 9: Cytochrome c oxidase subunit 6C

Chain V:



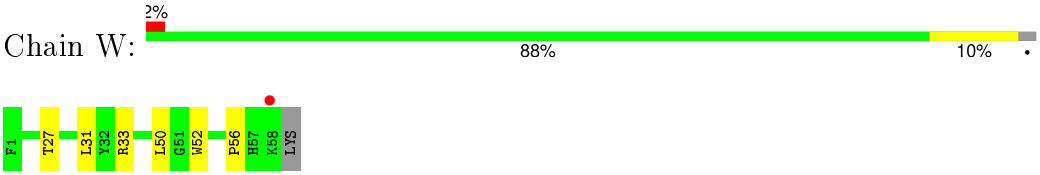
- Molecule 10: Cytochrome c oxidase subunit 7A1

Chain J:



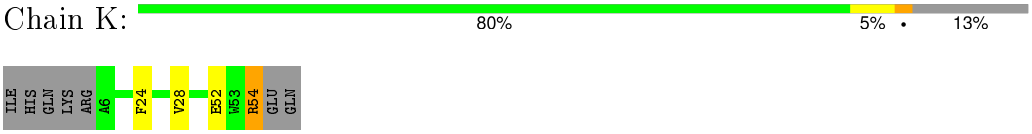
- Molecule 10: Cytochrome c oxidase subunit 7A1

Chain W:



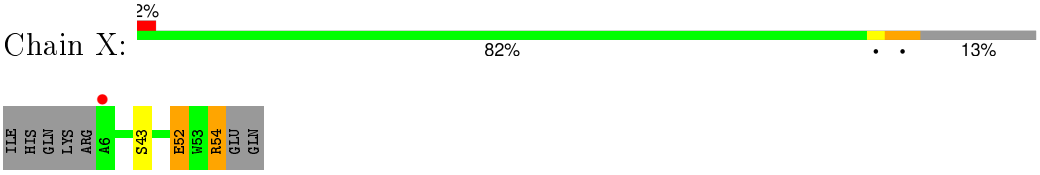
- Molecule 11: Cytochrome c oxidase subunit 7B

Chain K:



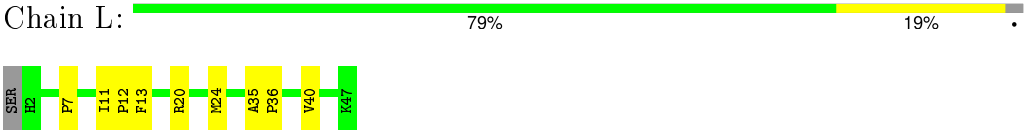
- Molecule 11: Cytochrome c oxidase subunit 7B

Chain X:



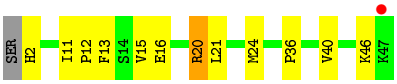
- Molecule 12: Cytochrome c oxidase subunit 7C

Chain L:



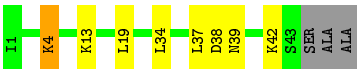
- Molecule 12: Cytochrome c oxidase subunit 7C

Chain Y:



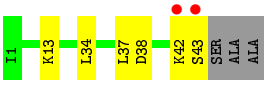
• Molecule 13: Cytochrome c oxidase subunit 8B

Chain M:



• Molecule 13: Cytochrome c oxidase subunit 8B

Chain Z:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	181.83Å 204.10Å 177.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 3.00 135.76 – 3.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (15.00-3.00) 100.0 (135.76-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	27.93 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.5	Depositor
R, R_{free}	0.150 , 0.187 0.162 , 0.195	Depositor DCC
R_{free} test set	6558 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	31.3	Xtriage
Anisotropy	0.637	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 54.9	EDS
Estimated twinning fraction	0.004 for l,-k,h	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 132529 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	32377	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.07% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.96	0/4156	0.91	13/5678 (0.2%)
1	N	0.92	0/4156	0.84	3/5678 (0.1%)
2	B	0.98	2/1860 (0.1%)	0.94	2/2534 (0.1%)
2	O	0.98	3/1860 (0.2%)	0.94	0/2534
3	C	0.96	1/2197 (0.0%)	0.81	2/3005 (0.1%)
3	P	0.92	0/2197	0.82	1/3005 (0.0%)
4	D	1.01	1/1229 (0.1%)	0.94	3/1658 (0.2%)
4	Q	0.97	2/1229 (0.2%)	0.85	2/1658 (0.1%)
5	E	0.94	1/871 (0.1%)	0.94	2/1182 (0.2%)
5	R	0.86	1/871 (0.1%)	0.85	3/1182 (0.3%)
6	F	0.91	0/765	0.97	1/1038 (0.1%)
6	S	1.06	2/765 (0.3%)	1.07	3/1038 (0.3%)
7	G	1.07	2/690 (0.3%)	0.92	0/937
7	T	1.00	2/690 (0.3%)	0.91	0/937
8	H	0.94	0/682	0.88	1/921 (0.1%)
8	U	0.86	0/682	0.88	2/921 (0.2%)
9	I	1.07	0/605	0.87	0/802
9	V	1.07	0/605	0.88	0/802
10	J	1.01	0/471	0.86	0/636
10	W	0.92	0/471	0.88	0/636
11	K	0.96	0/398	0.89	1/546 (0.2%)
11	X	1.00	1/398 (0.3%)	0.77	0/546
12	L	0.87	0/393	0.83	0/526
12	Y	1.08	1/393 (0.3%)	0.81	0/526
13	M	0.94	0/345	0.93	1/470 (0.2%)
13	Z	0.81	0/345	0.86	0/470
All	All	0.96	19/29324 (0.1%)	0.89	40/39866 (0.1%)

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	36	TRP	CB-CG	8.62	1.65	1.50
7	T	36	TRP	CB-CG	8.62	1.65	1.50
12	Y	16	GLU	CG-CD	8.15	1.64	1.51
2	O	198	GLU	C-O	6.50	1.35	1.23
2	B	198	GLU	C-O	6.47	1.35	1.23

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	136	LEU	CB-CG-CD2	-10.95	92.39	111.00
1	A	136	LEU	CA-CB-CG	8.60	135.08	115.30
1	A	136	LEU	CB-CG-CD1	8.13	124.81	111.00
8	H	27	ARG	NE-CZ-NH1	7.85	124.23	120.30
4	D	20	ARG	NE-CZ-NH2	-7.71	116.44	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	53	0
1	N	4027	0	4001	61	0
2	B	1824	0	1833	22	0
2	O	1824	0	1833	34	0
3	C	2110	0	2027	28	0
3	P	2110	0	2027	32	0
4	D	1195	0	1183	13	0
4	Q	1195	0	1183	18	0
5	E	852	0	845	6	0
5	R	852	0	845	8	0
6	F	748	0	728	13	0
6	S	748	0	728	27	0
7	G	675	0	644	31	0
7	T	675	0	644	33	0
8	H	662	0	623	11	0
8	U	662	0	623	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	I	601	0	613	7	0
9	V	601	0	613	10	0
10	J	460	0	459	2	0
10	W	460	0	459	6	0
11	K	384	0	366	2	0
11	X	384	0	366	6	0
12	L	380	0	380	12	0
12	Y	380	0	380	11	1
13	M	335	0	352	3	0
13	Z	335	0	352	1	0
14	A	120	0	108	10	0
14	N	120	0	108	8	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	63	0	110	6	0
18	D	63	0	110	5	0
18	L	63	0	110	14	0
18	N	189	0	330	22	0
19	A	102	0	152	13	0
19	C	102	0	152	10	0
19	N	102	0	152	9	0
19	P	102	0	152	7	0
20	B	2	0	0	0	0
20	O	2	0	0	0	0
21	B	52	0	80	11	0
21	O	52	0	80	17	0
22	B	29	0	39	2	0
22	C	58	0	78	2	0
22	G	29	0	39	0	0
22	J	29	0	38	2	0
22	P	58	0	78	2	0
22	W	29	0	38	3	0
23	C	1	0	0	0	0
23	P	1	0	0	0	0
24	C	106	0	154	8	0
24	G	53	0	77	10	0
24	P	106	0	154	13	0
24	T	53	0	77	12	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	C	100	0	156	19	0
25	G	100	0	156	20	0
25	P	100	0	156	9	0
25	T	100	0	156	24	0
26	F	1	0	0	0	0
26	S	1	0	0	0	0
27	M	33	0	39	0	0
27	Z	33	0	39	0	0
28	A	212	0	0	13	0
28	B	127	0	0	2	0
28	C	110	0	0	2	0
28	D	104	0	0	4	0
28	E	66	0	0	3	0
28	F	81	0	0	5	0
28	G	52	0	0	3	0
28	H	47	0	0	2	0
28	I	32	0	0	5	0
28	J	18	0	0	0	0
28	K	20	0	0	2	0
28	L	27	0	0	1	0
28	M	20	0	0	0	0
28	N	210	0	0	8	0
28	O	115	0	0	1	0
28	P	109	0	0	5	0
28	Q	60	0	0	4	0
28	R	45	0	0	0	0
28	S	79	0	0	4	0
28	T	42	0	0	4	0
28	U	47	0	0	0	0
28	V	24	0	0	5	1
28	W	17	0	0	1	0
28	X	18	0	0	1	0
28	Y	17	0	0	1	0
28	Z	12	0	0	0	0
All	All	32377	0	31226	521	1

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 8.

The worst 5 of 521 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)
24:P:1265:PEK:H383	25:T:1269:CDL:C27	1.54	1.35
24:P:1265:PEK:C38	25:T:1269:CDL:H273	1.66	1.25
24:C:265:PEK:H383	25:G:269:CDL:H273	1.20	1.19
6:S:52:ILE:O	6:S:94:HIS:CE1	1.96	1.18
28:N:4772:HOH:O	24:P:1264:PEK:H381	1.44	1.14

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Y:2:HIS:N	28:V:4556:HOH:O[2_685]	2.13	0.07

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	512/514 (100%)	494 (96%)	17 (3%)	1 (0%)	52 88
1	N	512/514 (100%)	497 (97%)	15 (3%)	0	100 100
2	B	225/227 (99%)	214 (95%)	10 (4%)	1 (0%)	39 80
2	O	225/227 (99%)	214 (95%)	10 (4%)	1 (0%)	39 80
3	C	257/261 (98%)	251 (98%)	6 (2%)	0	100 100
3	P	257/261 (98%)	250 (97%)	5 (2%)	2 (1%)	24 66
4	D	142/147 (97%)	136 (96%)	6 (4%)	0	100 100
4	Q	142/147 (97%)	138 (97%)	4 (3%)	0	100 100
5	E	103/109 (94%)	102 (99%)	1 (1%)	0	100 100
5	R	103/109 (94%)	103 (100%)	0	0	100 100
6	F	96/98 (98%)	87 (91%)	8 (8%)	1 (1%)	19 61
6	S	96/98 (98%)	88 (92%)	6 (6%)	2 (2%)	9 40
7	G	81/85 (95%)	65 (80%)	8 (10%)	8 (10%)	1 3

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
7	T	81/85 (95%)	66 (82%)	10 (12%)	5 (6%)	2 10
8	H	77/85 (91%)	69 (90%)	5 (6%)	3 (4%)	4 21
8	U	77/85 (91%)	71 (92%)	4 (5%)	2 (3%)	7 33
9	I	71/73 (97%)	68 (96%)	3 (4%)	0	100 100
9	V	71/73 (97%)	68 (96%)	2 (3%)	1 (1%)	14 51
10	J	56/59 (95%)	56 (100%)	0	0	100 100
10	W	56/59 (95%)	56 (100%)	0	0	100 100
11	K	47/56 (84%)	47 (100%)	0	0	100 100
11	X	47/56 (84%)	47 (100%)	0	0	100 100
12	L	44/47 (94%)	41 (93%)	3 (7%)	0	100 100
12	Y	44/47 (94%)	43 (98%)	1 (2%)	0	100 100
13	M	41/46 (89%)	41 (100%)	0	0	100 100
13	Z	41/46 (89%)	39 (95%)	2 (5%)	0	100 100
All	All	3504/3614 (97%)	3351 (96%)	126 (4%)	27 (1%)	24 66

5 of 27 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	95	GLN
7	G	4	ALA
7	G	7	ASP
7	G	8	HIS
7	G	39	SER

5.3.2 Protein sidechains (i)

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%)	418 (98%)	8 (2%)	65 90
1	N	426/426 (100%)	415 (97%)	11 (3%)	54 85
2	B	210/210 (100%)	199 (95%)	11 (5%)	29 68

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	O	210/210 (100%)	197 (94%)	13 (6%)	23 60
3	C	224/226 (99%)	218 (97%)	6 (3%)	52 85
3	P	224/226 (99%)	217 (97%)	7 (3%)	47 83
4	D	128/129 (99%)	126 (98%)	2 (2%)	70 92
4	Q	128/129 (99%)	123 (96%)	5 (4%)	39 77
5	E	92/95 (97%)	90 (98%)	2 (2%)	60 88
5	R	92/95 (97%)	90 (98%)	2 (2%)	60 88
6	F	81/81 (100%)	77 (95%)	4 (5%)	31 71
6	S	81/81 (100%)	76 (94%)	5 (6%)	23 60
7	G	67/68 (98%)	59 (88%)	8 (12%)	6 26
7	T	67/68 (98%)	61 (91%)	6 (9%)	12 41
8	H	71/75 (95%)	65 (92%)	6 (8%)	13 45
8	U	71/75 (95%)	66 (93%)	5 (7%)	19 55
9	I	57/57 (100%)	54 (95%)	3 (5%)	28 67
9	V	57/57 (100%)	54 (95%)	3 (5%)	28 67
10	J	49/50 (98%)	48 (98%)	1 (2%)	63 89
10	W	49/50 (98%)	48 (98%)	1 (2%)	63 89
11	K	39/46 (85%)	38 (97%)	1 (3%)	54 85
11	X	39/46 (85%)	38 (97%)	1 (3%)	54 85
12	L	39/40 (98%)	39 (100%)	0	100 100
12	Y	39/40 (98%)	38 (97%)	1 (3%)	54 85
13	M	37/38 (97%)	31 (84%)	6 (16%)	3 14
13	Z	37/38 (97%)	32 (86%)	5 (14%)	5 20
All	All	3040/3082 (99%)	2917 (96%)	123 (4%)	38 77

5 of 123 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	M	38	ASP
1	N	512	ASN
9	V	8	GLN
13	M	42	LYS
1	N	180	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
7	G	71	HIS
10	J	29	ASN
5	R	94	ASN
9	I	8	GLN
11	K	35	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	FME	A	1	1	8,9,10	0.73	0	6,9,11	5.04	3 (50%)
2	FME	B	1	2	8,9,10	1.03	0	6,9,11	6.35	3 (50%)
7	TPO	G	11	7	8,10,11	2.17	4 (50%)	7,14,16	1.12	1 (14%)
9	SAC	I	1	9	7,8,9	2.54	2 (28%)	7,9,11	1.79	2 (28%)
1	FME	N	1	1	8,9,10	0.62	0	6,9,11	6.13	3 (50%)
2	FME	O	1	2	8,9,10	0.72	0	6,9,11	5.35	2 (33%)
7	TPO	T	11	7	8,10,11	1.97	3 (37%)	7,14,16	1.55	2 (28%)
9	SAC	V	1	9	7,8,9	2.51	2 (28%)	7,9,11	3.96	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 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	11	TPO	CB-CA	2.03	1.57	1.54
7	T	11	TPO	P-OG1	2.05	1.66	1.60
7	G	11	TPO	P-O2P	2.42	1.63	1.54
7	T	11	TPO	P-O2P	2.42	1.63	1.54
7	G	11	TPO	P-OG1	3.00	1.69	1.60

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	N	1	FME	CA-N-CN	-14.36	100.73	122.82
2	B	1	FME	CA-N-CN	-14.25	100.91	122.82
2	O	1	FME	CA-N-CN	-12.59	103.45	122.82
1	A	1	FME	CA-N-CN	-11.19	105.61	122.82
9	V	1	SAC	CB-CA-N	-9.00	90.89	110.60

There are no chirality outliers.

All (4) torsion outliers are listed below:

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

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1	FME	2	0
2	O	1	FME	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	T	11	TPO	2	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 52 ligands modelled in this entry, 2 are unknown and 8 are monoatomic - leaving 42 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	1.13	3 (7%)	41,103,103	3.02	20 (48%)
14	HEA	A	516	1	40,67,67	1.15	4 (10%)	41,103,103	1.74	6 (14%)
18	TGL	A	521	-	62,62,62	1.24	6 (9%)	65,65,65	1.85	15 (23%)
19	PGV	A	522	-	50,50,50	0.83	2 (4%)	51,56,56	1.18	2 (3%)
19	PGV	A	524	-	50,50,50	1.25	2 (4%)	51,56,56	1.29	7 (13%)
22	CHD	B	1085	-	29,32,32	0.75	0	48,51,51	1.84	14 (29%)
20	CUA	B	228	2	0,1,1	0.00	-	0,0,0	0.00	-
21	PSC	B	229	-	51,51,51	1.18	3 (5%)	55,59,59	1.14	3 (5%)
24	PEK	C	264	-	51,52,52	0.97	4 (7%)	52,57,57	1.48	7 (13%)
24	PEK	C	265	-	51,52,52	1.25	2 (3%)	52,57,57	1.29	6 (11%)
19	PGV	C	267	-	50,50,50	0.83	3 (6%)	51,56,56	1.10	3 (5%)
19	PGV	C	268	-	50,50,50	1.22	2 (4%)	51,56,56	1.38	8 (15%)
25	CDL	C	270	-	99,99,99	1.33	13 (13%)	101,111,111	1.38	15 (14%)
22	CHD	C	271	-	29,32,32	0.58	0	48,51,51	2.24	20 (41%)
22	CHD	C	525	-	29,32,32	0.76	0	48,51,51	1.24	6 (12%)
18	TGL	D	523	-	62,62,62	1.34	6 (9%)	65,65,65	1.64	10 (15%)
24	PEK	G	1263	-	51,52,52	1.29	4 (7%)	52,57,57	1.35	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	CHD	G	229	-	29,32,32	0.53	0	48,51,51	1.23	2 (4%)
25	CDL	G	269	-	99,99,99	1.38	12 (12%)	101,111,111	1.37	12 (11%)
22	CHD	J	60	-	29,32,32	0.94	0	48,51,51	3.00	24 (50%)
18	TGL	L	522	-	62,62,62	1.36	7 (11%)	65,65,65	1.62	12 (18%)
27	DMU	M	526	-	34,34,34	0.93	2 (5%)	45,45,45	2.63	16 (35%)
19	PGV	N	1266	-	50,50,50	0.83	2 (4%)	51,56,56	1.40	6 (11%)
18	TGL	N	1521	-	62,62,62	1.24	6 (9%)	65,65,65	1.66	10 (15%)
18	TGL	N	1522	-	62,62,62	1.56	7 (11%)	65,65,65	1.65	14 (21%)
18	TGL	N	1523	-	62,62,62	1.35	6 (9%)	65,65,65	1.51	10 (15%)
19	PGV	N	1524	-	50,50,50	0.97	2 (4%)	51,56,56	1.26	8 (15%)
14	HEA	N	515	1	40,67,67	1.42	5 (12%)	41,103,103	3.38	20 (48%)
14	HEA	N	516	1	40,67,67	1.09	3 (7%)	41,103,103	1.69	11 (26%)
21	PSC	O	1229	-	51,51,51	1.15	3 (5%)	55,59,59	1.14	4 (7%)
20	CUA	O	228	2	0,1,1	0.00	-	0,0,0	0.00	-
24	PEK	P	1264	-	51,52,52	0.99	4 (7%)	52,57,57	1.43	10 (19%)
24	PEK	P	1265	-	51,52,52	1.31	5 (9%)	52,57,57	1.33	5 (9%)
19	PGV	P	1267	-	50,50,50	0.90	3 (6%)	51,56,56	1.09	3 (5%)
19	PGV	P	1268	-	50,50,50	1.20	2 (4%)	51,56,56	1.52	7 (13%)
25	CDL	P	1270	-	99,99,99	1.37	12 (12%)	101,111,111	1.45	17 (16%)
22	CHD	P	1271	-	29,32,32	0.60	0	48,51,51	2.17	19 (39%)
22	CHD	P	1525	-	29,32,32	0.66	0	48,51,51	1.60	9 (18%)
25	CDL	T	1269	-	99,99,99	1.33	12 (12%)	101,111,111	1.31	11 (10%)
24	PEK	T	263	-	51,52,52	1.29	4 (7%)	52,57,57	1.27	6 (11%)
22	CHD	W	1059	-	29,32,32	0.91	1 (3%)	48,51,51	3.36	21 (43%)
27	DMU	Z	1526	-	34,34,34	0.88	2 (5%)	45,45,45	2.58	17 (37%)

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	3/3/7/16	0/24/76/76	0/0/8/8
18	TGL	A	521	-	-	0/65/65/65	0/0/0/0
19	PGV	A	522	-	-	0/55/55/55	0/0/0/0
19	PGV	A	524	-	-	1/55/55/55	0/0/0/0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CHD	B	1085	-	-	0/7/74/74	0/4/4/4
20	CUA	B	228	2	-	0/0/0/0	0/0/0/0
21	PSC	B	229	-	-	0/55/55/55	0/0/0/0
24	PEK	C	264	-	-	0/56/56/56	0/0/0/0
24	PEK	C	265	-	-	0/56/56/56	0/0/0/0
19	PGV	C	267	-	-	0/55/55/55	0/0/0/0
19	PGV	C	268	-	-	0/55/55/55	0/0/0/0
25	CDL	C	270	-	-	0/110/110/110	0/0/0/0
22	CHD	C	271	-	-	0/7/74/74	0/4/4/4
22	CHD	C	525	-	-	0/7/74/74	0/4/4/4
18	TGL	D	523	-	-	0/65/65/65	0/0/0/0
24	PEK	G	1263	-	-	0/56/56/56	0/0/0/0
22	CHD	G	229	-	-	0/7/74/74	0/4/4/4
25	CDL	G	269	-	-	0/110/110/110	0/0/0/0
22	CHD	J	60	-	-	0/7/74/74	0/4/4/4
18	TGL	L	522	-	-	0/65/65/65	0/0/0/0
27	DMU	M	526	-	4/4/10/10	0/19/59/59	0/2/2/2
19	PGV	N	1266	-	-	0/55/55/55	0/0/0/0
18	TGL	N	1521	-	-	0/65/65/65	0/0/0/0
18	TGL	N	1522	-	-	0/65/65/65	0/0/0/0
18	TGL	N	1523	-	-	0/65/65/65	0/0/0/0
19	PGV	N	1524	-	-	1/55/55/55	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	3/3/7/16	0/24/76/76	0/0/8/8
21	PSC	O	1229	-	-	0/55/55/55	0/0/0/0
20	CUA	O	228	2	-	0/0/0/0	0/0/0/0
24	PEK	P	1264	-	-	0/56/56/56	0/0/0/0
24	PEK	P	1265	-	-	0/56/56/56	0/0/0/0
19	PGV	P	1267	-	-	0/55/55/55	0/0/0/0
19	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	-	-	0/7/74/74	0/4/4/4
22	CHD	P	1525	-	-	0/7/74/74	0/4/4/4
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	-	-	0/7/74/74	0/4/4/4
27	DMU	Z	1526	-	4/4/10/10	0/19/59/59	0/2/2/2

The worst 5 of 154 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	N	515	HEA	C4A-NA	-4.10	1.31	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	P	1270	CDL	C59-C58	-3.64	1.30	1.51
25	C	270	CDL	C59-C58	-3.53	1.31	1.51
18	L	522	TGL	C10-CB9	-3.50	1.31	1.51
18	L	522	TGL	C20-CA9	-3.42	1.31	1.51

The worst 5 of 422 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	515	HEA	C17-C18-C19	-10.20	105.58	127.76
14	N	515	HEA	C17-C18-C19	-9.89	106.25	127.76
22	W	1059	CHD	C18-C13-C12	-7.67	101.61	109.09
22	W	1059	CHD	C17-C13-C14	-6.82	93.16	100.05
22	J	60	CHD	C17-C13-C14	-5.99	94.00	100.05

5 of 20 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
14	N	515	HEA	ND
14	N	515	HEA	NA
14	N	515	HEA	NB
14	A	516	HEA	ND
14	A	516	HEA	NA

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	A	524	PGV	C02-O01-C1-C2
19	N	1524	PGV	C02-O01-C1-C2

There are no ring outliers.

36 monomers are involved in 242 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	A	515	HEA	7	0
14	A	516	HEA	3	0
18	A	521	TGL	6	0
19	A	522	PGV	1	0
19	A	524	PGV	12	0
22	B	1085	CHD	2	0
21	B	229	PSC	11	0
24	C	264	PEK	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	C	265	PEK	5	0
19	C	267	PGV	7	0
19	C	268	PGV	3	0
25	C	270	CDL	19	0
22	C	271	CHD	2	0
18	D	523	TGL	5	0
24	G	1263	PEK	10	0
25	G	269	CDL	20	0
22	J	60	CHD	2	0
18	L	522	TGL	14	0
19	N	1266	PGV	2	0
18	N	1521	TGL	7	0
18	N	1522	TGL	9	0
18	N	1523	TGL	6	0
19	N	1524	PGV	7	0
14	N	515	HEA	5	0
14	N	516	HEA	3	0
21	O	1229	PSC	17	0
24	P	1264	PEK	5	0
24	P	1265	PEK	8	0
19	P	1267	PGV	2	0
19	P	1268	PGV	5	0
25	P	1270	CDL	9	0
22	P	1271	CHD	1	0
22	P	1525	CHD	1	0
25	T	1269	CDL	24	0
24	T	263	PEK	12	0
22	W	1059	CHD	3	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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%)	-0.30	0 100 100	13, 17, 24, 50	0
1	N	513/514 (99%)	-0.33	0 100 100	13, 19, 26, 49	0
2	B	226/227 (99%)	-0.25	0 100 100	12, 21, 49, 70	0
2	O	226/227 (99%)	-0.13	2 (0%) 85 64	16, 24, 50, 68	0
3	C	259/261 (99%)	-0.43	0 100 100	13, 18, 30, 48	0
3	P	259/261 (99%)	-0.41	1 (0%) 93 80	14, 20, 33, 52	0
4	D	144/147 (97%)	-0.36	0 100 100	14, 20, 41, 64	0
4	Q	144/147 (97%)	0.17	7 (4%) 33 13	19, 31, 56, 99	0
5	E	105/109 (96%)	-0.47	1 (0%) 84 60	13, 20, 48, 85	0
5	R	105/109 (96%)	-0.34	2 (1%) 70 41	17, 24, 56, 88	0
6	F	98/98 (100%)	-0.03	5 (5%) 32 12	15, 24, 72, 108	0
6	S	98/98 (100%)	0.06	5 (5%) 32 12	14, 23, 74, 106	0
7	G	83/85 (97%)	0.10	5 (6%) 25 9	13, 24, 92, 96	0
7	T	83/85 (97%)	0.23	7 (8%) 14 5	16, 26, 92, 97	0
8	H	79/85 (92%)	-0.03	2 (2%) 61 30	16, 27, 76, 99	0
8	U	79/85 (92%)	-0.02	1 (1%) 79 53	19, 29, 76, 100	0
9	I	72/73 (98%)	-0.15	1 (1%) 78 51	16, 29, 54, 62	0
9	V	72/73 (98%)	0.01	0 100 100	16, 35, 55, 79	0
10	J	58/59 (98%)	-0.13	2 (3%) 49 21	19, 28, 55, 89	0
10	W	58/59 (98%)	-0.13	1 (1%) 73 45	18, 27, 61, 95	0
11	K	49/56 (87%)	-0.32	0 100 100	19, 26, 37, 49	0
11	X	49/56 (87%)	-0.06	1 (2%) 68 39	24, 32, 47, 61	0
12	L	46/47 (97%)	-0.27	0 100 100	17, 23, 46, 70	0
12	Y	46/47 (97%)	-0.22	1 (2%) 65 35	18, 24, 51, 73	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	M	43/46 (93%)	-0.11	0 100 100	15, 21, 66, 91	0
13	Z	43/46 (93%)	-0.13	2 (4%) 35 14	22, 26, 75, 94	0
All	All	3550/3614 (98%)	-0.22	46 (1%) 79 53	12, 21, 52, 108	0

The worst 5 of 46 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	Q	5	VAL	12.9
4	Q	4	SER	12.6
6	S	97	ALA	9.4
4	Q	6	VAL	7.7
4	Q	8	SER	6.8

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, 95^{th} 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
2	FME	O	1	10/11	0.97	0.26	-	23,24,32,39	0
7	TPO	T	11	11/12	0.72	0.41	-	64,70,88,88	0
2	FME	B	1	10/11	0.97	0.22	-	20,21,29,35	0
9	SAC	I	1	9/10	0.59	0.44	-	71,74,76,78	0
1	FME	N	1	10/11	0.95	0.31	-	35,35,51,53	0
9	SAC	V	1	9/10	0.73	0.52	-	84,85,86,86	0
1	FME	A	1	10/11	0.96	0.30	-	34,36,49,58	0
7	TPO	G	11	11/12	0.60	0.35	-	61,67,86,87	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, 95^{th} 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
25	CDL	P	1270	100/100	0.83	0.48	9.89	39,83,105,108	0
22	CHD	J	60	29/29	0.71	0.52	7.33	98,105,109,109	0
19	PGV	A	524	51/51	0.85	0.41	7.22	29,64,91,94	0
22	CHD	W	1059	29/29	0.65	0.47	6.84	91,103,105,105	0
18	TGL	A	521	63/63	0.88	0.35	6.59	40,64,86,90	0
18	TGL	L	522	63/63	0.86	0.36	6.57	32,55,78,82	0
25	CDL	G	269	100/100	0.76	0.57	6.48	56,82,107,111	0
25	CDL	C	270	100/100	0.86	0.52	6.44	38,80,104,106	0
19	PGV	N	1524	51/51	0.80	0.40	5.81	36,64,98,101	0
19	PGV	P	1268	51/51	0.76	0.46	5.63	74,86,100,101	0
18	TGL	N	1522	63/63	0.82	0.40	5.27	41,65,81,83	0
25	CDL	T	1269	100/100	0.76	0.50	5.16	51,83,107,108	0
18	TGL	D	523	63/63	0.83	0.33	4.46	44,64,89,90	0
18	TGL	N	1521	63/63	0.85	0.40	4.42	40,68,88,92	0
18	TGL	N	1523	63/63	0.75	0.40	4.17	45,70,89,91	0
19	PGV	N	1266	51/51	0.98	0.29	3.40	20,34,52,53	0
21	PSC	B	229	52/52	0.78	0.47	3.10	44,89,112,114	0
22	CHD	P	1271	29/29	0.85	0.37	3.04	78,87,88,88	0
21	PSC	O	1229	52/52	0.79	0.45	2.50	34,82,109,112	0
24	PEK	P	1265	53/53	0.74	0.45	2.29	34,86,99,100	0
19	PGV	A	522	51/51	0.98	0.27	2.27	14,25,49,51	0
19	PGV	P	1267	51/51	0.98	0.28	2.24	17,25,63,65	0
27	DMU	Z	1526	33/33	0.94	0.27	2.10	29,41,54,57	0
19	PGV	C	267	51/51	0.98	0.25	2.06	15,23,61,65	0
24	PEK	C	264	53/53	0.96	0.25	2.04	14,34,69,70	0
24	PEK	P	1264	53/53	0.96	0.24	1.89	14,35,68,70	0
14	HEA	N	515	60/60	0.96	0.25	1.76	22,41,66,70	0
24	PEK	C	265	53/53	0.74	0.39	1.44	36,87,96,98	0
19	PGV	C	268	51/51	0.80	0.46	1.34	57,84,99,100	0
24	PEK	T	263	53/53	0.70	0.52	1.20	38,90,112,114	0
22	CHD	C	271	29/29	0.86	0.38	1.12	76,85,87,88	0
24	PEK	G	1263	53/53	0.78	0.41	0.98	42,92,110,110	0
14	HEA	A	516	60/60	0.98	0.22	0.65	10,15,23,26	0
14	HEA	A	515	60/60	0.98	0.21	0.37	6,18,35,40	0
14	HEA	N	516	60/60	0.98	0.21	0.23	5,17,25,27	0
22	CHD	C	525	29/29	0.97	0.21	0.01	18,26,28,28	0
22	CHD	P	1525	29/29	0.96	0.20	-0.10	19,26,29,33	0
27	DMU	M	526	33/33	0.96	0.19	-0.43	26,34,43,43	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
22	CHD	B	1085	29/29	0.97	0.17	-0.62	7,13,15,22	0
22	CHD	G	229	29/29	0.98	0.17	-0.73	6,12,14,15	0
26	ZN	F	99	1/1	1.00	0.12	-2.05	22,22,22,22	0
17	NA	N	519	1/1	0.97	0.10	-2.06	21,21,21,21	0
20	CUA	B	228	2/2	0.99	0.10	-2.28	17,17,17,18	0
26	ZN	S	99	1/1	0.99	0.11	-2.29	22,22,22,22	0
17	NA	A	519	1/1	0.97	0.13	-2.73	18,18,18,18	0
20	CUA	O	228	2/2	0.99	0.10	-3.70	20,20,20,22	0
16	MG	N	518	1/1	0.95	0.12	-6.19	18,18,18,18	0
16	MG	A	518	1/1	0.99	0.10	-6.78	15,15,15,15	0
15	CU	N	517	1/1	0.98	0.16	-	24,24,24,24	0
15	CU	A	517	1/1	0.97	0.17	-	22,22,22,22	0
23	UNX	P	262	1/1	0.55	0.26	-	42,42,42,42	0
23	UNX	C	262	1/1	0.81	0.30	-	42,42,42,42	0

6.5 Other polymers (i)

There are no such residues in this entry.