



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 03:40 PM UTC

PDB ID : 1OCR / pdb_00001ocr
Title : BOVINE HEART CYTOCHROME C OXIDASE IN THE FULLY REDUCED STATE
Authors : Tsukihara, T.; Yao, M.
Deposited on : 1998-07-07
Resolution : 2.35 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 types of validation reports are described at

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

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

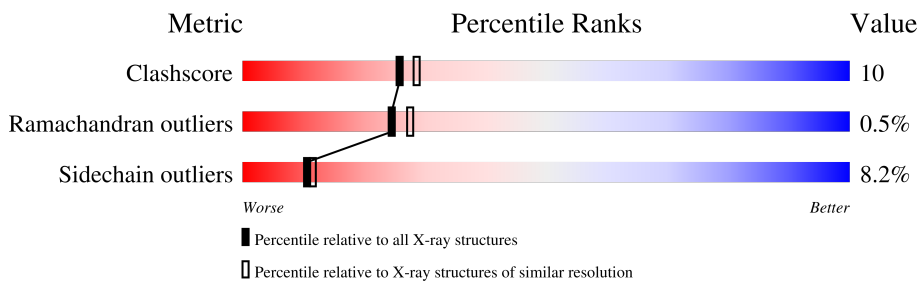
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)











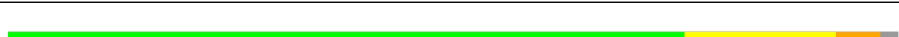


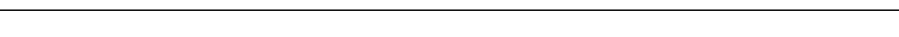
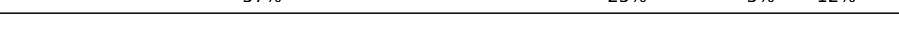
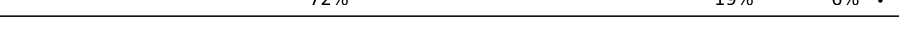

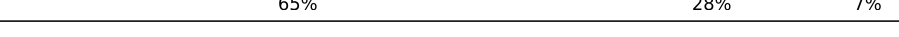
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	 79% 18%
5	R	109	 74% 22%
6	F	98	 70% 24% 5%
6	S	98	 70% 23% 6%
7	G	84	 65% 24% 8%
7	T	84	 64% 26% 7%
8	H	85	 67% 24% 7%
8	U	85	 68% 22% 7%
9	I	73	 79% 19%
9	V	73	 70% 29%
10	J	59	 76% 17% 5%
10	W	59	 73% 20% 5%
11	K	56	 62% 20% 5% 12%
11	X	56	 57% 25% 5% 12%
12	L	47	 72% 19% 6%
12	Y	47	 68% 23% 6%
13	M	46	 65% 28% 7%
13	Z	46	 63% 30% 7%

2 Entry composition [i](#)

There are 18 unique types of molecules in this entry. The entry contains 28926 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	4025	2690	623	677	35	0	0	0
1	N	514	4025	2690	623	677	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	1870	1212	289	351	18	0	6	0
2	O	227	1870	1212	289	351	18	0	6	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	2124	1420	338	353	13	0	0	0
3	P	261	2124	1420	338	353	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	1195	777	196	218	4	0	0	0
4	Q	144	1195	777	196	218	4	0	0	0

- 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	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 (CCD ID: 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		

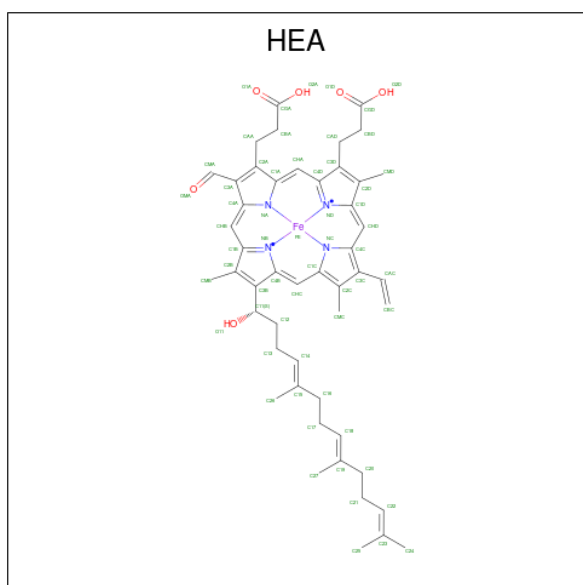
- Molecule 15 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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 (CCD ID: 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 (CCD ID: HEA) (formula: C₄₉H₅₆FeN₄O₆).



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 ZINC ION (CCD ID: ZN) (formula: Zn).

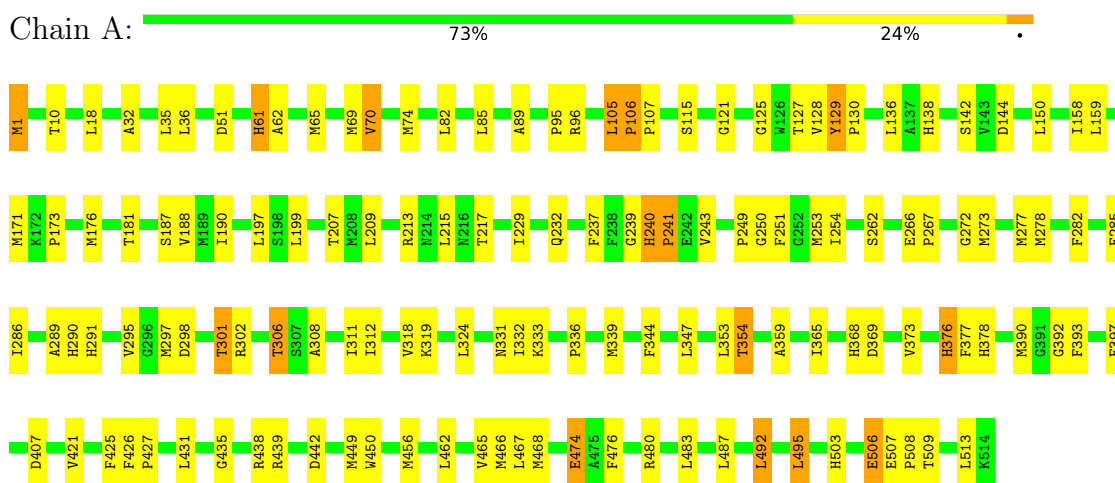
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	F	1	Total 1	Zn 1	0	0
18	S	1	Total 1	Zn 1	0	0

3 Residue-property plots [i](#)

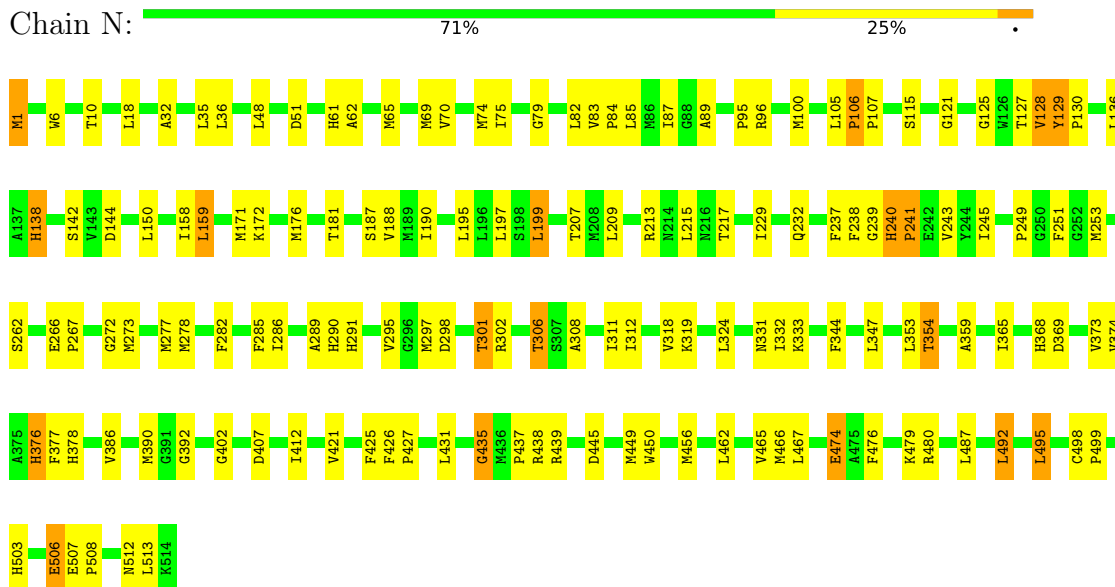
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

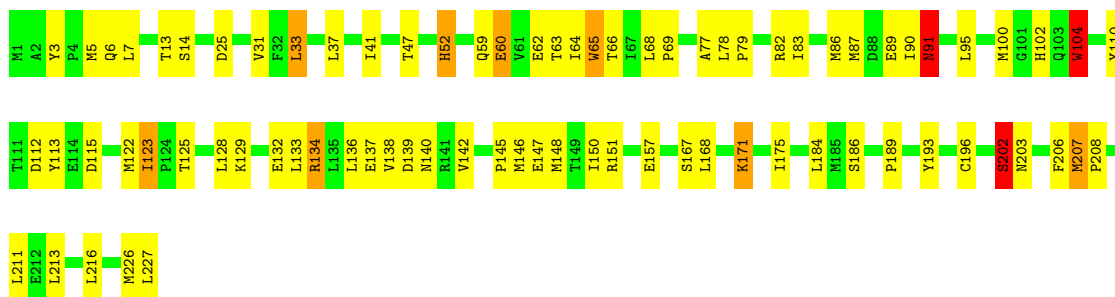


- Molecule 1: CYTOCHROME C OXIDASE



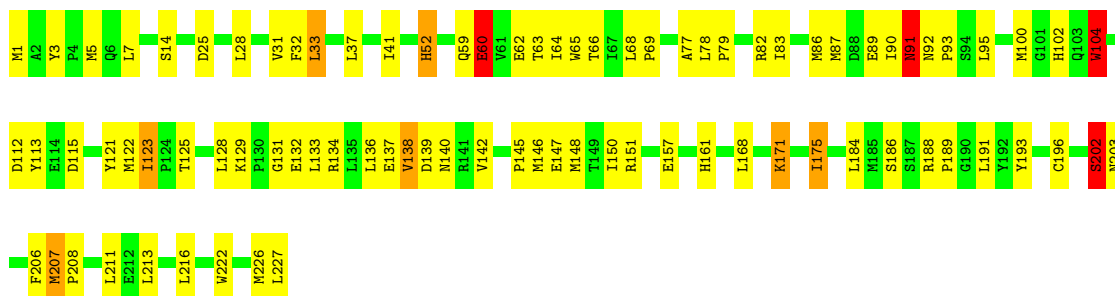
- Molecule 2: CYTOCHROME C OXIDASE

Chain B:  65% 30%



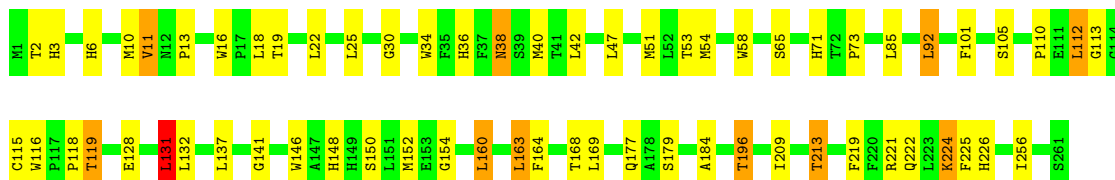
• Molecule 2: CYTOCHROME C OXIDASE

Chain O:  62% 33%




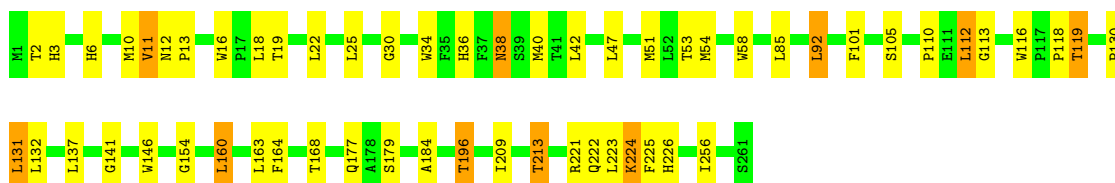
• Molecule 3: CYTOCHROME C OXIDASE

Chain C:  75% 20%



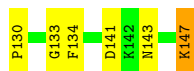
• Molecule 3: CYTOCHROME C OXIDASE

Chain P:  78% 18%

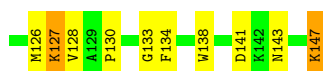
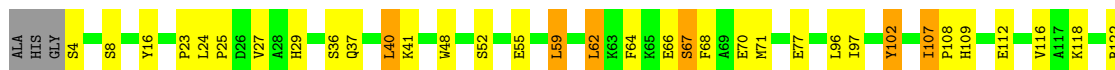


• Molecule 4: CYTOCHROME C OXIDASE

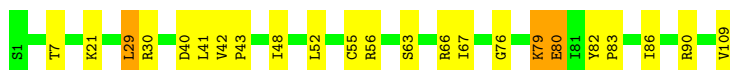
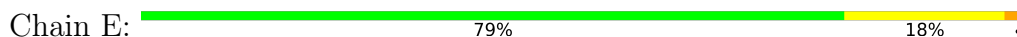
Chain D:  71% 22%



- Molecule 4: CYTOCHROME C OXIDASE



- Molecule 5: CYTOCHROME C OXIDASE



- Molecule 5: CYTOCHROME C OXIDASE



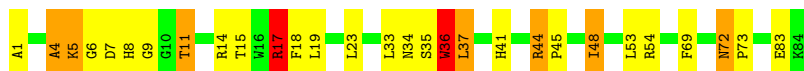
- Molecule 6: CYTOCHROME C OXIDASE



- Molecule 6: CYTOCHROME C OXIDASE



- Molecule 7: CYTOCHROME C OXIDASE



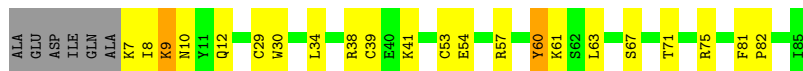
- Molecule 7: CYTOCHROME C OXIDASE

Chain T:  64% 26% 7%



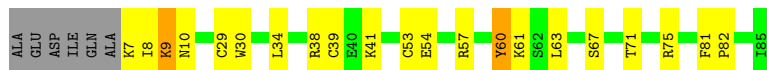
- Molecule 8: CYTOCHROME C OXIDASE

Chain H:  67% 24% 7%




- Molecule 8: CYTOCHROME C OXIDASE

Chain U:  68% 22% 7%



- Molecule 9: CYTOCHROME C OXIDASE

Chain I:  79% 19%



- Molecule 9: CYTOCHROME C OXIDASE

Chain V:  70% 29%




- Molecule 10: CYTOCHROME C OXIDASE

Chain J:  76% 17% 5%



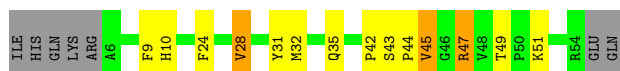
- Molecule 10: CYTOCHROME C OXIDASE

Chain W:  73% 20% 5%



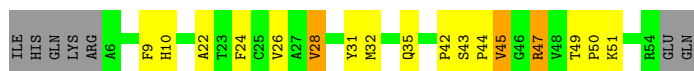
- Molecule 11: CYTOCHROME C OXIDASE

Chain K:  62% 20% 5% 12%



● Molecule 11: CYTOCHROME C OXIDASE

Chain X:  57% 25% 5% 12%



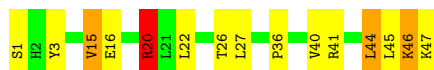
● Molecule 12: CYTOCHROME C OXIDASE

Chain L:  72% 19% 6% .



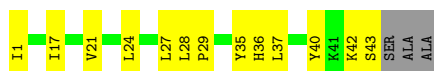
● Molecule 12: CYTOCHROME C OXIDASE

Chain Y:  68% 23% 6% .



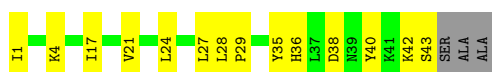
● Molecule 13: CYTOCHROME C OXIDASE

Chain M:  65% 28% 7%



● Molecule 13: CYTOCHROME C OXIDASE

Chain Z:  63% 30% 7%



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, α , β , γ	189.10Å 210.50Å 178.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.35	Depositor
% Data completeness (in resolution range)	89.8 (15.00-2.35)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.84	Depositor
R, R_{free}	0.203 , 0.247	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	28926	wwPDB-VP
Average B, all atoms (Å ²)	39.0	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, MG, ZN, 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	1.02	8/4164 (0.2%)	1.20	40/5688 (0.7%)
1	N	0.86	8/4164 (0.2%)	1.15	40/5688 (0.7%)
2	B	0.90	1/1917 (0.1%)	1.19	17/2612 (0.7%)
2	O	0.80	1/1917 (0.1%)	1.17	16/2612 (0.6%)
3	C	0.92	0/2211	1.02	11/3023 (0.4%)
3	P	0.79	0/2211	1.01	9/3023 (0.3%)
4	D	0.75	0/1229	0.99	4/1658 (0.2%)
4	Q	0.67	0/1229	1.04	4/1658 (0.2%)
5	E	0.79	0/898	1.08	7/1218 (0.6%)
5	R	0.69	0/898	1.09	8/1218 (0.7%)
6	F	0.82	0/765	1.20	7/1038 (0.7%)
6	S	0.75	0/765	1.16	4/1038 (0.4%)
7	G	0.81	0/699	1.22	12/950 (1.3%)
7	T	0.75	0/699	1.22	11/950 (1.2%)
8	H	0.82	0/682	1.14	7/921 (0.8%)
8	U	0.72	0/682	1.11	6/921 (0.7%)
9	I	0.85	0/611	0.97	2/810 (0.2%)
9	V	0.76	0/611	0.94	2/810 (0.2%)
10	J	0.78	0/471	0.96	0/636
10	W	0.68	0/471	0.93	0/636
11	K	0.95	0/398	1.11	0/546
11	X	0.73	0/398	1.08	0/546
12	L	0.91	0/399	1.04	2/534 (0.4%)
12	Y	0.71	0/399	1.04	3/534 (0.6%)
13	M	0.81	0/345	0.99	1/470 (0.2%)
13	Z	0.66	0/345	1.00	1/470 (0.2%)
All	All	0.84	18/29578 (0.1%)	1.11	214/40208 (0.5%)

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	B	0	1
All	All	0	3

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	376	HIS	ND1-CE1	9.63	1.42	1.32
1	A	61	HIS	CD2-NE2	9.27	1.48	1.37
1	N	376	HIS	ND1-CE1	9.07	1.41	1.32
1	N	378	HIS	ND1-CE1	8.96	1.41	1.32
1	A	378	HIS	ND1-CE1	8.90	1.41	1.32

The worst 5 of 214 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	Q	133	GLY	N-CA-C	14.89	130.50	112.49
1	A	61	HIS	ND1-CE1-NE2	10.43	118.83	108.40
1	A	378	HIS	ND1-CE1-NE2	9.79	118.19	108.40
1	A	376	HIS	ND1-CE1-NE2	8.90	117.30	108.40
1	N	332	ILE	N-CA-C	8.79	120.50	108.89

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	240	HIS	Sidechain
2	B	110	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	75	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	N	4025	0	4002	87	0
2	B	1870	0	1873	57	0
2	O	1870	0	1873	58	0
3	C	2124	0	2044	42	0
3	P	2124	0	2044	39	0
4	D	1195	0	1183	30	0
4	Q	1195	0	1183	36	0
5	E	878	0	868	15	0
5	R	878	0	868	18	0
6	F	748	0	728	18	0
6	S	748	0	728	17	0
7	G	672	0	645	21	0
7	T	672	0	645	25	0
8	H	662	0	623	11	0
8	U	662	0	625	11	0
9	I	598	0	612	8	0
9	V	598	0	612	14	0
10	J	460	0	459	9	0
10	W	460	0	459	9	0
11	K	384	0	366	12	0
11	X	384	0	366	14	0
12	L	386	0	388	8	0
12	Y	386	0	388	10	0
13	M	335	0	352	8	0
13	Z	335	0	352	10	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	9	0
17	N	120	0	108	6	0
18	F	1	0	0	0	0
18	S	1	0	0	0	0
All	All	28926	0	28504	544	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 10.

The worst 5 of 544 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)
6:S:10:GLU:HG2	6:S:25:ARG:HH22	1.30	0.94
6:F:10:GLU:HG2	6:F:25:ARG:HH22	1.30	0.94
1:A:176:MET:HE3	1:A:181:THR:HG22	1.58	0.85
3:C:101:PHE:HD1	3:C:196:THR:HG21	1.43	0.84
1:A:278:MET:HE2	7:T:18:PHE:HE2	1.42	0.84

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%)	491 (96%)	21 (4%)	0	100	100
1	N	512/514 (100%)	492 (96%)	20 (4%)	0	100	100
2	B	231/227 (102%)	208 (90%)	20 (9%)	3 (1%)	9	8
2	O	231/227 (102%)	207 (90%)	21 (9%)	3 (1%)	9	8
3	C	259/261 (99%)	252 (97%)	6 (2%)	1 (0%)	30	34
3	P	259/261 (99%)	252 (97%)	6 (2%)	1 (0%)	30	34
4	D	142/147 (97%)	137 (96%)	5 (4%)	0	100	100
4	Q	142/147 (97%)	135 (95%)	7 (5%)	0	100	100
5	E	107/109 (98%)	105 (98%)	2 (2%)	0	100	100
5	R	107/109 (98%)	105 (98%)	2 (2%)	0	100	100
6	F	96/98 (98%)	90 (94%)	5 (5%)	1 (1%)	12	12
6	S	96/98 (98%)	91 (95%)	4 (4%)	1 (1%)	12	12
7	G	82/84 (98%)	67 (82%)	11 (13%)	4 (5%)	1	0
7	T	82/84 (98%)	67 (82%)	11 (13%)	4 (5%)	1	0
8	H	77/85 (91%)	73 (95%)	4 (5%)	0	100	100
8	U	77/85 (91%)	74 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	I	71/73 (97%)	65 (92%)	6 (8%)	0	100	100
9	V	71/73 (97%)	65 (92%)	6 (8%)	0	100	100
10	J	56/59 (95%)	53 (95%)	3 (5%)	0	100	100
10	W	56/59 (95%)	52 (93%)	3 (5%)	1 (2%)	6	5
11	K	47/56 (84%)	45 (96%)	2 (4%)	0	100	100
11	X	47/56 (84%)	45 (96%)	2 (4%)	0	100	100
12	L	45/47 (96%)	42 (93%)	3 (7%)	0	100	100
12	Y	45/47 (96%)	43 (96%)	2 (4%)	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	3532/3612 (98%)	3338 (94%)	175 (5%)	19 (0%)	24	27

5 of 19 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	91[A]	ASN
2	B	91[B]	ASN
7	G	4	ALA
2	O	91[A]	ASN
2	O	91[B]	ASN

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%)	397 (93%)	30 (7%)	14	15
1	N	427/427 (100%)	394 (92%)	33 (8%)	12	13
2	B	217/211 (103%)	203 (94%)	14 (6%)	15	18
2	O	217/211 (103%)	203 (94%)	14 (6%)	15	18
3	C	226/226 (100%)	206 (91%)	20 (9%)	9	10
3	P	226/226 (100%)	207 (92%)	19 (8%)	10	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D	128/129 (99%)	116 (91%)	12 (9%)	8	8
4	Q	128/129 (99%)	116 (91%)	12 (9%)	8	8
5	E	95/95 (100%)	91 (96%)	4 (4%)	26	35
5	R	95/95 (100%)	91 (96%)	4 (4%)	26	35
6	F	81/81 (100%)	72 (89%)	9 (11%)	6	5
6	S	81/81 (100%)	72 (89%)	9 (11%)	6	5
7	G	68/68 (100%)	59 (87%)	9 (13%)	4	3
7	T	68/68 (100%)	60 (88%)	8 (12%)	5	5
8	H	71/75 (95%)	65 (92%)	6 (8%)	10	11
8	U	71/75 (95%)	65 (92%)	6 (8%)	10	11
9	I	58/58 (100%)	55 (95%)	3 (5%)	21	25
9	V	58/58 (100%)	54 (93%)	4 (7%)	14	16
10	J	49/50 (98%)	43 (88%)	6 (12%)	5	4
10	W	49/50 (98%)	42 (86%)	7 (14%)	3	3
11	K	39/46 (85%)	35 (90%)	4 (10%)	7	6
11	X	39/46 (85%)	35 (90%)	4 (10%)	7	6
12	L	40/40 (100%)	34 (85%)	6 (15%)	3	2
12	Y	40/40 (100%)	33 (82%)	7 (18%)	2	1
13	M	37/38 (97%)	35 (95%)	2 (5%)	20	24
13	Z	37/38 (97%)	35 (95%)	2 (5%)	20	24
All	All	3072/3088 (100%)	2818 (92%)	254 (8%)	10	11

5 of 254 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	K	47	ARG
7	T	37	LEU
1	N	312	ILE
7	T	33	LEU
10	W	30	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such sidechains are listed below:

Mol	Chain	Res	Type
4	Q	109	HIS
10	W	29	ASN
4	Q	119	GLN
8	U	10	ASN
13	Z	36	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 12 are monoatomic - leaving 4 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	67,67,67	1.15	6 (8%)	81,103,103	1.37	12 (14%)
17	HEA	A	516	1	67,67,67	1.50	9 (13%)	81,103,103	1.54	18 (22%)
17	HEA	A	515	1	67,67,67	1.34	8 (11%)	81,103,103	1.61	16 (19%)
17	HEA	N	515	1	67,67,67	1.14	4 (5%)	81,103,103	1.57	13 (16%)

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	516	1	-	6/36/76/76	-
17	HEA	A	516	1	-	6/36/76/76	-
17	HEA	A	515	1	-	10/36/76/76	-
17	HEA	N	515	1	-	10/36/76/76	-

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	C4C-NC	-4.64	1.30	1.39
17	A	516	HEA	C1D-C2D	4.25	1.53	1.44
17	A	516	HEA	FE-NA	4.12	2.08	1.95
17	A	516	HEA	CMA-C3A	-3.88	1.36	1.45
17	N	515	HEA	C11-C3B	-3.76	1.46	1.51

The worst 5 of 59 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	515	HEA	C13-C14-C15	-5.24	115.63	127.62
17	N	515	HEA	C13-C14-C15	-5.08	115.99	127.62
17	A	516	HEA	CMD-C2D-C1D	4.30	131.76	125.03
17	N	515	HEA	CMB-C2B-C3B	-3.93	122.67	130.28
17	N	516	HEA	CHB-C4A-NA	-3.86	120.25	124.45

There are no chirality outliers.

5 of 32 torsion outliers are listed below:

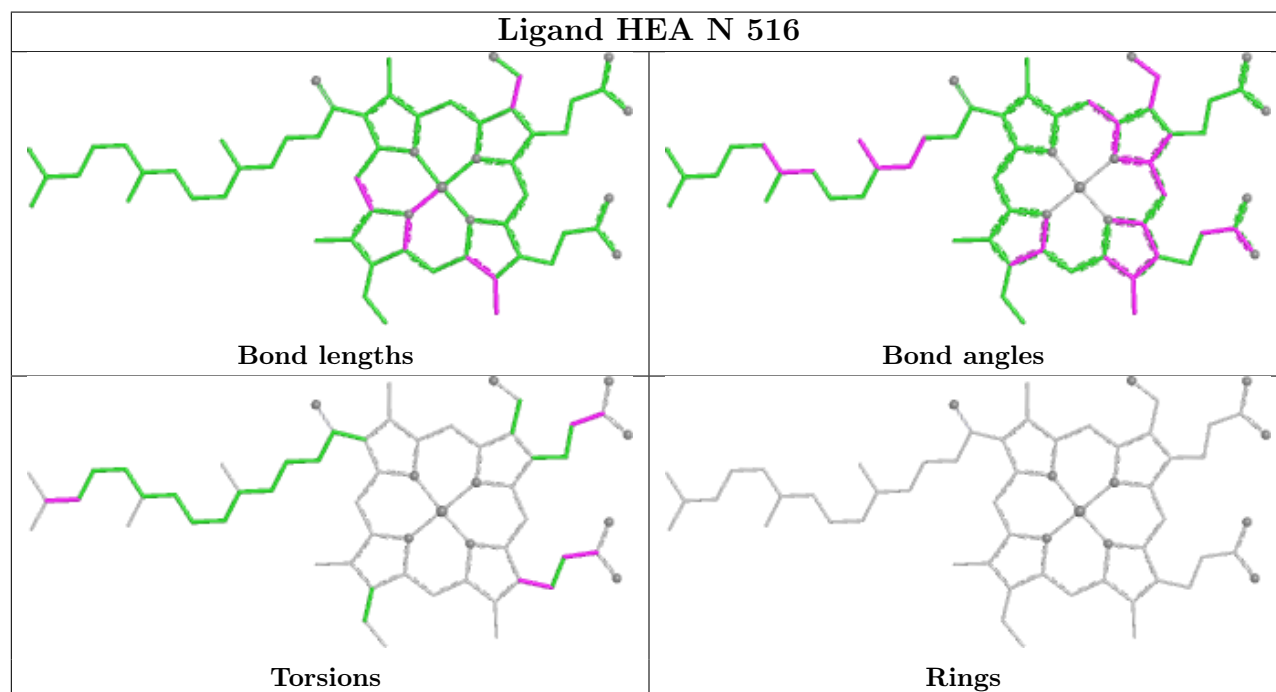
Mol	Chain	Res	Type	Atoms
17	N	516	HEA	C4D-C3D-CAD-CBD
17	A	516	HEA	C21-C22-C23-C25
17	N	516	HEA	C21-C22-C23-C25
17	A	516	HEA	C4D-C3D-CAD-CBD
17	A	515	HEA	C2A-C3A-CMA-OMA

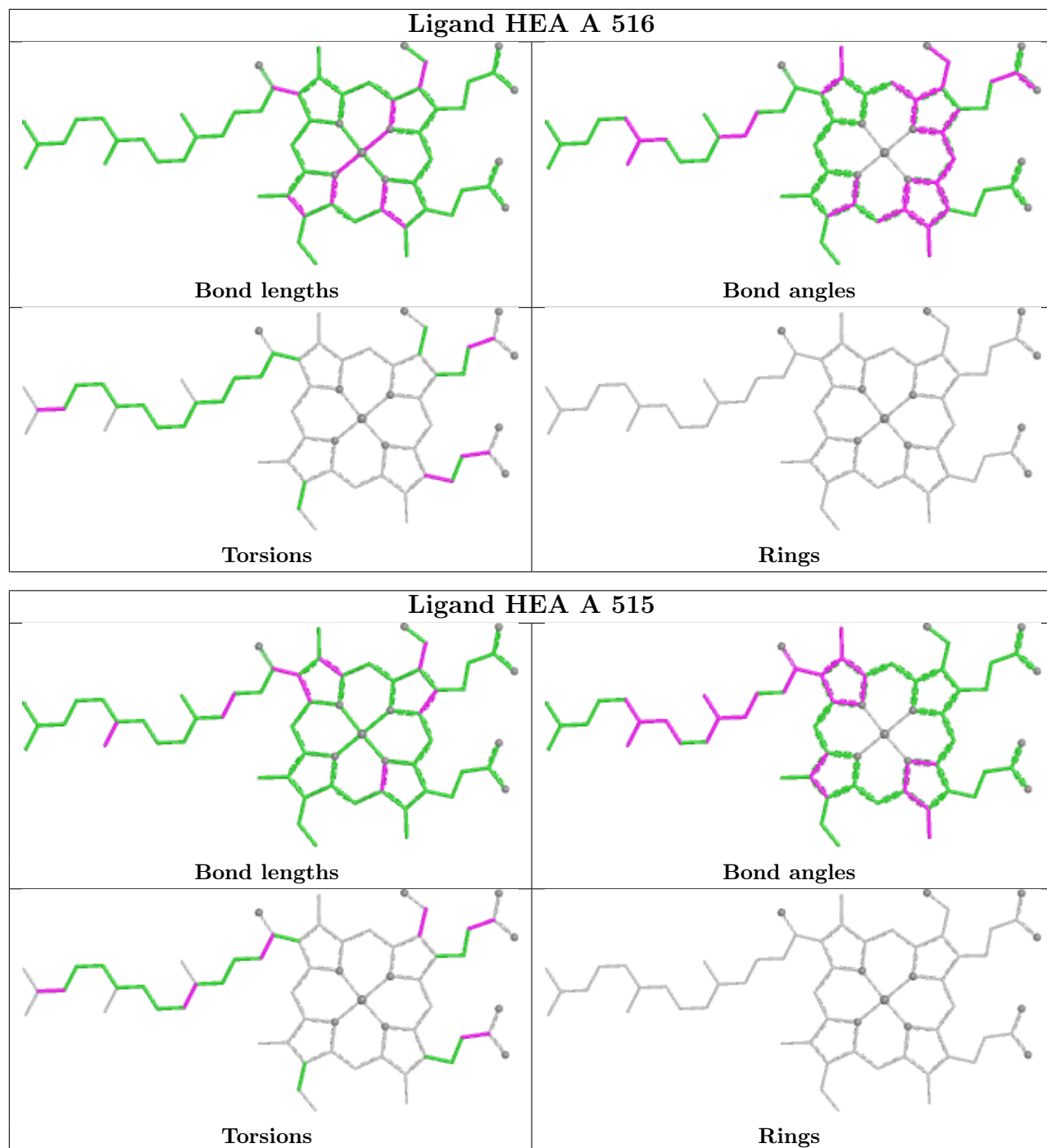
There are no ring outliers.

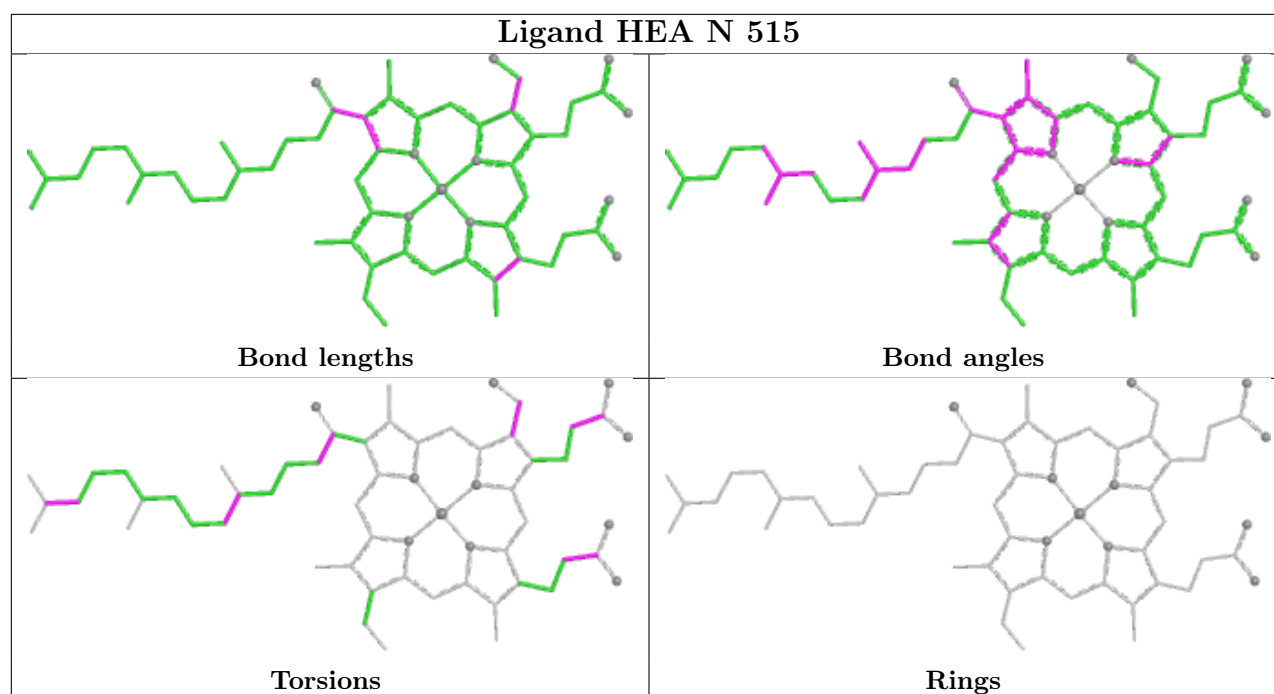
3 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	A	516	HEA	2	0
17	A	515	HEA	7	0
17	N	515	HEA	6	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	O	1
2	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	O	87:MET	C	88[A]:ASP	N	1.17
1	B	87:MET	C	88[A]:ASP	N	1.16

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.