wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 01:45 AM GMT

PDB ID	:	2DYS
Title	:	Bovine heart cytochrome C oxidase modified by DCCD
Authors	:	Shinzawa-Itoh, K.; Aoyama, H.; Muramoto, K.; Kurauchi, T.; Mizushima, T.; Yamashita, E.; Tsukihara, T.; Yoshikawa, S.
Deposited on	:	2006-09-16
Resolution	:	2.20 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:

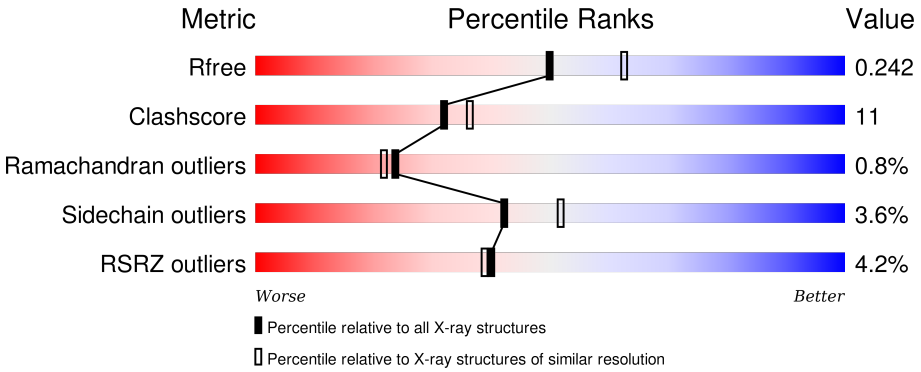
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.20 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	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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	84% 15%
1	N	514	82% 17%
2	B	227	74% 24%
2	O	227	% 67% 29%
3	C	261	82% 16%

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Mol	Chain	Length	Quality of chain
3	P	261	84% 15%
4	D	147	3% 85% 12%
4	Q	147	12% 78% 20%
5	E	109	2% 76% 19%
5	R	109	6% 72% 22%
6	F	98	8% 83% 14%
6	S	98	9% 84% 11%
7	G	85	21% 69% 22% 6%
7	T	85	20% 66% 26% 6%
8	H	85	11% 75% 16% 7%
8	U	85	16% 75% 14% 7%
9	I	73	86% 14%
9	V	73	10% 81% 19%
10	J	59	10% 81% 15%
10	W	59	7% 83% 14%
11	K	56	79% 9% 13%
11	X	56	9% 71% 14% 13%
12	L	47	81% 17%
12	Y	47	4% 79% 19%
13	M	46	7% 61% 30% 7%
13	Z	46	17% 65% 28% 7%

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
15	MG	A	602	-	-	-	X
15	MG	N	602	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
16	NA	A	603	-	-	-	X
16	NA	N	603	-	-	-	X
17	HEA	A	604	X	-	-	-
17	HEA	A	605	X	-	-	-
17	HEA	N	604	X	-	-	-
17	HEA	N	605	X	-	-	-
18	PGV	A	606	-	-	-	X
18	PGV	A	607	-	-	-	X
18	PGV	C	308	-	-	-	X
18	PGV	N	608	-	-	-	X
18	PGV	P	308	-	-	-	X
20	TGL	B	302	-	-	-	X
20	TGL	D	201	-	-	-	X
20	TGL	L	101	-	-	X	X
20	TGL	N	606	-	-	-	X
20	TGL	N	607	-	-	-	X
20	TGL	O	303	-	-	-	X
21	PSC	B	303	-	-	X	X
21	PSC	O	304	-	-	X	X
22	CHD	C	310	X	-	-	-
22	CHD	J	101	X	-	-	X
22	CHD	P	310	X	-	-	X
22	CHD	W	101	X	-	-	X
23	DCW	C	301	-	-	X	-
24	DMU	C	302	X	-	-	X
24	DMU	M	101	X	-	-	-
24	DMU	P	302	X	-	-	X
24	DMU	Z	101	X	-	-	X
26	PEK	G	102	-	-	-	X
26	PEK	T	101	-	-	-	X
27	CDL	C	309	-	-	-	X
27	CDL	G	101	-	-	-	X
27	CDL	P	309	-	-	-	X
27	CDL	T	102	-	-	X	X

2 Entry composition

There are 29 unique types of molecules in this entry. The entry contains 32170 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
			2109	1412	336	349	12			
3	P	259	Total	C	N	O	S	0	0	0
			2109	1412	336	349	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 polypeptide Va.

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 polypeptide Vb.

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 polypeptide VIa-heart.

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 VIb isoform 1.

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 polypeptide VIc.

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

- Molecule 10 is a protein called Cytochrome c oxidase polypeptide VIIa-heart.

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 polypeptide VIIb.

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 polypeptide VIIc.

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 polypeptide VIII-heart.

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

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

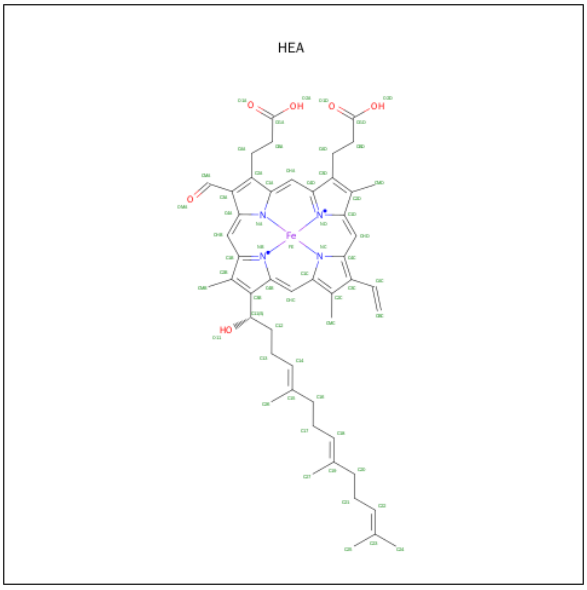
- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 16 is SODIUM ION (three-letter code: NA) (formula: Na).

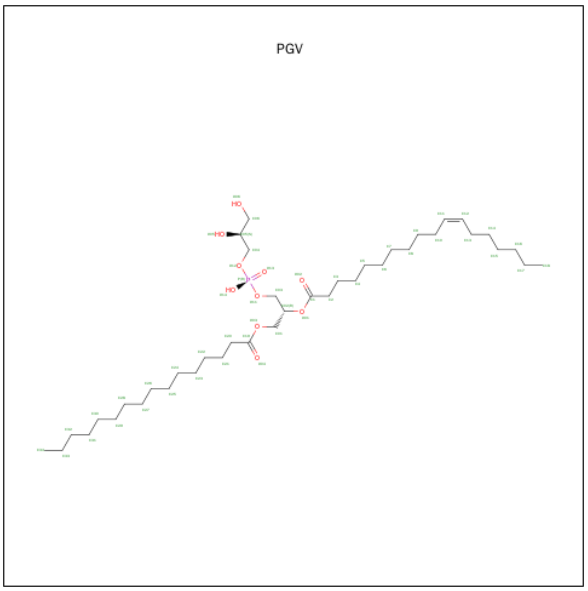
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	A	1	Total Na 1 1	0	0
16	N	1	Total Na 1 1	0	0

- Molecule 17 is HEME-A (three-letter code: HEA) (formula: $C_{49}H_{56}FeN_4O_6$).



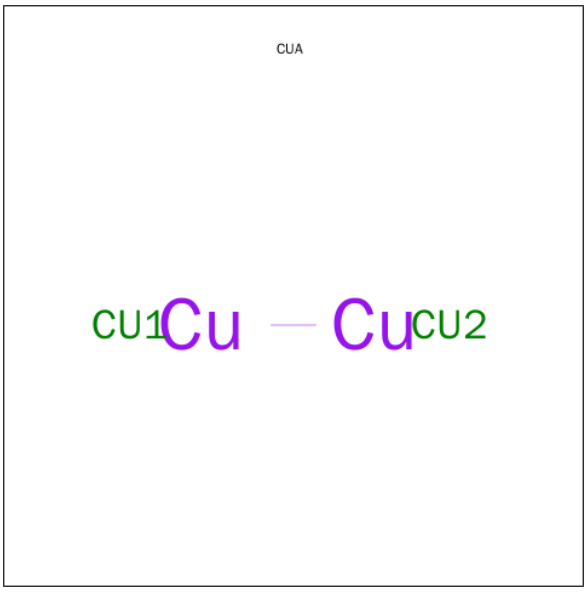
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	A	1	Total C Fe N O 60 49 1 4 6	0	0
17	A	1	Total C Fe N O 60 49 1 4 6	0	0
17	N	1	Total C Fe N O 60 49 1 4 6	0	0
17	N	1	Total C Fe N O 60 49 1 4 6	0	0

- Molecule 18 is (1R)-2-{[{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (three-letter code: PGV) (formula: $C_{40}H_{77}O_{10}P$).



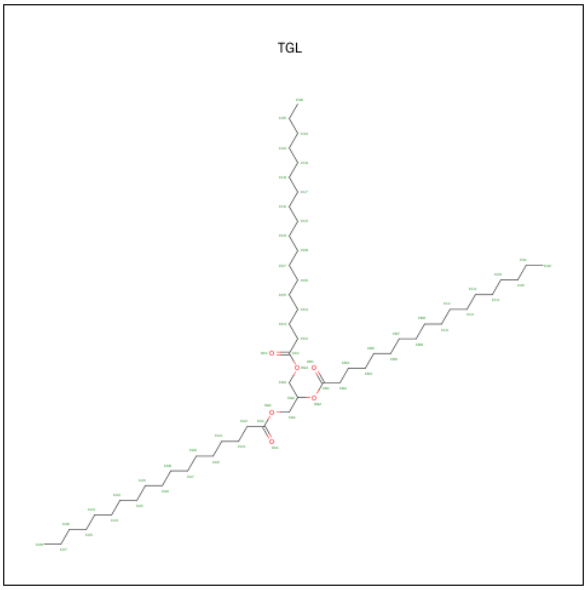
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
18	A	1	Total	C	O	P	0	0
			51	40	10	1		
18	A	1	Total	C	O	P	0	0
			51	40	10	1		
18	C	1	Total	C	O	P	0	0
			51	40	10	1		
18	C	1	Total	C	O	P	0	0
			51	40	10	1		
18	N	1	Total	C	O	P	0	0
			51	40	10	1		
18	N	1	Total	C	O	P	0	0
			51	40	10	1		
18	P	1	Total	C	O	P	0	0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

- Molecule 19 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu_2).



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

- Molecule 20 is TRISTEAROYLGLYCEROL (three-letter code: TGL) (formula: $C_{57}H_{110}O_6$).



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

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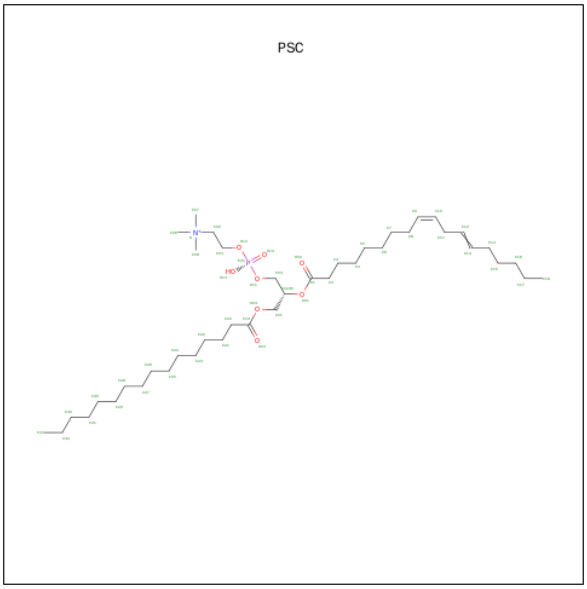
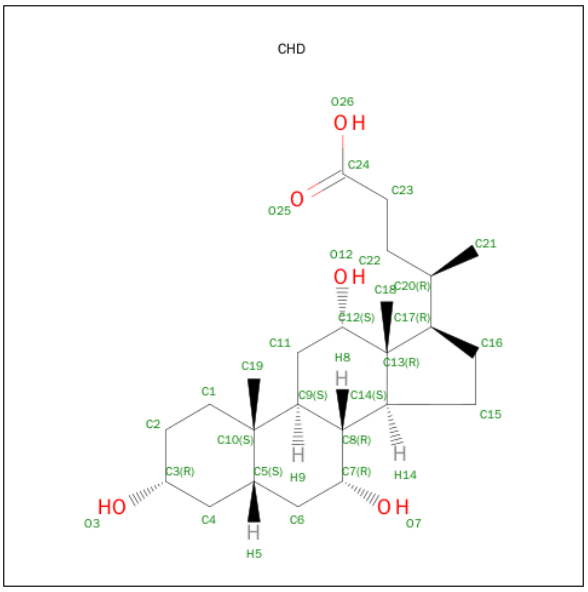
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	L	1	Total C O 63 57 6	0	0
20	N	1	Total C O 63 57 6	0	0
20	N	1	Total C O 63 57 6	0	0
20	O	1	Total C O 63 57 6	0	0

- 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: $C_{42}H_{81}NO_8P$).



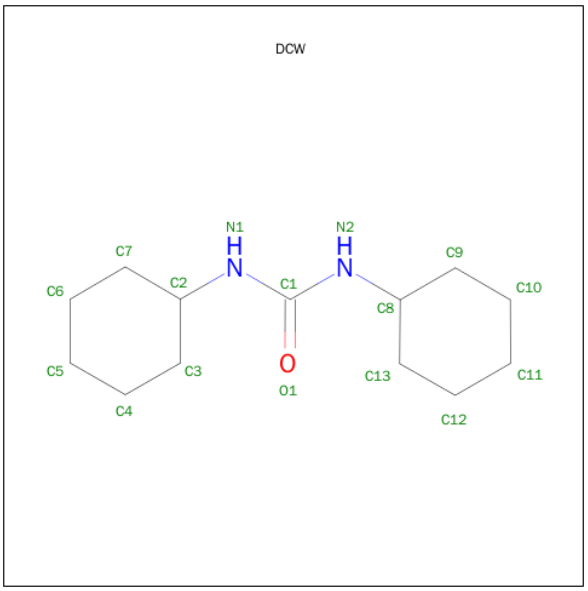
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	B	1	Total C N O P 52 42 1 8 1	0	0
21	O	1	Total C N O P 52 42 1 8 1	0	0

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



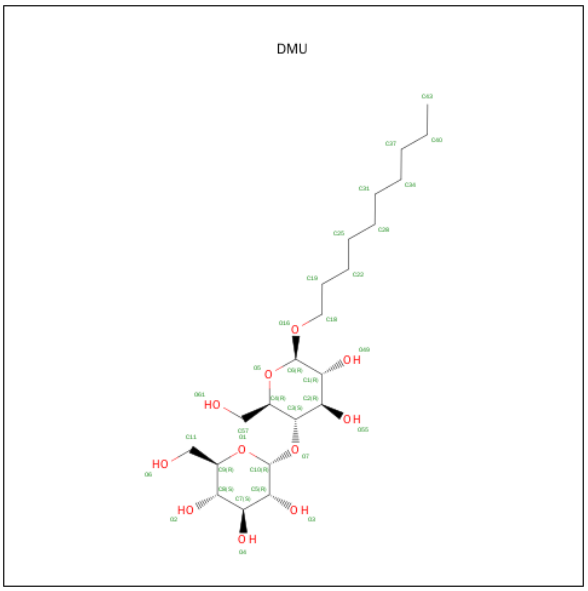
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	B	1	Total C O 29 24 5	0	0
22	C	1	Total C O 29 24 5	0	0
22	C	1	Total C O 29 24 5	0	0
22	J	1	Total C O 29 24 5	0	0
22	O	1	Total C O 29 24 5	0	0
22	P	1	Total C O 29 24 5	0	0
22	P	1	Total C O 29 24 5	0	0
22	W	1	Total C O 29 24 5	0	0

- Molecule 23 is DICYCLOHEXYLUREA (three-letter code: DCW) (formula: $C_{13}H_{24}N_2O$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
23	C	1	Total	C	N	O	0	0
			16	13	2	1		
23	P	1	Total	C	N	O	0	0
			16	13	2	1		

- Molecule 24 is SUGAR (DECYL-BETA-D-MALTOPYRANOSIDE) (three-letter code: DMU) (formula: $C_{22}H_{42}O_{11}$).



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

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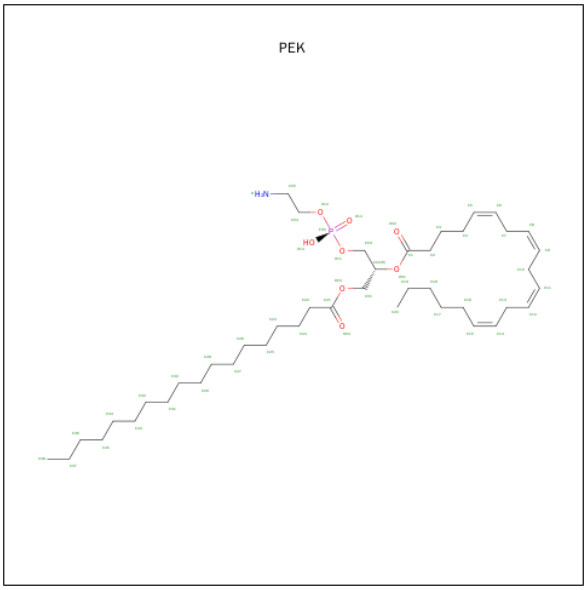
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	M	1	Total C O 33 22 11	0	0
24	P	1	Total C O 33 22 11	0	0
24	Z	1	Total C O 33 22 11	0	0

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

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

- Molecule 26 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
26	C	1	Total C N O P 53 43 1 8 1	0	0
26	C	1	Total C N O P 53 43 1 8 1	0	0
26	G	1	Total C N O P 53 43 1 8 1	0	0

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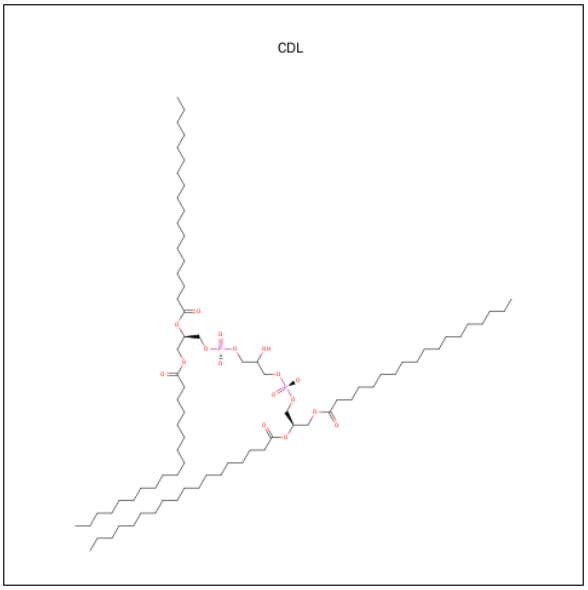
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
26	P	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
26	P	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
26	T	1	Total	C	N	O	P	0	0
			53	43	1	8	1		

- Molecule 27 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



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

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

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

- Molecule 29 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	A	199	Total O 199 199	0	0
29	B	119	Total O 119 119	0	0
29	C	82	Total O 82 82	0	0
29	D	79	Total O 79 79	0	0
29	E	58	Total O 58 58	0	0
29	F	64	Total O 64 64	0	0
29	G	35	Total O 35 35	0	0
29	H	39	Total O 39 39	0	0
29	I	29	Total O 29 29	0	0
29	J	14	Total O 14 14	0	0
29	K	21	Total O 21 21	0	0
29	L	17	Total O 17 17	0	0
29	M	14	Total O 14 14	0	0
29	N	176	Total O 176 176	0	0
29	O	103	Total O 103 103	0	0
29	P	74	Total O 74 74	0	0
29	Q	46	Total O 46 46	0	0
29	R	41	Total O 41 41	0	0
29	S	56	Total O 56 56	0	0
29	T	30	Total O 30 30	0	0
29	U	39	Total O 39 39	0	0

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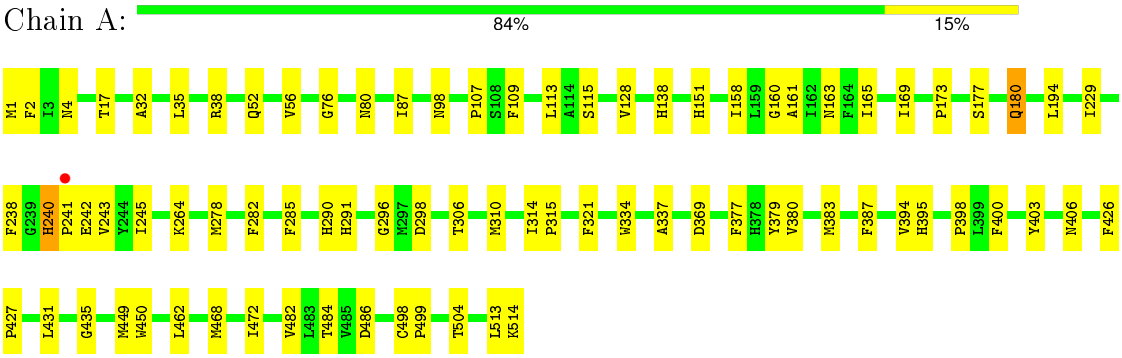
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	V	19	Total O 19 19	0	0
29	W	14	Total O 14 14	0	0
29	X	17	Total O 17 17	0	0
29	Y	13	Total O 13 13	0	0
29	Z	10	Total O 10 10	0	0

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.

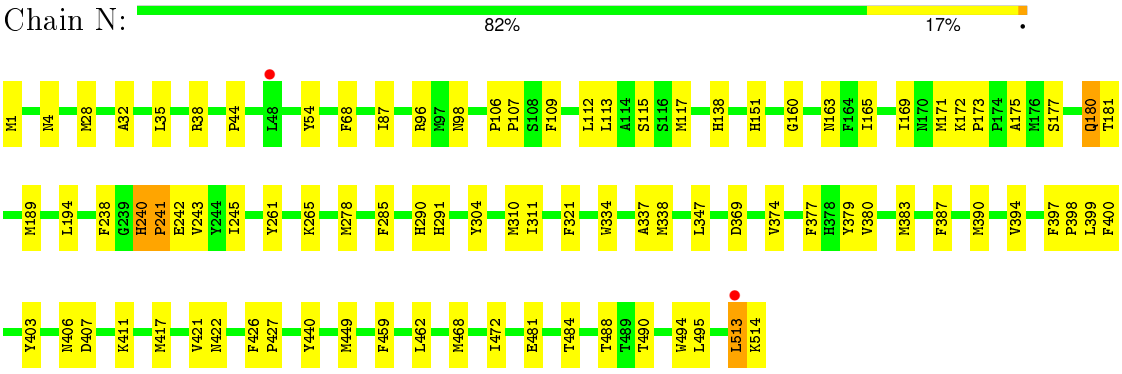
- Molecule 1: Cytochrome c oxidase subunit 1

Chain A:



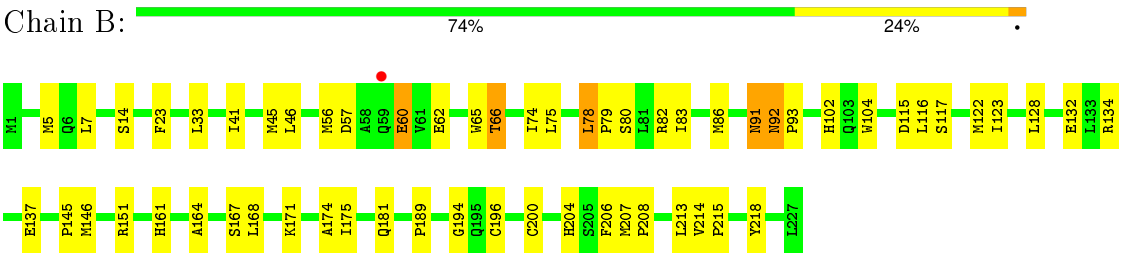
- Molecule 1: Cytochrome c oxidase subunit 1

Chain N:



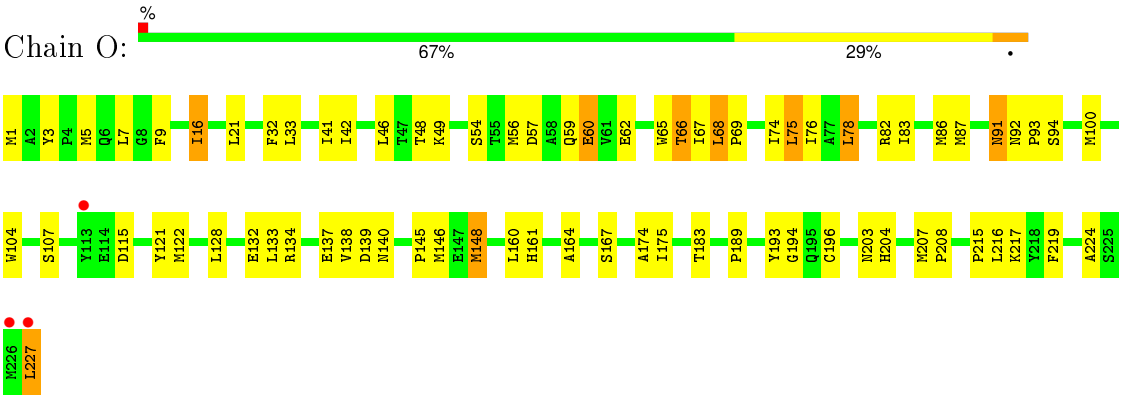
- Molecule 2: Cytochrome c oxidase subunit 2

Chain B:



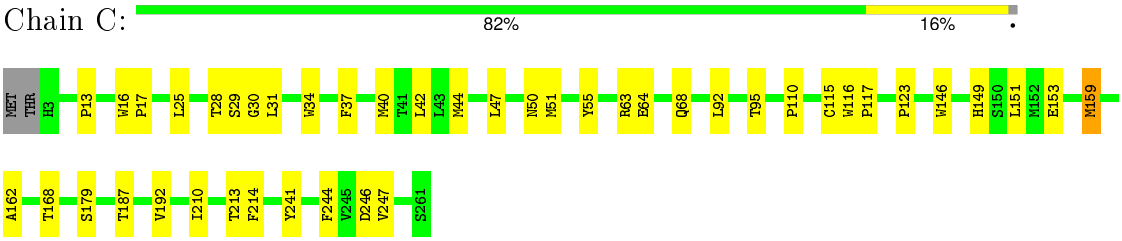
- Molecule 2: Cytochrome c oxidase subunit 2

Chain O:



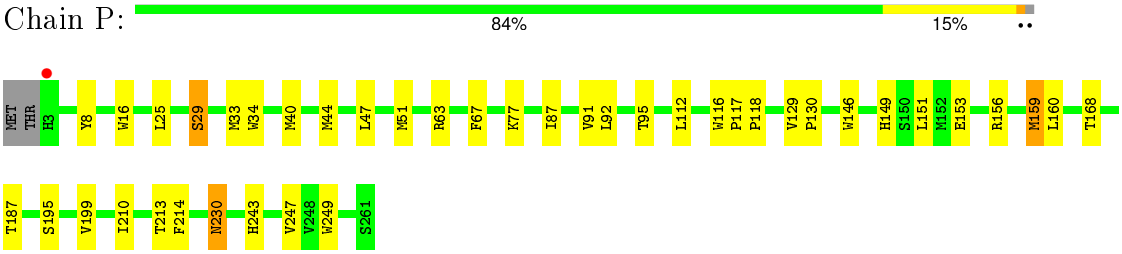
• Molecule 3: Cytochrome c oxidase subunit 3

Chain C:



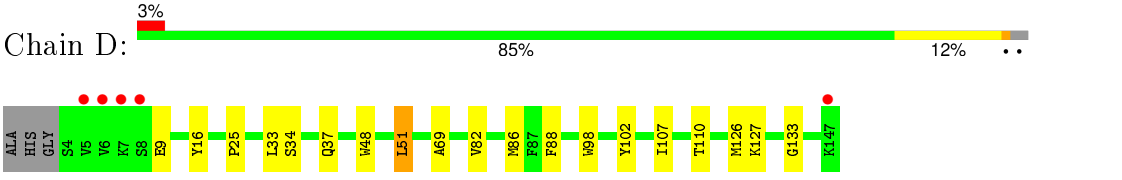
• Molecule 3: Cytochrome c oxidase subunit 3

Chain P:



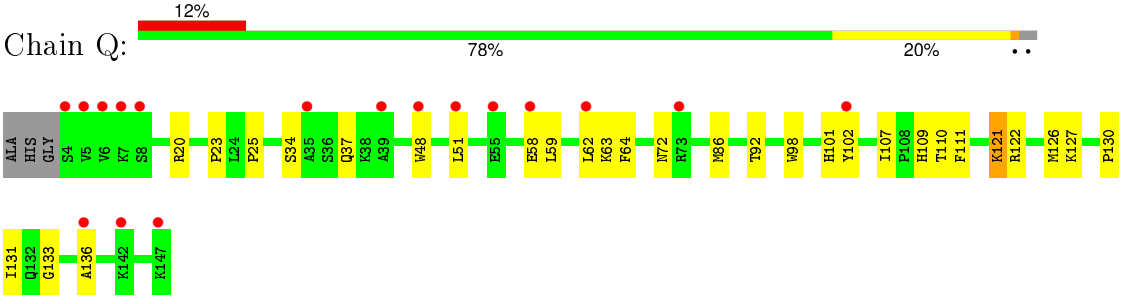
• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1

Chain D:



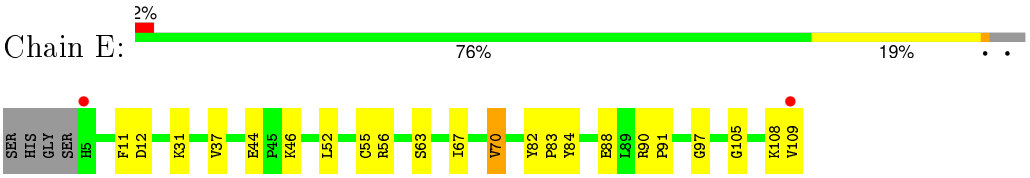
• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1

Chain Q:



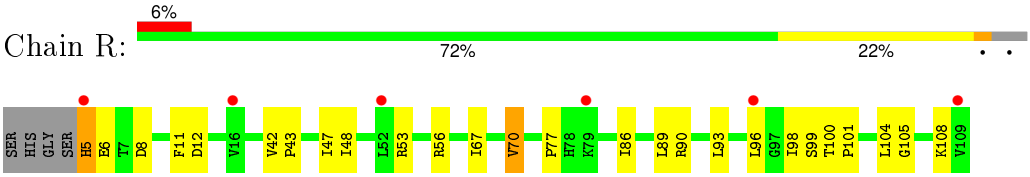
• Molecule 5: Cytochrome c oxidase polypeptide Va

Chain E:



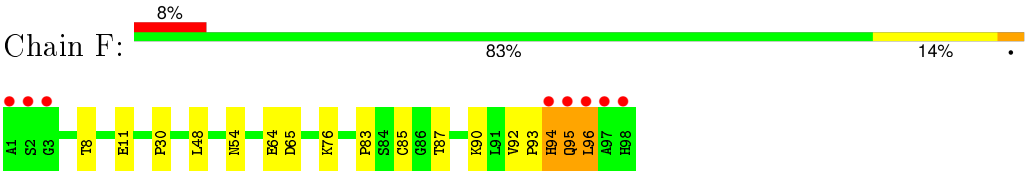
• Molecule 5: Cytochrome c oxidase polypeptide Va

Chain R:



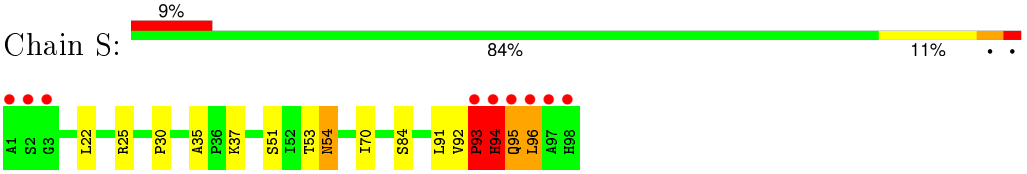
• Molecule 6: Cytochrome c oxidase polypeptide Vb

Chain F:



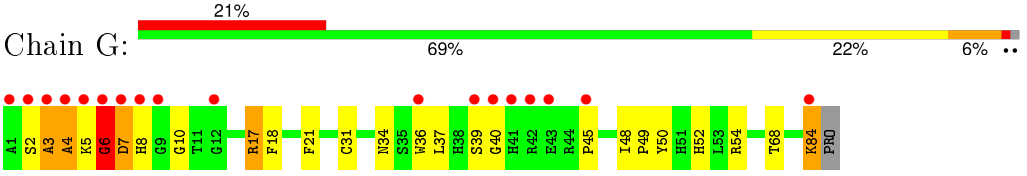
• Molecule 6: Cytochrome c oxidase polypeptide Vb

Chain S:



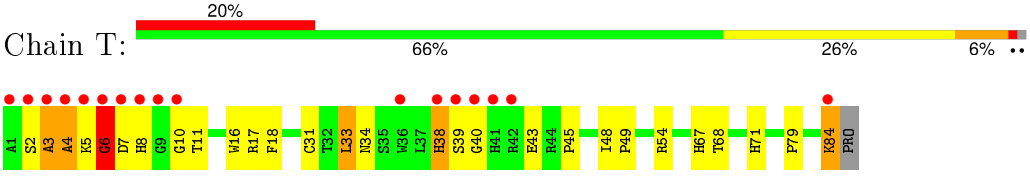
• Molecule 7: Cytochrome c oxidase polypeptide VIa-heart

Chain G:



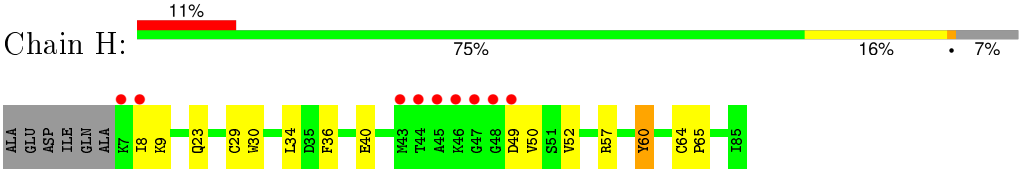
• Molecule 7: Cytochrome c oxidase polypeptide VIa-heart

Chain T:



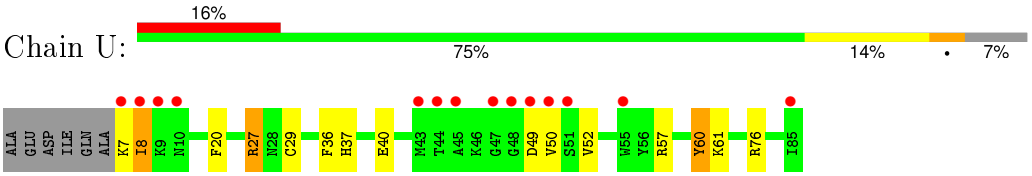
• Molecule 8: Cytochrome c oxidase subunit VIb isoform 1

Chain H:



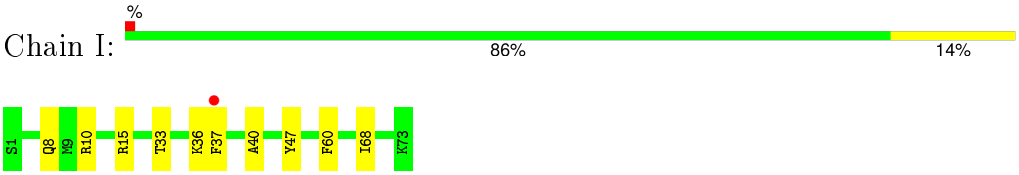
• Molecule 8: Cytochrome c oxidase subunit VIb isoform 1

Chain U:



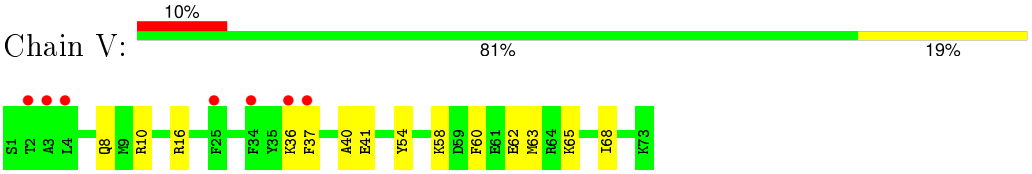
• Molecule 9: Cytochrome c oxidase polypeptide VIc

Chain I:



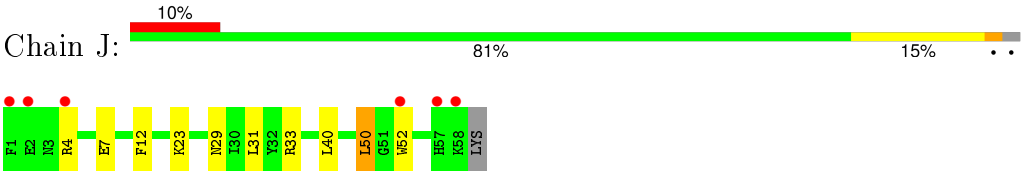
• Molecule 9: Cytochrome c oxidase polypeptide VIc

Chain V:



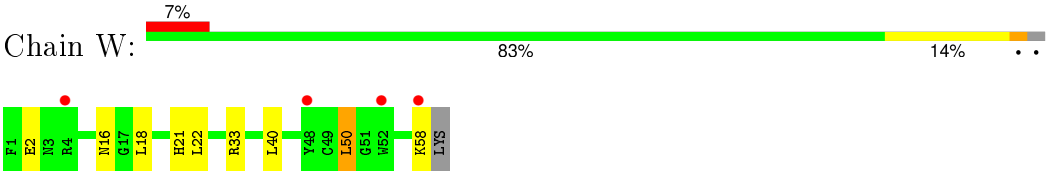
• Molecule 10: Cytochrome c oxidase polypeptide VIIa-heart

Chain J:



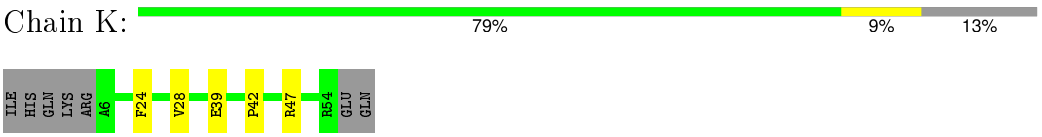
• Molecule 10: Cytochrome c oxidase polypeptide VIIa-heart

Chain W:



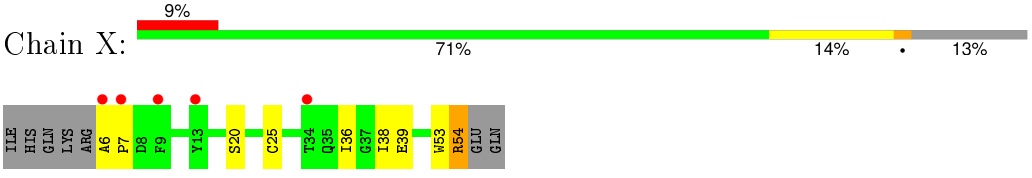
• Molecule 11: Cytochrome c oxidase polypeptide VIIb

Chain K:



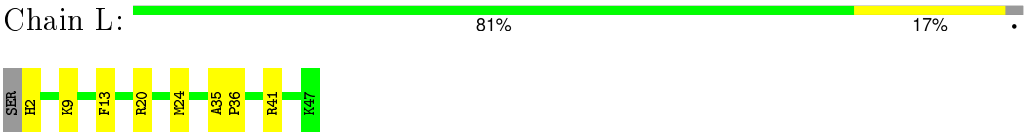
• Molecule 11: Cytochrome c oxidase polypeptide VIIb

Chain X:



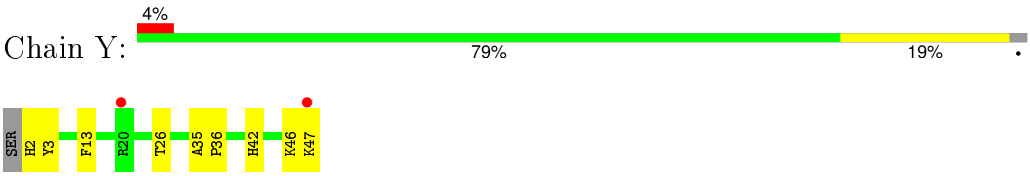
• Molecule 12: Cytochrome c oxidase polypeptide VIIc

Chain L:



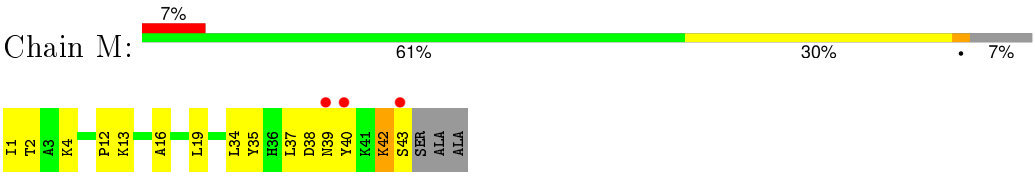
• Molecule 12: Cytochrome c oxidase polypeptide VIIc

Chain Y:



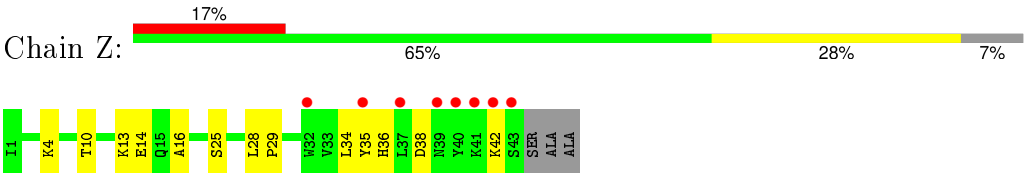
• Molecule 13: Cytochrome c oxidase polypeptide VIII-heart

Chain M:



• Molecule 13: Cytochrome c oxidase polypeptide VIII-heart

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	184.13Å 207.23Å 178.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.20 58.85 – 2.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-2.20) 99.3 (58.85-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.57 (at 2.20Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.197 , 0.242 0.206 , 0.242	Depositor DCC
R_{free} test set	16858 reflections (5.21%)	DCC
Wilson B-factor (Å^2)	33.2	Xtriage
Anisotropy	0.058	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 62.0	EDS
Estimated twinning fraction	0.006 for l,-k,h	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 340546 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	32170	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.63% 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, DCW, 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	0.59	0/4156	0.72	1/5678 (0.0%)
1	N	0.55	0/4156	0.69	0/5678
2	B	0.56	0/1860	0.79	0/2534
2	O	0.55	0/1860	0.80	1/2534 (0.0%)
3	C	0.59	0/2196	0.64	0/3003
3	P	0.56	0/2196	0.64	0/3003
4	D	0.59	0/1229	0.73	2/1658 (0.1%)
4	Q	0.59	0/1229	0.69	1/1658 (0.1%)
5	E	0.53	0/871	0.69	0/1182
5	R	0.54	0/871	0.71	1/1182 (0.1%)
6	F	0.54	0/765	0.84	2/1038 (0.2%)
6	S	0.54	0/765	0.85	2/1038 (0.2%)
7	G	0.61	0/690	0.76	1/937 (0.1%)
7	T	0.60	0/690	0.79	2/937 (0.2%)
8	H	0.53	0/682	0.70	0/921
8	U	0.49	0/682	0.68	0/921
9	I	0.56	0/605	0.65	0/802
9	V	0.57	0/605	0.62	0/802
10	J	0.51	0/471	0.67	0/636
10	W	0.51	0/471	0.72	0/636
11	K	0.56	0/398	0.70	0/546
11	X	0.50	0/398	0.68	0/546
12	L	0.59	0/393	0.61	0/526
12	Y	0.52	0/393	0.64	0/526
13	M	0.55	0/345	0.65	0/470
13	Z	0.53	0/345	0.66	0/470
All	All	0.56	0/29322	0.71	13/39862 (0.0%)

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

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	N	0	2
9	I	0	1
All	All	0	4

There are no bond length outliers.

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	T	33	LEU	CA-CB-CG	6.86	131.08	115.30
6	S	94	HIS	N-CA-C	6.48	128.49	111.00
6	F	94	HIS	N-CA-C	6.21	127.75	111.00
4	D	51	LEU	CA-CB-CG	6.02	129.15	115.30
6	F	93	PRO	N-CA-C	5.85	127.30	112.10

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	240	HIS	Sidechain
9	I	47	TYR	Sidechain
1	N	240	HIS	Sidechain
1	N	304	TYR	Sidechain

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	69	0
1	N	4027	0	4001	72	0
2	B	1824	0	1833	44	0
2	O	1824	0	1833	57	0
3	C	2109	0	2027	40	0
3	P	2109	0	2027	40	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	1195	0	1183	17	0
4	Q	1195	0	1183	25	0
5	E	852	0	845	15	0
5	R	852	0	845	16	0
6	F	748	0	728	9	0
6	S	748	0	728	12	0
7	G	675	0	644	24	0
7	T	675	0	644	28	0
8	H	662	0	623	9	0
8	U	662	0	623	12	0
9	I	601	0	613	6	0
9	V	601	0	613	12	0
10	J	460	0	459	8	0
10	W	460	0	459	8	0
11	K	384	0	366	4	0
11	X	384	0	366	10	0
12	L	380	0	380	13	0
12	Y	380	0	380	9	0
13	M	335	0	352	10	0
13	Z	335	0	352	8	0
14	A	1	0	0	0	0
14	N	1	0	0	0	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	120	0	108	5	0
17	N	120	0	108	6	0
18	A	102	0	152	16	0
18	C	102	0	152	9	0
18	N	102	0	152	13	0
18	P	102	0	152	9	0
19	B	2	0	0	0	0
19	O	2	0	0	0	0
20	B	63	0	110	6	0
20	D	63	0	110	6	0
20	L	63	0	110	23	0
20	N	126	0	220	19	0
20	O	63	0	110	7	0
21	B	52	0	80	23	0
21	O	52	0	80	21	0
22	B	29	0	39	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	C	58	0	77	1	0
22	J	29	0	39	2	0
22	O	29	0	39	0	0
22	P	58	0	78	2	0
22	W	29	0	39	4	0
23	C	16	0	23	9	0
23	P	16	0	23	8	0
24	C	33	0	37	5	0
24	M	33	0	37	1	0
24	P	33	0	37	5	0
24	Z	33	0	37	1	0
25	C	1	0	0	0	0
25	P	1	0	0	0	0
26	C	106	0	154	18	0
26	G	53	0	77	10	0
26	P	106	0	154	17	0
26	T	53	0	77	8	0
27	C	100	0	156	15	0
27	G	100	0	156	15	0
27	P	100	0	156	14	0
27	T	100	0	156	21	0
28	F	1	0	0	0	0
28	S	1	0	0	0	0
29	A	199	0	0	6	0
29	B	119	0	0	2	0
29	C	82	0	0	2	0
29	D	79	0	0	2	0
29	E	58	0	0	3	0
29	F	64	0	0	2	0
29	G	35	0	0	1	0
29	H	39	0	0	1	0
29	I	29	0	0	4	0
29	J	14	0	0	1	0
29	K	21	0	0	0	0
29	L	17	0	0	2	0
29	M	14	0	0	1	0
29	N	176	0	0	3	0
29	O	103	0	0	5	0
29	P	74	0	0	3	0
29	Q	46	0	0	2	0
29	R	41	0	0	1	0
29	S	56	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	T	30	0	0	2	0
29	U	39	0	0	0	0
29	V	19	0	0	0	0
29	W	14	0	0	2	0
29	X	17	0	0	0	0
29	Y	13	0	0	0	0
29	Z	10	0	0	1	0
All	All	32170	0	31343	655	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

The worst 5 of 655 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)
10:W:33:ARG:HG2	22:W:101:CHD:H152	1.31	1.10
21:B:303:PSC:H343	21:B:303:PSC:H142	1.31	1.07
21:O:304:PSC:H142	21:O:304:PSC:H343	1.28	1.06
7:G:84:LYS:HD2	7:G:84:LYS:H	1.22	1.05
12:L:20:ARG:HH12	20:L:101:TGL:HC61	1.15	1.05

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	512/514 (100%)	493 (96%)	19 (4%)	0	100	100
1	N	512/514 (100%)	493 (96%)	19 (4%)	0	100	100
2	B	225/227 (99%)	209 (93%)	14 (6%)	2 (1%)	21	19
2	O	225/227 (99%)	206 (92%)	18 (8%)	1 (0%)	39	42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	257/261 (98%)	251 (98%)	6 (2%)	0	100	100
3	P	257/261 (98%)	251 (98%)	6 (2%)	0	100	100
4	D	142/147 (97%)	140 (99%)	2 (1%)	0	100	100
4	Q	142/147 (97%)	138 (97%)	4 (3%)	0	100	100
5	E	103/109 (94%)	101 (98%)	2 (2%)	0	100	100
5	R	103/109 (94%)	100 (97%)	3 (3%)	0	100	100
6	F	96/98 (98%)	87 (91%)	6 (6%)	3 (3%)	5	2
6	S	96/98 (98%)	87 (91%)	5 (5%)	4 (4%)	3	1
7	G	81/85 (95%)	64 (79%)	9 (11%)	8 (10%)	1	0
7	T	81/85 (95%)	65 (80%)	8 (10%)	8 (10%)	1	0
8	H	77/85 (91%)	70 (91%)	6 (8%)	1 (1%)	15	11
8	U	77/85 (91%)	70 (91%)	6 (8%)	1 (1%)	15	11
9	I	71/73 (97%)	67 (94%)	4 (6%)	0	100	100
9	V	71/73 (97%)	67 (94%)	4 (6%)	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%)	43 (98%)	1 (2%)	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%)	41 (100%)	0	0	100	100
All	All	3504/3614 (97%)	3329 (95%)	147 (4%)	28 (1%)	24	22

5 of 28 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	G	4	ALA
7	G	7	ASP
7	G	8	HIS
7	G	39	SER
6	S	94	HIS

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%)	416 (98%)	10 (2%)	58 71
1	N	426/426 (100%)	414 (97%)	12 (3%)	51 63
2	B	210/210 (100%)	201 (96%)	9 (4%)	35 43
2	O	210/210 (100%)	195 (93%)	15 (7%)	18 19
3	C	224/226 (99%)	217 (97%)	7 (3%)	47 59
3	P	224/226 (99%)	219 (98%)	5 (2%)	60 72
4	D	128/129 (99%)	127 (99%)	1 (1%)	86 93
4	Q	128/129 (99%)	127 (99%)	1 (1%)	86 93
5	E	92/95 (97%)	89 (97%)	3 (3%)	45 56
5	R	92/95 (97%)	88 (96%)	4 (4%)	35 43
6	F	81/81 (100%)	80 (99%)	1 (1%)	78 88
6	S	81/81 (100%)	78 (96%)	3 (4%)	41 50
7	G	67/68 (98%)	62 (92%)	5 (8%)	17 17
7	T	67/68 (98%)	61 (91%)	6 (9%)	12 11
8	H	71/75 (95%)	69 (97%)	2 (3%)	51 63
8	U	71/75 (95%)	68 (96%)	3 (4%)	36 44
9	I	57/57 (100%)	54 (95%)	3 (5%)	28 32
9	V	57/57 (100%)	56 (98%)	1 (2%)	66 79
10	J	49/50 (98%)	47 (96%)	2 (4%)	37 45
10	W	49/50 (98%)	48 (98%)	1 (2%)	63 76
11	K	39/46 (85%)	39 (100%)	0	100 100
11	X	39/46 (85%)	37 (95%)	2 (5%)	29 34
12	L	39/40 (98%)	38 (97%)	1 (3%)	54 66
12	Y	39/40 (98%)	39 (100%)	0	100 100
13	M	37/38 (97%)	29 (78%)	8 (22%)	1 1
13	Z	37/38 (97%)	33 (89%)	4 (11%)	8 7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3040/3082 (99%)	2931 (96%)	109 (4%)	42 52

5 of 109 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	M	39	ASN
1	N	369	ASP
8	U	60	TYR
13	M	42	LYS
1	N	115	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 43 such sidechains are listed below:

Mol	Chain	Res	Type
1	N	151	HIS
2	O	10	GLN
7	T	66	ASN
1	N	178	GLN
1	N	180	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	0.67	0	6,9,11	1.56	1 (16%)
2	FME	B	1	2	8,9,10	0.91	0	6,9,11	1.38	1 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	TPO	G	11	7	8,10,11	1.83	1 (12%)	7,14,16	1.11	1 (14%)
9	SAC	I	1	9	7,8,9	2.48	2 (28%)	7,9,11	2.03	2 (28%)
1	FME	N	1	1	8,9,10	0.74	0	6,9,11	1.29	2 (33%)
2	FME	O	1	2	8,9,10	0.59	0	6,9,11	1.23	1 (16%)
7	TPO	T	11	7	8,10,11	1.33	1 (12%)	7,14,16	1.06	1 (14%)
9	SAC	V	1	9	7,8,9	2.86	2 (28%)	7,9,11	2.13	4 (57%)

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 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	T	11	TPO	CB-CA	2.48	1.58	1.54
9	I	1	SAC	CA-N	3.97	1.52	1.46
7	G	11	TPO	CB-CA	4.33	1.61	1.54
9	I	1	SAC	OAC-C1A	5.01	1.34	1.23
9	V	1	SAC	OAC-C1A	5.08	1.35	1.23

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1	FME	CA-N-CN	-2.97	118.25	122.82
9	I	1	SAC	CA-N-C1A	-2.89	111.56	121.37
9	V	1	SAC	CA-N-C1A	-2.83	111.76	121.37
2	B	1	FME	CA-N-CN	-2.76	118.58	122.82
9	V	1	SAC	OAC-C1A-C2A	-2.54	117.40	122.06

There are no chirality outliers.

All (4) torsion outliers are listed below:

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

There are no ring outliers.

4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1	FME	4	0
1	N	1	FME	1	0
2	O	1	FME	5	0
7	T	11	TPO	1	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
17	HEA	A	604	1	40,67,67	1.14	2 (5%)	41,103,103	1.99	13 (31%)
17	HEA	A	605	1	40,67,67	1.56	8 (20%)	41,103,103	1.46	6 (14%)
18	PGV	A	606	-	50,50,50	1.17	3 (6%)	51,56,56	1.05	4 (7%)
18	PGV	A	607	-	50,50,50	1.01	3 (6%)	51,56,56	1.11	2 (3%)
19	CUA	B	301	2	0,1,1	0.00	-	0,0,0	0.00	-
20	TGL	B	302	-	62,62,62	0.77	2 (3%)	65,65,65	1.67	12 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
21	PSC	B	303	-	51,51,51	1.32	6 (11%)	55,59,59	1.13	1 (1%)
22	CHD	B	304	-	29,32,32	0.85	1 (3%)	48,51,51	1.89	12 (25%)
23	DCW	C	301	3	17,17,17	1.31	2 (11%)	21,21,21	1.00	0
24	DMU	C	302	-	34,34,34	2.70	14 (41%)	45,45,45	4.27	18 (40%)
22	CHD	C	304	-	29,32,32	0.89	2 (6%)	48,51,51	1.96	12 (25%)
26	PEK	C	305	-	51,52,52	1.44	5 (9%)	52,57,57	1.10	3 (5%)
26	PEK	C	306	-	51,52,52	1.68	9 (17%)	52,57,57	1.13	4 (7%)
18	PGV	C	307	-	50,50,50	0.98	3 (6%)	51,56,56	1.02	5 (9%)
18	PGV	C	308	-	50,50,50	1.42	5 (10%)	51,56,56	0.84	2 (3%)
27	CDL	C	309	-	99,99,99	0.88	3 (3%)	101,111,111	0.94	5 (4%)
22	CHD	C	310	-	29,32,32	0.97	1 (3%)	48,51,51	3.52	26 (54%)
20	TGL	D	201	-	62,62,62	0.96	4 (6%)	65,65,65	1.49	11 (16%)
27	CDL	G	101	-	99,99,99	1.15	8 (8%)	101,111,111	0.96	8 (7%)
26	PEK	G	102	-	51,52,52	1.93	12 (23%)	52,57,57	1.21	4 (7%)
22	CHD	J	101	-	29,32,32	0.94	2 (6%)	48,51,51	3.72	25 (52%)
20	TGL	L	101	-	62,62,62	1.28	6 (9%)	65,65,65	1.78	12 (18%)
24	DMU	M	101	-	34,34,34	3.13	8 (23%)	45,45,45	4.27	19 (42%)
17	HEA	N	604	1	40,67,67	1.41	7 (17%)	41,103,103	1.97	12 (29%)
17	HEA	N	605	1	40,67,67	1.52	8 (20%)	41,103,103	1.54	8 (19%)
20	TGL	N	606	-	62,62,62	1.40	6 (9%)	65,65,65	1.75	13 (20%)
20	TGL	N	607	-	62,62,62	0.86	2 (3%)	65,65,65	1.46	10 (15%)
18	PGV	N	608	-	50,50,50	1.21	4 (8%)	51,56,56	1.03	3 (5%)
18	PGV	N	609	-	50,50,50	1.13	5 (10%)	51,56,56	1.17	3 (5%)
19	CUA	O	301	2	0,1,1	0.00	-	0,0,0	0.00	-
22	CHD	O	302	-	29,32,32	0.68	0	48,51,51	1.88	14 (29%)
20	TGL	O	303	-	62,62,62	0.85	2 (3%)	65,65,65	1.62	9 (13%)
21	PSC	O	304	-	51,51,51	1.29	4 (7%)	55,59,59	1.14	3 (5%)
23	DCW	P	301	3	17,17,17	1.58	2 (11%)	21,21,21	0.88	0
24	DMU	P	302	-	34,34,34	2.58	13 (38%)	45,45,45	4.37	18 (40%)
22	CHD	P	304	-	29,32,32	0.69	1 (3%)	48,51,51	1.86	12 (25%)
26	PEK	P	305	-	51,52,52	1.54	7 (13%)	52,57,57	1.19	7 (13%)
26	PEK	P	306	-	51,52,52	1.65	8 (15%)	52,57,57	1.14	4 (7%)
18	PGV	P	307	-	50,50,50	0.95	3 (6%)	51,56,56	0.89	2 (3%)
18	PGV	P	308	-	50,50,50	1.41	5 (10%)	51,56,56	0.88	3 (5%)
27	CDL	P	309	-	99,99,99	0.93	5 (5%)	101,111,111	0.95	4 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	CHD	P	310	-	29,32,32	0.87	1 (3%)	48,51,51	3.59	26 (54%)
26	PEK	T	101	-	51,52,52	2.07	12 (23%)	52,57,57	1.20	3 (5%)
27	CDL	T	102	-	99,99,99	1.14	10 (10%)	101,111,111	0.99	9 (8%)
22	CHD	W	101	-	29,32,32	1.08	2 (6%)	48,51,51	3.77	25 (52%)
24	DMU	Z	101	-	34,34,34	3.02	10 (29%)	45,45,45	4.19	19 (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
17	HEA	A	604	1	3/3/7/16	0/24/76/76	0/0/8/8
17	HEA	A	605	1	3/3/7/16	0/24/76/76	0/0/8/8
18	PGV	A	606	-	-	1/55/55/55	0/0/0/0
18	PGV	A	607	-	-	0/55/55/55	0/0/0/0
19	CUA	B	301	2	-	0/0/0/0	0/0/0/0
20	TGL	B	302	-	-	0/65/65/65	0/0/0/0
21	PSC	B	303	-	-	0/55/55/55	0/0/0/0
22	CHD	B	304	-	-	0/7/74/74	0/4/4/4
23	DCW	C	301	3	-	0/8/24/24	0/2/2/2
24	DMU	C	302	-	6/6/10/10	0/19/59/59	0/2/2/2
22	CHD	C	304	-	-	0/7/74/74	0/4/4/4
26	PEK	C	305	-	-	0/56/56/56	0/0/0/0
26	PEK	C	306	-	-	0/56/56/56	0/0/0/0
18	PGV	C	307	-	-	0/55/55/55	0/0/0/0
18	PGV	C	308	-	-	0/55/55/55	0/0/0/0
27	CDL	C	309	-	-	0/110/110/110	0/0/0/0
22	CHD	C	310	-	5/5/12/12	0/7/74/74	0/4/4/4
20	TGL	D	201	-	-	0/65/65/65	0/0/0/0
27	CDL	G	101	-	-	0/110/110/110	0/0/0/0
26	PEK	G	102	-	-	0/56/56/56	0/0/0/0
22	CHD	J	101	-	5/5/12/12	0/7/74/74	0/4/4/4
20	TGL	L	101	-	-	0/65/65/65	0/0/0/0
24	DMU	M	101	-	5/5/10/10	0/19/59/59	0/2/2/2
17	HEA	N	604	1	3/3/7/16	0/24/76/76	0/0/8/8
17	HEA	N	605	1	3/3/7/16	0/24/76/76	0/0/8/8
20	TGL	N	606	-	-	0/65/65/65	0/0/0/0
20	TGL	N	607	-	-	0/65/65/65	0/0/0/0
18	PGV	N	608	-	-	1/55/55/55	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	PGV	N	609	-	-	0/55/55/55	0/0/0/0
19	CUA	O	301	2	-	0/0/0/0	0/0/0/0
22	CHD	O	302	-	-	0/7/74/74	0/4/4/4
20	TGL	O	303	-	-	0/65/65/65	0/0/0/0
21	PSC	O	304	-	-	0/55/55/55	0/0/0/0
23	DCW	P	301	3	-	0/8/24/24	0/2/2/2
24	DMU	P	302	-	6/6/10/10	0/19/59/59	0/2/2/2
22	CHD	P	304	-	-	0/7/74/74	0/4/4/4
26	PEK	P	305	-	-	0/56/56/56	0/0/0/0
26	PEK	P	306	-	-	0/56/56/56	0/0/0/0
18	PGV	P	307	-	-	0/55/55/55	0/0/0/0
18	PGV	P	308	-	-	0/55/55/55	0/0/0/0
27	CDL	P	309	-	-	0/110/110/110	0/0/0/0
22	CHD	P	310	-	5/5/12/12	0/7/74/74	0/4/4/4
26	PEK	T	101	-	-	0/56/56/56	0/0/0/0
27	CDL	T	102	-	-	0/110/110/110	0/0/0/0
22	CHD	W	101	-	5/5/12/12	0/7/74/74	0/4/4/4
24	DMU	Z	101	-	5/5/10/10	0/19/59/59	0/2/2/2

The worst 5 of 226 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	M	101	DMU	O7-C3	-7.71	1.24	1.43
24	Z	101	DMU	O7-C3	-7.22	1.25	1.43
24	M	101	DMU	O16-C6	-6.70	1.28	1.40
24	M	101	DMU	O1-C9	-6.56	1.27	1.44
24	Z	101	DMU	O16-C18	-6.48	1.24	1.42

The worst 5 of 411 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	P	310	CHD	C17-C13-C12	-10.11	108.72	117.68
22	C	310	CHD	C17-C13-C12	-9.52	109.24	117.68
24	M	101	DMU	C8-C7-C5	-7.63	96.55	110.79
24	Z	101	DMU	C8-C7-C5	-7.45	96.89	110.79
22	P	310	CHD	C19-C10-C9	-6.37	101.63	111.18

5 of 54 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
24	C	302	DMU	C5

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Mol	Chain	Res	Type	Atom
24	C	302	DMU	C6
24	C	302	DMU	C9
24	C	302	DMU	C4
24	C	302	DMU	C2

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	A	606	PGV	P-O11-C03-C02
18	N	608	PGV	P-O11-C03-C02

There are no ring outliers.

41 monomers are involved in 284 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	A	604	HEA	2	0
17	A	605	HEA	3	0
18	A	606	PGV	8	0
18	A	607	PGV	8	0
20	B	302	TGL	6	0
21	B	303	PSC	23	0
22	B	304	CHD	1	0
23	C	301	DCW	9	0
24	C	302	DMU	5	0
26	C	305	PEK	11	0
26	C	306	PEK	7	0
18	C	307	PGV	8	0
18	C	308	PGV	1	0
27	C	309	CDL	15	0
22	C	310	CHD	1	0
20	D	201	TGL	6	0
27	G	101	CDL	15	0
26	G	102	PEK	10	0
22	J	101	CHD	2	0
20	L	101	TGL	23	0
24	M	101	DMU	1	0
17	N	604	HEA	4	0
17	N	605	HEA	2	0
20	N	606	TGL	14	0
20	N	607	TGL	5	0
18	N	608	PGV	7	0
18	N	609	PGV	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	O	303	TGL	7	0
21	O	304	PSC	21	0
23	P	301	DCW	8	0
24	P	302	DMU	5	0
26	P	305	PEK	11	0
26	P	306	PEK	6	0
18	P	307	PGV	8	0
18	P	308	PGV	1	0
27	P	309	CDL	14	0
22	P	310	CHD	2	0
26	T	101	PEK	8	0
27	T	102	CDL	21	0
22	W	101	CHD	4	0
24	Z	101	DMU	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	-0.09	1 (0%) 95 95	16, 25, 36, 67	0
1	N	513/514 (99%)	-0.17	2 (0%) 93 93	20, 32, 45, 70	0
2	B	226/227 (99%)	-0.52	1 (0%) 93 93	16, 31, 65, 95	0
2	O	226/227 (99%)	-0.43	3 (1%) 79 78	27, 41, 71, 96	0
3	C	259/261 (99%)	-0.54	0 100 100	20, 30, 50, 83	0
3	P	259/261 (99%)	-0.55	1 (0%) 93 93	23, 33, 56, 89	0
4	D	144/147 (97%)	-0.41	5 (3%) 48 46	24, 36, 63, 90	0
4	Q	144/147 (97%)	0.80	17 (11%) 6 6	35, 53, 78, 108	0
5	E	105/109 (96%)	-0.10	2 (1%) 70 68	26, 36, 68, 109	0
5	R	105/109 (96%)	0.39	6 (5%) 27 27	32, 45, 70, 111	0
6	F	98/98 (100%)	0.22	8 (8%) 14 14	22, 37, 100, 118	0
6	S	98/98 (100%)	0.49	9 (9%) 11 10	26, 43, 103, 115	0
7	G	83/85 (97%)	0.72	18 (21%) 1 1	23, 39, 103, 112	0
7	T	83/85 (97%)	0.78	17 (20%) 1 1	26, 45, 103, 113	0
8	H	79/85 (92%)	0.17	9 (11%) 7 6	25, 41, 99, 105	0
8	U	79/85 (92%)	0.68	14 (17%) 2 2	32, 48, 99, 109	0
9	I	72/73 (98%)	0.16	1 (1%) 78 77	27, 45, 74, 83	0
9	V	72/73 (98%)	0.50	7 (9%) 10 9	34, 56, 80, 97	0
10	J	58/59 (98%)	0.15	6 (10%) 9 8	27, 41, 79, 106	0
10	W	58/59 (98%)	0.41	4 (6%) 20 19	34, 49, 87, 110	0
11	K	49/56 (87%)	-0.29	0 100 100	29, 41, 57, 74	0
11	X	49/56 (87%)	0.68	5 (10%) 9 8	44, 56, 74, 88	0
12	L	46/47 (97%)	-0.44	0 100 100	21, 32, 55, 92	0
12	Y	46/47 (97%)	-0.29	2 (4%) 39 38	34, 43, 69, 98	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	M	43/46 (93%)	-0.14	3 (6%) 19 19	23, 32, 97, 108	0
13	Z	43/46 (93%)	0.34	8 (18%) 2 1	39, 47, 101, 112	0
All	All	3550/3614 (98%)	-0.06	149 (4%) 40 39	16, 35, 74, 118	0

The worst 5 of 149 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	Q	5	VAL	18.6
4	Q	6	VAL	15.5
6	S	97	ALA	15.1
6	S	96	LEU	15.1
4	Q	8	SER	11.2

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	0.95	0.14	-	40,42,47,54	0
7	TPO	G	11	11/12	0.55	0.32	-	89,96,117,119	0
2	FME	B	1	10/11	0.95	0.13	-	25,33,44,53	0
9	SAC	V	1	9/10	0.49	0.64	-	101,107,109,110	0
1	FME	N	1	10/11	0.92	0.21	-	57,61,85,85	0
7	TPO	T	11	11/12	0.49	0.29	-	87,93,112,113	0
9	SAC	I	1	9/10	0.80	0.27	-	89,93,96,97	0
1	FME	A	1	10/11	0.87	0.14	-	50,60,76,86	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
24	DMU	C	302	33/33	0.65	0.41	16.74	88,116,120,120	0
22	CHD	W	101	29/29	0.75	0.34	13.35	89,100,103,108	0
22	CHD	J	101	29/29	0.81	0.37	7.84	91,99,104,107	0
18	PGV	A	606	51/51	0.75	0.30	7.76	32,75,113,120	0
16	NA	A	603	1/1	0.78	0.20	7.50	44,44,44,44	0
24	DMU	P	302	33/33	0.64	0.41	7.32	91,116,120,120	0
20	TGL	D	201	63/63	0.74	0.25	6.46	45,70,82,87	0
27	CDL	P	309	100/100	0.74	0.39	6.00	37,90,108,118	0
20	TGL	O	303	63/63	0.76	0.26	5.61	46,70,91,96	0
27	CDL	C	309	100/100	0.75	0.36	5.60	43,92,103,109	0
20	TGL	L	101	63/63	0.76	0.29	5.09	36,67,81,84	0
18	PGV	N	608	51/51	0.79	0.36	5.00	38,80,114,119	0
20	TGL	N	606	63/63	0.68	0.34	4.88	39,68,86,88	0
15	MG	N	602	1/1	0.94	0.16	4.51	35,35,35,35	0
20	TGL	B	302	63/63	0.82	0.22	4.21	41,67,89,94	0
16	NA	N	603	1/1	0.81	0.19	3.74	50,50,50,50	0
18	PGV	C	308	51/51	0.69	0.39	3.74	61,87,113,116	0
24	DMU	Z	101	33/33	0.82	0.33	3.36	50,72,86,92	0
15	MG	A	602	1/1	0.95	0.17	2.88	23,23,23,23	0
20	TGL	N	607	63/63	0.73	0.22	2.79	48,69,85,92	0
27	CDL	T	102	100/100	0.62	0.35	2.74	47,86,112,120	0
27	CDL	G	101	100/100	0.64	0.34	2.73	55,88,111,120	0
21	PSC	B	303	52/52	0.57	0.36	2.52	47,90,120,120	0
21	PSC	O	304	52/52	0.64	0.39	2.43	48,88,120,120	0
18	PGV	P	308	51/51	0.68	0.39	2.43	66,90,112,116	0
22	CHD	P	310	29/29	0.85	0.24	2.42	78,91,94,99	0
18	PGV	A	607	51/51	0.97	0.15	2.07	22,41,66,76	0
18	PGV	N	609	51/51	0.97	0.14	1.95	25,43,64,77	0
24	DMU	M	101	33/33	0.85	0.20	1.93	45,63,80,87	0
26	PEK	P	306	53/53	0.66	0.35	1.80	40,89,110,114	0
18	PGV	P	307	51/51	0.96	0.13	1.79	23,36,68,73	0
26	PEK	T	101	53/53	0.46	0.46	1.71	50,90,115,120	0
26	PEK	G	102	53/53	0.54	0.41	1.60	50,89,115,120	0
18	PGV	C	307	51/51	0.96	0.12	1.40	22,33,65,72	0
22	CHD	C	310	29/29	0.84	0.26	1.35	75,92,97,101	0
26	PEK	C	306	53/53	0.56	0.30	1.16	46,91,115,120	0
26	PEK	P	305	53/53	0.94	0.14	0.88	24,46,73,77	0
17	HEA	N	604	60/60	0.98	0.17	0.81	20,32,50,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
19	CUA	B	301	2/2	0.99	0.14	0.69	24,24,24,27	0
17	HEA	A	604	60/60	0.99	0.17	0.64	16,25,49,54	0
26	PEK	C	305	53/53	0.95	0.13	0.59	17,43,71,73	0
28	ZN	F	101	1/1	0.99	0.09	0.54	32,32,32,32	0
17	HEA	N	605	60/60	0.98	0.17	0.51	16,27,34,36	0
17	HEA	A	605	60/60	0.98	0.16	0.39	10,24,31,33	0
23	DCW	P	301	16/16	0.93	0.15	0.34	52,59,70,70	0
23	DCW	C	301	16/16	0.90	0.17	0.19	46,50,53,54	0
22	CHD	C	304	29/29	0.97	0.12	-0.15	25,31,37,39	0
22	CHD	P	304	29/29	0.96	0.12	-0.26	25,32,40,46	0
19	CUA	O	301	2/2	0.98	0.10	-0.38	36,36,36,36	0
22	CHD	O	302	29/29	0.97	0.10	-0.38	17,29,37,40	0
22	CHD	B	304	29/29	0.97	0.08	-0.54	20,27,34,38	0
28	ZN	S	101	1/1	0.99	0.06	-1.12	34,34,34,34	0
25	UNX	P	303	1/1	0.67	0.26	-	50,50,50,50	0
14	CU	A	601	1/1	0.99	0.12	-	23,23,23,23	0
14	CU	N	601	1/1	0.99	0.15	-	28,28,28,28	0
25	UNX	C	303	1/1	0.75	0.39	-	45,45,45,45	0

6.5 Other polymers (i)

There are no such residues in this entry.