wwPDB X-ray Structure Validation Summary Report (i)

Jan 31, 2016 – 09:24 PM GMT

PDB ID	:	1OCO
Title	:	BOVINE HEART CYTOCHROME C OXIDASE IN CARBON MONOXIDE-BOUND STATE
Authors	:	Tsukihara, T.; Yao, M.
Deposited on	:	1998-07-09
Resolution	:	2.80 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 (i)) were used in the production of this report:

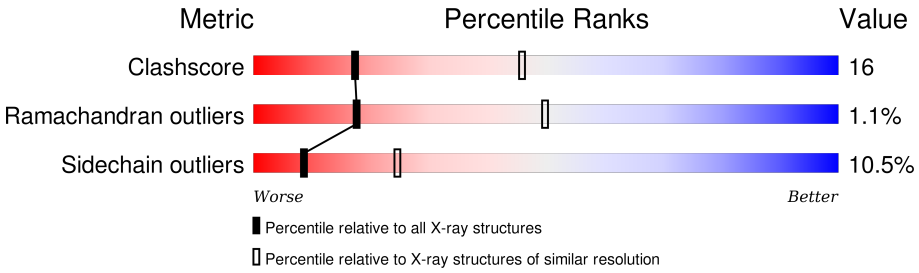
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 2.80 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))
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	514	68% 29% ·
1	N	514	69% 28% ·
2	B	227	56% 37% 6%
2	O	227	57% 36% 7%
3	C	261	70% 24% 6%
3	P	261	67% 27% 5% ·
4	D	147	60% 33% 5% ·

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Mol	Chain	Length	Quality of chain
4	Q	147	61% 33%
5	E	109	63% 32% 5%
5	R	109	63% 33%
6	F	98	56% 36% 6%
6	S	98	50% 42% 6%
7	G	84	64% 25% 11%
7	T	84	62% 29% 10%
8	H	85	52% 25% 12% 12%
8	U	85	54% 22% 12% 12%
9	I	73	62% 33% 5%
9	V	73	56% 38% 5%
10	J	59	61% 25% 8% 5%
10	W	59	64% 22% 8% 5%
11	K	56	61% 25% 13%
11	X	56	57% 29% 13%
12	L	47	64% 32%
12	Y	47	66% 30%
13	M	46	67% 24% 7%
13	Z	46	65% 26% 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
18	HEA	A	515	X	-	-	-
18	HEA	A	516	X	-	-	-
18	HEA	N	515	X	-	-	-
18	HEA	N	516	X	-	-	-

2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 28810 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	514	Total	C	N	O	S	0	0	0
			4025	2690	623	677	35			
1	N	514	Total	C	N	O	S	0	0	0
			4025	2690	623	677	35			

- Molecule 2 is a protein called CYTOCHROME C OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	227	Total	C	N	O	S	0	5	0
			1863	1207	288	350	18			
2	O	227	Total	C	N	O	S	0	5	0
			1863	1207	288	350	18			

- Molecule 3 is a protein called CYTOCHROME C OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	261	Total	C	N	O	S	0	0	0
			2124	1420	338	353	13			
3	P	261	Total	C	N	O	S	0	0	0
			2124	1420	338	353	13			

- Molecule 4 is a protein called CYTOCHROME C OXIDASE.

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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	109	Total	C	N	O	S	0	0	0
			878	558	150	168	2			
5	R	109	Total	C	N	O	S	0	0	0
			878	558	150	168	2			

- Molecule 6 is a protein called CYTOCHROME C OXIDASE.

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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	84	Total	C	N	O	S	0	0	0
			672	431	129	111	1			
7	T	84	Total	C	N	O	S	0	0	0
			672	431	129	111	1			

- Molecule 8 is a protein called CYTOCHROME C OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	75	Total	C	N	O	S	0	0	0
			628	395	114	114	5			
8	U	75	Total	C	N	O	S	0	0	0
			628	395	114	114	5			

- Molecule 9 is a protein called CYTOCHROME C OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	73	Total	C	N	O	S	0	0	0
			598	388	107	99	4			
9	V	73	Total	C	N	O	S	0	0	0
			598	388	107	99	4			

- Molecule 10 is a protein called CYTOCHROME C OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	56	Total	C	N	O	S	0	0	0
			441	285	73	80	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	W	56	Total	C	N	O	S	0	0	0
			441	285	73	80	3			

- Molecule 11 is a protein called CYTOCHROME C OXIDASE.

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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	47	Total	C	N	O	S	0	0	0
			386	257	65	62	2			
12	Y	47	Total	C	N	O	S	0	0	0
			386	257	65	62	2			

- Molecule 13 is a protein called CYTOCHROME C OXIDASE.

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	O	2	Total	Cu	0	0
			2	2		
14	B	2	Total	Cu	0	0
			2	2		
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 1 1	0	0
15	N	1	Total Mg 1 1	0	0

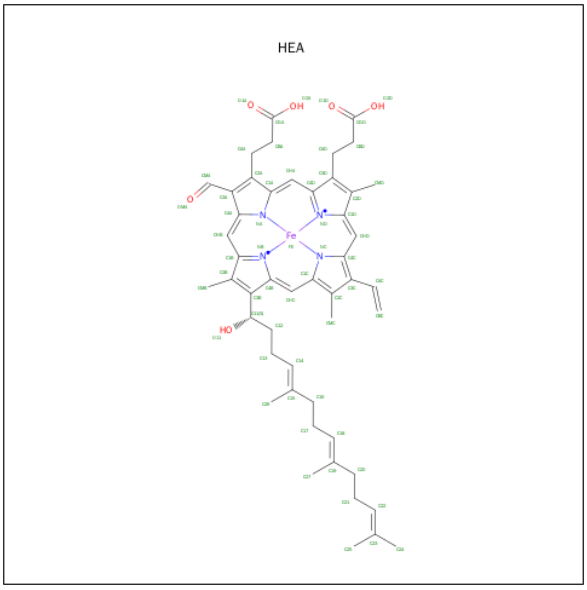
- Molecule 16 is SODIUM ION (three-letter code: NA) (formula: Na).

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

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

- Molecule 18 is HEME-A (three-letter code: HEA) (formula: $C_{49}H_{56}FeN_4O_6$).



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

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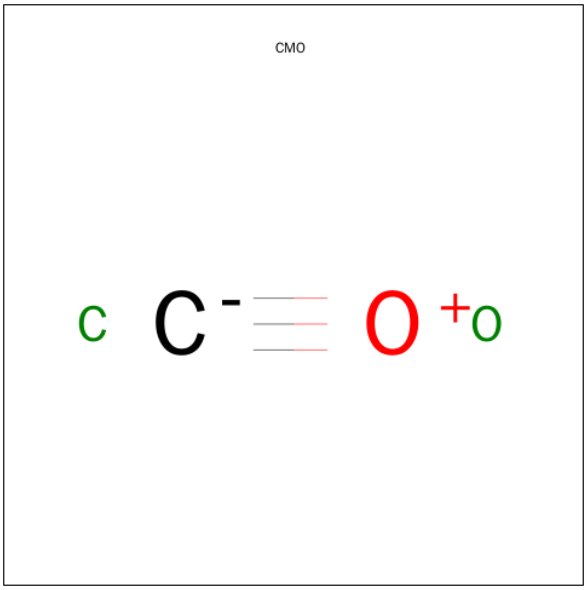
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	A	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
18	N	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
18	N	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		

- Molecule 19 is CARBON MONOXIDE (three-letter code: CMO) (formula: CO).



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

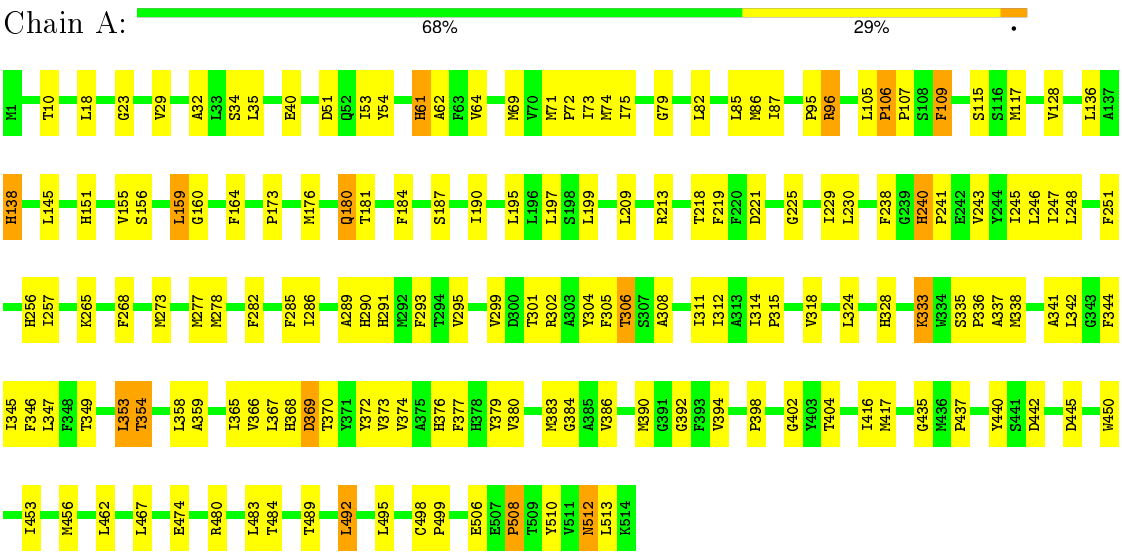
3 Residue-property plots (i)

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.

Note EDS was not executed.

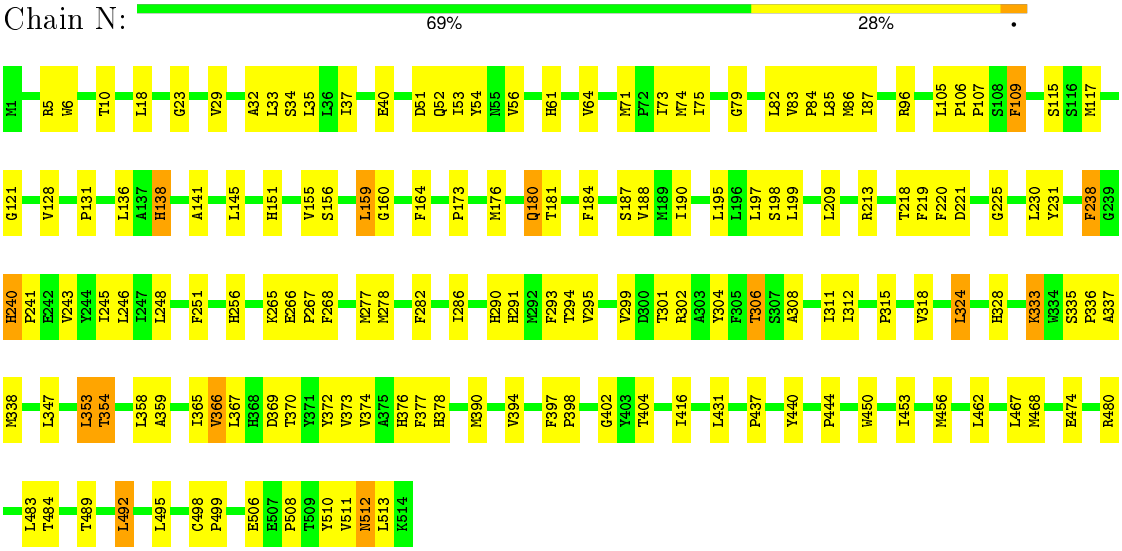
• Molecule 1: CYTOCHROME C OXIDASE

Chain A:



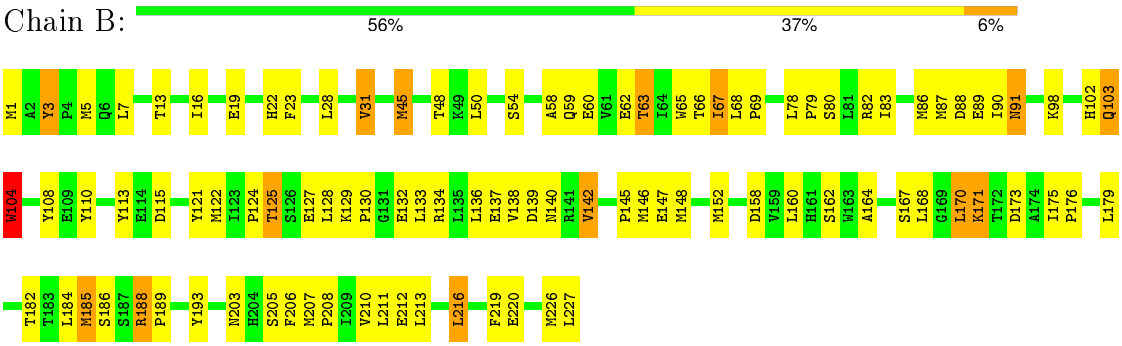
• Molecule 1: CYTOCHROME C OXIDASE

Chain N:



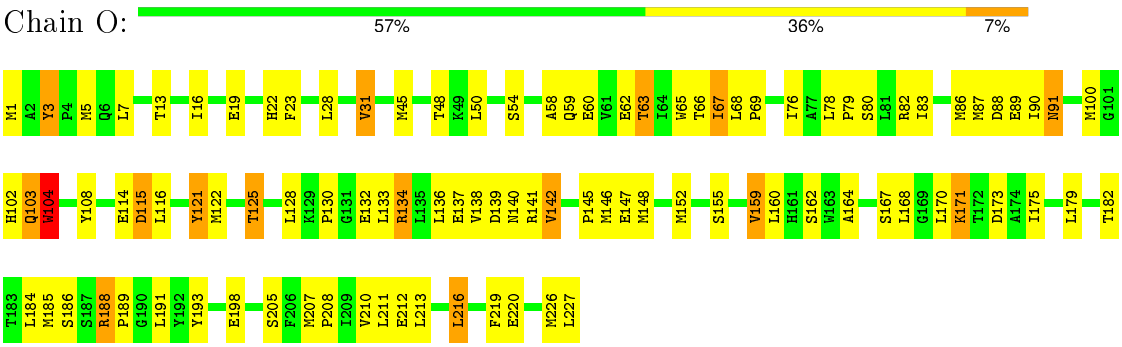
- Molecule 2: CYTOCHROME C OXIDASE

Chain B:



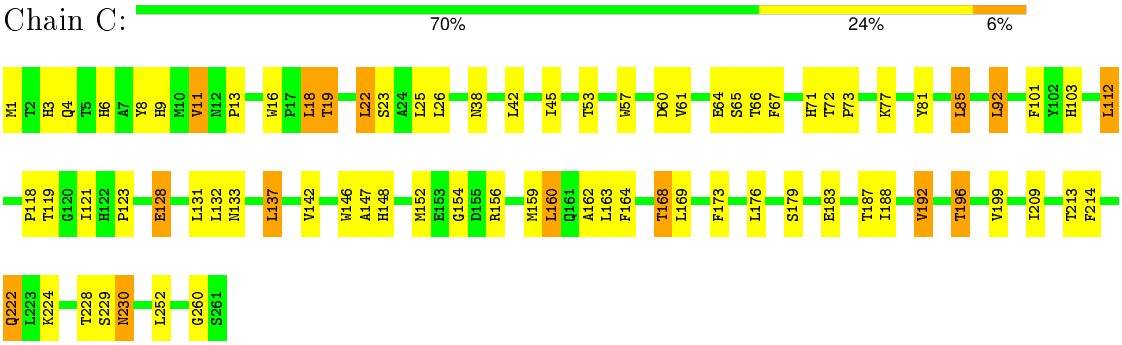
- Molecule 2: CYTOCHROME C OXIDASE

Chain O:



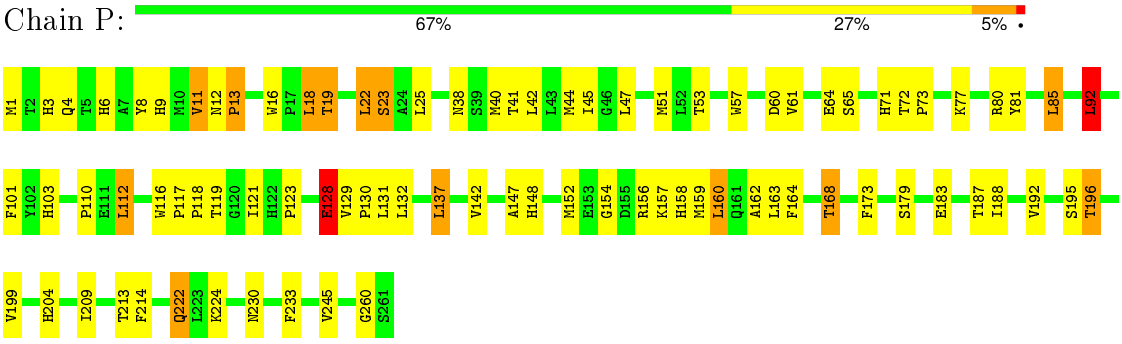
- Molecule 3: CYTOCHROME C OXIDASE

Chain C:



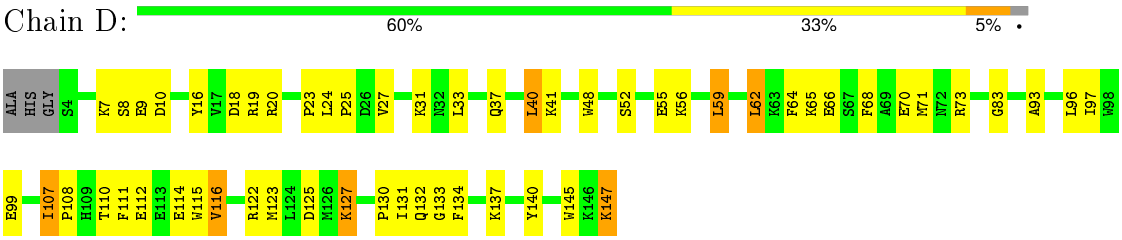
- Molecule 3: CYTOCHROME C OXIDASE

Chain P:



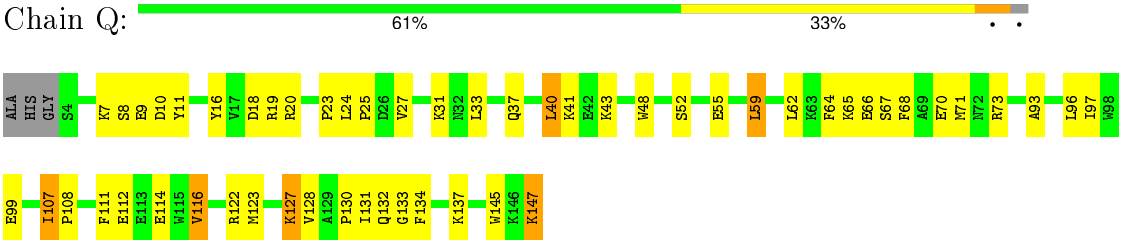
- Molecule 4: CYTOCHROME C OXIDASE

Chain D:



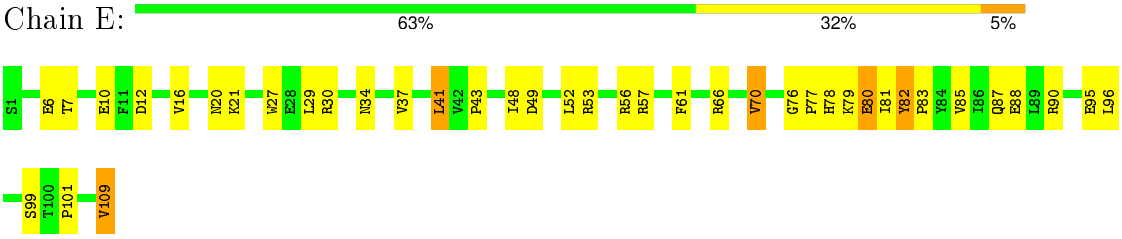
- Molecule 4: CYTOCHROME C OXIDASE

Chain Q:



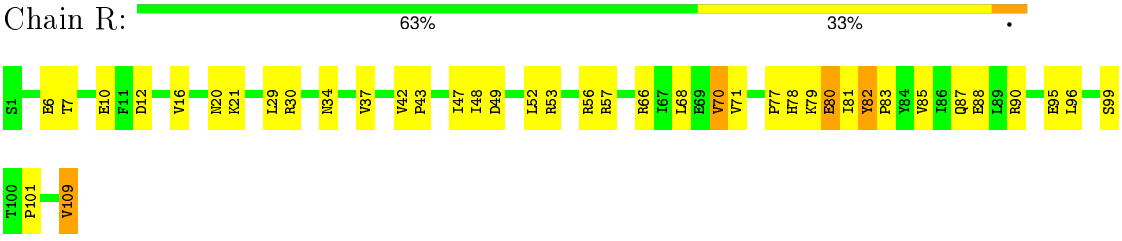
- Molecule 5: CYTOCHROME C OXIDASE

Chain E:



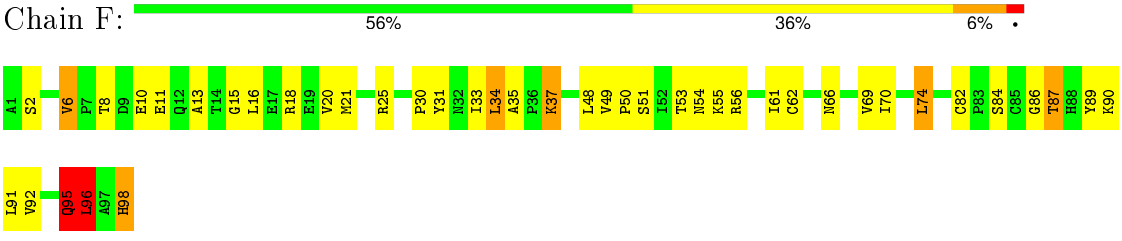
- Molecule 5: CYTOCHROME C OXIDASE

Chain R:



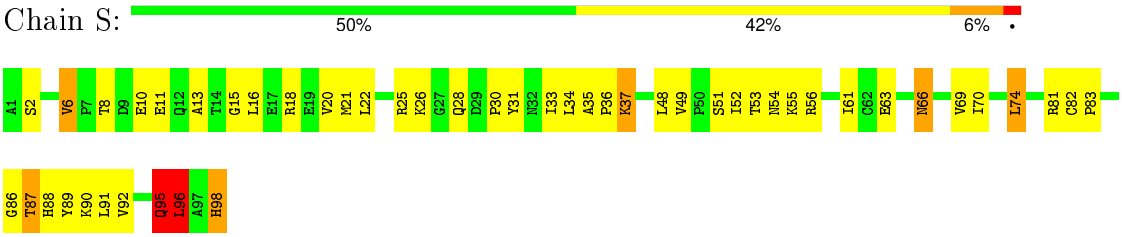
- Molecule 6: CYTOCHROME C OXIDASE

Chain F:



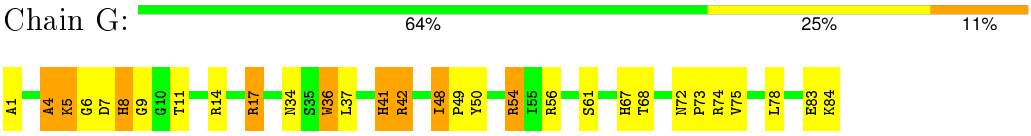
- Molecule 6: CYTOCHROME C OXIDASE

Chain S:



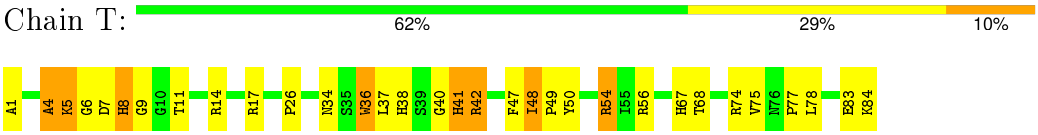
• Molecule 7: CYTOCHROME C OXIDASE

Chain G:



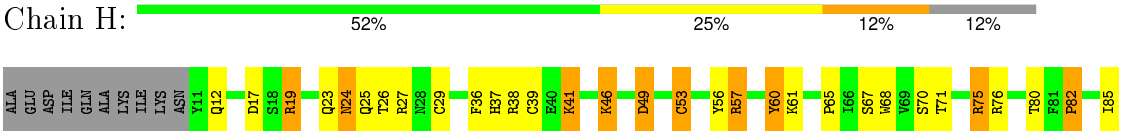
• Molecule 7: CYTOCHROME C OXIDASE

Chain T:



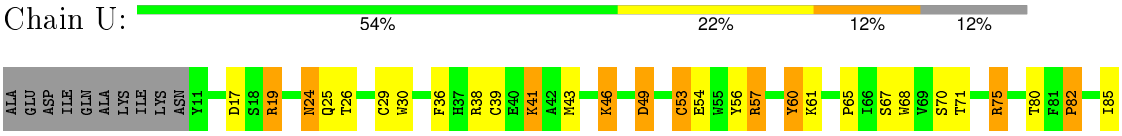
• Molecule 8: CYTOCHROME C OXIDASE

Chain H:



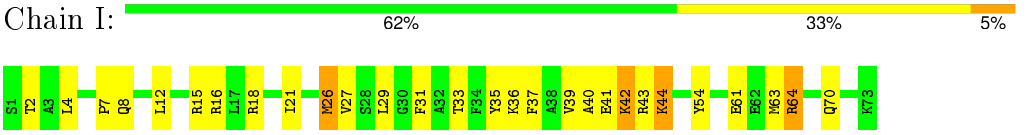
• Molecule 8: CYTOCHROME C OXIDASE

Chain U:



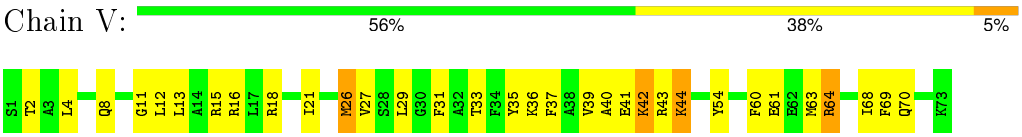
• Molecule 9: CYTOCHROME C OXIDASE

Chain I:



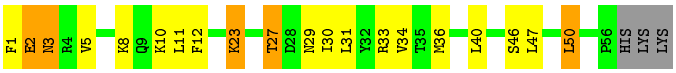
• Molecule 9: CYTOCHROME C OXIDASE

Chain V:



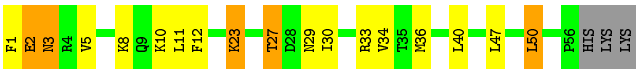
• Molecule 10: CYTOCHROME C OXIDASE

Chain J:



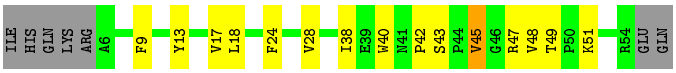
• Molecule 10: CYTOCHROME C OXIDASE

Chain W:



• Molecule 11: CYTOCHROME C OXIDASE

Chain K:



• Molecule 11: CYTOCHROME C OXIDASE

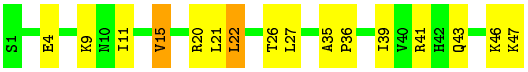
Chain X:

• Molecule 12: CYTOCHROME C OXIDASE

Chain L:

• Molecule 12: CYTOCHROME C OXIDASE

Chain Y:

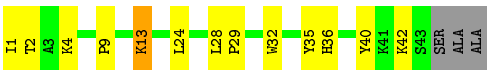


• Molecule 13: CYTOCHROME C OXIDASE

Chain M:

• Molecule 13: CYTOCHROME C OXIDASE

Chain Z:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	189.10Å 210.50Å 178.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	7.00 – 2.80	Depositor
% Data completeness (in resolution range)	97.3 (7.00-2.80)	Depositor
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.84	Depositor
R, R_{free}	0.213 , 0.256	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	28810	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CMO, MG, NA, ZN, HEA, CU

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	0.76	1/4164 (0.0%)	0.86	2/5688 (0.0%)
1	N	0.69	2/4164 (0.0%)	0.84	1/5688 (0.0%)
2	B	0.70	0/1909	0.91	1/2601 (0.0%)
2	O	0.65	1/1909 (0.1%)	0.88	1/2601 (0.0%)
3	C	0.67	0/2211	0.77	1/3023 (0.0%)
3	P	0.66	0/2211	0.77	1/3023 (0.0%)
4	D	0.65	0/1229	0.72	1/1658 (0.1%)
4	Q	0.61	0/1229	0.70	1/1658 (0.1%)
5	E	0.59	0/898	0.72	0/1218
5	R	0.56	0/898	0.72	0/1218
6	F	0.68	0/765	0.86	0/1038
6	S	0.64	0/765	0.87	0/1038
7	G	0.66	0/699	0.85	1/950 (0.1%)
7	T	0.63	0/699	0.86	1/950 (0.1%)
8	H	0.67	0/648	0.78	0/877
8	U	0.61	0/648	0.77	0/877
9	I	0.67	0/611	0.73	0/810
9	V	0.71	0/611	0.73	0/810
10	J	0.64	0/451	0.76	0/610
10	W	0.66	0/451	0.75	0/610
11	K	0.66	0/398	0.70	0/546
11	X	0.58	0/398	0.67	0/546
12	L	0.70	0/399	0.65	0/534
12	Y	0.66	0/399	0.64	0/534
13	M	0.60	0/345	0.74	0/470
13	Z	0.58	0/345	0.70	0/470
All	All	0.67	4/29454 (0.0%)	0.80	11/40046 (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	2
1	N	0	2
2	B	0	2
2	O	0	1
3	C	0	1
3	P	0	1
5	E	0	1
5	R	0	1
All	All	0	11

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	O	198	GLU	CG-CD	6.00	1.60	1.51
1	N	61	HIS	CG-CD2	5.63	1.45	1.35
1	N	378	HIS	CG-CD2	5.43	1.45	1.35
1	A	61	HIS	CG-CD2	5.18	1.44	1.35

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	133	GLY	N-CA-C	6.20	128.60	113.10
3	C	92	LEU	CA-CB-CG	-6.11	101.25	115.30
1	N	61	HIS	CG-ND1-CE1	-5.94	97.98	105.70
3	P	92	LEU	CA-CB-CG	-5.85	101.85	115.30
4	Q	133	GLY	N-CA-C	5.72	127.41	113.10

There are no chirality outliers.

5 of 11 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	240	HIS	Sidechain
1	A	304	TYR	Sidechain
2	B	110	TYR	Sidechain
2	B	121	TYR	Sidechain
3	C	8	TYR	Sidechain

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	4025	0	4002	128	0
1	N	4025	0	4002	125	0
2	B	1863	0	1867	82	0
2	O	1863	0	1867	81	0
3	C	2124	0	2044	64	0
3	P	2124	0	2044	74	0
4	D	1195	0	1183	44	0
4	Q	1195	0	1183	44	0
5	E	878	0	868	33	0
5	R	878	0	868	30	0
6	F	748	0	728	39	0
6	S	748	0	728	48	0
7	G	672	0	645	34	0
7	T	672	0	645	33	0
8	H	628	0	582	46	0
8	U	628	0	582	45	0
9	I	598	0	612	28	0
9	V	598	0	612	28	0
10	J	441	0	439	13	0
10	W	441	0	439	11	0
11	K	384	0	366	12	0
11	X	384	0	366	15	0
12	L	386	0	388	14	0
12	Y	386	0	388	13	0
13	M	335	0	352	15	0
13	Z	335	0	352	15	0
14	A	1	0	0	0	0
14	B	2	0	0	0	0
14	N	1	0	0	0	0
14	O	2	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	F	1	0	0	0	0
17	S	1	0	0	0	0
18	A	120	0	107	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	N	120	0	107	8	0
19	A	2	0	0	0	0
19	N	2	0	0	0	0
All	All	28810	0	28366	920	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 16.

The worst 5 of 920 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)
8:H:57:ARG:HH11	8:H:57:ARG:HB3	1.23	1.03
8:U:57:ARG:HB3	8:U:57:ARG:HH11	1.20	1.01
2:B:86:MET:O	2:B:89[B]:GLU:HG2	1.65	0.96
1:A:35:LEU:HD11	1:A:462:LEU:HD13	1.53	0.90
2:O:86:MET:O	2:O:89[B]:GLU:HG2	1.71	0.89

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%)	477 (93%)	33 (6%)	2 (0%)	39 74
1	N	512/514 (100%)	476 (93%)	36 (7%)	0	100 100
2	B	230/227 (101%)	202 (88%)	24 (10%)	4 (2%)	11 36
2	O	230/227 (101%)	202 (88%)	23 (10%)	5 (2%)	8 28
3	C	259/261 (99%)	249 (96%)	8 (3%)	2 (1%)	24 58
3	P	259/261 (99%)	250 (96%)	8 (3%)	1 (0%)	39 74
4	D	142/147 (97%)	134 (94%)	7 (5%)	1 (1%)	26 62

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
4	Q	142/147 (97%)	133 (94%)	8 (6%)	1 (1%)	26 62
5	E	107/109 (98%)	103 (96%)	4 (4%)	0	100 100
5	R	107/109 (98%)	103 (96%)	4 (4%)	0	100 100
6	F	96/98 (98%)	85 (88%)	6 (6%)	5 (5%)	2 7
6	S	96/98 (98%)	86 (90%)	5 (5%)	5 (5%)	2 7
7	G	82/84 (98%)	65 (79%)	14 (17%)	3 (4%)	4 14
7	T	82/84 (98%)	64 (78%)	16 (20%)	2 (2%)	7 25
8	H	73/85 (86%)	64 (88%)	8 (11%)	1 (1%)	14 42
8	U	73/85 (86%)	62 (85%)	10 (14%)	1 (1%)	14 42
9	I	71/73 (97%)	66 (93%)	5 (7%)	0	100 100
9	V	71/73 (97%)	66 (93%)	5 (7%)	0	100 100
10	J	54/59 (92%)	49 (91%)	2 (4%)	3 (6%)	2 6
10	W	54/59 (92%)	50 (93%)	1 (2%)	3 (6%)	2 6
11	K	47/56 (84%)	40 (85%)	7 (15%)	0	100 100
11	X	47/56 (84%)	41 (87%)	6 (13%)	0	100 100
12	L	45/47 (96%)	41 (91%)	4 (9%)	0	100 100
12	Y	45/47 (96%)	42 (93%)	3 (7%)	0	100 100
13	M	41/46 (89%)	40 (98%)	1 (2%)	0	100 100
13	Z	41/46 (89%)	40 (98%)	0	1 (2%)	7 25
All	All	3518/3612 (97%)	3230 (92%)	248 (7%)	40 (1%)	17 50

5 of 40 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	91[A]	ASN
2	B	91[B]	ASN
4	D	20	ARG
6	F	87	THR
6	F	96	LEU

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	427/427 (100%)	395 (92%)	32 (8%)	17	43
1	N	427/427 (100%)	395 (92%)	32 (8%)	17	43
2	B	216/211 (102%)	189 (88%)	27 (12%)	6	17
2	O	216/211 (102%)	191 (88%)	25 (12%)	7	20
3	C	226/226 (100%)	199 (88%)	27 (12%)	6	19
3	P	226/226 (100%)	199 (88%)	27 (12%)	6	19
4	D	128/129 (99%)	117 (91%)	11 (9%)	13	36
4	Q	128/129 (99%)	118 (92%)	10 (8%)	16	41
5	E	95/95 (100%)	86 (90%)	9 (10%)	11	30
5	R	95/95 (100%)	87 (92%)	8 (8%)	14	37
6	F	81/81 (100%)	73 (90%)	8 (10%)	10	28
6	S	81/81 (100%)	74 (91%)	7 (9%)	13	36
7	G	68/68 (100%)	56 (82%)	12 (18%)	2	7
7	T	68/68 (100%)	55 (81%)	13 (19%)	2	5
8	H	67/75 (89%)	54 (81%)	13 (19%)	2	5
8	U	67/75 (89%)	55 (82%)	12 (18%)	2	6
9	I	58/58 (100%)	51 (88%)	7 (12%)	6	18
9	V	58/58 (100%)	51 (88%)	7 (12%)	6	18
10	J	47/50 (94%)	40 (85%)	7 (15%)	4	11
10	W	47/50 (94%)	40 (85%)	7 (15%)	4	11
11	K	39/46 (85%)	37 (95%)	2 (5%)	29	63
11	X	39/46 (85%)	37 (95%)	2 (5%)	29	63
12	L	40/40 (100%)	35 (88%)	5 (12%)	6	17
12	Y	40/40 (100%)	34 (85%)	6 (15%)	3	11
13	M	37/38 (97%)	34 (92%)	3 (8%)	15	39
13	Z	37/38 (97%)	34 (92%)	3 (8%)	15	39
All	All	3058/3088 (99%)	2736 (90%)	322 (10%)	8	24

5 of 322 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	I	64	ARG
1	N	312	ILE
9	V	2	THR
10	J	10	LYS
1	N	18	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 36 such sidechains are listed below:

Mol	Chain	Res	Type
11	K	10	HIS
1	N	512	ASN
11	X	10	HIS
13	M	39	ASN
3	P	71	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 18 ligands modelled in this entry, 12 are monoatomic - leaving 6 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	$\#\|Z\|>2$
18	HEA	A	515	1	40,67,67	1.80	6 (15%)	41,103,103	2.56	17 (41%)
18	HEA	A	516	19,1	40,67,67	2.06	10 (25%)	41,103,103	1.63	10 (24%)
19	CMO	A	520	18,14	0,1,1	0.00	-	0,0,0	0.00	-
18	HEA	N	515	1	40,67,67	1.42	5 (12%)	41,103,103	2.35	16 (39%)
18	HEA	N	516	19,1	40,67,67	2.00	8 (20%)	41,103,103	1.72	12 (29%)
19	CMO	N	520	18,14	0,1,1	0.00	-	0,0,0	0.00	-

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
18	HEA	A	515	1	3/3/7/16	0/24/76/76	0/0/8/8
18	HEA	A	516	19,1	3/3/7/16	0/24/76/76	0/0/8/8
19	CMO	A	520	18,14	-	0/0/0/0	0/0/0/0
18	HEA	N	515	1	3/3/7/16	0/24/76/76	0/0/8/8
18	HEA	N	516	19,1	3/3/7/16	0/24/76/76	0/0/8/8
19	CMO	N	520	18,14	-	0/0/0/0	0/0/0/0

The worst 5 of 29 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	N	516	HEA	C3C-C2C	-8.29	1.29	1.40
18	A	516	HEA	C3C-C2C	-6.31	1.32	1.40
18	A	516	HEA	C3A-C2A	-5.86	1.32	1.40
18	N	515	HEA	C3A-C2A	-4.03	1.35	1.40
18	A	516	HEA	C3B-C2B	-3.77	1.27	1.41

The worst 5 of 55 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	N	515	HEA	C13-C14-C15	-5.73	115.31	127.76
18	A	515	HEA	C13-C14-C15	-5.50	115.81	127.76
18	A	515	HEA	O11-C11-C12	-5.08	97.32	109.73
18	A	515	HEA	C17-C18-C19	-4.66	117.63	127.76
18	A	515	HEA	CMB-C2B-C1B	-4.21	121.40	128.36

5 of 12 chirality outliers are listed below:

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

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	A	515	HEA	8	0
18	A	516	HEA	4	0
18	N	515	HEA	6	0
18	N	516	HEA	2	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.