



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jul 31, 2023 – 10:50 PM EDT

PDB ID : 2OCC  
Title : BOVINE HEART CYTOCHROME C OXIDASE AT THE FULLY OXIDIZED STATE  
Authors : Tsukihara, T.; Yao, M.  
Deposited on : 1998-05-26  
Resolution : 2.30 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](mailto: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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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)  
Xtrriage (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) : 2.34

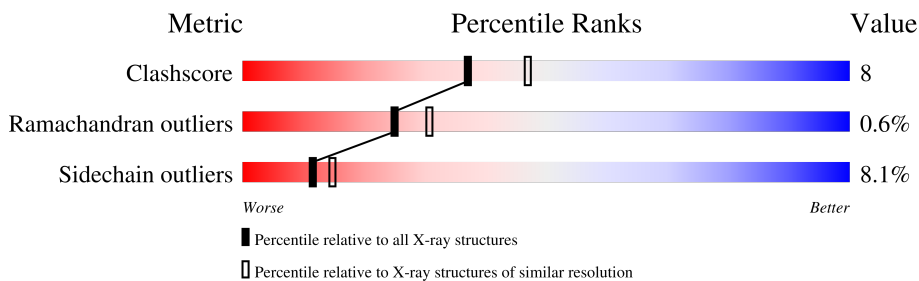
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	
1	N	514	
2	B	227	
2	O	227	
3	C	261	
3	P	261	
4	D	147	
4	Q	147	

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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	HEA	A	515	X	-	-	-
17	HEA	A	516	X	-	-	-
17	HEA	N	515	X	-	-	-
17	HEA	N	516	X	-	-	-

## 2 Entry composition [i](#)

There are 19 unique types of molecules in this entry. The entry contains 28864 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
			Total	C	N	O	S			
1	A	514	Total 4025	C 2690	N 623	O 677	S 35	0	0	0
1	N	514	Total 4025	C 2690	N 623	O 677	S 35	0	0	0

- Molecule 2 is a protein called CYTOCHROME C OXIDASE.

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

- Molecule 3 is a protein called CYTOCHROME C OXIDASE.

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

- Molecule 4 is a protein called CYTOCHROME C OXIDASE.

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

- Molecule 5 is a protein called CYTOCHROME C OXIDASE.

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.

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	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.

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	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.

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	A	1	Total	Cu	0	0
			1	1		
14	B	2	Total	Cu	0	0
			2	2		
14	N	1	Total	Cu	0	0
			1	1		
14	O	2	Total	Cu	0	0
			2	2		

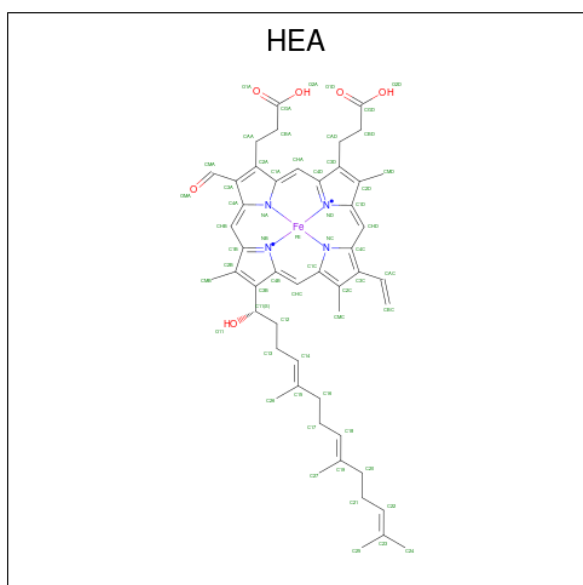
- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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).

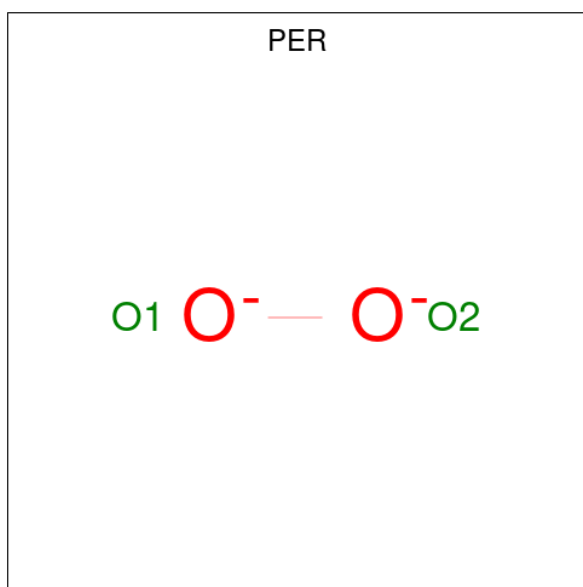
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	A	1	Total Na 1 1	0	0
16	N	1	Total Na 1 1	0	0

- Molecule 17 is HEME-A (three-letter code: HEA) (formula: C<sub>49</sub>H<sub>56</sub>FeN<sub>4</sub>O<sub>6</sub>).



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 PEROXIDE ION (three-letter code: PER) (formula: O<sub>2</sub>).



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

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

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

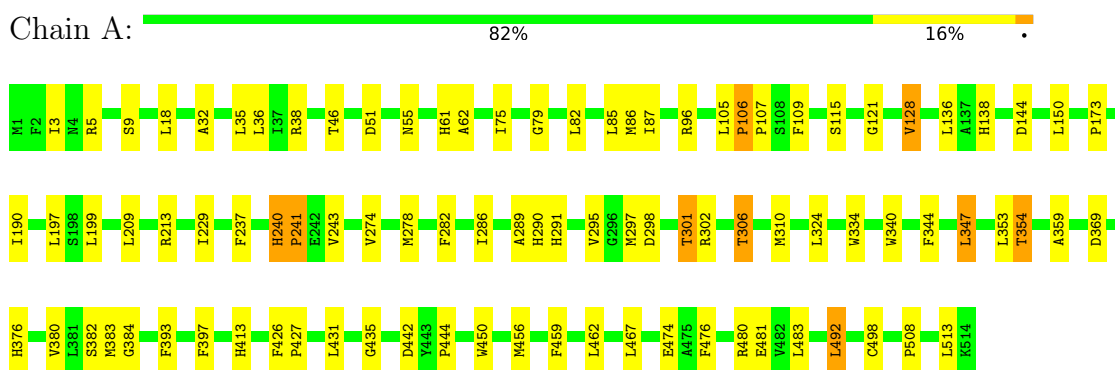


### 3 Residue-property plots [i](#)

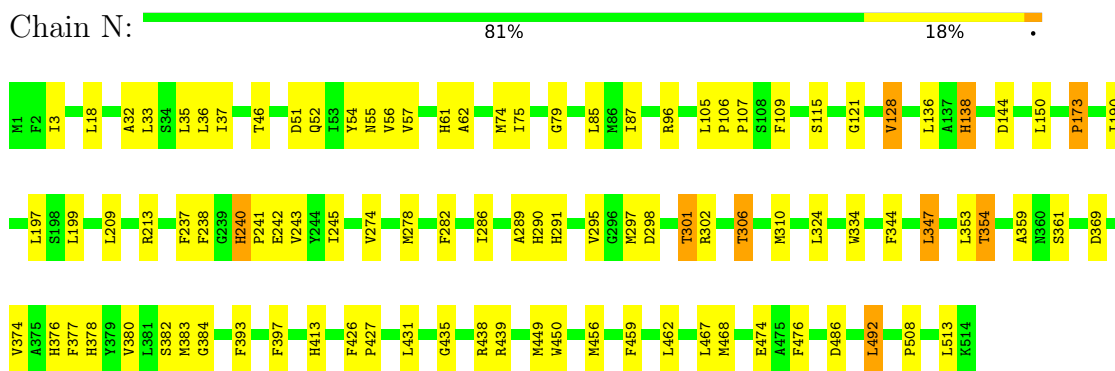
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

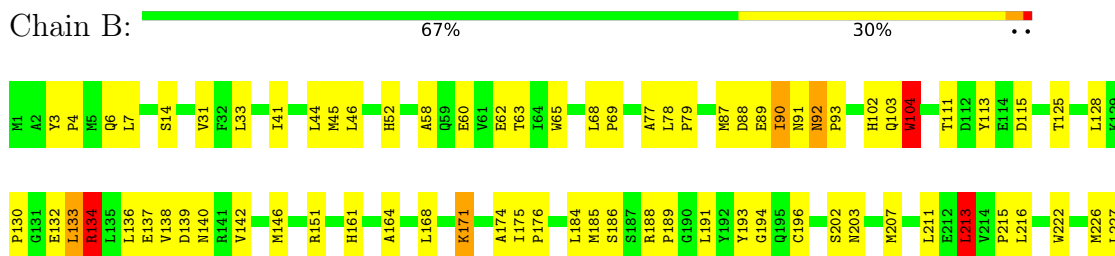
- Molecule 1: CYTOCHROME C OXIDASE



- Molecule 1: CYTOCHROME C OXIDASE

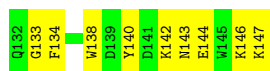


- Molecule 2: CYTOCHROME C OXIDASE

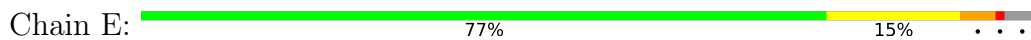


- Molecule 2: CYTOCHROME C OXIDASE





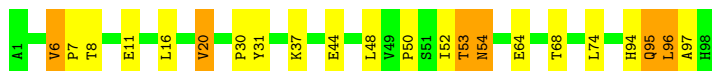
- Molecule 5: CYTOCHROME C OXIDASE



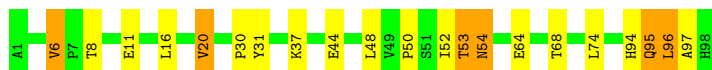
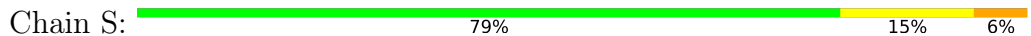
- Molecule 5: CYTOCHROME C OXIDASE



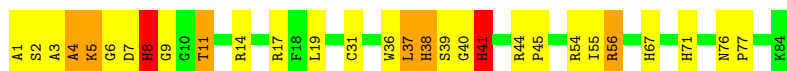
- Molecule 6: CYTOCHROME C OXIDASE



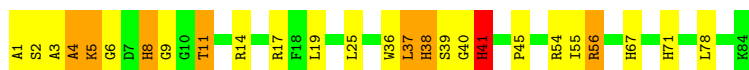
- Molecule 6: CYTOCHROME C OXIDASE



- Molecule 7: CYTOCHROME C OXIDASE

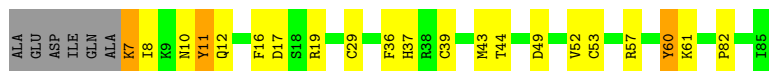


- Molecule 7: CYTOCHROME C OXIDASE



- Molecule 8: CYTOCHROME C OXIDASE

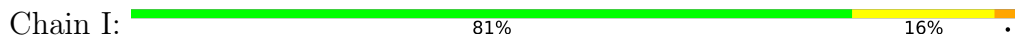




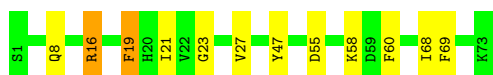
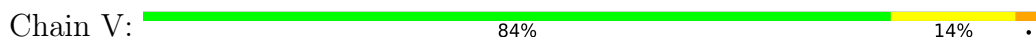
- Molecule 8: CYTOCHROME C OXIDASE



- Molecule 9: CYTOCHROME C OXIDASE



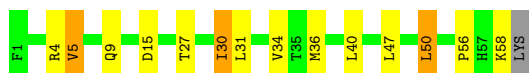
- Molecule 9: CYTOCHROME C OXIDASE



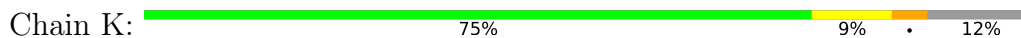
- Molecule 10: CYTOCHROME C OXIDASE



- Molecule 10: CYTOCHROME C OXIDASE



- Molecule 11: CYTOCHROME C OXIDASE

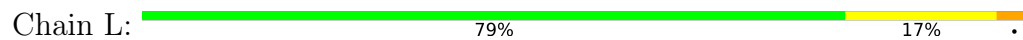


- Molecule 11: CYTOCHROME C OXIDASE

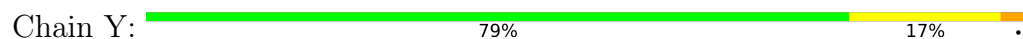




- Molecule 12: CYTOCHROME C OXIDASE



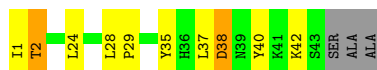
- Molecule 12: CYTOCHROME C OXIDASE



- Molecule 13: CYTOCHROME C OXIDASE



- Molecule 13: CYTOCHROME C OXIDASE



## 4 Data and refinement statistics

Xtrriage (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, $\alpha$ , $\beta$ , $\gamma$	189.10Å 210.50Å 178.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.30	Depositor
% Data completeness (in resolution range)	88.9 (15.00-2.30)	Depositor
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR 3.84	Depositor
R, $R_{free}$	0.209 , 0.244	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	28864	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	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: NA, ZN, PER, MG, CU, HEA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.72	1/4164 (0.0%)	0.80	2/5688 (0.0%)
1	N	0.62	1/4164 (0.0%)	0.77	2/5688 (0.0%)
2	B	0.70	0/1909	0.91	5/2601 (0.2%)
2	O	0.64	0/1909	0.89	3/2601 (0.1%)
3	C	0.68	0/2211	0.71	1/3023 (0.0%)
3	P	0.61	0/2211	0.70	1/3023 (0.0%)
4	D	0.63	0/1229	0.72	1/1658 (0.1%)
4	Q	0.60	0/1229	0.70	1/1658 (0.1%)
5	E	0.62	0/871	0.71	1/1182 (0.1%)
5	R	0.55	0/871	0.70	1/1182 (0.1%)
6	F	0.63	0/765	0.79	0/1038
6	S	0.60	0/765	0.79	0/1038
7	G	0.80	1/699 (0.1%)	0.84	1/950 (0.1%)
7	T	0.74	0/699	0.84	1/950 (0.1%)
8	H	0.63	0/682	0.69	0/921
8	U	0.60	0/682	0.67	0/921
9	I	0.70	0/611	0.69	0/810
9	V	0.65	0/611	0.67	0/810
10	J	0.66	0/471	0.69	0/636
10	W	0.65	0/471	0.69	0/636
11	K	0.70	0/398	0.75	0/546
11	X	0.60	0/398	0.72	0/546
12	L	0.75	0/399	0.64	0/534
12	Y	0.65	0/399	0.63	0/534
13	M	0.63	0/345	0.70	0/470
13	Z	0.59	0/345	0.70	0/470
All	All	0.66	3/29508 (0.0%)	0.76	20/40114 (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	1
2	O	0	1
3	C	0	1
3	P	0	1
4	D	0	1
4	Q	0	1
8	H	0	1
8	U	0	1
All	All	0	9

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	31	CYS	CB-SG	-5.89	1.72	1.81
1	N	61	HIS	CG-CD2	5.13	1.44	1.35
1	A	498	CYS	CB-SG	-5.00	1.73	1.81

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	Q	133	GLY	N-CA-C	7.12	130.91	113.10
4	D	133	GLY	N-CA-C	7.06	130.74	113.10
5	E	41	LEU	CA-CB-CG	6.75	130.83	115.30
1	A	480	ARG	NE-CZ-NH2	-6.70	116.95	120.30
2	O	103	GLN	CA-C-N	-6.54	102.80	117.20

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	240	HIS	Sidechain
3	C	182	TYR	Sidechain
4	D	140	TYR	Sidechain
8	H	11	TYR	Sidechain
1	N	240	HIS	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	4025	0	4002	62	0
1	N	4025	0	4002	66	0
2	B	1863	0	1867	48	0
2	O	1863	0	1867	45	0
3	C	2124	0	2044	28	0
3	P	2124	0	2044	28	0
4	D	1195	0	1183	35	0
4	Q	1195	0	1183	39	0
5	E	852	0	845	17	0
5	R	852	0	845	18	0
6	F	748	0	728	15	0
6	S	748	0	728	13	0
7	G	672	0	645	18	0
7	T	672	0	645	16	0
8	H	662	0	623	13	0
8	U	662	0	623	13	0
9	I	598	0	612	11	0
9	V	598	0	612	9	0
10	J	460	0	459	5	0
10	W	460	0	459	7	0
11	K	384	0	366	8	0
11	X	384	0	366	10	0
12	L	386	0	388	7	0
12	Y	386	0	388	8	0
13	M	335	0	352	8	0
13	Z	335	0	352	9	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	120	0	108	5	0
17	N	120	0	108	4	0
18	A	2	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	N	2	0	0	1	0
19	F	1	0	0	0	0
19	S	1	0	0	0	0
All	All	28864	0	28444	443	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 8.

The worst 5 of 443 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)
18:A:520:PER:O2	18:A:520:PER:O1	1.69	1.11
18:N:520:PER:O1	18:N:520:PER:O2	1.63	1.11
3:P:2:THR:HG23	6:S:96:LEU:HD12	1.58	0.85
3:C:2:THR:HG23	6:F:96:LEU:HD12	1.61	0.82
1:N:306:THR:HB	1:N:359:ALA:O	1.82	0.79

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%)	494 (96%)	18 (4%)	0	100	100
1	N	512/514 (100%)	495 (97%)	17 (3%)	0	100	100
2	B	230/227 (101%)	208 (90%)	20 (9%)	2 (1%)	17	20
2	O	230/227 (101%)	208 (90%)	20 (9%)	2 (1%)	17	20
3	C	259/261 (99%)	252 (97%)	6 (2%)	1 (0%)	34	42
3	P	259/261 (99%)	252 (97%)	6 (2%)	1 (0%)	34	42
4	D	142/147 (97%)	138 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	Q	142/147 (97%)	137 (96%)	5 (4%)	0	100	100
5	E	103/109 (94%)	101 (98%)	2 (2%)	0	100	100
5	R	103/109 (94%)	101 (98%)	2 (2%)	0	100	100
6	F	96/98 (98%)	91 (95%)	3 (3%)	2 (2%)	7	5
6	S	96/98 (98%)	91 (95%)	3 (3%)	2 (2%)	7	5
7	G	82/84 (98%)	65 (79%)	12 (15%)	5 (6%)	1	0
7	T	82/84 (98%)	66 (80%)	11 (13%)	5 (6%)	1	0
8	H	77/85 (91%)	72 (94%)	5 (6%)	0	100	100
8	U	77/85 (91%)	72 (94%)	5 (6%)	0	100	100
9	I	71/73 (97%)	68 (96%)	3 (4%)	0	100	100
9	V	71/73 (97%)	68 (96%)	3 (4%)	0	100	100
10	J	56/59 (95%)	54 (96%)	1 (2%)	1 (2%)	8	7
10	W	56/59 (95%)	55 (98%)	0	1 (2%)	8	7
11	K	47/56 (84%)	43 (92%)	4 (8%)	0	100	100
11	X	47/56 (84%)	42 (89%)	5 (11%)	0	100	100
12	L	45/47 (96%)	44 (98%)	1 (2%)	0	100	100
12	Y	45/47 (96%)	44 (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	3522/3612 (98%)	3343 (95%)	157 (4%)	22 (1%)	25	31

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	G	4	ALA
2	O	134	ARG
7	T	4	ALA
2	B	104	TRP
2	B	134	ARG

### 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%)	402 (94%)	25 (6%)	19	27
1	N	427/427 (100%)	401 (94%)	26 (6%)	18	25
2	B	216/211 (102%)	193 (89%)	23 (11%)	6	7
2	O	216/211 (102%)	195 (90%)	21 (10%)	8	9
3	C	226/226 (100%)	209 (92%)	17 (8%)	13	17
3	P	226/226 (100%)	208 (92%)	18 (8%)	12	15
4	D	128/129 (99%)	120 (94%)	8 (6%)	18	24
4	Q	128/129 (99%)	120 (94%)	8 (6%)	18	24
5	E	92/95 (97%)	85 (92%)	7 (8%)	13	16
5	R	92/95 (97%)	85 (92%)	7 (8%)	13	16
6	F	81/81 (100%)	71 (88%)	10 (12%)	4	5
6	S	81/81 (100%)	71 (88%)	10 (12%)	4	5
7	G	68/68 (100%)	59 (87%)	9 (13%)	4	4
7	T	68/68 (100%)	58 (85%)	10 (15%)	3	3
8	H	71/75 (95%)	65 (92%)	6 (8%)	10	13
8	U	71/75 (95%)	65 (92%)	6 (8%)	10	13
9	I	58/58 (100%)	55 (95%)	3 (5%)	23	32
9	V	58/58 (100%)	55 (95%)	3 (5%)	23	32
10	J	49/50 (98%)	42 (86%)	7 (14%)	3	3
10	W	49/50 (98%)	42 (86%)	7 (14%)	3	3
11	K	39/46 (85%)	37 (95%)	2 (5%)	24	33
11	X	39/46 (85%)	37 (95%)	2 (5%)	24	33
12	L	40/40 (100%)	35 (88%)	5 (12%)	4	5
12	Y	40/40 (100%)	35 (88%)	5 (12%)	4	5
13	M	37/38 (97%)	33 (89%)	4 (11%)	6	7
13	Z	37/38 (97%)	33 (89%)	4 (11%)	6	7
All	All	3064/3088 (99%)	2811 (92%)	253 (8%)	11	14

5 of 253 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	K	43	SER
7	T	39	SER
1	N	347	LEU
7	T	36	TRP
10	W	5	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
6	S	54	ASN
7	T	71	HIS
1	N	55	ASN
1	N	413	HIS
1	N	503	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 monosaccharides 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
17	HEA	N	516	1,18	57,67,67	1.28	6 (10%)	61,103,103	1.68	14 (22%)
17	HEA	A	516	1,18	57,67,67	1.56	7 (12%)	61,103,103	1.89	15 (24%)
17	HEA	A	515	1	57,67,67	1.34	8 (14%)	61,103,103	1.44	9 (14%)
18	PER	N	520	17,14	0,1,1	-	-	-	-	-
17	HEA	N	515	1	57,67,67	1.18	6 (10%)	61,103,103	1.46	8 (13%)
18	PER	A	520	17,14	0,1,1	-	-	-	-	-

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	N	515	1	2/2/7/16	9/32/76/76	-
17	HEA	A	516	1,18	2/2/7/16	2/32/76/76	-
17	HEA	A	515	1	2/2/7/16	9/32/76/76	-
17	HEA	N	516	1,18	2/2/7/16	4/32/76/76	-

The worst 5 of 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	516	HEA	C3C-C2C	-4.40	1.34	1.40
17	A	516	HEA	C3A-CMA	-4.26	1.36	1.46
17	A	516	HEA	C3A-C2A	-3.69	1.35	1.40
17	A	516	HEA	C4B-NB	3.67	1.46	1.40
17	A	515	HEA	C3A-CMA	-3.61	1.38	1.46

The worst 5 of 46 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	516	HEA	C4B-NB-C1B	-5.57	99.32	105.07
17	N	515	HEA	C13-C14-C15	-5.50	114.41	127.66
17	A	515	HEA	C13-C14-C15	-5.06	115.47	127.66
17	N	516	HEA	C1D-C2D-C3D	-4.24	102.50	106.96
17	A	516	HEA	C2D-C1D-ND	4.22	114.84	109.84

5 of 8 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
17	A	515	HEA	NB

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

5 of 24 torsion outliers are listed below:

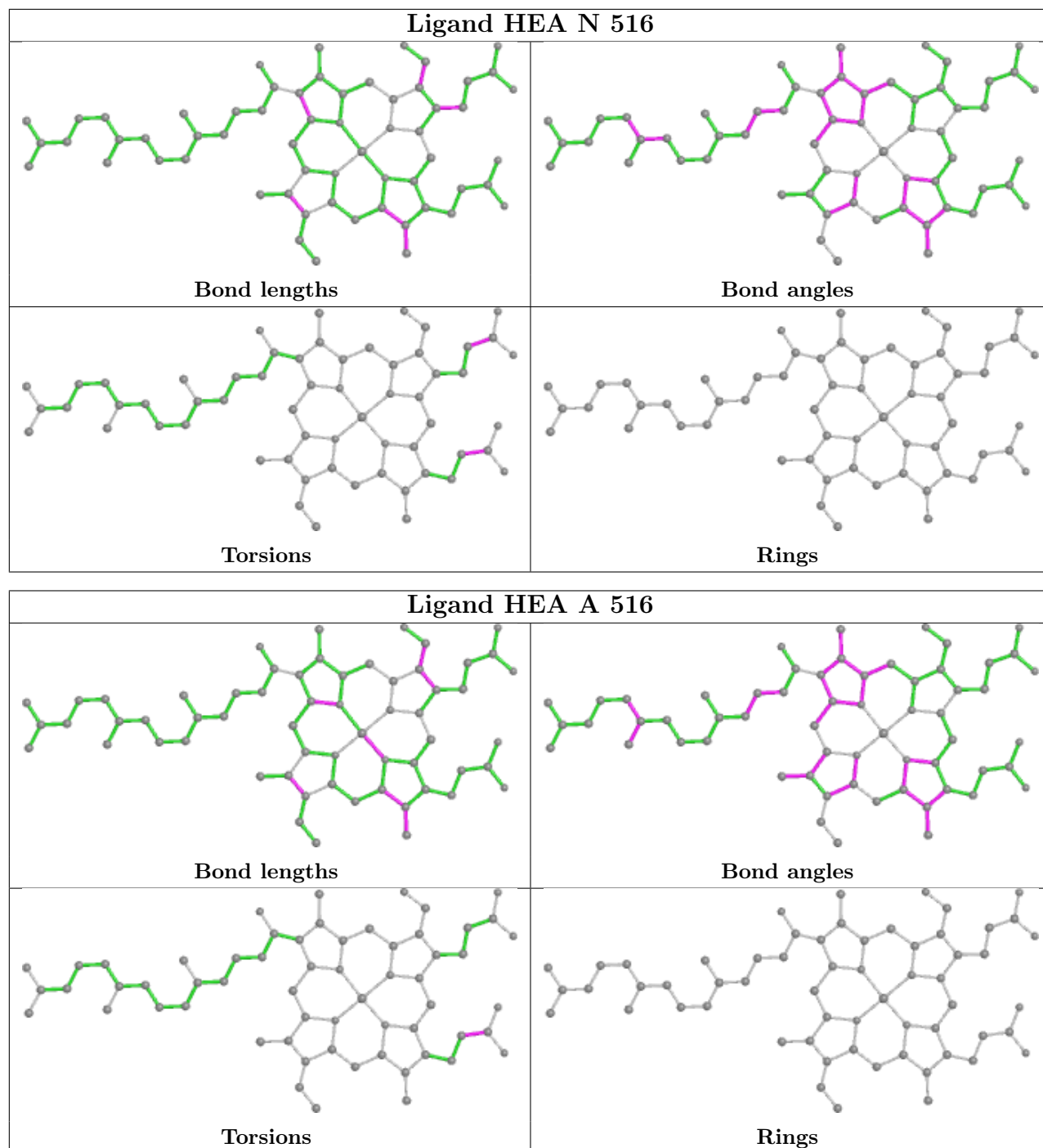
Mol	Chain	Res	Type	Atoms
17	N	515	HEA	C12-C11-C3B-C2B
17	A	515	HEA	C15-C16-C17-C18
17	N	515	HEA	C15-C16-C17-C18
17	A	515	HEA	C26-C15-C16-C17
17	N	515	HEA	C26-C15-C16-C17

There are no ring outliers.

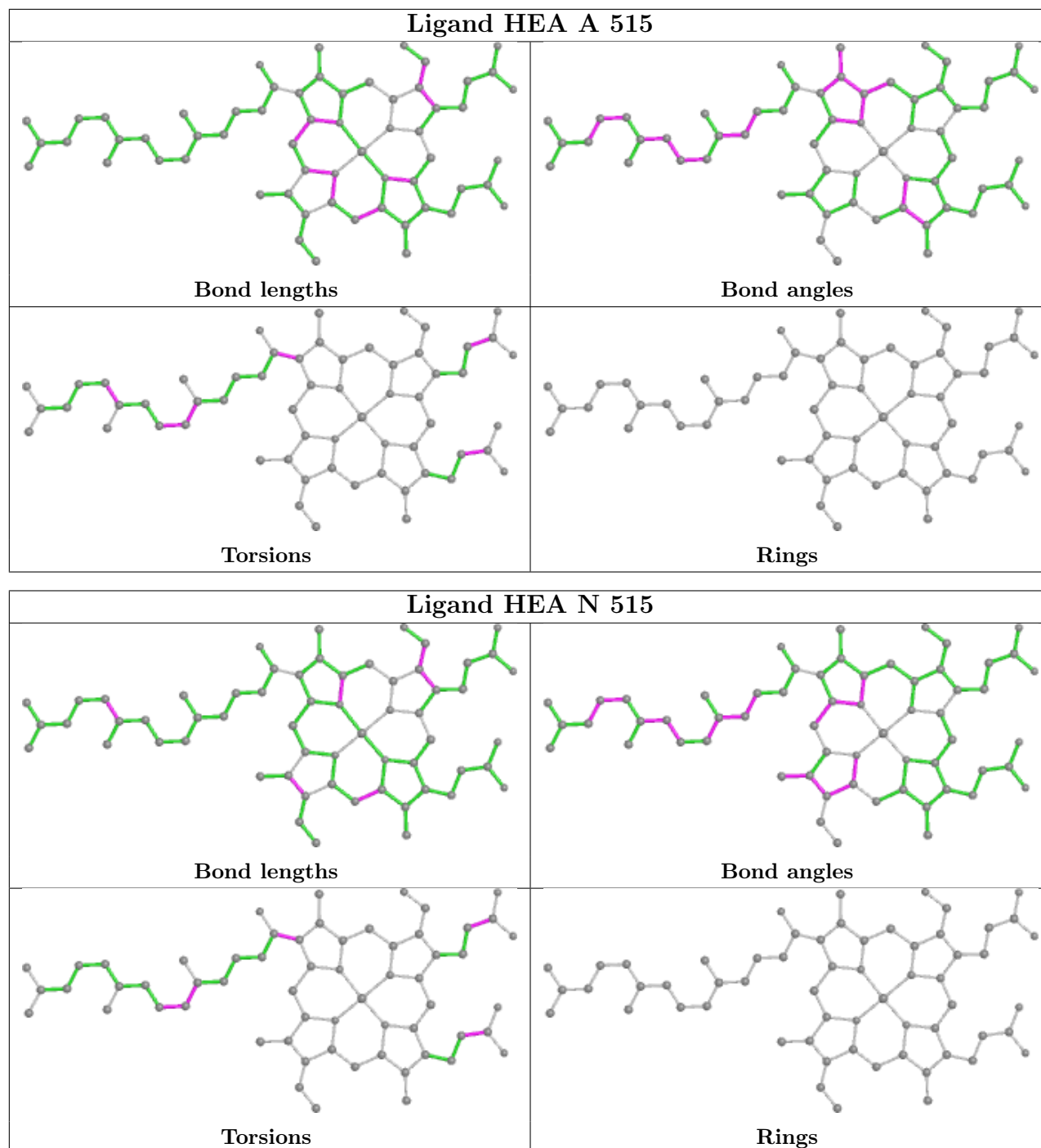
5 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	N	516	HEA	1	0
17	A	515	HEA	5	0
18	N	520	PER	1	0
17	N	515	HEA	3	0
18	A	520	PER	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.