



wwPDB X-ray Structure Validation Summary Report ⓘ

May 17, 2020 – 03:44 pm BST

PDB ID : 1AR1
Title : Structure at 2.7 Angstrom Resolution of the Paracoccus Denitrificans two-subunit Cytochrome C Oxidase Complexed with an Antibody Fv Fragment
Authors : Ostermeier, C.; Harrenga, A.; Ermler, U.; Michel, H.
Deposited on : 1997-08-08
Resolution : 2.70 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

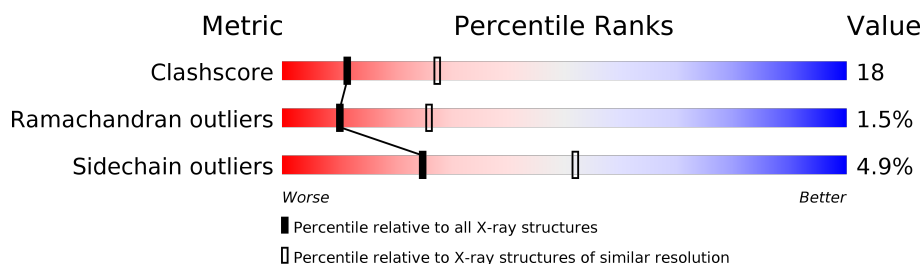
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)

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	558	
2	B	298	
3	C	127	
4	D	120	

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
8	HEA	A	562	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	HEA	A	563	X	-	-	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 8243 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	529	Total	C	N	O	S	0	0	0
			4183	2807	654	689	33			

- Molecule 2 is a protein called CYTOCHROME C OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	252	Total	C	N	O	S	0	0	0
			1976	1295	319	354	8			

- Molecule 3 is a protein called ANTIBODY FV FRAGMENT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	118	Total	C	N	O	S	0	0	0
			932	586	156	184	6			

- Molecule 4 is a protein called ANTIBODY FV FRAGMENT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	108	Total	C	N	O	S	0	0	0
			831	530	135	164	2			

- Molecule 5 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	2	Total	Cu	0	0
			2	2		
5	A	1	Total	Cu	0	0
			1	1		

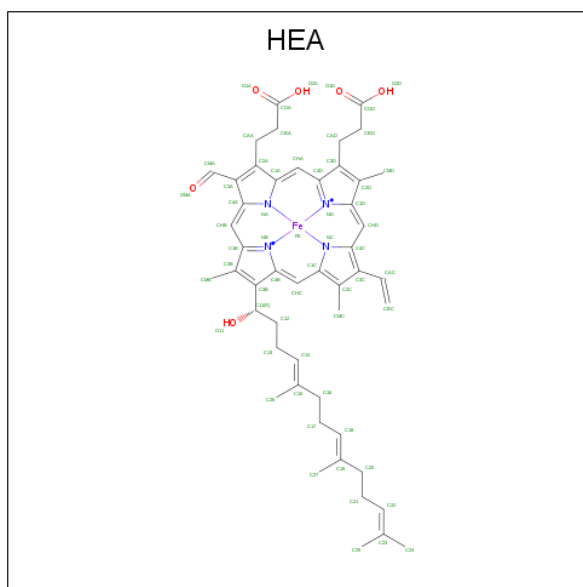
- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Mg 1 1	0	0

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

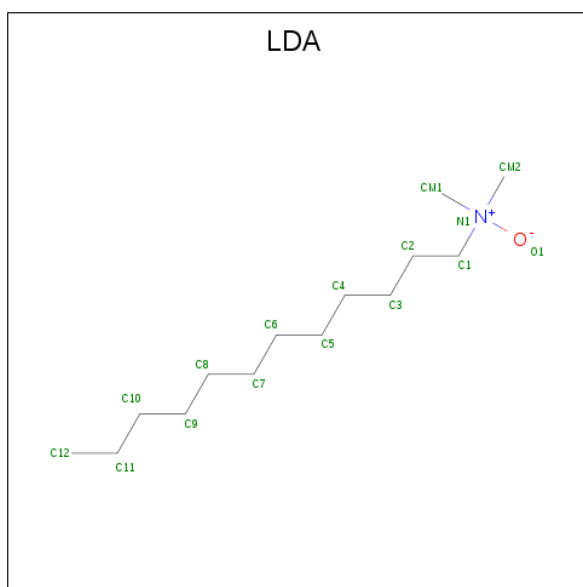
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Ca 1 1	0	0

- Molecule 8 is HEME-A (three-letter code: HEA) (formula: C₄₉H₅₆FeN₄O₆).



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

- Molecule 9 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: C₁₄H₃₁NO).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	1	Total	C	N	O	0	0
			16	14	1	1		
9	A	1	Total	C	N	O	0	0
			16	14	1	1		
9	A	1	Total	C	N	O	0	0
			16	14	1	1		
9	A	1	Total	C	N	O	0	0
			16	14	1	1		
9	A	1	Total	C	N	O	0	0
			16	14	1	1		
9	A	1	Total	C	N	O	0	0
			16	14	1	1		
9	B	1	Total	C	N	O	0	0
			16	14	1	1		
9	B	1	Total	C	N	O	0	0
			16	14	1	1		
9	B	1	Total	C	N	O	0	0
			16	14	1	1		

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	21	Total	O	0	0
			21	21		
10	B	21	Total	O	0	0
			21	21		
10	C	5	Total	O	0	0
			5	5		

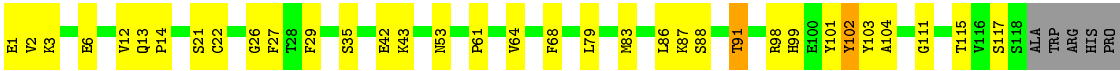
Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	D	5	Total	O	0	0
			5	5		

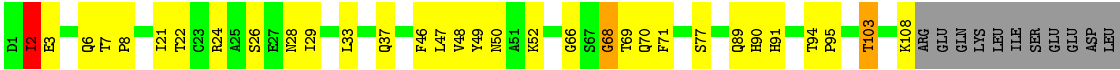
VAL
LYS
LEU
ALA
SER
ALA
GLU

● Molecule 3: ANTIBODY FV FRAGMENT



GLN
PHE
GLY
GLY

● Molecule 4: ANTIBODY FV FRAGMENT



MET

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	93.50 Å 151.00 Å 156.70 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.70	Depositor
% Data completeness (in resolution range)	93.1 (30.00-2.70)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.207 , 0.261	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8243	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, LDA, CA, 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	0.51	0/4339	0.64	0/5923
2	B	0.52	0/2033	0.69	0/2787
3	C	0.47	0/954	0.65	0/1291
4	D	0.48	0/852	0.62	0/1156
All	All	0.51	0/8178	0.66	0/11157

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	280	TYR	Sidechain
1	A	339	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	4183	0	4103	182	0
2	B	1976	0	1963	67	0
3	C	932	0	889	23	0
4	D	831	0	807	23	0
5	A	1	0	0	0	0
5	B	2	0	0	0	0
6	A	1	0	0	0	0
7	A	1	0	0	0	0
8	A	120	0	108	20	0
9	A	96	0	186	4	0
9	B	48	0	93	5	0
10	A	21	0	0	2	0
10	B	21	0	0	1	0
10	C	5	0	0	1	0
10	D	5	0	0	0	0
All	All	8243	0	8149	287	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 18.

The worst 5 of 287 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)
1:A:153:GLY:HA2	1:A:176:GLY:H	1.23	1.03
1:A:23:PHE:HB3	1:A:136:TRP:HZ2	1.35	0.91
8:A:562:HEA:HBC1	8:A:562:HEA:HMC1	1.56	0.88
4:D:50:ASN:H	4:D:91:HIS:HE1	1.24	0.86
1:A:300:LYS:HD2	1:A:364:GLY:HA3	1.57	0.85

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	527/558 (94%)	478 (91%)	43 (8%)	6 (1%)	14	34
2	B	250/298 (84%)	223 (89%)	22 (9%)	5 (2%)	7	19
3	C	116/127 (91%)	111 (96%)	4 (3%)	1 (1%)	17	40
4	D	106/120 (88%)	96 (91%)	7 (7%)	3 (3%)	5	11
All	All	999/1103 (91%)	908 (91%)	76 (8%)	15 (2%)	10	26

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	365	GLY
2	B	120	GLN
1	A	175	ALA
1	A	207	MET
2	B	154	TYR

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	432/454 (95%)	411 (95%)	21 (5%)	25	52
2	B	211/243 (87%)	203 (96%)	8 (4%)	33	62
3	C	101/107 (94%)	98 (97%)	3 (3%)	41	70
4	D	92/104 (88%)	83 (90%)	9 (10%)	8	18
All	All	836/908 (92%)	795 (95%)	41 (5%)	25	52

5 of 41 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	408	VAL
2	B	3	VAL
4	D	52	LYS
1	A	499	SER
1	A	518	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	518	ASN
2	B	21	GLN
2	B	215	GLN
1	A	486	ASN
2	B	208	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 16 ligands modelled in this entry, 5 are monoatomic - leaving 11 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	$\# Z > 2$
9	LDA	B	272	-	12,15,15	2.26	1 (8%)	14,17,17	0.62	0
8	HEA	A	563	1	44,67,67	1.51	8 (18%)	37,103,103	1.10	3 (8%)
9	LDA	A	564	-	12,15,15	2.28	1 (8%)	14,17,17	0.82	1 (7%)
9	LDA	A	569	-	12,15,15	2.35	1 (8%)	14,17,17	0.75	0
9	LDA	B	273	-	12,15,15	2.10	1 (8%)	14,17,17	0.34	0
8	HEA	A	562	1	44,67,67	1.52	8 (18%)	37,103,103	1.18	5 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	LDA	A	567	-	12,15,15	2.41	1 (8%)	14,17,17	0.42	0
9	LDA	A	568	-	12,15,15	1.81	1 (8%)	14,17,17	0.55	0
9	LDA	A	566	-	12,15,15	2.38	1 (8%)	14,17,17	0.50	0
9	LDA	B	274	-	12,15,15	1.93	1 (8%)	14,17,17	0.64	0
9	LDA	A	565	-	12,15,15	2.48	1 (8%)	14,17,17	0.58	0

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
9	LDA	B	272	-	-	1/13/13/13	-
8	HEA	A	563	1	3/3/7/16	6/24/76/76	-
9	LDA	A	564	-	-	0/13/13/13	-
9	LDA	A	569	-	-	0/13/13/13	-
9	LDA	B	273	-	-	3/13/13/13	-
8	HEA	A	562	1	3/3/7/16	5/24/76/76	-
9	LDA	A	567	-	-	1/13/13/13	-
9	LDA	A	568	-	-	4/13/13/13	-
9	LDA	A	566	-	-	1/13/13/13	-
9	LDA	B	274	-	-	0/13/13/13	-
9	LDA	A	565	-	-	0/13/13/13	-

The worst 5 of 25 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	565	LDA	O1-N1	-8.53	1.22	1.42
9	A	567	LDA	O1-N1	-8.16	1.23	1.42
9	A	566	LDA	O1-N1	-8.01	1.23	1.42
9	B	272	LDA	O1-N1	-7.76	1.24	1.42
9	A	564	LDA	O1-N1	-7.75	1.24	1.42

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	563	HEA	C3C-C4C-NC	2.79	112.81	109.21
8	A	562	HEA	C17-C18-C19	-2.75	121.03	127.66
9	A	564	LDA	C12-C11-C10	2.50	132.42	113.42
8	A	562	HEA	C13-C14-C15	-2.29	122.13	127.66

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	562	HEA	C1B-C2B-C3B	-2.19	105.47	107.00

5 of 6 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
8	A	563	HEA	ND
8	A	563	HEA	NA
8	A	563	HEA	NB
8	A	562	HEA	ND
8	A	562	HEA	NA

5 of 21 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	563	HEA	C15-C16-C17-C18
8	A	563	HEA	C21-C22-C23-C25
9	B	273	LDA	C2-C1-N1-CM2
8	A	563	HEA	C21-C22-C23-C24
8	A	563	HEA	C27-C19-C20-C21

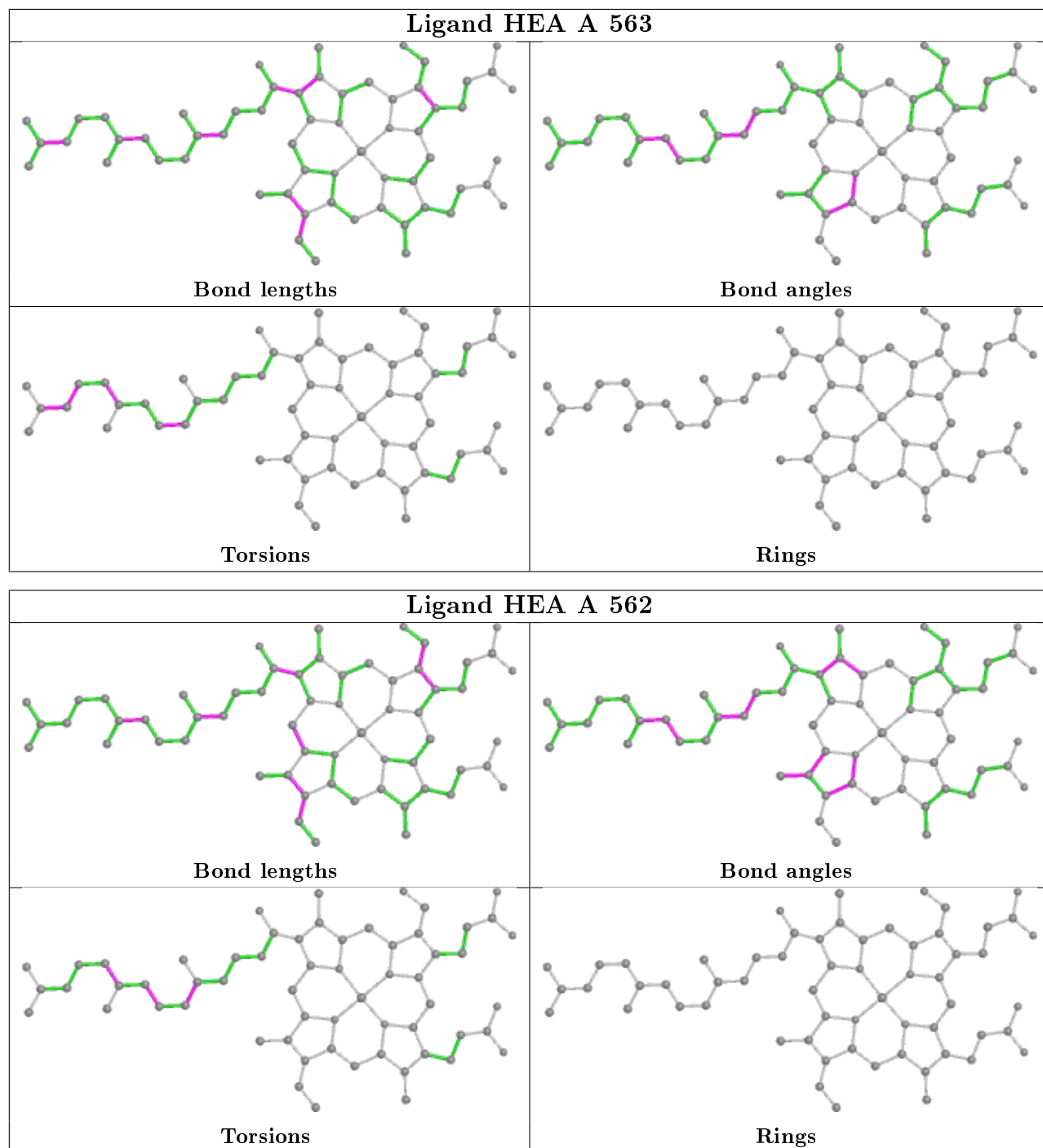
There are no ring outliers.

8 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	272	LDA	2	0
8	A	563	HEA	13	0
9	A	569	LDA	1	0
9	B	273	LDA	1	0
8	A	562	HEA	7	0
9	A	566	LDA	2	0
9	B	274	LDA	2	0
9	A	565	LDA	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 ⓘ

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.