



wwPDB X-ray Structure Validation Summary Report ⓘ

May 13, 2020 – 01:54 pm BST

PDB ID : 1OCZ
Title : BOVINE HEART CYTOCHROME C OXIDASE IN AZIDE-BOUND STATE
Authors : Tsukihara, T.; Yao, M.
Deposited on : 1998-07-13
Resolution : 2.90 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

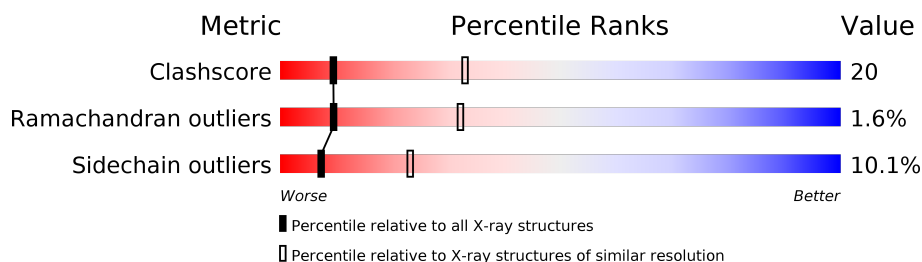
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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))
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)







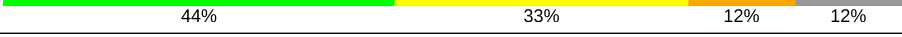



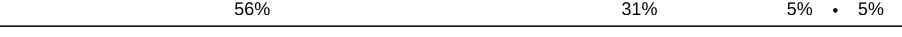







The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	514	63% 34% .
1	N	514	63% 35% .
2	B	227	51% 42% 6%
2	O	227	51% 43% 6%
3	C	261	68% 25% 6% .
3	P	261	65% 29% 5% .
4	D	147	58% 35% 5% .
4	Q	147	56% 37% 5% .

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Mol	Chain	Length	Quality of chain
5	E	109	
5	R	109	
6	F	98	
6	S	98	
7	G	84	
7	T	84	
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
17	AZI	N	521	-	-	X	-
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 28818 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		

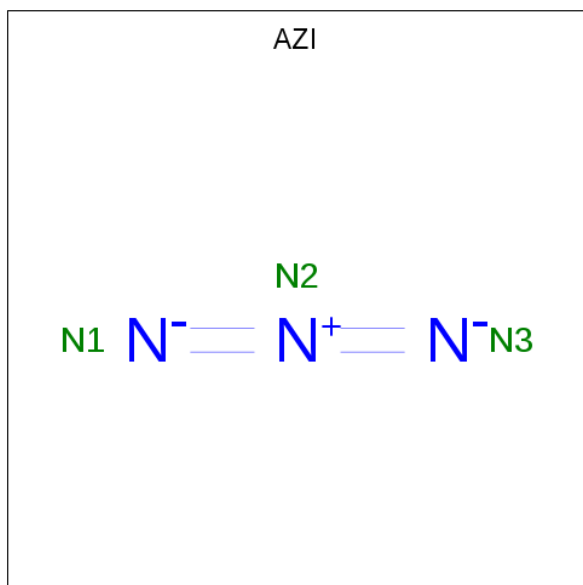
- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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).

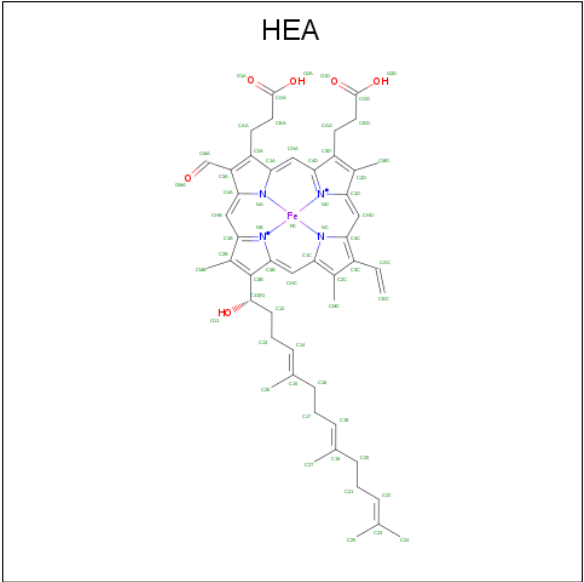
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	A	1	Total Na 1 1	0	0
16	N	1	Total Na 1 1	0	0

- Molecule 17 is AZIDE ION (three-letter code: AZI) (formula: N₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	A	1	Total N 3 3	0	0
17	A	1	Total N 3 3	0	0
17	N	1	Total N 3 3	0	0
17	N	1	Total N 3 3	0	0

- Molecule 18 is HEME-A (three-letter code: HEA) (formula: C₄₉H₅₆FeN₄O₆).



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

- Molecule 19 is ZINC ION (three-letter code: ZN) (formula: Zn).

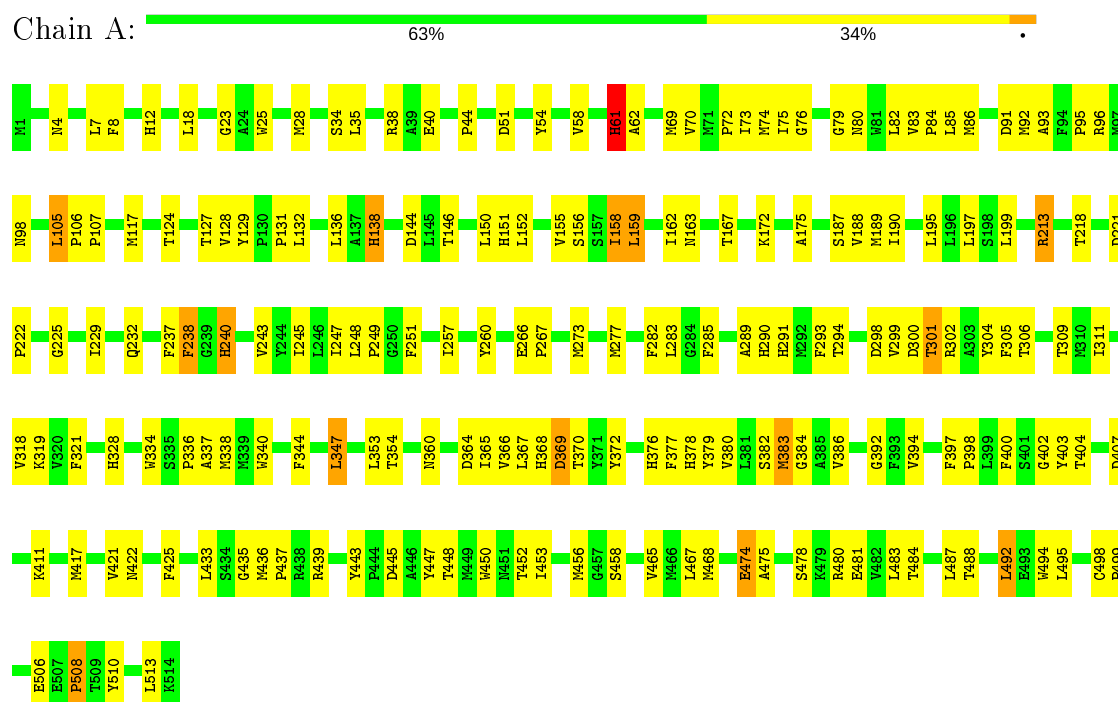
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	S	1	Total	Zn	0	0
			1	1		
19	F	1	Total	Zn	0	0
			1	1		

3 Residue-property plots [i](#)

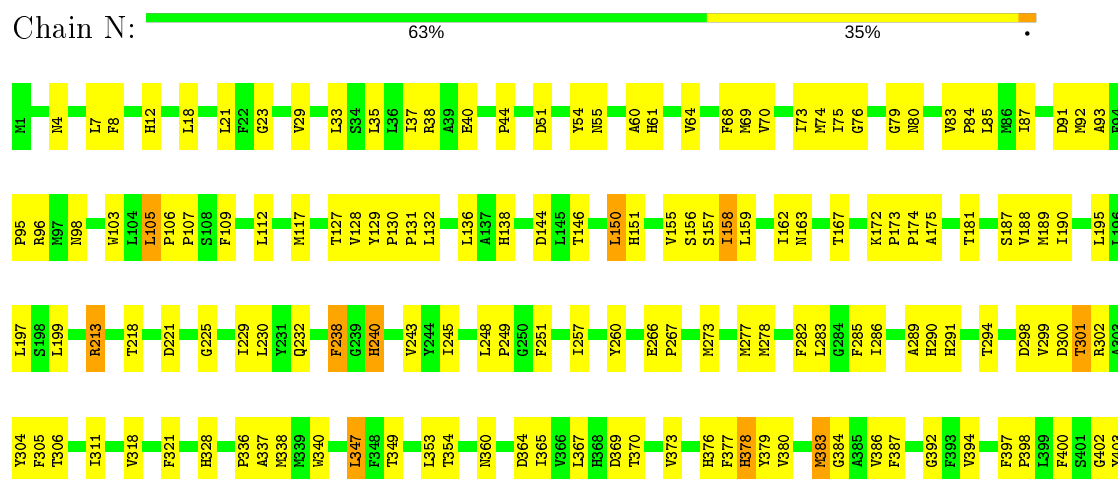
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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. 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.

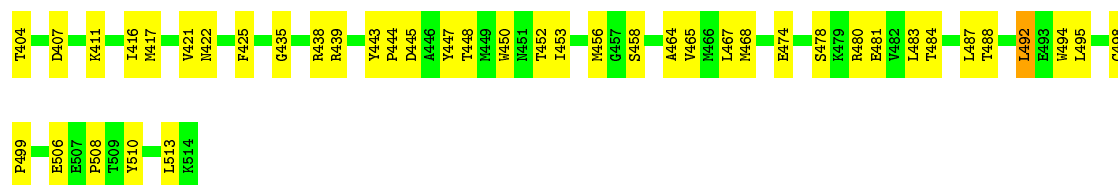
Note EDS was not executed.

• Molecule 1: CYTOCHROME C OXIDASE



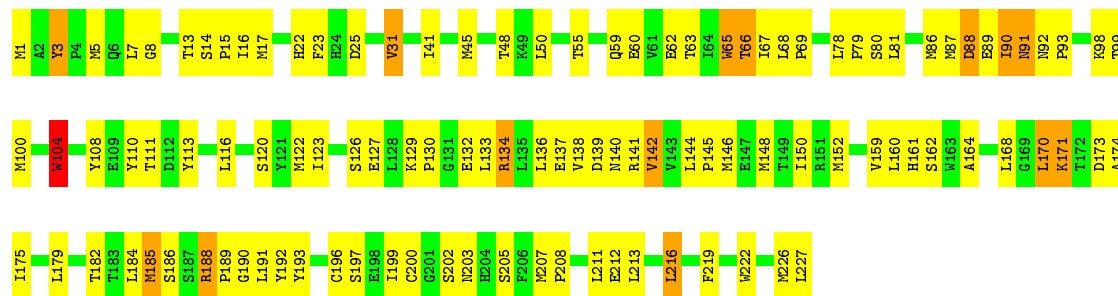
• Molecule 1: CYTOCHROME C OXIDASE





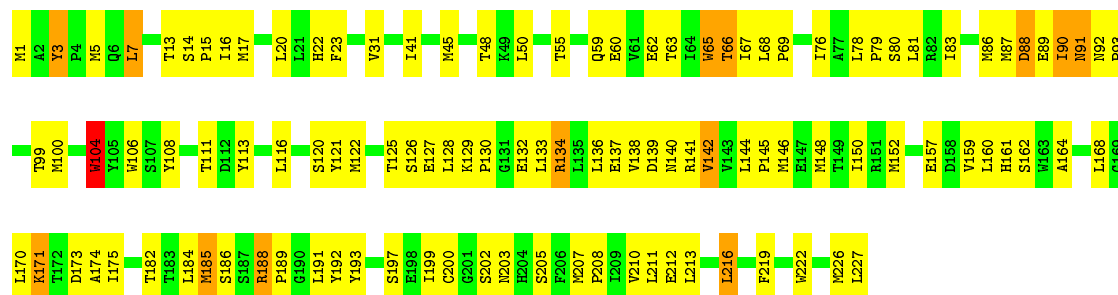
• Molecule 2: CYTOCHROME C OXIDASE

Chain B: 51% 42% 6%



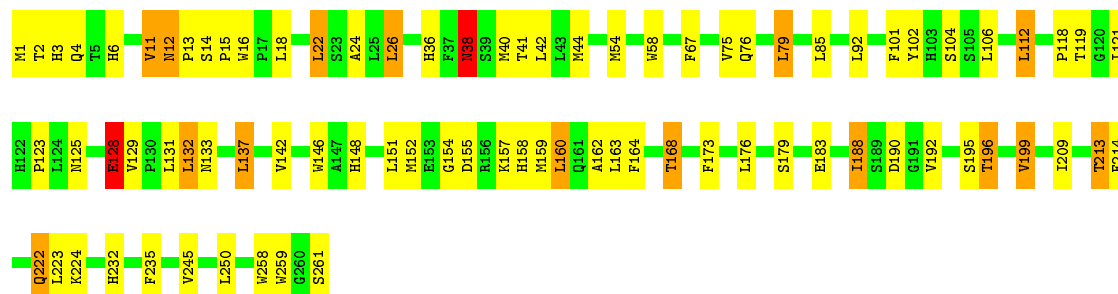
• Molecule 2: CYTOCHROME C OXIDASE

Chain O: 51% 43% 6%



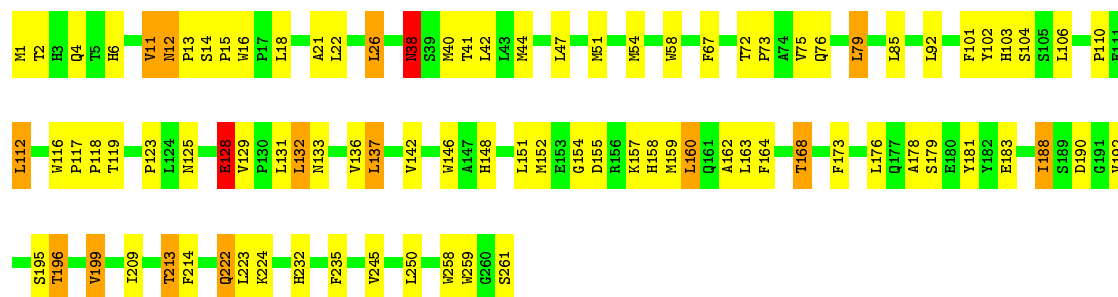
• Molecule 3: CYTOCHROME C OXIDASE

Chain C: 68% 25% 6%



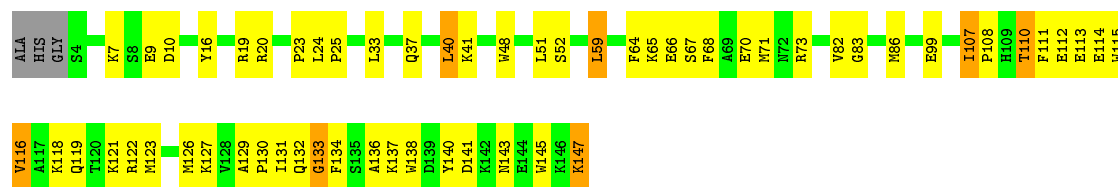
• Molecule 3: CYTOCHROME C OXIDASE

Chain P: 65% 29% 5%



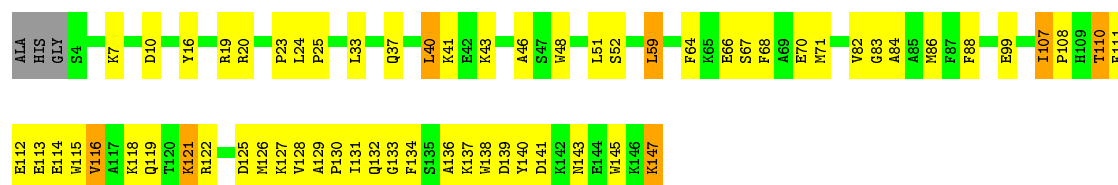
• Molecule 4: CYTOCHROME C OXIDASE

Chain D: 58% 35% 5%



• Molecule 4: CYTOCHROME C OXIDASE

Chain Q: 56% 37% 5%



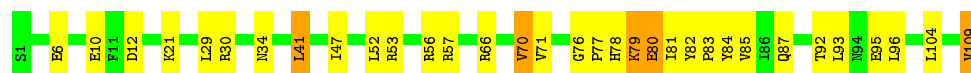
• Molecule 5: CYTOCHROME C OXIDASE

Chain E: 70% 26% 5%



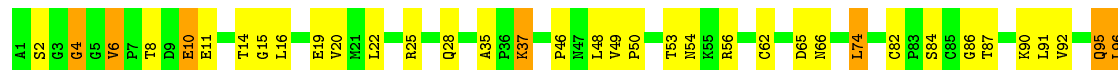
• Molecule 5: CYTOCHROME C OXIDASE

Chain R: 70% 26% 5%



• Molecule 6: CYTOCHROME C OXIDASE

Chain F: 61% 31% 8%



A97
H98

- Molecule 6: CYTOCHROME C OXIDASE

Chain S: 57% 34% 9%

A1	S2	G3	G4	G5	V6	P7	T8	D9	E10	E11	T14	G15	L16	E17	R18	E19	V20	L21	L22	R25	Q28	A35	P36	R37	L48	V49	F50	T53	N54	K55	R56	C62	D65	N66	L74	C82	P83	S84	C85	G86	T87	R88	Y89	K90	L91	V92	Q95	L96
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A97
H98

- Molecule 7: CYTOCHROME C OXIDASE

Chain G: 57% 31% 11%

A1	S2	A3	A4	K5	G6	D7	H8	G9	G10	T11	R14	R17	F18	L19	L23	P26	K36	S39	G40	R41	R42	E43	R44	F47	I48	P49	Y50	L53	R54	R56	H67	T68	P69	F70	R74	V75	L78	G81	K84
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- Molecule 7: CYTOCHROME C OXIDASE

Chain T: 60% 29% 11%

A1	S2	A3	A4	K5	G6	D7	H8	G9	G10	T11	R14	R17	F18	L19	L23	P26	L33	K36	S39	G40	R41	R42	E43	R44	F47	I48	P49	Y50	L53	R54	R56	H67	T68	R74	V75	L78	G81	K84
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- Molecule 8: CYTOCHROME C OXIDASE

Chain H: 44% 33% 12% 12%

ALA	GLU	ASP	ILE	GLN	ALA	LYS	ILE	LYS	LYS	ASN	Y11	Q12	D17	S18	R19	F20	P21	R27	R28	C29	F36	H37	R38	C39	M43	K46	G47	G48	D49	V50	S51	V52	C53	Y56	R57	R58	V59	Y60	K61	P65	I66	S67	H68	V69	S70	T71	R75	R76	T80	F81	P82
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G83
R84
I85

- Molecule 8: CYTOCHROME C OXIDASE

Chain U: 45% 34% 9% 12%

ALA	GLU	ASP	ILE	GLN	ALA	LYS	ILE	LYS	LYS	ASN	Y11	Q12	D17	S18	R19	F20	P21	R27	R28	C29	V30	F36	H37	R38	C39	M43	K46	G47	G48	D49	V50	S51	V52	C53	Y56	R57	R58	V59	Y60	K61	P65	I66	S67	H68	V69	S70	T71	R75	R76	T80	F81	P82
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G83
R84
I85

- Molecule 9: CYTOCHROME C OXIDASE

Chain I: 51% 44% 5%

S1	P7	Q8	G11	L12	L13	A14	R15	L16	L17	R18	F19	H20	L21	M26	V27	S28	L29	G30	F31	A32	T33	K36	F37	A38	V39	A40	E41	K42	R43	K44	Y51	Y54	D55	K58	D59	P60	E61	E62	M63	R64	F69	Q70	S71	A72	K73
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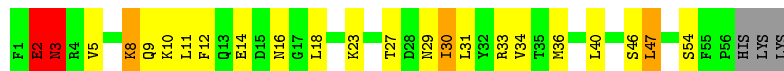
- Molecule 9: CYTOCHROME C OXIDASE

Chain V: 



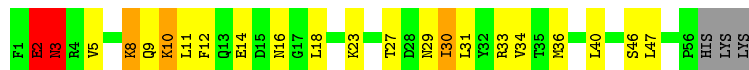
- Molecule 10: CYTOCHROME C OXIDASE

Chain J: 



- Molecule 10: CYTOCHROME C OXIDASE

Chain W: 



- Molecule 11: CYTOCHROME C OXIDASE

Chain K: 



- Molecule 11: CYTOCHROME C OXIDASE

Chain X: 



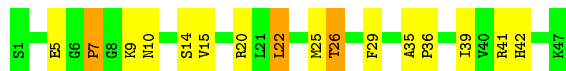
- Molecule 12: CYTOCHROME C OXIDASE

Chain L: 



- Molecule 12: CYTOCHROME C OXIDASE

Chain Y: 



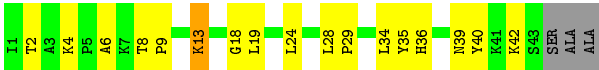
- Molecule 13: CYTOCHROME C OXIDASE

Chain M:

57%

35%

• 7%



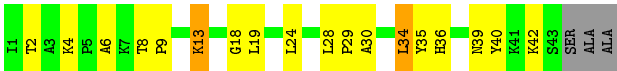
● Molecule 13: CYTOCHROME C OXIDASE

Chain Z:

54%

35%

• 7%



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	189.20Å 210.60Å 178.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	7.00 – 2.90	Depositor
% Data completeness (in resolution range)	80.2 (7.00-2.90)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.84	Depositor
R, R_{free}	0.195 , 0.255	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	28818	wwPDB-VP
Average B, all atoms (Å ²)	38.0	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: AZI, 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	0.70	1/4164 (0.0%)	0.84	2/5688 (0.0%)
1	N	0.64	1/4164 (0.0%)	0.82	1/5688 (0.0%)
2	B	0.66	0/1909	0.89	2/2601 (0.1%)
2	O	0.62	0/1909	0.85	1/2601 (0.0%)
3	C	0.65	0/2211	0.77	1/3023 (0.0%)
3	P	0.61	0/2211	0.75	1/3023 (0.0%)
4	D	0.63	0/1229	0.71	1/1658 (0.1%)
4	Q	0.59	0/1229	0.69	1/1658 (0.1%)
5	E	0.60	0/898	0.72	0/1218
5	R	0.55	0/898	0.71	0/1218
6	F	0.63	0/765	0.86	0/1038
6	S	0.58	0/765	0.85	0/1038
7	G	0.59	0/699	0.81	1/950 (0.1%)
7	T	0.61	0/699	0.83	1/950 (0.1%)
8	H	0.62	0/648	0.73	0/877
8	U	0.62	0/648	0.73	0/877
9	I	0.65	0/611	0.70	0/810
9	V	0.64	0/611	0.70	0/810
10	J	0.64	0/451	0.73	0/610
10	W	0.62	0/451	0.70	0/610
11	K	0.68	0/398	0.70	0/546
11	X	0.54	0/398	0.69	0/546
12	L	0.65	0/399	0.68	0/534
12	Y	0.61	0/399	0.67	0/534
13	M	0.61	0/345	0.76	0/470
13	Z	0.57	0/345	0.73	0/470
All	All	0.64	2/29454 (0.0%)	0.79	12/40046 (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	4
1	N	0	3
2	B	0	1
All	All	0	8

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	378	HIS	CG-CD2	6.05	1.46	1.35
1	A	334	TRP	CB-CG	-5.31	1.40	1.50

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	92	LEU	CA-CB-CG	-7.17	98.81	115.30
3	P	92	LEU	CA-CB-CG	-6.78	99.71	115.30
4	D	133	GLY	N-CA-C	5.96	127.99	113.10
7	G	7	ASP	N-CA-C	5.90	126.93	111.00
1	N	435	GLY	N-CA-C	5.77	127.52	113.10

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	240	HIS	Sidechain
1	A	304	TYR	Sidechain
1	A	372	TYR	Sidechain
1	A	61	HIS	Sidechain
2	B	110	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	164	0
1	N	4025	0	4002	167	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1863	0	1867	100	0
2	O	1863	0	1867	104	0
3	C	2124	0	2044	75	0
3	P	2124	0	2044	82	0
4	D	1195	0	1183	57	0
4	Q	1195	0	1183	60	0
5	E	878	0	868	31	0
5	R	878	0	868	30	0
6	F	748	0	728	32	0
6	S	748	0	728	38	0
7	G	672	0	645	53	0
7	T	672	0	645	50	0
8	H	628	0	582	49	0
8	U	628	0	582	51	0
9	I	598	0	612	37	0
9	V	598	0	612	36	0
10	J	441	0	439	20	0
10	W	441	0	439	22	0
11	K	384	0	366	12	0
11	X	384	0	366	15	0
12	L	386	0	388	13	0
12	Y	386	0	388	15	0
13	M	335	0	352	13	0
13	Z	335	0	352	14	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	A	6	0	0	1	0
17	N	6	0	0	3	0
18	A	120	0	108	18	0
18	N	120	0	108	15	0
19	F	1	0	0	0	0
19	S	1	0	0	0	0
All	All	28818	0	28368	1117	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 20.

The worst 5 of 1117 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)
2:O:86:MET:O	2:O:89[B]:GLU:HG2	1.20	1.32
2:B:86:MET:O	2:B:89[B]:GLU:HG2	1.32	1.27
2:B:59:GLN:HA	2:B:62:GLU:HB2	1.30	1.07
2:O:59:GLN:HA	2:O:62:GLU:HB2	1.32	1.06
3:P:12:ASN:HD22	3:P:12:ASN:H	1.02	0.99

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%)	469 (92%)	39 (8%)	4 (1%)	19	51
1	N	512/514 (100%)	470 (92%)	38 (7%)	4 (1%)	19	51
2	B	230/227 (101%)	197 (86%)	27 (12%)	6 (3%)	5	20
2	O	230/227 (101%)	197 (86%)	27 (12%)	6 (3%)	5	20
3	C	259/261 (99%)	249 (96%)	7 (3%)	3 (1%)	13	40
3	P	259/261 (99%)	248 (96%)	8 (3%)	3 (1%)	13	40
4	D	142/147 (97%)	131 (92%)	10 (7%)	1 (1%)	22	54
4	Q	142/147 (97%)	129 (91%)	12 (8%)	1 (1%)	22	54
5	E	107/109 (98%)	101 (94%)	6 (6%)	0	100	100
5	R	107/109 (98%)	103 (96%)	4 (4%)	0	100	100
6	F	96/98 (98%)	82 (85%)	7 (7%)	7 (7%)	1	3
6	S	96/98 (98%)	79 (82%)	10 (10%)	7 (7%)	1	3
7	G	82/84 (98%)	64 (78%)	13 (16%)	5 (6%)	1	4
7	T	82/84 (98%)	65 (79%)	12 (15%)	5 (6%)	1	4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	H	73/85 (86%)	61 (84%)	10 (14%)	2 (3%)	5	19
8	U	73/85 (86%)	61 (84%)	10 (14%)	2 (3%)	5	19
9	I	71/73 (97%)	67 (94%)	3 (4%)	1 (1%)	11	36
9	V	71/73 (97%)	67 (94%)	4 (6%)	0	100	100
10	J	54/59 (92%)	47 (87%)	5 (9%)	2 (4%)	3	13
10	W	54/59 (92%)	47 (87%)	5 (9%)	2 (4%)	3	13
11	K	47/56 (84%)	35 (74%)	12 (26%)	0	100	100
11	X	47/56 (84%)	36 (77%)	11 (23%)	0	100	100
12	L	45/47 (96%)	42 (93%)	3 (7%)	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%)	1 (2%)	0	100	100
All	All	3518/3612 (97%)	3169 (90%)	288 (8%)	61 (2%)	9	31

5 of 61 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	328	HIS
2	B	88[A]	ASP
2	B	88[B]	ASP
2	B	91[A]	ASN
2	B	91[B]	ASN

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	427/427 (100%)	399 (93%)	28 (7%)	16	44
1	N	427/427 (100%)	394 (92%)	33 (8%)	13	35
2	B	216/211 (102%)	192 (89%)	24 (11%)	6	19
2	O	216/211 (102%)	192 (89%)	24 (11%)	6	19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	226/226 (100%)	196 (87%)	30 (13%)	4	11
3	P	226/226 (100%)	196 (87%)	30 (13%)	4	11
4	D	128/129 (99%)	118 (92%)	10 (8%)	12	34
4	Q	128/129 (99%)	118 (92%)	10 (8%)	12	34
5	E	95/95 (100%)	89 (94%)	6 (6%)	18	46
5	R	95/95 (100%)	89 (94%)	6 (6%)	18	46
6	F	81/81 (100%)	72 (89%)	9 (11%)	6	19
6	S	81/81 (100%)	73 (90%)	8 (10%)	8	24
7	G	68/68 (100%)	59 (87%)	9 (13%)	4	12
7	T	68/68 (100%)	57 (84%)	11 (16%)	2	7
8	H	67/75 (89%)	54 (81%)	13 (19%)	1	4
8	U	67/75 (89%)	56 (84%)	11 (16%)	2	7
9	I	58/58 (100%)	52 (90%)	6 (10%)	7	22
9	V	58/58 (100%)	51 (88%)	7 (12%)	5	15
10	J	47/50 (94%)	40 (85%)	7 (15%)	3	9
10	W	47/50 (94%)	40 (85%)	7 (15%)	3	9
11	K	39/46 (85%)	35 (90%)	4 (10%)	7	22
11	X	39/46 (85%)	35 (90%)	4 (10%)	7	22
12	L	40/40 (100%)	37 (92%)	3 (8%)	13	37
12	Y	40/40 (100%)	36 (90%)	4 (10%)	7	23
13	M	37/38 (97%)	32 (86%)	5 (14%)	4	11
13	Z	37/38 (97%)	32 (86%)	5 (14%)	4	11
All	All	3058/3088 (99%)	2744 (90%)	314 (10%)	7	22

5 of 314 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	K	7	PRO
1	N	338	MET
9	V	41	GLU
12	L	15	VAL
1	N	130	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
10	J	3	ASN
1	N	368	HIS
9	V	53	ASN
12	L	42	HIS
1	N	12	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 20 ligands modelled in this entry, 12 are monoatomic - leaving 8 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	N	515	1	44,67,67	1.79	7 (15%)	37,103,103	1.97	12 (32%)
17	AZI	N	521	1	0,2,2	0.00	-	0,1,1	0.00	-
18	HEA	A	516	1,17	44,67,67	1.91	8 (18%)	37,103,103	1.75	9 (24%)
18	HEA	N	516	1,17	44,67,67	1.74	8 (18%)	37,103,103	1.79	8 (21%)
18	HEA	A	515	1	44,67,67	1.59	7 (15%)	37,103,103	2.49	14 (37%)
17	AZI	N	520	18,14	0,2,2	0.00	-	0,1,1	0.00	-
17	AZI	A	520	18,14	0,2,2	0.00	-	0,1,1	0.00	-
17	AZI	A	521	-	0,2,2	0.00	-	0,1,1	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	N	516	1,17	1/1/7/16	4/24/76/76	-
18	HEA	N	515	1	3/3/7/16	4/24/76/76	-
18	HEA	A	515	1	3/3/7/16	4/24/76/76	-
18	HEA	A	516	1,17	1/1/7/16	5/24/76/76	-

The worst 5 of 30 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	N	515	HEA	C3B-C11	-7.93	1.46	1.52
18	A	515	HEA	C3B-C11	-6.73	1.47	1.52
18	N	516	HEA	C3B-C11	-5.88	1.48	1.52
18	A	516	HEA	C3C-C2C	-5.74	1.32	1.40
18	N	516	HEA	C3C-C2C	-5.17	1.33	1.40

The worst 5 of 43 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	515	HEA	C4B-C3B-C2B	-7.64	101.53	106.87
18	N	516	HEA	C4B-C3B-C2B	-5.78	102.83	106.87
18	A	515	HEA	C1B-C2B-C3B	5.63	110.91	107.00
18	A	516	HEA	CBD-CAD-C3D	5.09	121.87	112.49
18	A	516	HEA	C4B-C3B-C2B	-4.75	103.55	106.87

5 of 8 chirality outliers are listed below:

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

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	N	516	HEA	C2D-C3D-CAD-CBD
18	N	516	HEA	C4D-C3D-CAD-CBD

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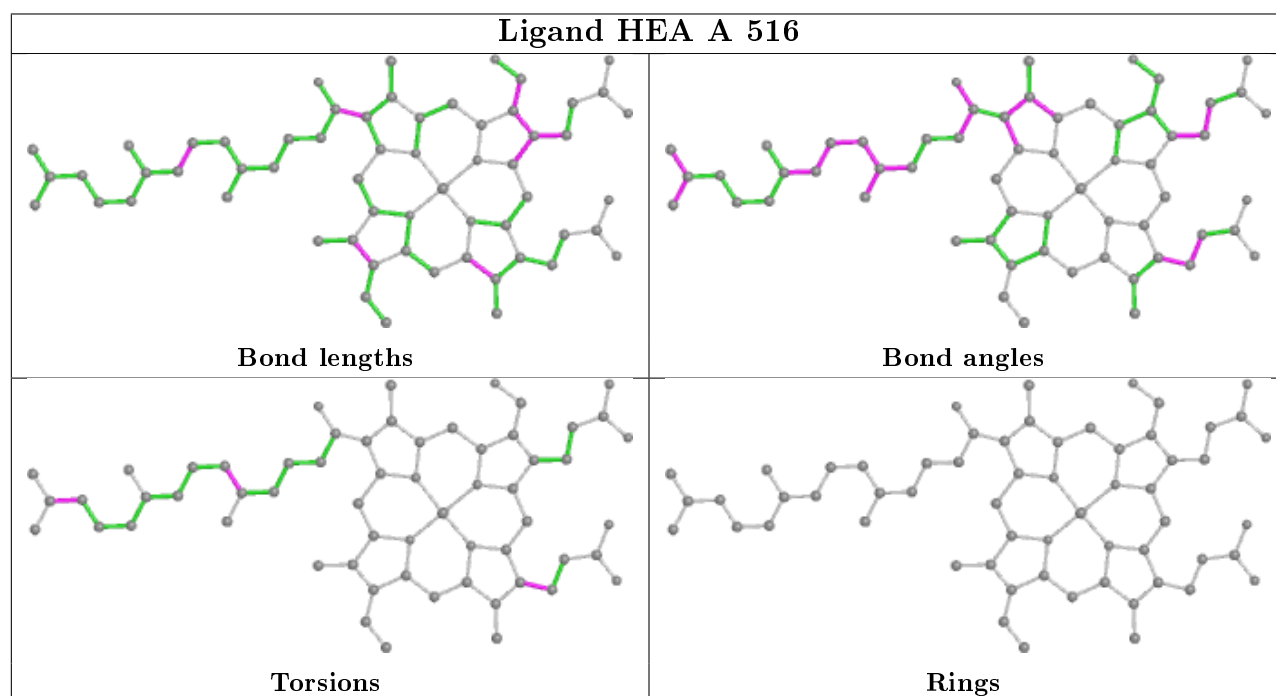
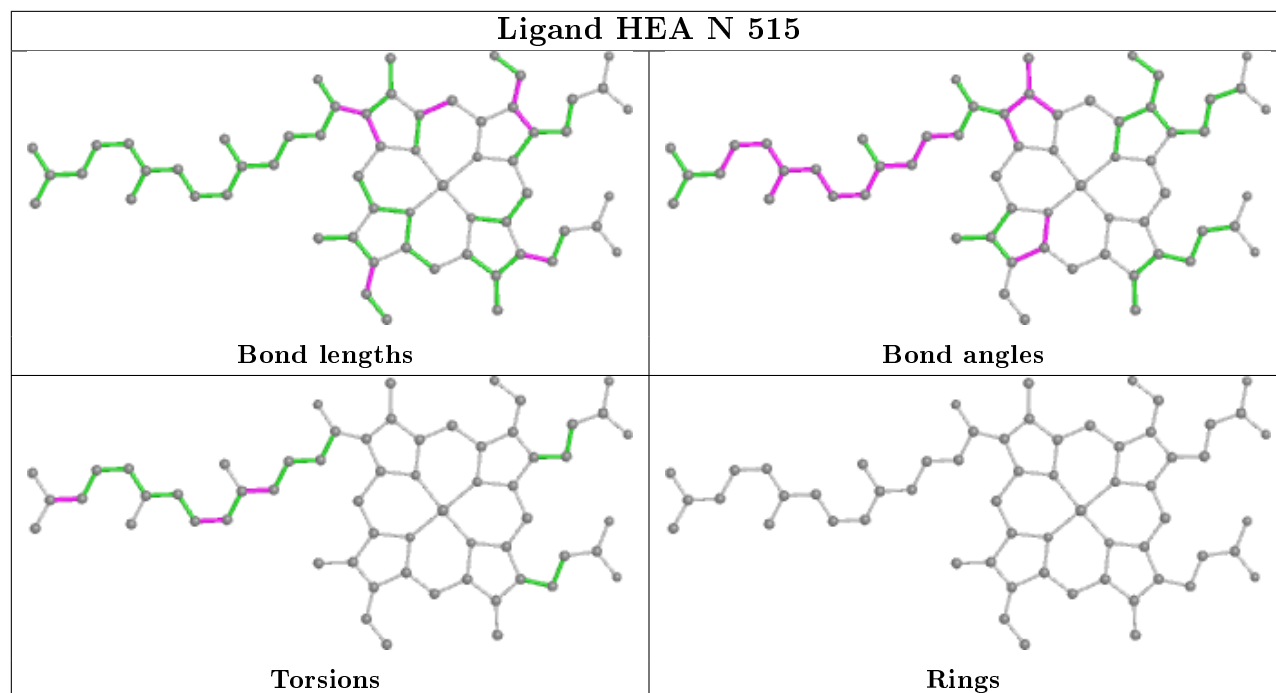
Mol	Chain	Res	Type	Atoms
18	N	516	HEA	C21-C22-C23-C25
18	A	516	HEA	C2D-C3D-CAD-CBD
18	A	516	HEA	C4D-C3D-CAD-CBD

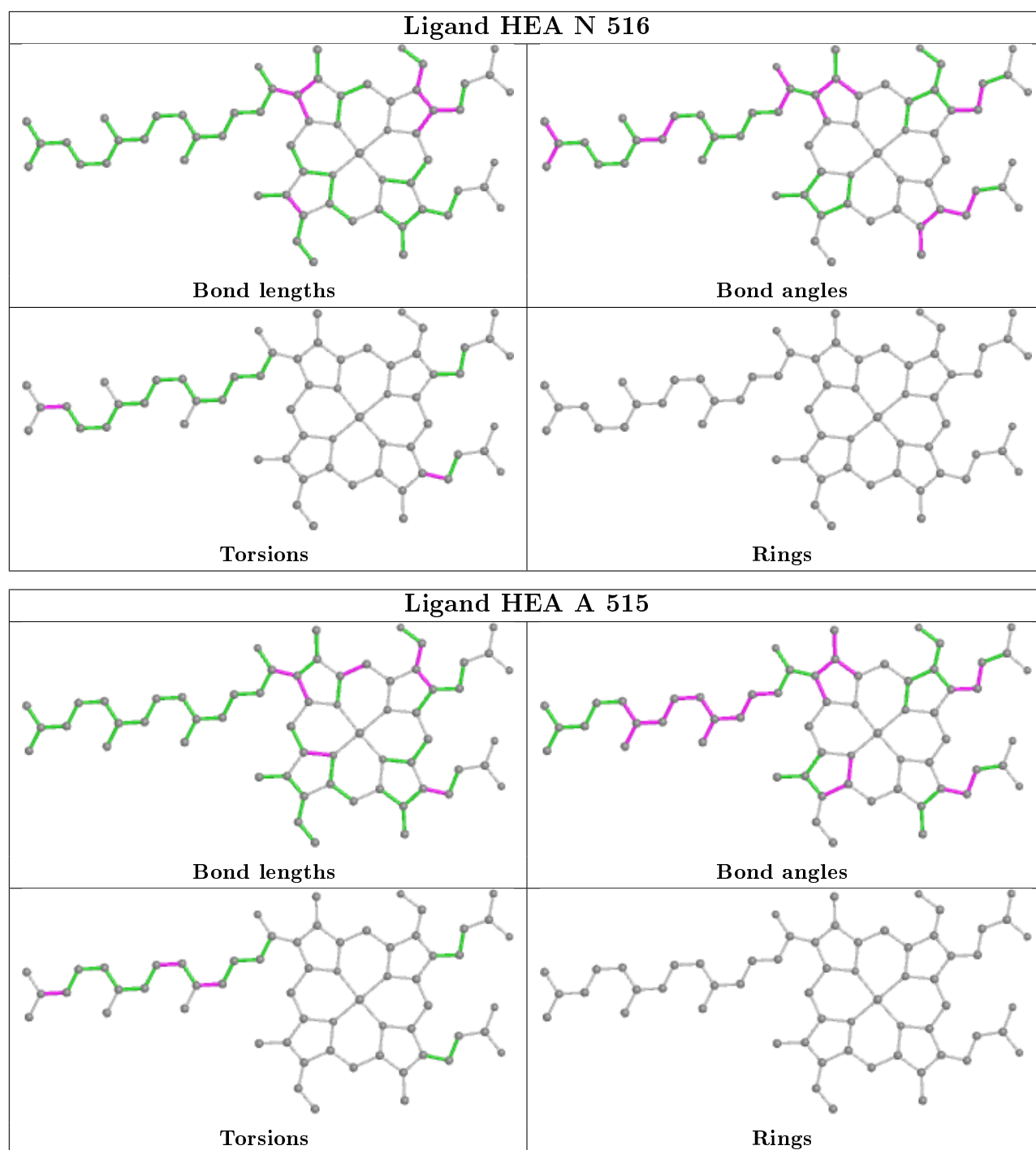
There are no ring outliers.

6 monomers are involved in 37 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	N	515	HEA	6	0
17	N	521	AZI	3	0
18	A	516	HEA	10	0
18	N	516	HEA	9	0
18	A	515	HEA	8	0
17	A	520	AZI	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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 is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.