



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 15, 2018 – 05:14 PM EST

PDB ID : 3WG7
Title : A 1.9 angstrom radiation damage free X-ray structure of large (420KDa) protein by femtosecond crystallography
Authors : Hirata, K.; Shinzawa-Itoh, K.; Yano, N.; Takemura, S.; Kato, K.; Hatanaka, M.; Muramoto, K.; Kawahara, T.; Tsukihara, T.; Yamashita, E.; Tono, K.; Ueno, G.; Hikima, T.; Murakami, H.; Inubushi, Y.; Yabashi, M.; Ishikawa, T.; Yamamoto, M.; Ogura, T.; Sugimoto, H.; Shen, J.R.; Yoshikawa, S.; Ago, H.
Deposited on : 2013-07-29
Resolution : 1.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030736
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030736

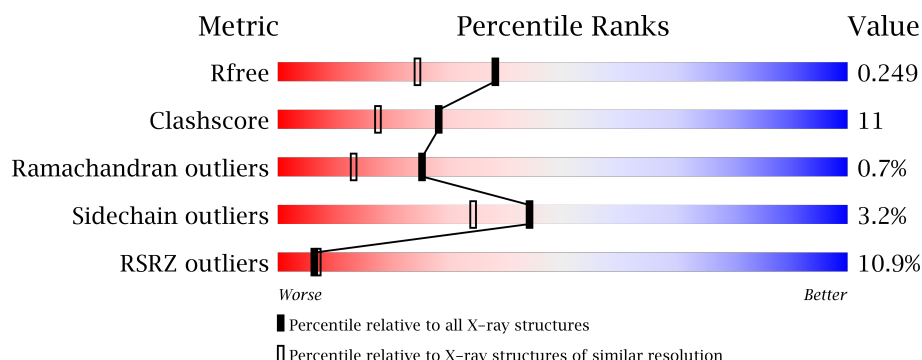
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 Å.

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



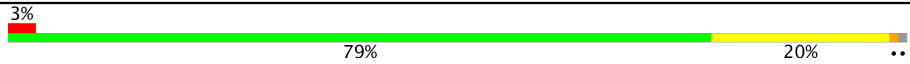

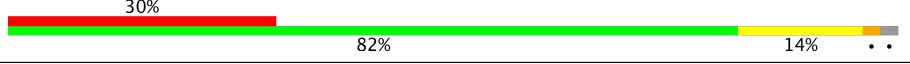
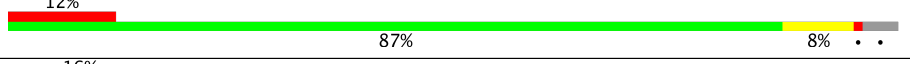

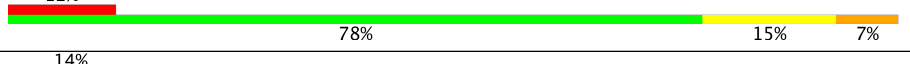


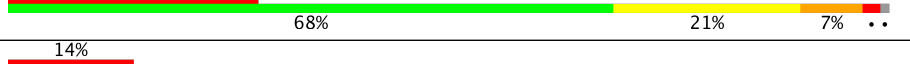


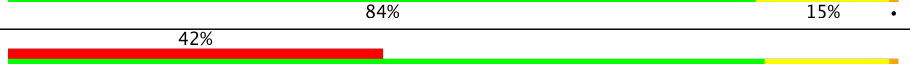

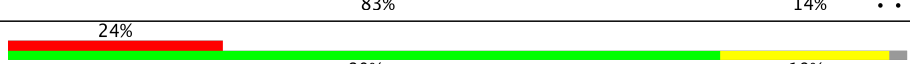
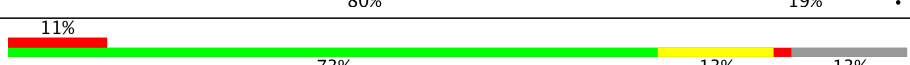
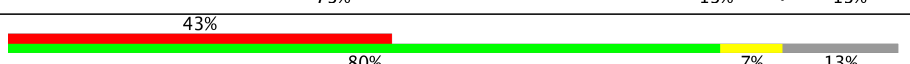
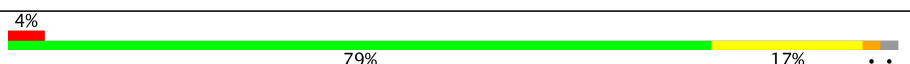
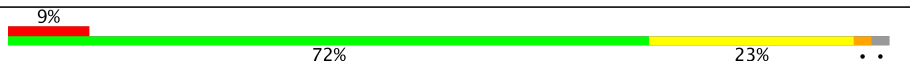
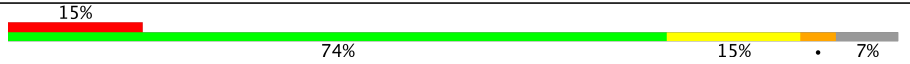


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	5047 (1.90-1.90)
Clashscore	112137	5731 (1.90-1.90)
Ramachandran outliers	110173	5669 (1.90-1.90)
Sidechain outliers	110143	5670 (1.90-1.90)
RSRZ outliers	101464	5100 (1.90-1.90)

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>3%</div> <div>84%</div> <div>16%</div> <div>.</div> </div>
1	N	514	<div> <div>2%</div> <div>82%</div> <div>16%</div> <div>.</div> </div>
2	B	227	<div> <div>5%</div> <div>75%</div> <div>22%</div> <div>.</div> </div>
2	O	227	<div> <div>10%</div> <div>74%</div> <div>25%</div> <div>.</div> </div>
3	C	261	<div> <div>3%</div> <div>84%</div> <div>15%</div> <div>.</div> </div>

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

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

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

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	HEA	N	601	X	-	-	-
14	HEA	N	602	X	-	-	-
16	MG	N	604	-	-	-	X
18	PER	A	606[A]	-	-	-	X
18	PER	A	606[B]	-	-	-	X
19	PGV	A	607	-	-	-	X
19	PGV	A	608	-	-	-	X
19	PGV	C	303	-	-	-	X
19	PGV	C	308	-	-	-	X
19	PGV	N	607	-	-	-	X
19	PGV	N	608	-	-	-	X
19	PGV	P	301	-	-	-	X
19	PGV	P	304	-	-	-	X
2	FME	O	1	-	-	X	-
20	TGL	B	301	-	-	-	X
20	TGL	D	201	-	-	-	X
20	TGL	L	101	-	-	-	X
20	TGL	N	609	-	-	-	X
20	TGL	Q	201	-	-	-	X
20	TGL	Y	101	-	-	-	X
22	CHD	C	305	-	-	-	X
22	CHD	J	101	-	-	-	X
22	CHD	W	101	-	-	-	X
23	PSC	N	610	-	-	X	-
24	PEK	C	302	-	-	-	X
25	CDL	C	304	-	-	X	X
25	CDL	G	101	-	-	X	-
25	CDL	P	305	-	-	-	X
25	CDL	T	102	-	-	X	X
27	DMU	M	101	X	-	-	-
27	DMU	Z	101	X	-	-	-

2 Entry composition

There are 28 unique types of molecules in this entry. The entry contains 33302 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	6	0
			4074	2725	629	684	36			
1	N	514	Total	C	N	O	S	0	6	0
			4074	2725	629	684	36			

- 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	1	0
			1832	1189	282	343	18			
2	O	227	Total	C	N	O	S	0	0	0
			1824	1185	281	340	18			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	259	Total	C	N	O	S	0	3	0
			2134	1427	339	353	15			
3	P	259	Total	C	N	O	S	0	3	0
			2134	1427	339	353	15			

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	84	Total	C	N	O	P	S	0	0
			675	431	129	113	1	1		
7	T	84	Total	C	N	O	P	S	0	0
			675	431	129	113	1	1		

- Molecule 8 is a protein called Cytochrome c oxidase subunit 6B1.

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

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

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

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

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

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

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

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

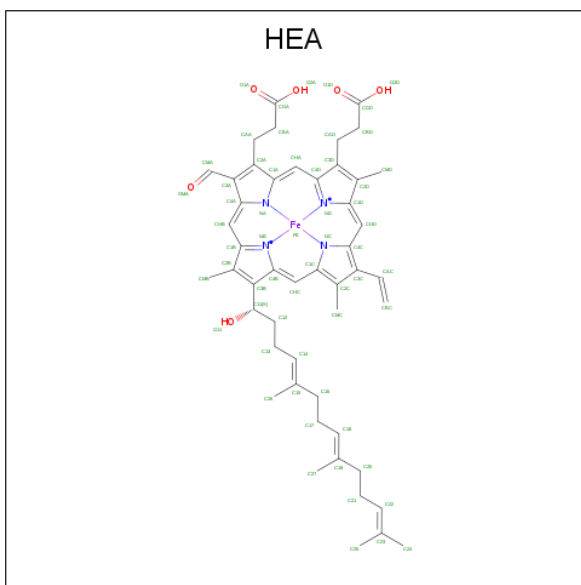
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

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

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

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

- Molecule 14 is HEME-A (three-letter code: HEA) (formula: C₄₉H₅₆FeN₄O₆).



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

- 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		

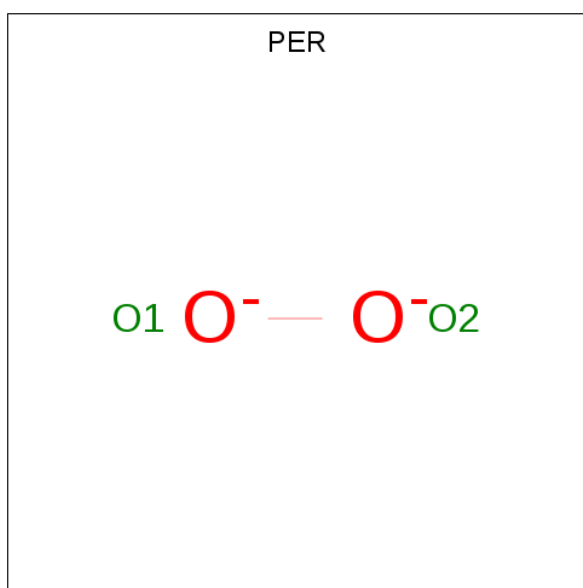
- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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).

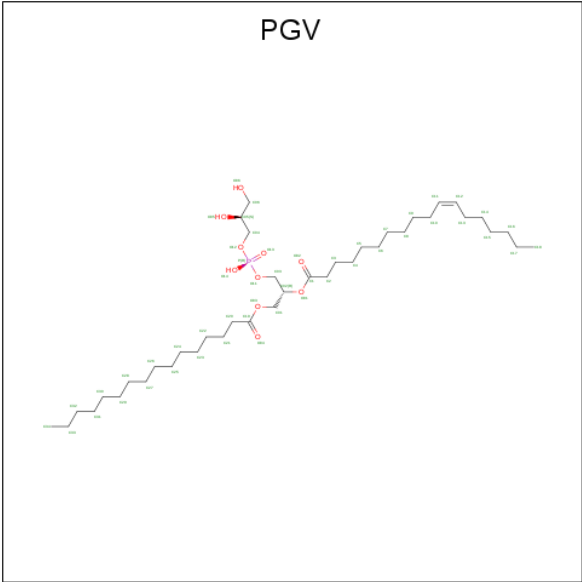
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	P	1	Total Na 1 1	0	0
17	A	1	Total Na 1 1	0	0
17	C	1	Total Na 1 1	0	0
17	N	1	Total Na 1 1	0	0

- Molecule 18 is PEROXIDE ION (three-letter code: PER) (formula: O₂).



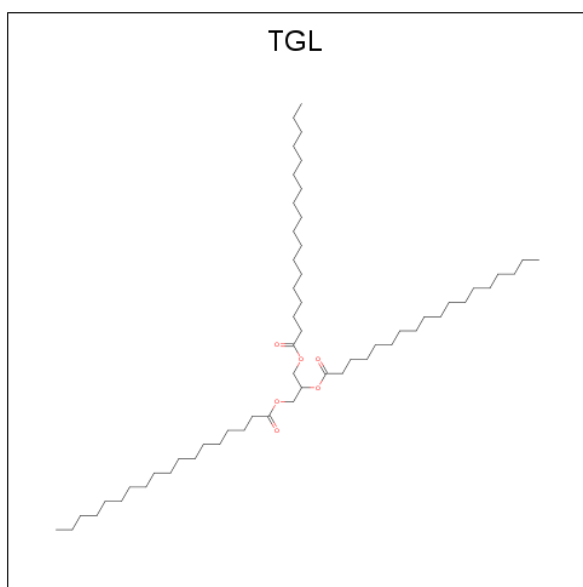
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	A	1	Total O 4 4	0	1
18	N	1	Total O 4 4	0	1

- 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: C₄₀H₇₇O₁₀P).



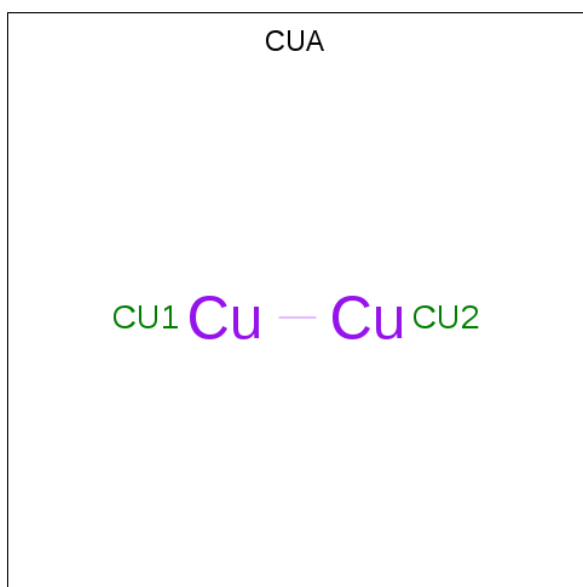
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
19	A	1	Total	C	O	P	0	0
			51	40	10	1		
19	A	1	Total	C	O	P	0	0
			51	40	10	1		
19	C	1	Total	C	O	P	0	0
			51	40	10	1		
19	C	1	Total	C	O	P	0	0
			51	40	10	1		
19	N	1	Total	C	O	P	0	0
			51	40	10	1		
19	N	1	Total	C	O	P	0	0
			51	40	10	1		
19	P	1	Total	C	O	P	0	0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

- Molecule 20 is TRISTEAROYLGLYCEROL (three-letter code: TGL) (formula: C₅₇H₁₁₀O₆).



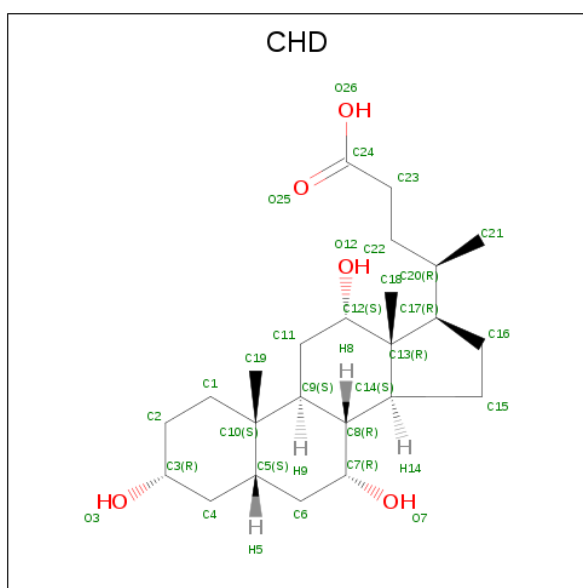
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
20	B	1	Total	C	O	0	0
			63	57	6		
20	D	1	Total	C	O	0	0
			63	57	6		
20	L	1	Total	C	O	0	0
			63	57	6		
20	N	1	Total	C	O	0	0
			63	57	6		
20	Q	1	Total	C	O	0	0
			63	57	6		
20	Y	1	Total	C	O	0	0
			63	57	6		

- 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: $C_{24}H_{40}O_5$).



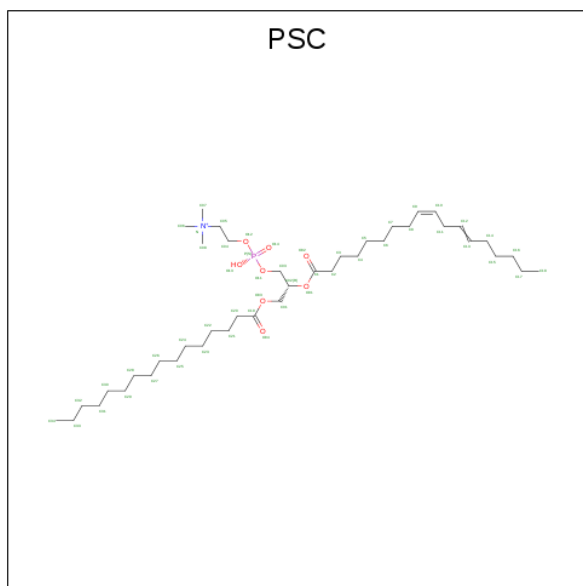
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	B	1	Total	C	O	0	0
			29	24	5		
22	C	1	Total	C	O	0	0
			29	24	5		

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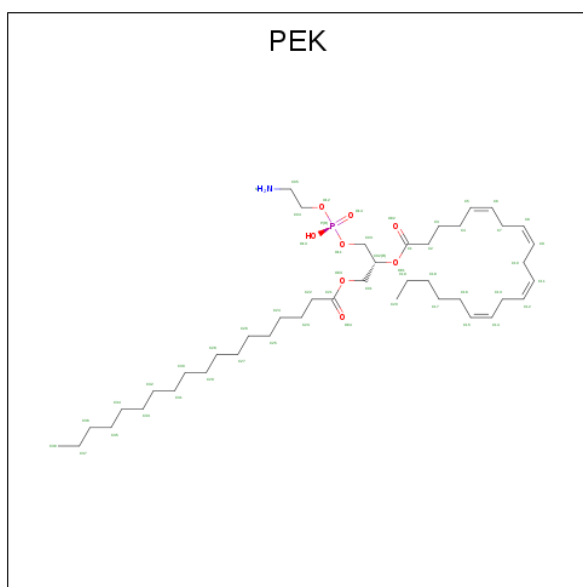
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	C	1	Total	C	O	0	0
			29	24	5		
22	G	1	Total	C	O	0	0
			29	24	5		
22	J	1	Total	C	O	0	0
			29	24	5		
22	P	1	Total	C	O	0	0
			29	24	5		
22	P	1	Total	C	O	0	0
			29	24	5		
22	W	1	Total	C	O	0	0
			29	24	5		

- Molecule 23 is (7R,17E,20E)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSA-17,20-DIEN-1-AMINIUM 4-OXIDE (three-letter code: PSC) (formula: C₄₂H₈₁NO₈P).



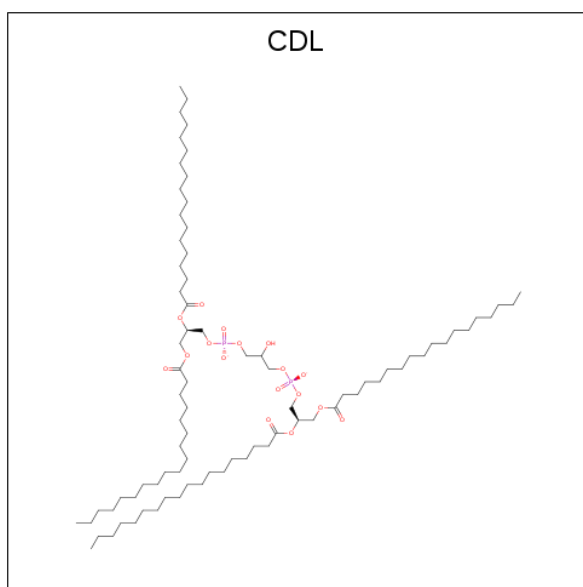
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
23	N	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

- 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	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	P	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
24	P	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: $C_{81}H_{156}O_{17}P_2$).

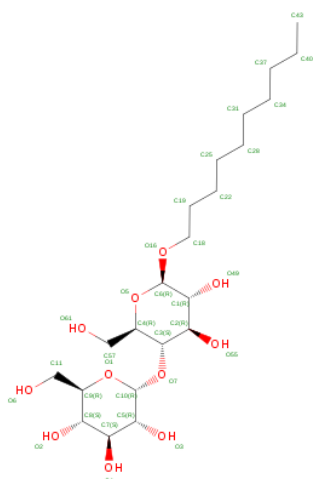


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
25	C	1	Total	C	O	P	0	0
			100	81	17	2		
25	G	1	Total	C	O	P	0	0
			100	81	17	2		
25	P	1	Total	C	O	P	0	0
			100	81	17	2		
25	T	1	Total	C	O	P	0	0
			100	81	17	2		

- Molecule 26 is 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 DECYL-BETA-D-MALTOPYRANOSIDE (three-letter code: DMU) (formula: C₂₂H₄₂O₁₁).



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

- Molecule 28 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	A	265	Total O 265 265	0	0
28	B	194	Total O 194 194	0	0
28	C	141	Total O 141 141	0	0
28	D	160	Total O 160 160	0	0
28	E	125	Total O 125 125	0	0
28	F	112	Total O 112 112	0	0
28	G	70	Total O 70 70	0	0
28	H	70	Total O 70 70	0	0
28	I	52	Total O 52 52	0	0
28	J	31	Total O 31 31	0	0

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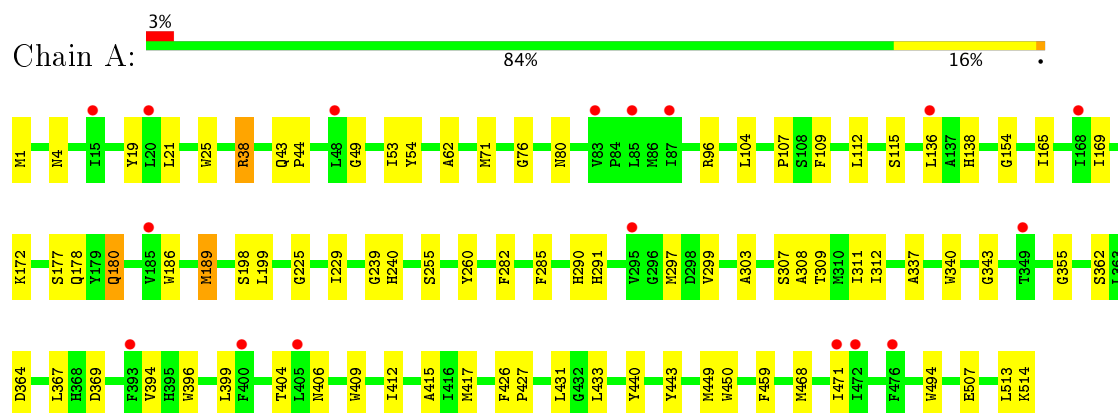
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
28	K	40	Total 40	O 40	0	0
28	L	31	Total 31	O 31	0	0
28	M	31	Total 31	O 31	0	0
28	N	259	Total 259	O 259	0	0
28	O	157	Total 157	O 157	0	0
28	P	143	Total 143	O 143	0	0
28	Q	90	Total 90	O 90	0	0
28	R	103	Total 103	O 103	0	0
28	S	122	Total 122	O 122	0	0
28	T	56	Total 56	O 56	0	0
28	U	51	Total 51	O 51	0	0
28	V	42	Total 42	O 42	0	0
28	W	38	Total 38	O 38	0	0
28	X	34	Total 34	O 34	0	0
28	Y	37	Total 37	O 37	0	0
28	Z	24	Total 24	O 24	0	0

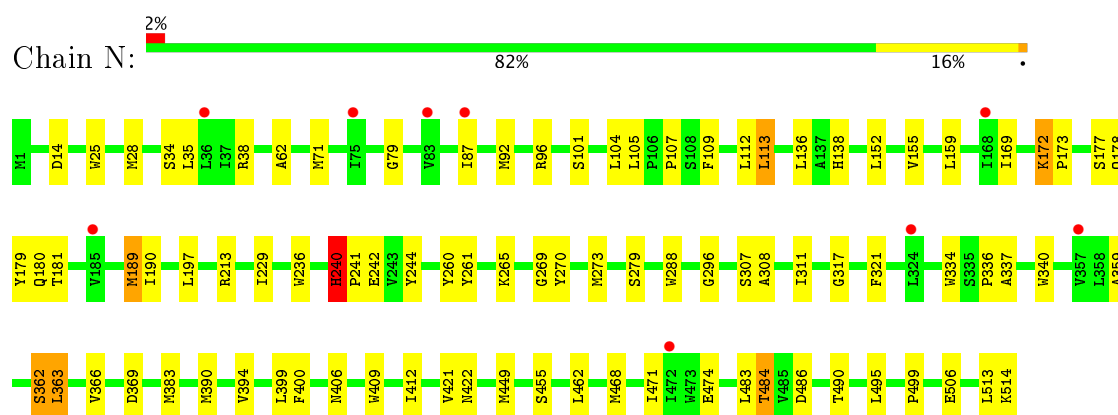
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

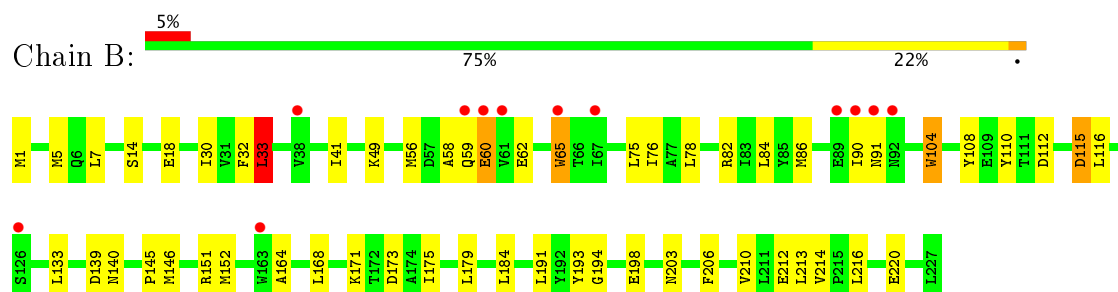
• Molecule 1: Cytochrome c oxidase subunit 1



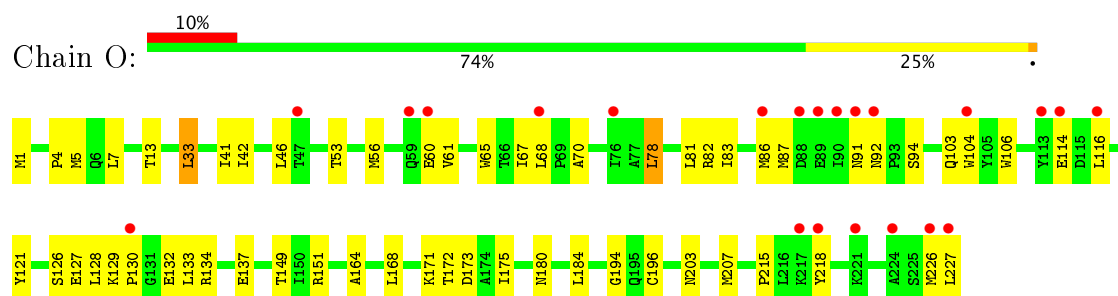
• Molecule 1: Cytochrome c oxidase subunit 1



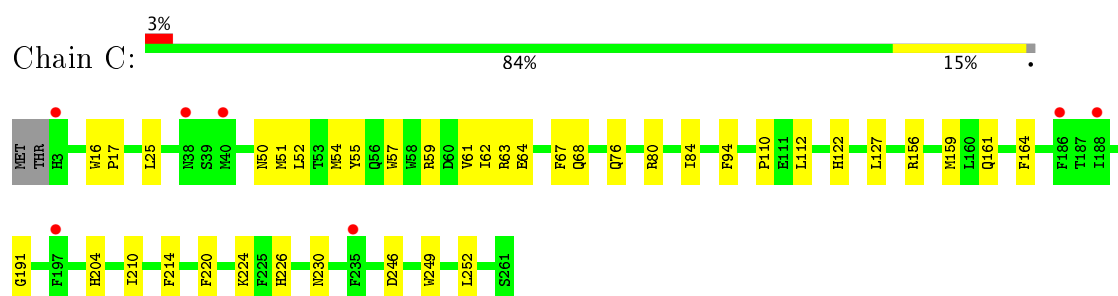
• Molecule 2: Cytochrome c oxidase subunit 2



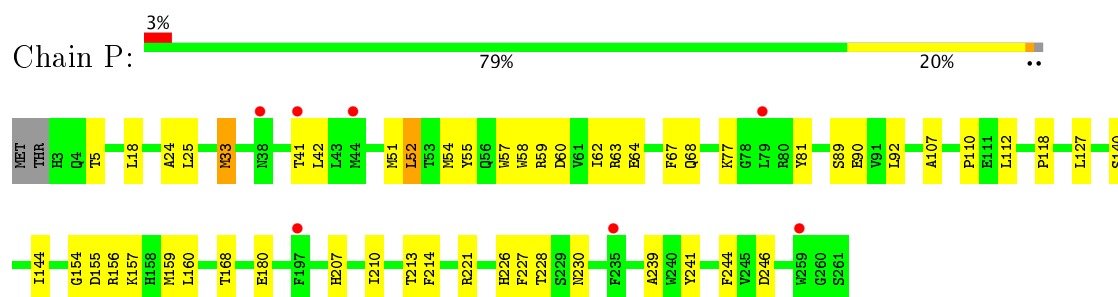
- Molecule 2: Cytochrome c oxidase subunit 2



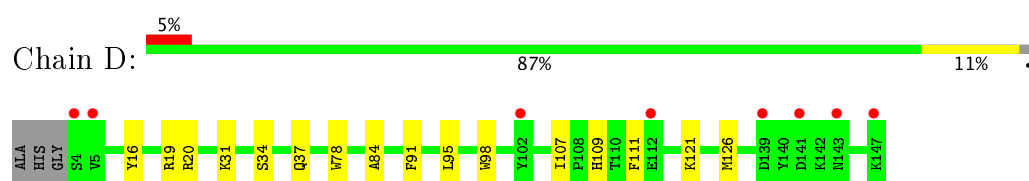
- Molecule 3: Cytochrome c oxidase subunit 3



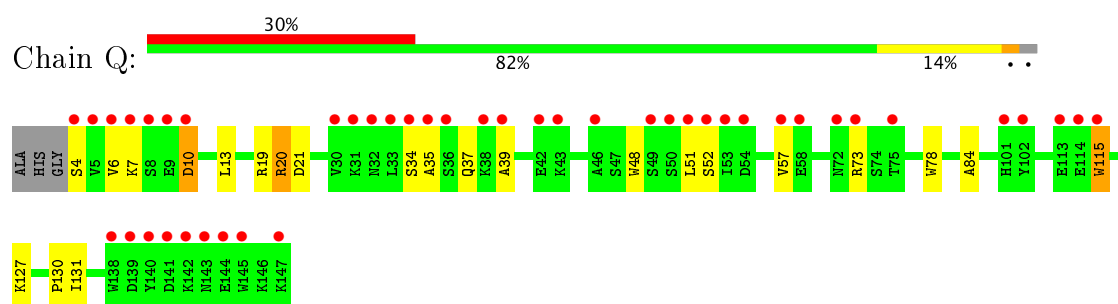
- Molecule 3: Cytochrome c oxidase subunit 3



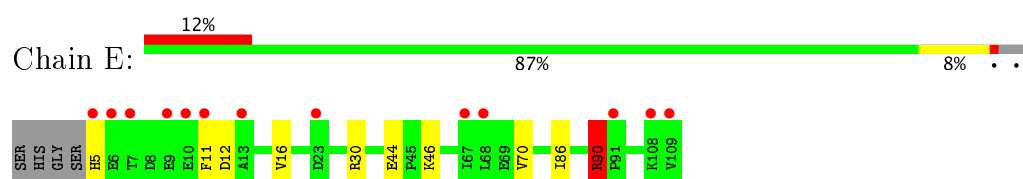
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial



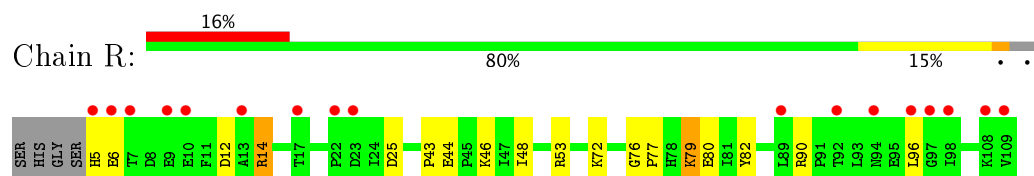
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial



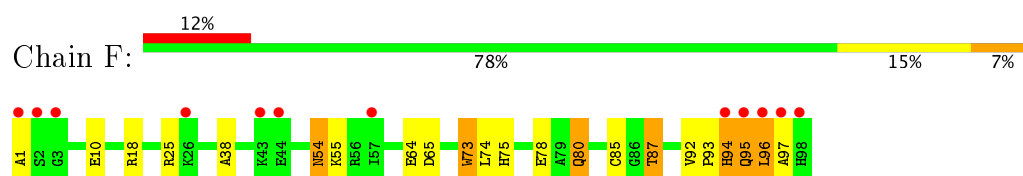
- Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial



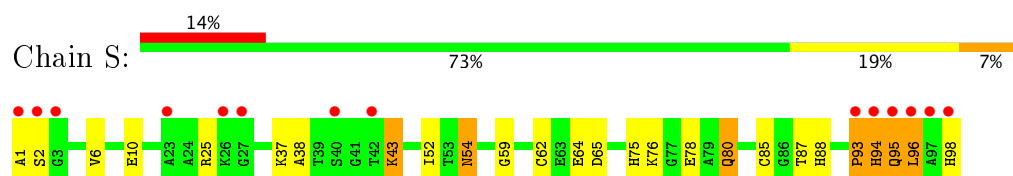
- Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial



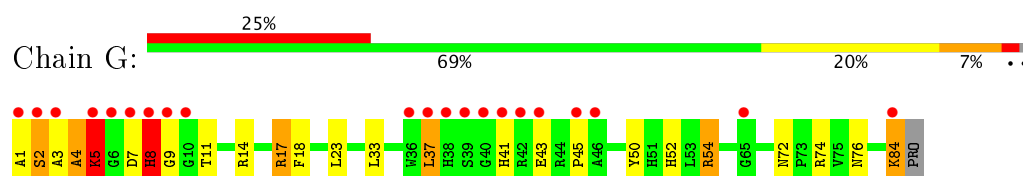
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



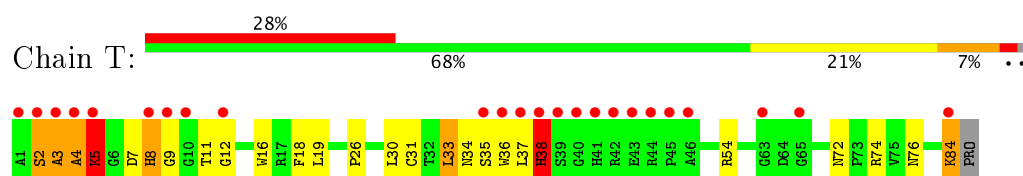
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



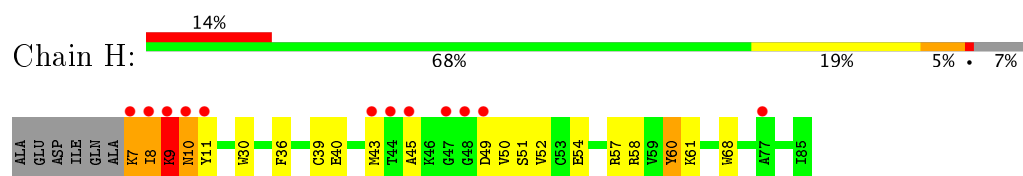
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



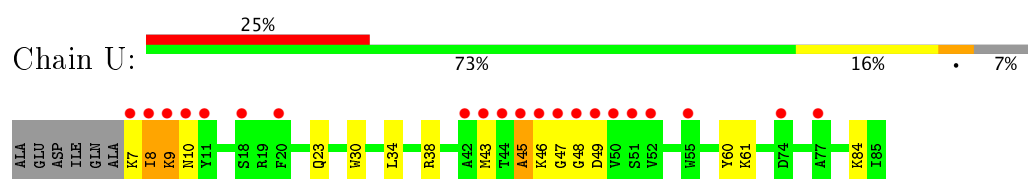
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



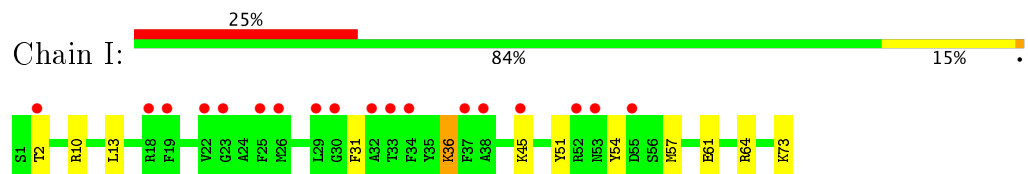
- Molecule 8: Cytochrome c oxidase subunit 6B1



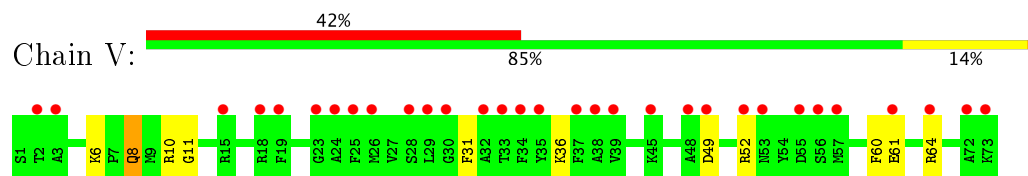
- Molecule 8: Cytochrome c oxidase subunit 6B1



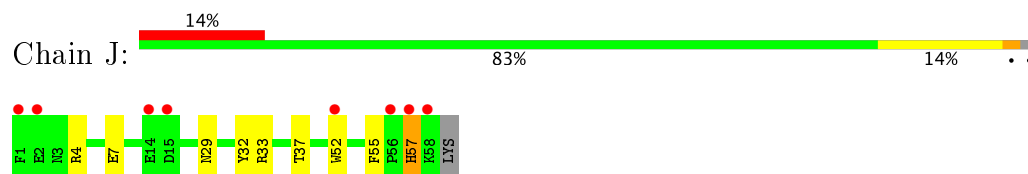
- Molecule 9: Cytochrome c oxidase subunit 6C



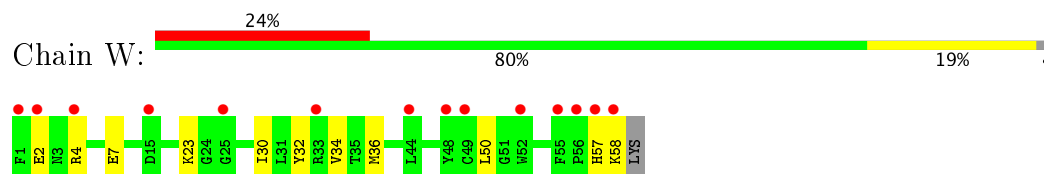
- Molecule 9: Cytochrome c oxidase subunit 6C



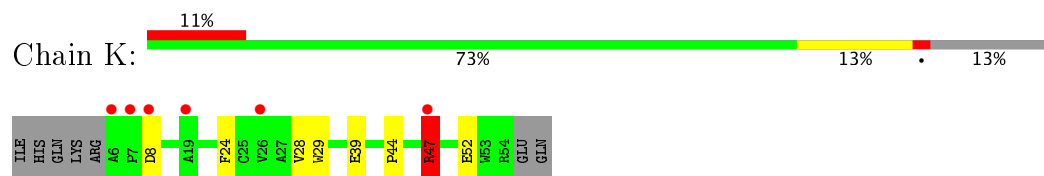
- Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial



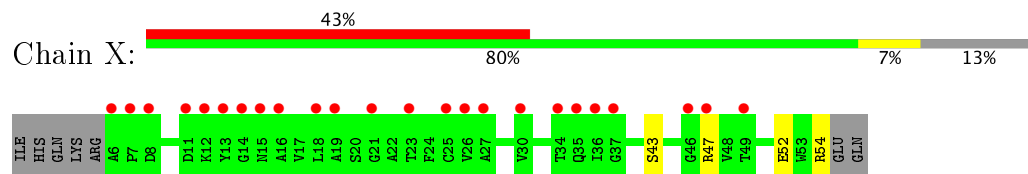
- Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial



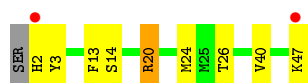
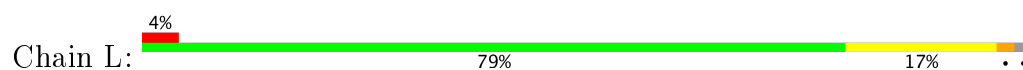
- Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial



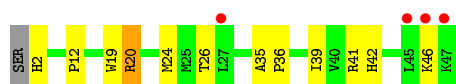
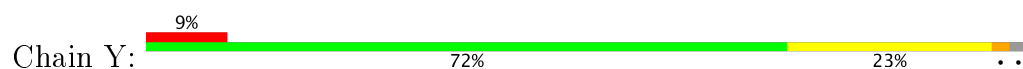
- Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial



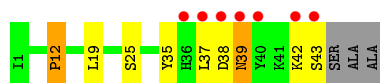
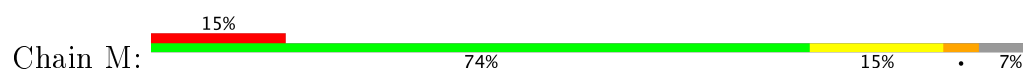
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial



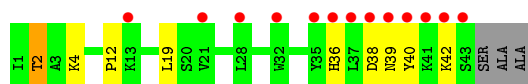
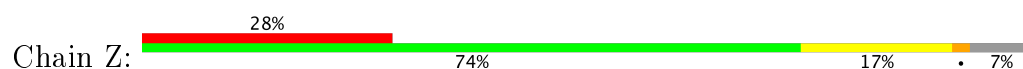
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	182.60Å 204.51Å 178.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 1.90 27.31 – 1.89	Depositor EDS
% Data completeness (in resolution range)	96.0 (40.00-1.90) 95.3 (27.31-1.89)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.49 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.8.0048	Depositor
R, R_{free}	0.195 , 0.230 0.220 , 0.249	Depositor DCC
R_{free} test set	25150 reflections (5.31%)	DCC
Wilson B-factor (Å ²)	24.9	Xtriage
Anisotropy	0.252	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.44 , 77.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.011 for l,-k,h	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	33302	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.91% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.46	22/4203 (0.5%)	1.15	11/5742 (0.2%)
1	N	1.40	17/4203 (0.4%)	1.14	17/5742 (0.3%)
2	B	1.24	4/1868 (0.2%)	1.13	8/2545 (0.3%)
2	O	1.11	2/1860 (0.1%)	1.06	3/2534 (0.1%)
3	C	1.32	3/2221 (0.1%)	0.98	2/3035 (0.1%)
3	P	1.29	7/2221 (0.3%)	1.02	4/3035 (0.1%)
4	D	1.20	2/1229 (0.2%)	1.05	4/1658 (0.2%)
4	Q	0.99	1/1229 (0.1%)	0.90	1/1658 (0.1%)
5	E	1.18	1/871 (0.1%)	1.02	2/1182 (0.2%)
5	R	1.00	0/871	1.07	7/1182 (0.6%)
6	F	1.08	1/765 (0.1%)	1.07	2/1038 (0.2%)
6	S	1.18	1/765 (0.1%)	1.05	0/1038
7	G	1.16	0/690	1.04	5/937 (0.5%)
7	T	1.12	1/690 (0.1%)	1.01	3/937 (0.3%)
8	H	1.14	2/682 (0.3%)	0.95	1/921 (0.1%)
8	U	0.97	0/682	0.95	0/921
9	I	0.94	0/605	1.01	3/802 (0.4%)
9	V	0.87	0/605	0.93	0/802
10	J	0.96	0/471	1.01	1/636 (0.2%)
10	W	0.97	0/471	1.00	0/636
11	K	1.11	1/398 (0.3%)	1.04	1/546 (0.2%)
11	X	0.96	0/398	0.84	0/546
12	L	1.20	0/393	1.20	2/526 (0.4%)
12	Y	1.13	0/393	0.95	1/526 (0.2%)
13	M	1.21	1/345 (0.3%)	1.01	1/470 (0.2%)
13	Z	1.09	0/345	0.90	0/470
All	All	1.24	66/29474 (0.2%)	1.06	79/40065 (0.2%)

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

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	N	0	1
6	F	0	1
6	S	0	1
8	H	0	1
10	J	0	1
10	W	0	1
All	All	0	6

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	T	36	TRP	CB-CG	8.63	1.65	1.50
1	N	242	GLU	CD-OE1	8.41	1.34	1.25
1	A	154	GLY	N-CA	7.80	1.57	1.46
1	N	236	TRP	CE3-CZ3	7.54	1.51	1.38
1	N	260	TYR	CG-CD2	7.26	1.48	1.39

The worst 5 of 79 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	96	ARG	NE-CZ-NH2	-13.88	113.36	120.30
5	R	90	ARG	NE-CZ-NH2	-10.73	114.94	120.30
11	K	47	ARG	NE-CZ-NH1	10.01	125.31	120.30
12	L	20	ARG	NE-CZ-NH2	-9.56	115.52	120.30
4	D	20	ARG	NE-CZ-NH2	9.53	125.06	120.30

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	F	93	PRO	Peptide
8	H	9	LYS	Peptide
10	J	57	HIS	Peptide
1	N	240	HIS	Sidechain
6	S	93	PRO	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	4074	0	4058	53	0
1	N	4074	0	4058	73	0
2	B	1832	0	1836	36	0
2	O	1824	0	1833	51	2
3	C	2134	0	2051	39	0
3	P	2134	0	2051	46	0
4	D	1195	0	1183	15	0
4	Q	1195	0	1183	30	0
5	E	852	0	845	7	0
5	R	852	0	845	10	2
6	F	748	0	728	16	1
6	S	748	0	728	36	7
7	G	675	0	643	29	0
7	T	675	0	643	34	0
8	H	662	0	623	19	0
8	U	662	0	623	11	0
9	I	601	0	613	8	2
9	V	601	0	613	8	0
10	J	460	0	459	8	0
10	W	460	0	459	8	0
11	K	384	0	366	7	0
11	X	384	0	366	4	0
12	L	380	0	380	14	0
12	Y	380	0	380	16	0
13	M	335	0	352	10	0
13	Z	335	0	352	9	0
14	A	120	0	108	10	0
14	N	120	0	108	6	0
15	A	1	0	0	0	0
15	N	1	0	0	0	0
16	A	1	0	0	0	0
16	N	1	0	0	0	0
17	A	1	0	0	0	0
17	C	1	0	0	1	0
17	N	1	0	0	0	0
17	P	1	0	0	0	0
18	A	4	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	N	4	0	0	1	0
19	A	102	0	152	10	0
19	C	102	0	152	5	0
19	N	102	0	152	16	0
19	P	102	0	152	10	0
20	B	63	0	110	3	0
20	D	63	0	110	13	0
20	L	63	0	110	12	0
20	N	63	0	110	4	0
20	Q	63	0	110	11	0
20	Y	63	0	110	16	0
21	B	2	0	0	0	0
21	O	2	0	0	0	0
22	B	29	0	39	1	0
22	C	58	0	78	4	0
22	G	29	0	39	0	0
22	J	29	0	39	5	0
22	P	58	0	78	5	0
22	W	29	0	38	5	0
23	B	52	0	80	13	0
23	N	52	0	80	21	0
24	C	106	0	154	23	0
24	G	53	0	77	6	0
24	P	106	0	154	22	0
24	T	53	0	77	12	0
25	C	100	0	156	23	0
25	G	100	0	156	37	0
25	P	100	0	156	17	0
25	T	100	0	156	29	0
26	F	1	0	0	0	0
26	S	1	0	0	0	0
27	M	33	0	42	1	0
27	Z	33	0	42	0	0
28	A	265	0	0	8	0
28	B	194	0	0	10	2
28	C	141	0	0	8	0
28	D	160	0	0	1	1
28	E	125	0	0	3	0
28	F	112	0	0	2	1
28	G	70	0	0	6	0
28	H	70	0	0	5	0
28	I	52	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	J	31	0	0	2	0
28	K	40	0	0	3	1
28	L	31	0	0	1	0
28	M	31	0	0	1	2
28	N	259	0	0	11	0
28	O	157	0	0	11	6
28	P	143	0	0	8	0
28	Q	90	0	0	5	0
28	R	103	0	0	3	0
28	S	122	0	0	7	1
28	T	56	0	0	2	0
28	U	51	0	0	2	0
28	V	42	0	0	5	0
28	W	38	0	0	2	0
28	X	34	0	0	3	0
28	Y	37	0	0	4	0
28	Z	24	0	0	1	0
All	All	33302	0	31396	691	14

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 691 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)
6:S:76:LYS:CE	6:S:93:PRO:HG2	1.47	1.41
6:S:43:LYS:CD	6:S:43:LYS:H	1.28	1.39
6:S:43:LYS:N	6:S:43:LYS:HD3	1.33	1.29
6:S:76:LYS:HD3	28:S:271:HOH:O	1.36	1.25
18:A:606[A]:PER:O2	18:A:606[A]:PER:O1	1.55	1.22

The worst 5 of 14 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)
28:F:294:HOH:O	28:K:114:HOH:O[2_585]	1.63	0.57
9:I:2:THR:CG2	5:R:80:GLU:OE1[3_647]	1.83	0.37
28:B:586:HOH:O	28:M:2318:HOH:O[2_584]	1.90	0.30
2:O:126:SER:O	6:S:94:HIS:CB[2_684]	1.93	0.27
6:S:95:GLN:N	28:O:535:HOH:O[2_685]	1.95	0.25

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	518/514 (101%)	500 (96%)	18 (4%)	0	100	100
1	N	518/514 (101%)	501 (97%)	17 (3%)	0	100	100
2	B	226/227 (100%)	213 (94%)	13 (6%)	0	100	100
2	O	225/227 (99%)	214 (95%)	10 (4%)	1 (0%)	38	26
3	C	260/261 (100%)	254 (98%)	6 (2%)	0	100	100
3	P	260/261 (100%)	255 (98%)	5 (2%)	0	100	100
4	D	142/147 (97%)	138 (97%)	4 (3%)	0	100	100
4	Q	142/147 (97%)	136 (96%)	5 (4%)	1 (1%)	25	13
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%)	91 (95%)	2 (2%)	3 (3%)	5	1
6	S	96/98 (98%)	90 (94%)	3 (3%)	3 (3%)	5	1
7	G	81/85 (95%)	69 (85%)	7 (9%)	5 (6%)	2	0
7	T	81/85 (95%)	68 (84%)	8 (10%)	5 (6%)	2	0
8	H	77/85 (91%)	71 (92%)	3 (4%)	3 (4%)	3	0
8	U	77/85 (91%)	70 (91%)	4 (5%)	3 (4%)	3	0
9	I	71/73 (97%)	69 (97%)	2 (3%)	0	100	100
9	V	71/73 (97%)	70 (99%)	1 (1%)	0	100	100
10	J	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
10	W	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
11	K	47/56 (84%)	46 (98%)	1 (2%)	0	100	100
11	X	47/56 (84%)	46 (98%)	1 (2%)	0	100	100
12	L	44/47 (94%)	42 (96%)	2 (4%)	0	100	100
12	Y	44/47 (94%)	41 (93%)	3 (7%)	0	100	100
13	M	41/46 (89%)	38 (93%)	3 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	Z	41/46 (89%)	39 (95%)	2 (5%)	0	100	100
All	All	3523/3614 (98%)	3376 (96%)	123 (4%)	24 (1%)	25	13

5 of 24 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	94	HIS
6	F	96	LEU
7	G	4	ALA
7	G	8	HIS
8	H	8	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	432/426 (101%)	426 (99%)	6 (1%)	71	69
1	N	432/426 (101%)	424 (98%)	8 (2%)	62	57
2	B	211/210 (100%)	199 (94%)	12 (6%)	24	13
2	O	210/210 (100%)	202 (96%)	8 (4%)	38	27
3	C	227/226 (100%)	223 (98%)	4 (2%)	64	60
3	P	227/226 (100%)	221 (97%)	6 (3%)	51	43
4	D	128/129 (99%)	127 (99%)	1 (1%)	85	85
4	Q	128/129 (99%)	125 (98%)	3 (2%)	56	49
5	E	92/95 (97%)	89 (97%)	3 (3%)	43	33
5	R	92/95 (97%)	89 (97%)	3 (3%)	43	33
6	F	81/81 (100%)	76 (94%)	5 (6%)	21	10
6	S	81/81 (100%)	78 (96%)	3 (4%)	39	28
7	G	67/68 (98%)	62 (92%)	5 (8%)	16	6
7	T	67/68 (98%)	58 (87%)	9 (13%)	4	1
8	H	71/75 (95%)	66 (93%)	5 (7%)	18	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	U	71/75 (95%)	68 (96%)	3 (4%)	34	23
9	I	57/57 (100%)	56 (98%)	1 (2%)	64	60
9	V	57/57 (100%)	54 (95%)	3 (5%)	26	15
10	J	49/50 (98%)	49 (100%)	0	100	100
10	W	49/50 (98%)	48 (98%)	1 (2%)	60	55
11	K	39/46 (85%)	38 (97%)	1 (3%)	51	43
11	X	39/46 (85%)	39 (100%)	0	100	100
12	L	39/40 (98%)	38 (97%)	1 (3%)	51	43
12	Y	39/40 (98%)	36 (92%)	3 (8%)	15	6
13	M	37/38 (97%)	34 (92%)	3 (8%)	14	5
13	Z	37/38 (97%)	35 (95%)	2 (5%)	26	14
All	All	3059/3082 (99%)	2960 (97%)	99 (3%)	44	34

5 of 99 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	M	12	PRO
2	O	33	LEU
9	V	36	LYS
13	M	39	ASN
1	N	362	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 40 such sidechains are listed below:

Mol	Chain	Res	Type
10	J	29	ASN
1	N	180	GLN
7	T	76	ASN
11	K	35	GLN
2	O	10	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
1	FME	A	1	1	9,9,10	0.57	0	7,9,11	1.41	1 (14%)
2	FME	B	1	2	9,9,10	1.80	2 (22%)	7,9,11	8.03	3 (42%)
7	TPO	G	11	7	9,10,11	1.70	3 (33%)	10,14,16	1.57	2 (20%)
9	SAC	I	1	9	8,8,9	2.42	3 (37%)	6,9,11	1.14	1 (16%)
1	FME	N	1	1	9,9,10	1.09	1 (11%)	7,9,11	1.30	1 (14%)
2	FME	O	1	2	9,9,10	0.93	0	7,9,11	1.88	3 (42%)
7	TPO	T	11	7	9,10,11	1.88	2 (22%)	10,14,16	1.50	1 (10%)
9	SAC	V	1	9	8,8,9	2.17	3 (37%)	6,9,11	1.69	2 (33%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	FME	A	1	1	-	0/6/9/11	0/0/0/0
2	FME	B	1	2	-	1/6/9/11	0/0/0/0
7	TPO	G	11	7	-	1/8/11/13	0/0/0/0
9	SAC	I	1	9	-	0/6/8/10	0/0/0/0
1	FME	N	1	1	-	0/6/9/11	0/0/0/0
2	FME	O	1	2	-	0/6/9/11	0/0/0/0
7	TPO	T	11	7	-	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 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	FME	O1-CN	-3.45	1.12	1.22
2	B	1	FME	CA-C	-2.90	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	1	FME	CA-C	2.11	1.53	1.50
9	V	1	SAC	CA-C	2.16	1.53	1.50
7	G	11	TPO	P-OG1	2.49	1.63	1.59

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	FME	CA-N-CN	-20.41	91.43	122.82
2	B	1	FME	O-C-CA	-3.42	117.18	125.15
2	O	1	FME	CG-CB-CA	-2.86	104.68	112.97
2	O	1	FME	O1-CN-N	-2.76	117.51	125.20
1	N	1	FME	O-C-CA	-2.47	119.39	125.15

There are no chirality outliers.

All (2) torsion outliers are listed below:

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

There are no ring outliers.

5 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1	FME	2	0
2	B	1	FME	2	0
7	G	11	TPO	1	0
2	O	1	FME	9	0
7	T	11	TPO	3	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 56 ligands modelled in this entry, 10 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	601	1	44,67,67	1.50	6 (13%)	37,103,103	2.34	11 (29%)
14	HEA	A	602	1,18	44,67,67	1.89	14 (31%)	37,103,103	1.95	10 (27%)
18	PER	A	606[A]	15,14	0,1,1	0.00	-	0,0,0	0.00	-
18	PER	A	606[B]	15	0,1,1	0.00	-	0,0,0	0.00	-
19	PGV	A	607	-	50,50,50	1.12	4 (8%)	51,56,56	1.32	5 (9%)
19	PGV	A	608	-	50,50,50	1.20	2 (4%)	51,56,56	1.50	6 (11%)
20	TGL	B	301	-	62,62,62	1.29	6 (9%)	65,65,65	1.75	11 (16%)
21	CUA	B	302	2	0,1,1	0.00	-	0,0,0	0.00	-
22	CHD	B	303	-	29,32,32	1.43	4 (13%)	47,51,51	1.90	12 (25%)
23	PSC	B	304	-	51,51,51	1.20	3 (5%)	56,59,59	1.20	4 (7%)
24	PEK	C	302	-	52,52,52	0.99	2 (3%)	54,57,57	1.16	6 (11%)
19	PGV	C	303	-	50,50,50	0.94	2 (4%)	51,56,56	1.43	8 (15%)
25	CDL	C	304	-	99,99,99	1.41	13 (13%)	101,111,111	1.54	12 (11%)
22	CHD	C	305	-	29,32,32	0.67	0	47,51,51	2.19	17 (36%)
22	CHD	C	306	-	29,32,32	1.18	3 (10%)	47,51,51	1.81	12 (25%)
24	PEK	C	307	-	52,52,52	1.09	2 (3%)	54,57,57	1.28	5 (9%)
19	PGV	C	308	-	50,50,50	1.17	3 (6%)	51,56,56	1.27	4 (7%)
20	TGL	D	201	-	62,62,62	1.53	7 (11%)	65,65,65	1.68	13 (20%)
25	CDL	G	101	-	99,99,99	1.35	12 (12%)	101,111,111	1.35	9 (8%)
24	PEK	G	102	-	52,52,52	1.12	2 (3%)	54,57,57	1.33	6 (11%)
22	CHD	G	103	-	29,32,32	1.52	5 (17%)	47,51,51	2.56	17 (36%)
22	CHD	J	101	-	29,32,32	0.65	0	47,51,51	2.70	25 (53%)
20	TGL	L	101	-	62,62,62	1.39	6 (9%)	65,65,65	1.49	8 (12%)
27	DMU	M	101	-	34,34,34	0.69	0	45,45,45	2.50	14 (31%)
14	HEA	N	601	1	44,67,67	1.18	6 (13%)	37,103,103	1.69	8 (21%)
14	HEA	N	602	1,18	44,67,67	1.40	6 (13%)	37,103,103	1.65	8 (21%)
18	PER	N	606[A]	15,14	0,1,1	0.00	-	0,0,0	0.00	-
18	PER	N	606[B]	15	0,1,1	0.00	-	0,0,0	0.00	-
19	PGV	N	607	-	50,50,50	1.01	2 (4%)	51,56,56	1.35	8 (15%)
19	PGV	N	608	-	50,50,50	1.03	2 (4%)	51,56,56	1.55	6 (11%)
20	TGL	N	609	-	62,62,62	1.33	6 (9%)	65,65,65	1.67	9 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	PSC	N	610	-	51,51,51	1.24	3 (5%)	56,59,59	1.32	4 (7%)
21	CUA	O	301	2	0,1,1	0.00	-	0,0,0	0.00	-
19	PGV	P	301	-	50,50,50	1.04	2 (4%)	51,56,56	1.25	5 (9%)
24	PEK	P	303	-	52,52,52	1.08	3 (5%)	54,57,57	1.51	5 (9%)
19	PGV	P	304	-	50,50,50	0.96	2 (4%)	51,56,56	1.06	1 (1%)
25	CDL	P	305	-	99,99,99	1.37	14 (14%)	101,111,111	1.43	11 (10%)
22	CHD	P	306	-	29,32,32	0.85	1 (3%)	47,51,51	2.46	18 (38%)
22	CHD	P	307	-	29,32,32	1.30	3 (10%)	47,51,51	1.37	6 (12%)
24	PEK	P	308	-	52,52,52	1.13	2 (3%)	54,57,57	1.13	4 (7%)
20	TGL	Q	201	-	62,62,62	1.54	7 (11%)	65,65,65	1.35	11 (16%)
24	PEK	T	101	-	52,52,52	1.04	2 (3%)	54,57,57	1.29	4 (7%)
25	CDL	T	102	-	99,99,99	1.33	12 (12%)	101,111,111	1.38	13 (12%)
22	CHD	W	101	-	29,32,32	0.78	0	47,51,51	3.12	18 (38%)
20	TGL	Y	101	-	62,62,62	1.37	6 (9%)	65,65,65	1.60	11 (16%)
27	DMU	Z	101	-	34,34,34	0.76	1 (2%)	45,45,45	1.89	12 (26%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	HEA	A	601	1	2/2/7/16	0/24/76/76	0/0/8/8
14	HEA	A	602	1,18	1/1/7/16	0/24/76/76	0/0/8/8
18	PER	A	606[A]	15,14	-	0/0/0/0	0/0/0/0
18	PER	A	606[B]	15	-	0/0/0/0	0/0/0/0
19	PGV	A	607	-	-	0/55/55/55	0/0/0/0
19	PGV	A	608	-	-	0/55/55/55	0/0/0/0
20	TGL	B	301	-	-	0/65/65/65	0/0/0/0
21	CUA	B	302	2	-	0/0/0/0	0/0/0/0
22	CHD	B	303	-	-	0/7/74/74	0/4/4/4
23	PSC	B	304	-	-	0/55/55/55	0/0/0/0
24	PEK	C	302	-	-	0/56/56/56	0/0/0/0
19	PGV	C	303	-	-	0/55/55/55	0/0/0/0
25	CDL	C	304	-	-	0/110/110/110	0/0/0/0
22	CHD	C	305	-	-	0/7/74/74	0/4/4/4
22	CHD	C	306	-	-	0/7/74/74	0/4/4/4
24	PEK	C	307	-	-	0/56/56/56	0/0/0/0
19	PGV	C	308	-	-	0/55/55/55	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	TGL	D	201	-	-	0/65/65/65	0/0/0/0
25	CDL	G	101	-	-	0/110/110/110	0/0/0/0
24	PEK	G	102	-	-	0/56/56/56	0/0/0/0
22	CHD	G	103	-	-	0/7/74/74	0/4/4/4
22	CHD	J	101	-	-	0/7/74/74	0/4/4/4
20	TGL	L	101	-	-	0/65/65/65	0/0/0/0
27	DMU	M	101	-	2/2/10/10	0/19/59/59	0/2/2/2
14	HEA	N	601	1	3/3/7/16	0/24/76/76	0/0/8/8
14	HEA	N	602	1,18	2/2/7/16	0/24/76/76	0/0/8/8
18	PER	N	606[A]	15,14	-	0/0/0/0	0/0/0/0
18	PER	N	606[B]	15	-	0/0/0/0	0/0/0/0
19	PGV	N	607	-	-	0/55/55/55	0/0/0/0
19	PGV	N	608	-	-	0/55/55/55	0/0/0/0
20	TGL	N	609	-	-	0/65/65/65	0/0/0/0
23	PSC	N	610	-	-	0/55/55/55	0/0/0/0
21	CUA	O	301	2	-	0/0/0/0	0/0/0/0
19	PGV	P	301	-	-	0/55/55/55	0/0/0/0
24	PEK	P	303	-	-	0/56/56/56	0/0/0/0
19	PGV	P	304	-	-	0/55/55/55	0/0/0/0
25	CDL	P	305	-	-	0/110/110/110	0/0/0/0
22	CHD	P	306	-	-	0/7/74/74	0/4/4/4
22	CHD	P	307	-	-	0/7/74/74	0/4/4/4
24	PEK	P	308	-	-	0/56/56/56	0/0/0/0
20	TGL	Q	201	-	-	0/65/65/65	0/0/0/0
24	PEK	T	101	-	-	0/56/56/56	0/0/0/0
25	CDL	T	102	-	-	1/110/110/110	0/0/0/0
22	CHD	W	101	-	-	0/7/74/74	0/4/4/4
20	TGL	Y	101	-	-	0/65/65/65	0/0/0/0
27	DMU	Z	101	-	2/2/10/10	0/19/59/59	0/2/2/2

The worst 5 of 176 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	601	HEA	C1A-NA	-4.97	1.30	1.36
14	N	602	HEA	C1A-NA	-4.55	1.31	1.36
25	T	102	CDL	C42-C41	-3.71	1.30	1.51
22	G	103	CHD	C10-C5	-3.54	1.49	1.55
25	C	304	CDL	C59-C58	-3.42	1.32	1.51

The worst 5 of 377 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	G	103	CHD	C1-C2-C3	-9.86	97.84	110.42
22	C	305	CHD	C23-C22-C20	-8.64	103.09	114.72
22	W	101	CHD	C18-C13-C12	-7.81	101.13	109.08
27	M	101	DMU	O7-C10-C5	-7.31	91.64	108.11
22	W	101	CHD	C17-C13-C14	-7.17	92.79	100.08

5 of 12 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
27	Z	101	DMU	C5
27	Z	101	DMU	C9
14	N	602	HEA	ND
14	N	602	HEA	NB
14	N	601	HEA	ND

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	T	102	CDL	CA4-OA6-CA5-C11

There are no ring outliers.

40 monomers are involved in 319 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	A	601	HEA	7	0
14	A	602	HEA	3	0
18	A	606[A]	PER	1	0
19	A	607	PGV	2	0
19	A	608	PGV	8	0
20	B	301	TGL	3	0
22	B	303	CHD	1	0
23	B	304	PSC	13	0
24	C	302	PEK	6	0
19	C	303	PGV	4	0
25	C	304	CDL	23	0
22	C	305	CHD	3	0
22	C	306	CHD	1	0
24	C	307	PEK	17	0
19	C	308	PGV	1	0
20	D	201	TGL	13	0
25	G	101	CDL	37	0
24	G	102	PEK	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	J	101	CHD	5	0
20	L	101	TGL	12	0
27	M	101	DMU	1	0
14	N	601	HEA	5	0
14	N	602	HEA	1	0
18	N	606[A]	PER	1	0
19	N	607	PGV	10	0
19	N	608	PGV	6	0
20	N	609	TGL	4	0
23	N	610	PSC	21	0
19	P	301	PGV	7	0
24	P	303	PEK	9	0
19	P	304	PGV	3	0
25	P	305	CDL	17	0
22	P	306	CHD	2	0
22	P	307	CHD	3	0
24	P	308	PEK	13	0
20	Q	201	TGL	11	0
24	T	101	PEK	12	0
25	T	102	CDL	29	0
22	W	101	CHD	5	0
20	Y	101	TGL	16	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	513/514 (99%)	0.40	17 (3%) 47 50	12, 15, 22, 51	0
1	N	513/514 (99%)	0.10	9 (1%) 69 72	9, 14, 20, 51	0
2	B	226/227 (99%)	0.31	12 (5%) 27 31	9, 18, 39, 65	0
2	O	226/227 (99%)	0.53	22 (9%) 8 9	11, 17, 41, 62	0
3	C	259/261 (99%)	0.18	7 (2%) 55 59	11, 17, 26, 59	0
3	P	259/261 (99%)	0.13	7 (2%) 55 59	10, 16, 26, 46	0
4	D	144/147 (97%)	0.31	8 (5%) 25 28	12, 18, 35, 57	0
4	Q	144/147 (97%)	1.60	44 (30%) 0 0	13, 23, 48, 106	0
5	E	105/109 (96%)	0.59	13 (12%) 4 5	11, 17, 41, 88	0
5	R	105/109 (96%)	1.08	17 (16%) 2 2	13, 18, 36, 89	0
6	F	98/98 (100%)	0.97	12 (12%) 5 5	15, 23, 68, 118	0
6	S	98/98 (100%)	0.90	14 (14%) 3 3	13, 20, 61, 97	0
7	G	83/85 (97%)	1.23	21 (25%) 1 1	11, 20, 73, 90	0
7	T	83/85 (97%)	1.54	24 (28%) 1 0	10, 20, 77, 101	0
8	H	79/85 (92%)	1.00	12 (15%) 2 3	16, 24, 62, 76	0
8	U	79/85 (92%)	1.34	21 (26%) 1 1	14, 22, 63, 76	0
9	I	72/73 (98%)	1.17	18 (25%) 1 1	15, 26, 53, 63	0
9	V	72/73 (98%)	2.05	31 (43%) 0 0	13, 26, 47, 58	0
10	J	58/59 (98%)	0.76	8 (13%) 3 3	17, 25, 45, 86	0
10	W	58/59 (98%)	1.25	14 (24%) 1 1	13, 22, 51, 91	0
11	K	49/56 (87%)	0.96	6 (12%) 5 5	16, 22, 36, 42	0
11	X	49/56 (87%)	2.16	24 (48%) 0 0	16, 21, 37, 43	0
12	L	46/47 (97%)	0.34	2 (4%) 36 39	15, 19, 37, 64	0
12	Y	46/47 (97%)	0.67	4 (8%) 11 12	12, 19, 38, 71	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	43/46 (93%)	0.72	7 (16%) 2 2	14, 18, 44, 77	0
13	Z	43/46 (93%)	1.57	13 (30%) 1 0	12, 18, 48, 66	0
All	All	3550/3614 (98%)	0.63	387 (10%) 6 7	9, 17, 43, 118	0

The worst 5 of 387 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	Q	5	VAL	16.3
6	S	97	ALA	15.1
6	F	97	ALA	14.9
4	Q	6	VAL	13.6
6	F	98	HIS	12.9

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
1	FME	A	1	10/11	0.94	0.18	-	25,33,52,71	0
9	SAC	I	1	9/10	0.66	0.50	-	43,49,64,67	0
9	SAC	V	1	9/10	0.34	0.70	-	63,69,72,74	0
7	TPO	G	11	11/12	0.60	0.43	-	65,74,106,115	0
2	FME	O	1	10/11	0.97	0.12	-	15,16,24,24	0
2	FME	B	1	10/11	0.96	0.15	-	15,16,24,33	0
1	FME	N	1	10/11	0.93	0.21	-	18,28,48,58	0
7	TPO	T	11	11/12	0.52	0.34	-	52,69,96,97	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
22	CHD	J	101	29/29	0.44	0.37	8.88	56,93,101,102	0
19	PGV	A	608	51/51	0.67	0.27	7.73	24,51,72,84	0
19	PGV	N	607	51/51	0.58	0.29	5.43	27,49,103,114	0
22	CHD	W	101	29/29	0.58	0.39	4.81	52,82,95,101	0
16	MG	N	604	1/1	0.90	0.14	4.51	17,17,17,17	0
18	PER	A	606[A]	2/2	0.99	0.17	4.41	10,10,10,12	0
25	CDL	P	305	100/100	0.70	0.27	4.11	28,60,102,116	0
19	PGV	C	308	51/51	0.68	0.26	4.10	34,64,99,101	0
18	PER	A	606[B]	2/2	0.99	0.17	3.96	11,11,11,11	2
20	TGL	L	101	63/63	0.53	0.30	3.92	28,44,70,80	0
20	TGL	Y	101	63/63	0.47	0.33	3.80	33,49,76,81	0
20	TGL	D	201	63/63	0.71	0.21	3.78	23,45,66,74	0
20	TGL	B	301	63/63	0.75	0.20	3.74	28,51,75,84	0
22	CHD	C	305	29/29	0.77	0.29	3.70	41,47,53,59	0
20	TGL	N	609	63/63	0.74	0.20	3.66	31,54,73,76	0
25	CDL	C	304	100/100	0.74	0.23	3.63	26,59,88,108	0
19	PGV	N	608	51/51	0.95	0.24	3.13	12,30,49,58	0
25	CDL	T	102	100/100	0.56	0.29	2.96	31,67,118,128	0
19	PGV	A	607	51/51	0.95	0.24	2.91	13,26,49,57	0
19	PGV	P	301	51/51	0.65	0.25	2.89	45,70,102,114	0
19	PGV	P	304	51/51	0.93	0.24	2.37	12,27,51,54	0
19	PGV	C	303	51/51	0.94	0.23	2.21	13,22,55,63	0
24	PEK	C	302	53/53	0.93	0.20	2.21	13,33,60,65	0
20	TGL	Q	201	63/63	0.60	0.26	2.19	30,47,66,71	0
24	PEK	P	303	53/53	0.91	0.18	1.90	13,29,70,77	0
27	DMU	Z	101	33/33	0.72	0.27	1.65	18,31,34,39	0
24	PEK	G	102	53/53	0.56	0.30	1.60	37,71,111,121	0
27	DMU	M	101	33/33	0.68	0.22	1.60	25,29,39,40	0
25	CDL	G	101	100/100	0.63	0.24	1.51	34,66,99,138	0
23	PSC	B	304	52/52	0.48	0.36	1.50	36,84,130,137	0
18	PER	N	606[A]	2/2	0.99	0.12	1.38	10,10,10,12	0
24	PEK	T	101	53/53	0.53	0.32	1.36	36,76,114,118	0
14	HEA	N	601	60/60	0.94	0.15	1.28	10,13,32,39	0
18	PER	N	606[B]	2/2	0.99	0.12	1.22	11,11,11,11	2
24	PEK	P	308	53/53	0.50	0.27	0.99	25,55,100,118	0
24	PEK	C	307	53/53	0.56	0.24	0.86	34,59,94,103	0
23	PSC	N	610	52/52	0.71	0.29	0.85	24,61,117,126	0
22	CHD	P	306	29/29	0.82	0.20	0.71	34,44,49,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
14	HEA	N	602	60/60	0.96	0.14	0.64	9,12,18,21	0
14	HEA	A	601	60/60	0.96	0.15	0.49	10,12,37,46	0
14	HEA	A	602	60/60	0.95	0.16	0.47	9,12,18,19	0
16	MG	A	604	1/1	0.97	0.10	-0.16	14,14,14,14	0
22	CHD	G	103	29/29	0.95	0.09	-0.51	8,10,12,16	0
22	CHD	B	303	29/29	0.95	0.09	-0.57	8,10,13,19	0
17	NA	A	605	1/1	0.98	0.09	-0.90	14,14,14,14	0
22	CHD	P	307	29/29	0.94	0.09	-0.97	12,19,23,26	0
22	CHD	C	306	29/29	0.94	0.09	-1.25	17,21,25,29	0
21	CUA	O	301	2/2	0.98	0.05	-2.15	14,14,14,15	0
17	NA	N	605	1/1	0.98	0.04	-2.47	12,12,12,12	0
21	CUA	B	302	2/2	0.99	0.04	-2.99	14,14,14,15	0
26	ZN	F	101	1/1	1.00	0.02	-3.16	19,19,19,19	0
26	ZN	S	101	1/1	0.99	0.04	-3.54	18,18,18,18	0
15	CU	N	603	1/1	1.00	0.07	-	14,14,14,14	0
17	NA	C	301	1/1	0.94	0.25	-	37,37,37,37	0
17	NA	P	302	1/1	0.92	0.11	-	29,29,29,29	0
15	CU	A	603	1/1	1.00	0.09	-	15,15,15,15	0

6.5 Other polymers [i](#)

There are no such residues in this entry.