



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 13, 2020 – 10:22 am BST

PDB ID : 1OCR  
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](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.

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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) : 2.11

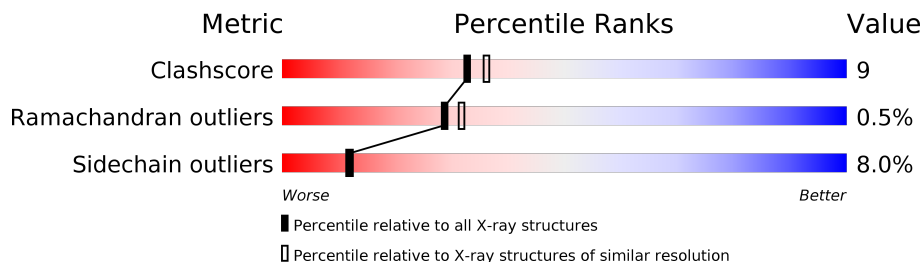
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.35 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	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)











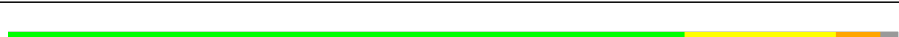


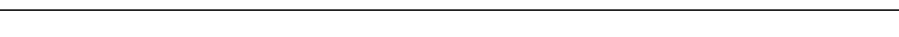
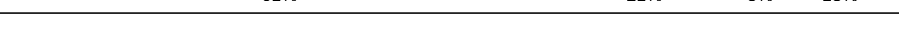
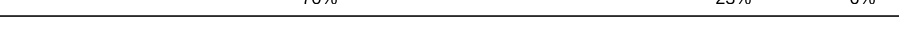

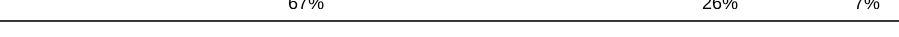
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria 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 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	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 1870	C 1212	N 289	O 351	S 18	0	6	0
2	O	227	Total 1870	C 1212	N 289	O 351	S 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	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	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 (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		

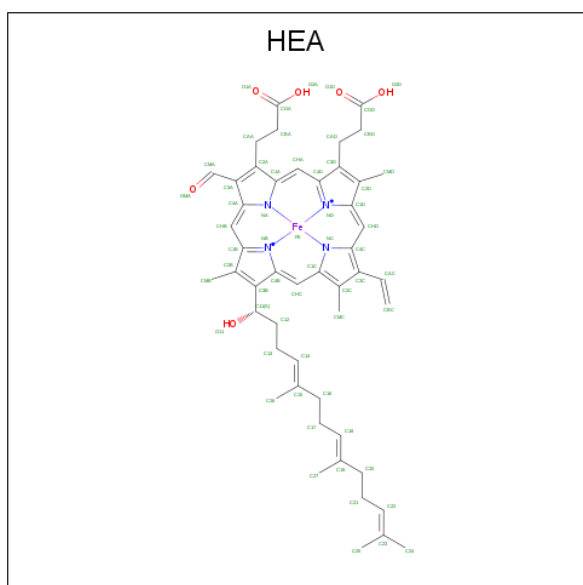
- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
18	S	1	Total 1	Zn 1	0	0
18	F	1	Total 1	Zn 1	0	0

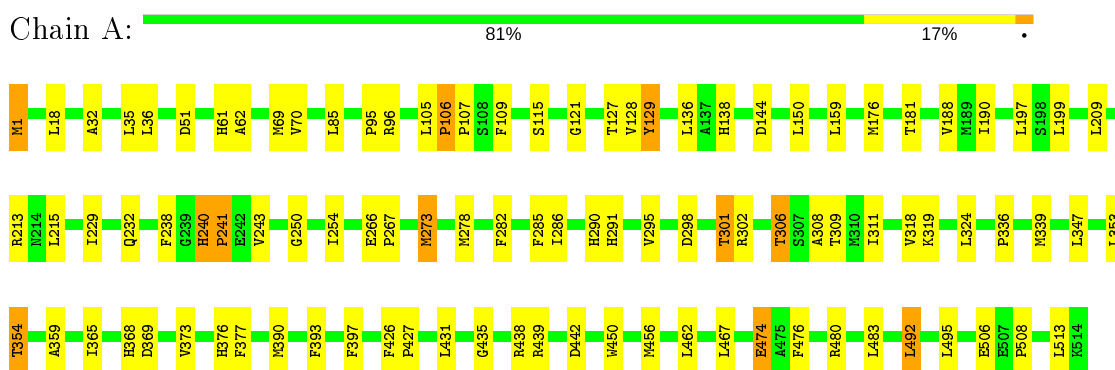


### 3 Residue-property plots [i](#)

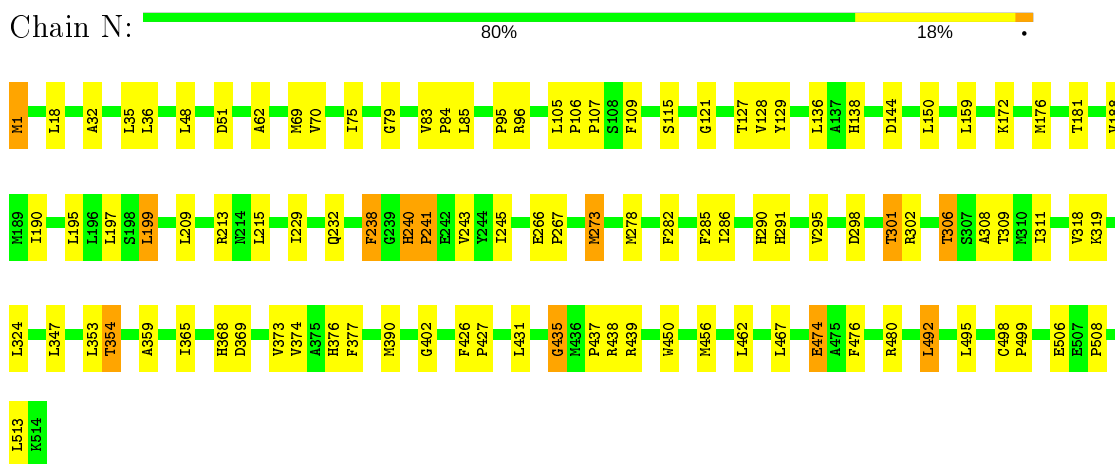
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according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

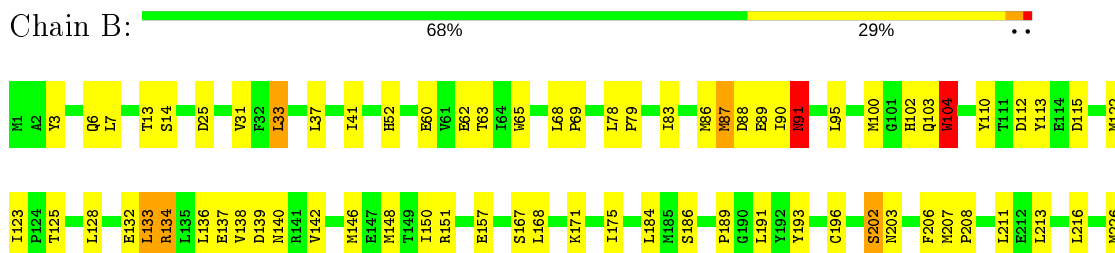
- Molecule 1: CYTOCHROME C OXIDASE



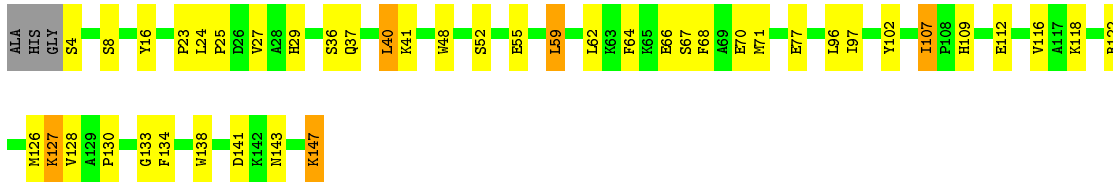
- Molecule 1: CYTOCHROME C OXIDASE



- Molecule 2: CYTOCHROME C OXIDASE







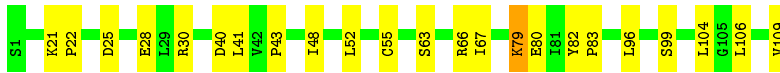
- Molecule 5: CYTOCHROME C OXIDASE

Chain E: 84% 15%



- Molecule 5: CYTOCHROME C OXIDASE

Chain R: 79% 20%



- Molecule 6: CYTOCHROME C OXIDASE

Chain F: 74% 22%



- Molecule 6: CYTOCHROME C OXIDASE

Chain S: 72% 22% 5%



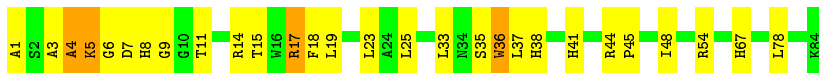
- Molecule 7: CYTOCHROME C OXIDASE

Chain G: 69% 26% 5%



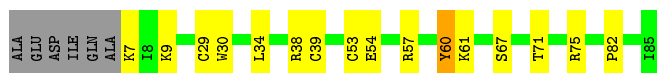
- Molecule 7: CYTOCHROME C OXIDASE

Chain T: 67% 29% 5%



- Molecule 8: CYTOCHROME C OXIDASE

Chain H:  74% 18% 7%




• Molecule 8: CYTOCHROME C OXIDASE

Chain U:  74% 18% 7%



• Molecule 9: CYTOCHROME C OXIDASE

Chain I:  82% 16%



• Molecule 9: CYTOCHROME C OXIDASE

Chain V:  74% 25%



• Molecule 10: CYTOCHROME C OXIDASE

Chain J:  76% 17% 5%



• Molecule 10: CYTOCHROME C OXIDASE

Chain W:  73% 22%



• Molecule 11: CYTOCHROME C OXIDASE

Chain K:  64% 18% 5% 13%



• Molecule 11: CYTOCHROME C OXIDASE

Chain X:  61% 21% 5% 13%



- Molecule 12: CYTOCHROME C OXIDASE

Chain L: 70% 23% 6%



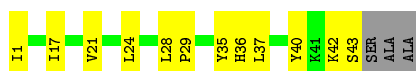
- Molecule 12: CYTOCHROME C OXIDASE

Chain Y: 70% 23% 6%



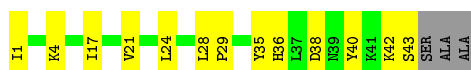
- Molecule 13: CYTOCHROME C OXIDASE

Chain M: 67% 26% 7%



- Molecule 13: CYTOCHROME C OXIDASE

Chain Z: 65% 28% 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, $\alpha$ , $\beta$ , $\gamma$	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 <sup>2</sup> )	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	0.70	0/4164	0.79	2/5688 (0.0%)
1	N	0.62	0/4164	0.77	1/5688 (0.0%)
2	B	0.71	1/1917 (0.1%)	0.92	4/2612 (0.2%)
2	O	0.66	1/1917 (0.1%)	0.91	3/2612 (0.1%)
3	C	0.67	0/2211	0.70	1/3023 (0.0%)
3	P	0.61	0/2211	0.70	1/3023 (0.0%)
4	D	0.62	0/1229	0.69	1/1658 (0.1%)
4	Q	0.59	0/1229	0.67	1/1658 (0.1%)
5	E	0.63	0/898	0.69	0/1218
5	R	0.57	0/898	0.69	0/1218
6	F	0.65	0/765	0.84	0/1038
6	S	0.63	0/765	0.83	0/1038
7	G	0.65	0/699	0.82	0/950
7	T	0.62	0/699	0.82	0/950
8	H	0.64	0/682	0.73	0/921
8	U	0.59	0/682	0.72	0/921
9	I	0.73	0/611	0.73	0/810
9	V	0.71	0/611	0.72	0/810
10	J	0.65	0/471	0.70	0/636
10	W	0.63	0/471	0.70	0/636
11	K	0.71	0/398	0.73	0/546
11	X	0.60	0/398	0.71	0/546
12	L	0.70	0/399	0.67	0/534
12	Y	0.64	0/399	0.65	0/534
13	M	0.59	0/345	0.69	0/470
13	Z	0.56	0/345	0.71	0/470
All	All	0.65	2/29578 (0.0%)	0.77	14/40208 (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	B	0	1
All	All	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	87	MET	C-N	-7.75	1.16	1.34
2	O	87	MET	C-N	-7.37	1.17	1.34

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	92	LEU	CA-CB-CG	-7.07	99.05	115.30
4	Q	133	GLY	N-CA-C	6.96	130.50	113.10
4	D	133	GLY	N-CA-C	6.94	130.46	113.10
3	P	92	LEU	CA-CB-CG	-6.72	99.85	115.30
2	B	133	LEU	CA-CB-CG	-5.86	101.81	115.30

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	67	0
1	N	4025	0	4002	74	0
2	B	1870	0	1872	52	0
2	O	1870	0	1872	52	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	2124	0	2044	37	0
3	P	2124	0	2044	33	0
4	D	1195	0	1183	31	0
4	Q	1195	0	1183	35	0
5	E	878	0	868	13	0
5	R	878	0	868	16	0
6	F	748	0	728	17	0
6	S	748	0	728	17	0
7	G	672	0	645	19	0
7	T	672	0	645	23	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	8	0
10	W	460	0	459	8	0
11	K	384	0	366	11	0
11	X	384	0	366	13	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	12	0
17	N	120	0	108	10	0
18	F	1	0	0	0	0
18	S	1	0	0	0	0
All	All	28926	0	28502	500	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 9.

The worst 5 of 500 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
3:C:101:PHE:HD1	3:C:196:THR:HG21	1.43	0.84
2:B:78:LEU:HB2	2:B:79:PRO:HD3	1.60	0.83
2:O:78:LEU:HB2	2:O:79:PRO:HD3	1.62	0.81

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%)	12	10
2	O	231/227 (102%)	207 (90%)	21 (9%)	3 (1%)	12	10
3	C	259/261 (99%)	252 (97%)	6 (2%)	1 (0%)	34	38
3	P	259/261 (99%)	252 (97%)	6 (2%)	1 (0%)	34	38
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%)	15	15
6	S	96/98 (98%)	91 (95%)	4 (4%)	1 (1%)	15	15
7	G	82/84 (98%)	67 (82%)	11 (13%)	4 (5%)	2	0
7	T	82/84 (98%)	67 (82%)	11 (13%)	4 (5%)	2	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%)	8	6
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%)	29	32

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%)	15	15
1	N	427/427 (100%)	398 (93%)	29 (7%)	16	16
2	B	217/211 (103%)	202 (93%)	15 (7%)	15	15
2	O	217/211 (103%)	202 (93%)	15 (7%)	15	15
3	C	226/226 (100%)	208 (92%)	18 (8%)	12	12
3	P	226/226 (100%)	207 (92%)	19 (8%)	11	10

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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%)	117 (91%)	11 (9%)	10	9
5	E	95/95 (100%)	92 (97%)	3 (3%)	39	47
5	R	95/95 (100%)	92 (97%)	3 (3%)	39	47
6	F	81/81 (100%)	73 (90%)	8 (10%)	8	7
6	S	81/81 (100%)	72 (89%)	9 (11%)	6	5
7	G	68/68 (100%)	57 (84%)	11 (16%)	2	1
7	T	68/68 (100%)	57 (84%)	11 (16%)	2	1
8	H	71/75 (95%)	66 (93%)	5 (7%)	15	15
8	U	71/75 (95%)	66 (93%)	5 (7%)	15	15
9	I	58/58 (100%)	55 (95%)	3 (5%)	23	27
9	V	58/58 (100%)	55 (95%)	3 (5%)	23	27
10	J	49/50 (98%)	43 (88%)	6 (12%)	5	4
10	W	49/50 (98%)	43 (88%)	6 (12%)	5	4
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%)	33 (82%)	7 (18%)	2	1
12	Y	40/40 (100%)	33 (82%)	7 (18%)	2	1
13	M	37/38 (97%)	35 (95%)	2 (5%)	22	25
13	Z	37/38 (97%)	35 (95%)	2 (5%)	22	25
All	All	3072/3088 (100%)	2824 (92%)	248 (8%)	12	11

5 of 248 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	K	45	VAL
1	N	273	MET
10	W	4	ARG
12	L	9	LYS
1	N	18	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
13	M	36	HIS
2	O	203	ASN
7	T	51	HIS
7	G	51	HIS
7	G	71	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

Of 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	44,67,67	1.41	6 (13%)	37,103,103	1.31	7 (18%)
17	HEA	N	515	1	44,67,67	1.78	6 (13%)	37,103,103	1.86	8 (21%)
17	HEA	A	515	1	44,67,67	1.80	10 (22%)	37,103,103	1.85	9 (24%)
17	HEA	A	516	1	44,67,67	1.77	6 (13%)	37,103,103	1.38	6 (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	3/3/7/16	3/24/76/76	-
17	HEA	N	515	1	2/2/7/16	4/24/76/76	-
17	HEA	A	515	1	2/2/7/16	5/24/76/76	-
17	HEA	A	516	1	3/3/7/16	3/24/76/76	-

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	N	515	HEA	C3B-C11	-7.88	1.46	1.52
17	A	515	HEA	C3B-C11	-7.42	1.47	1.52
17	A	516	HEA	C3A-C2A	-5.23	1.33	1.40
17	A	516	HEA	C1D-C2D	4.67	1.53	1.42
17	A	516	HEA	C3C-C2C	-4.55	1.34	1.40

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	515	HEA	C13-C14-C15	-5.00	115.63	127.66
17	N	515	HEA	C13-C14-C15	-4.85	115.99	127.66
17	A	515	HEA	C20-C19-C18	3.74	128.69	121.12
17	A	515	HEA	C4B-C3B-C2B	-3.72	104.27	106.87
17	N	515	HEA	C4B-C3B-C2B	-3.44	104.46	106.87

5 of 10 chirality outliers are listed below:

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

5 of 15 torsion outliers are listed below:

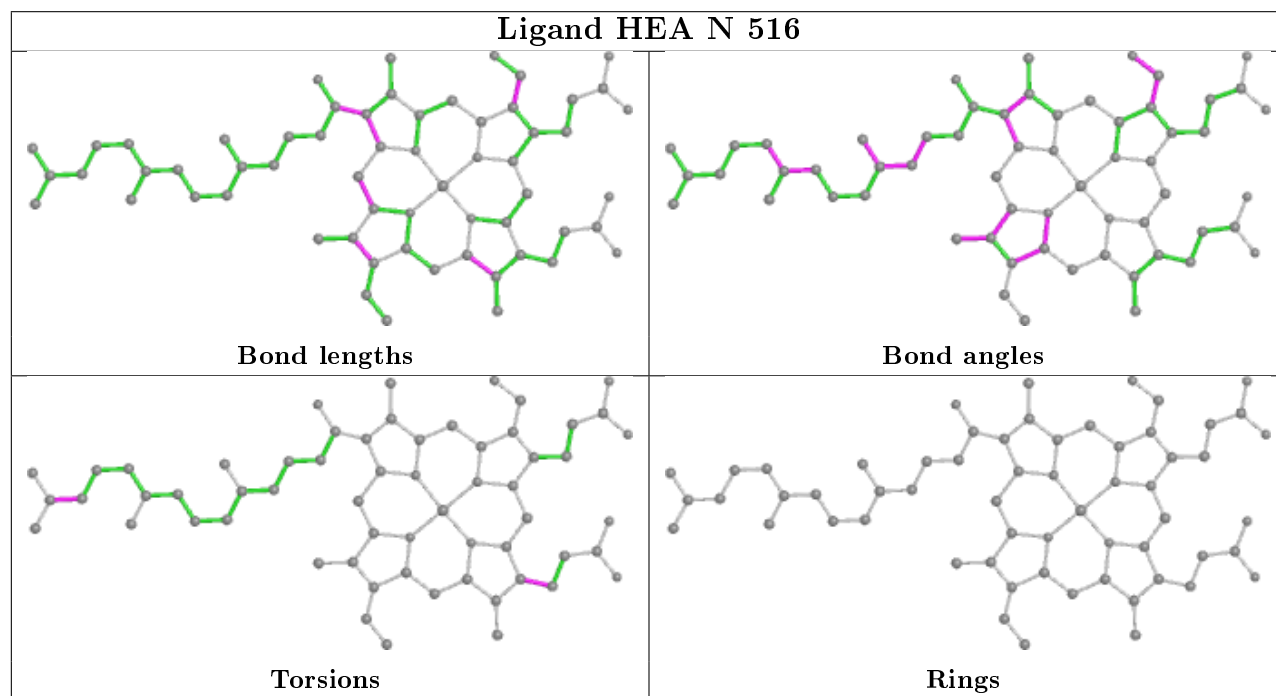
Mol	Chain	Res	Type	Atoms
17	N	516	HEA	C4D-C3D-CAD-CBD
17	A	516	HEA	C21-C22-C23-C25
17	N	516	HEA	C21-C22-C23-C25
17	A	515	HEA	C26-C15-C16-C17
17	N	515	HEA	C26-C15-C16-C17

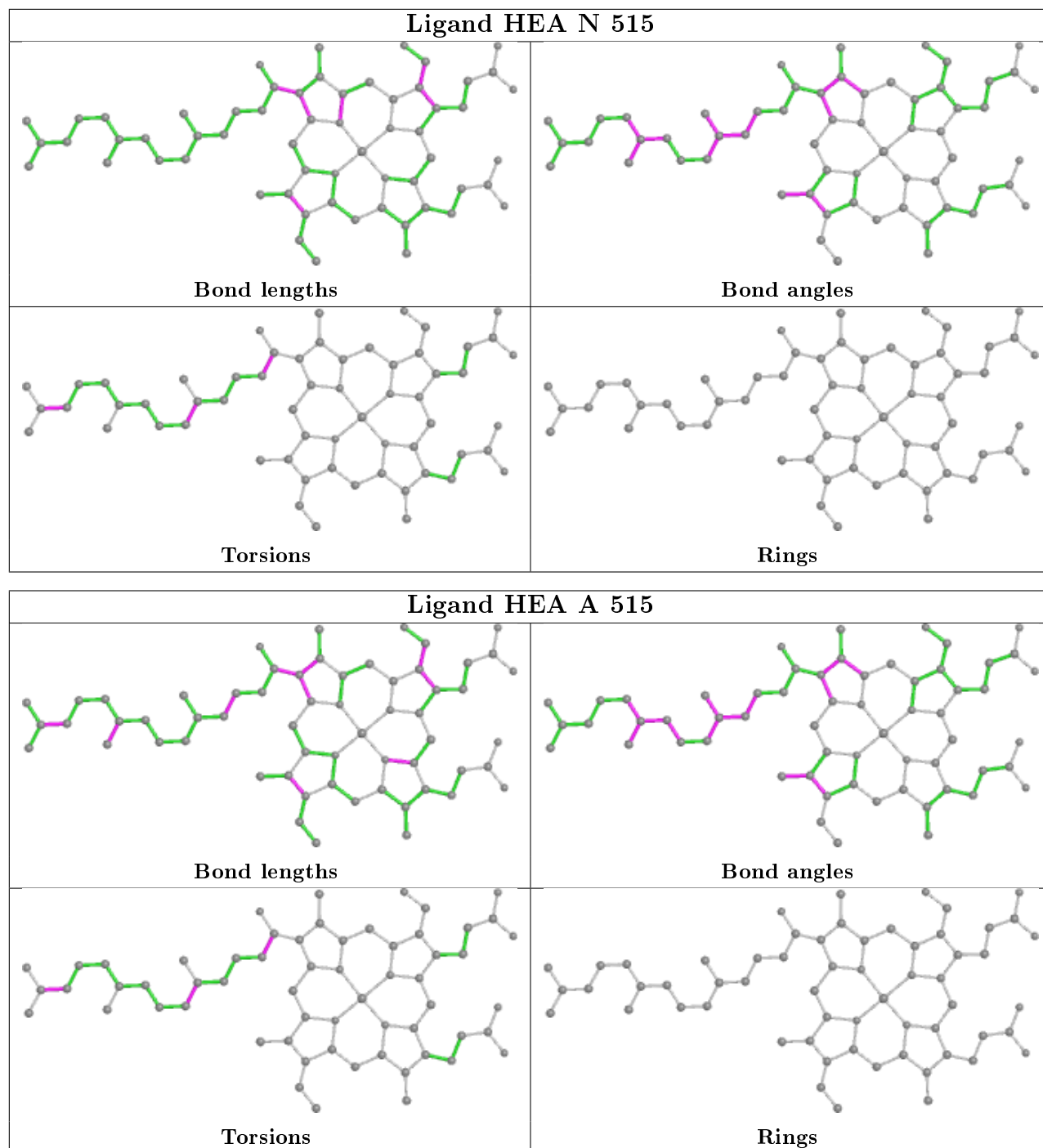
There are no ring outliers.

4 monomers are involved in 22 short contacts:

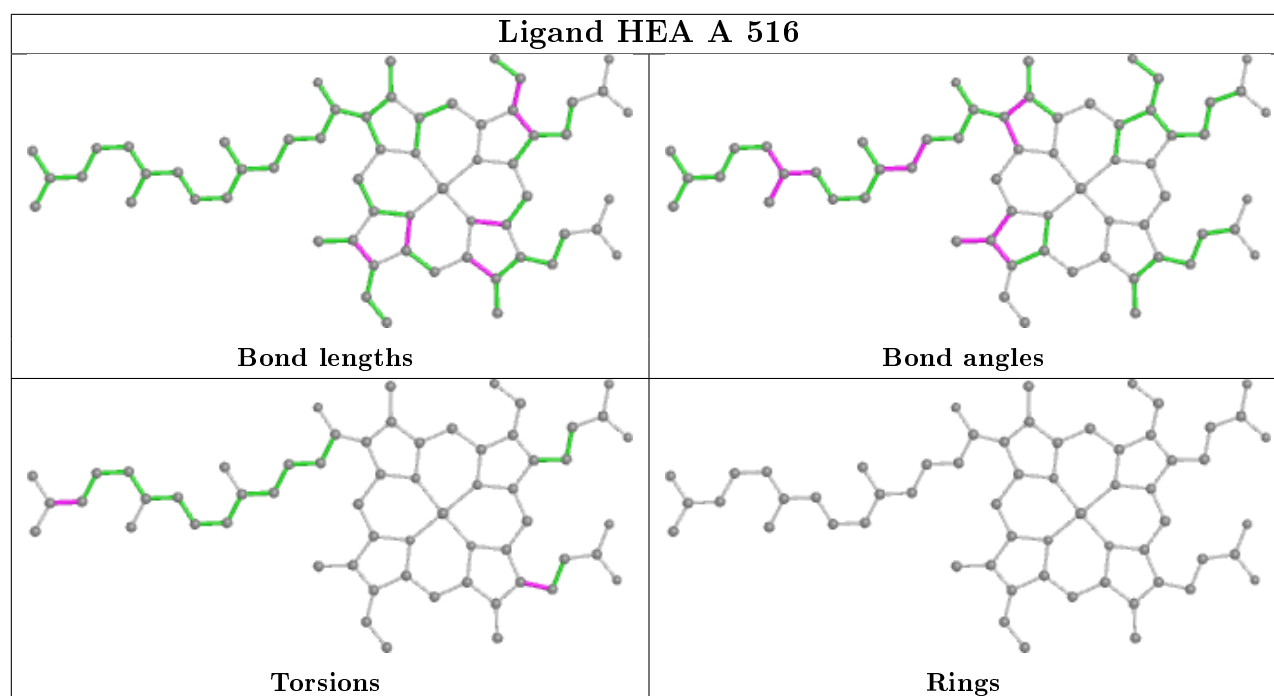
Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	N	516	HEA	2	0
17	N	515	HEA	8	0
17	A	515	HEA	8	0
17	A	516	HEA	4	0

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

### 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.