



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 18, 2024 – 04:49 PM JST

PDB ID : 6KOB  
Title : X-ray Structure of the proton-pumping cytochrome aa3-600 menaquinol oxidase from *Bacillus subtilis*  
Authors : Xu, J.; Ding, Z.; Liu, B.; Li, J.; Gennis, R.B.; Zhu, J.  
Deposited on : 2019-08-09  
Resolution : 3.60 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)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

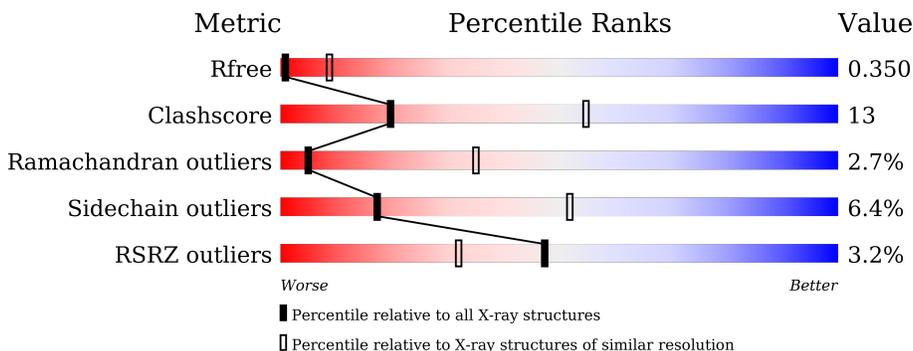
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.60 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))
$R_{free}$	130704	1257 (3.70-3.50)
Clashscore	141614	1353 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)
RSRZ outliers	127900	1161 (3.70-3.50)

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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	655	
1	E	655	
2	B	296	
2	F	296	
3	C	204	
3	G	204	

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Mol	Chain	Length	Quality of chain
4	D	124	<p>%</p> <p>44% 12% 44%</p>
4	H	124	<p>%</p> <p>46% 10% 44%</p>

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
7	MQ7	E	1004	-	-	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 17944 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 AA3-600 quinol oxidase subunit I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	607	4855	3270	752	792	41	0	0	0
1	E	607	4855	3270	752	792	41	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	650	HIS	-	expression tag	UNP A0A063X8D0
A	651	HIS	-	expression tag	UNP A0A063X8D0
A	652	HIS	-	expression tag	UNP A0A063X8D0
A	653	HIS	-	expression tag	UNP A0A063X8D0
A	654	HIS	-	expression tag	UNP A0A063X8D0
A	655	HIS	-	expression tag	UNP A0A063X8D0
E	650	HIS	-	expression tag	UNP A0A063X8D0
E	651	HIS	-	expression tag	UNP A0A063X8D0
E	652	HIS	-	expression tag	UNP A0A063X8D0
E	653	HIS	-	expression tag	UNP A0A063X8D0
E	654	HIS	-	expression tag	UNP A0A063X8D0
E	655	HIS	-	expression tag	UNP A0A063X8D0

- Molecule 2 is a protein called Quinol oxidase subunit 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	256	2073	1348	328	390	7	0	0	0
2	F	256	2073	1348	328	390	7	0	0	0

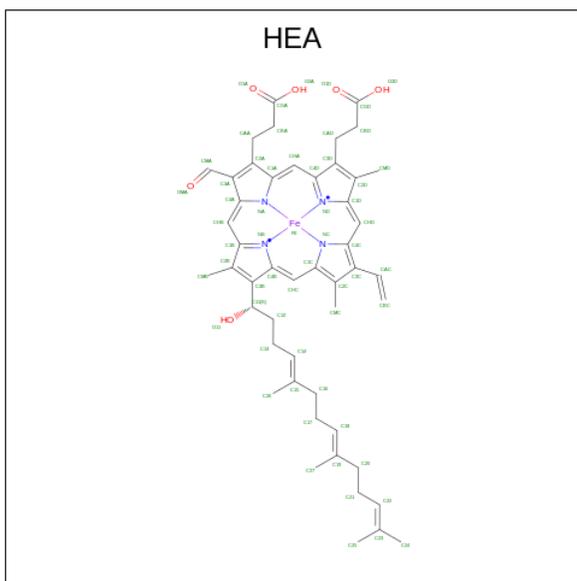
- Molecule 3 is a protein called AA3-600 quinol oxidase subunit IIII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	178	Total 1411	C 953	N 222	O 231	S 5	0	0	0
3	G	178	Total 1411	C 953	N 222	O 231	S 5	0	0	0

- Molecule 4 is a protein called AA3-600 quinol oxidase subunit IV, Quinol oxidase subunit 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	70	Total 482	C 317	N 78	O 84	S 3	0	0	0
4	H	70	Total 482	C 317	N 78	O 84	S 3	0	0	0

- Molecule 5 is HEME-A (three-letter code: HEA) (formula:  $C_{49}H_{56}FeN_4O_6$ ).

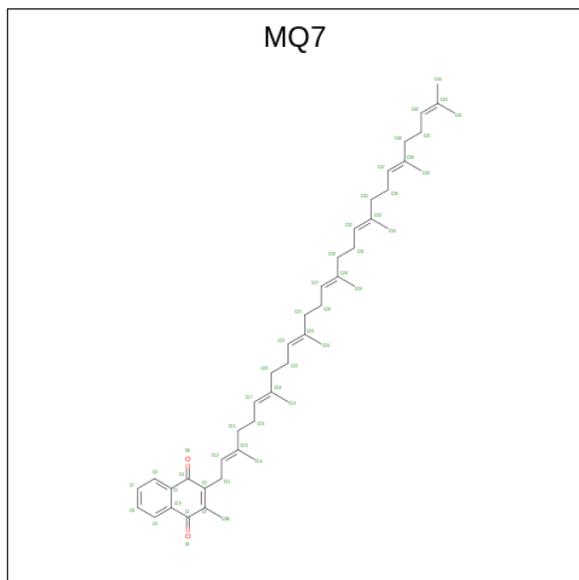


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
5	A	1	Total 60	C 49	Fe 1	N 4	O 6	0	0
5	A	1	Total 60	C 49	Fe 1	N 4	O 6	0	0
5	E	1	Total 60	C 49	Fe 1	N 4	O 6	0	0
5	E	1	Total 60	C 49	Fe 1	N 4	O 6	0	0

- Molecule 6 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Cu 1 1	0	0
6	E	1	Total Cu 1 1	0	0

- Molecule 7 is MENAQUINONE-7 (three-letter code: MQ7) (formula: C<sub>46</sub>H<sub>64</sub>O<sub>2</sub>).

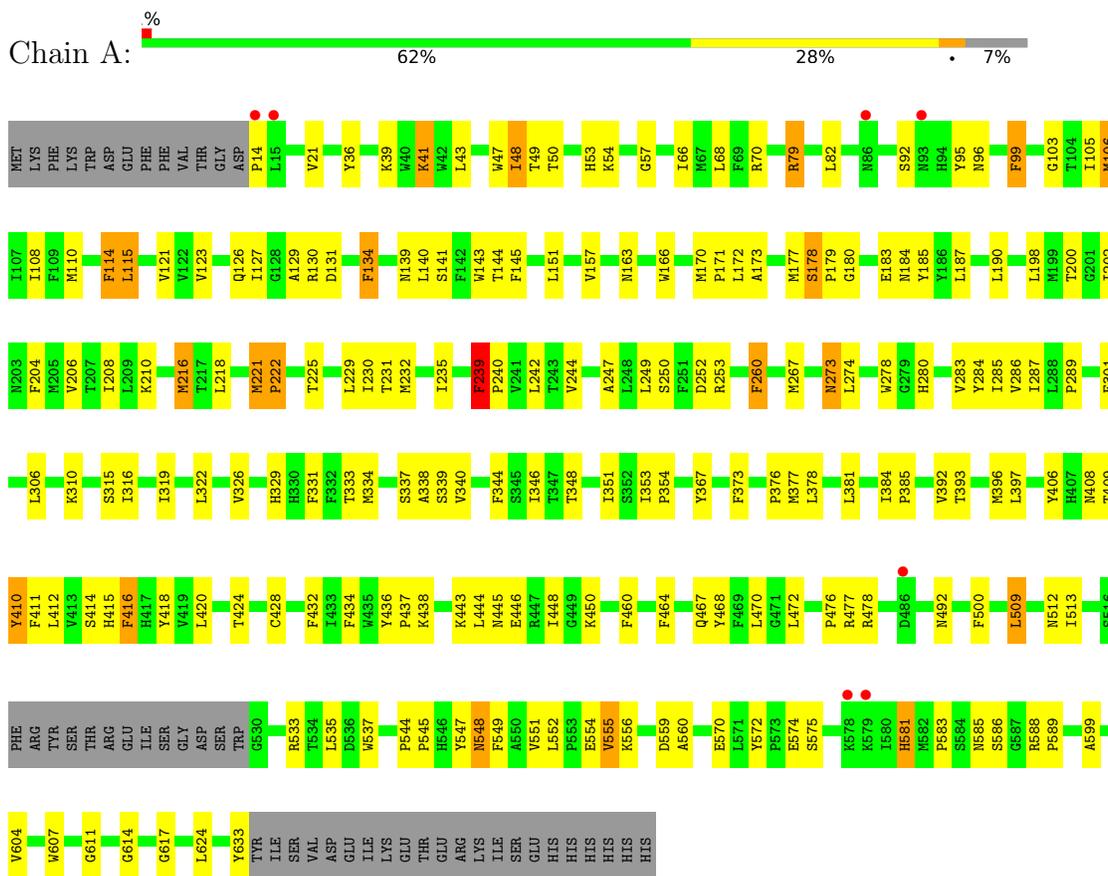


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 30 28 2	0	0
7	E	1	Total C O 30 28 2	0	0

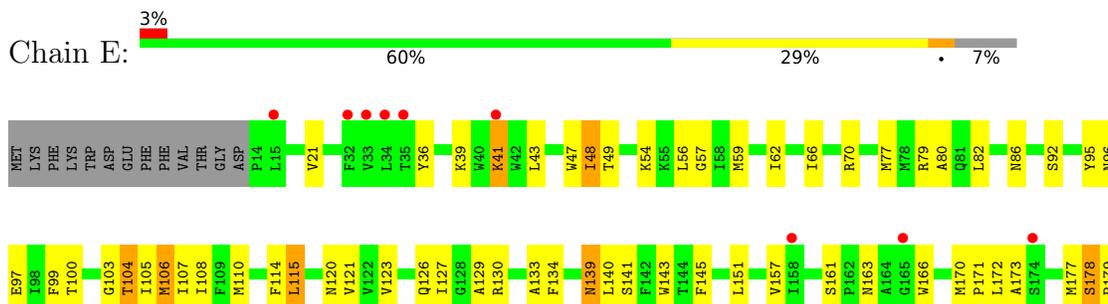
### 3 Residue-property plots

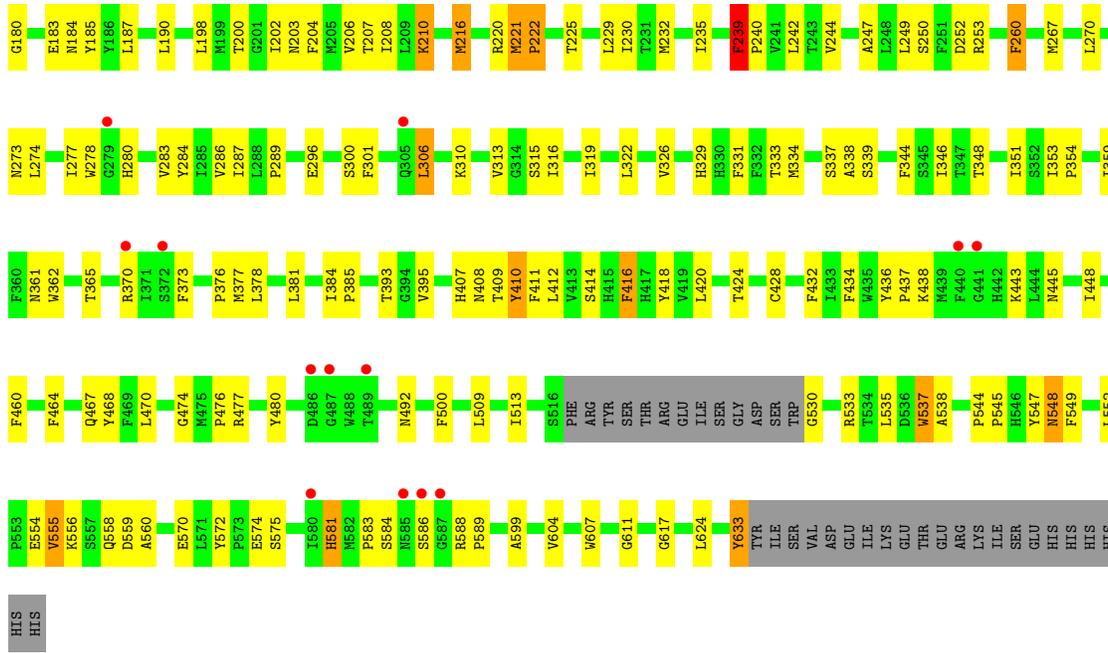
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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.

- Molecule 1: AA3-600 quinol oxidase subunit I

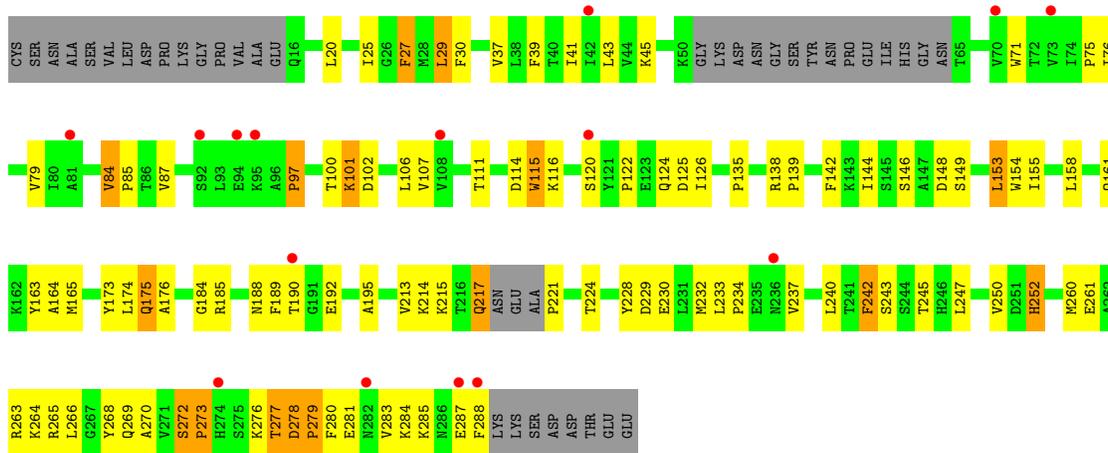


- Molecule 1: AA3-600 quinol oxidase subunit I

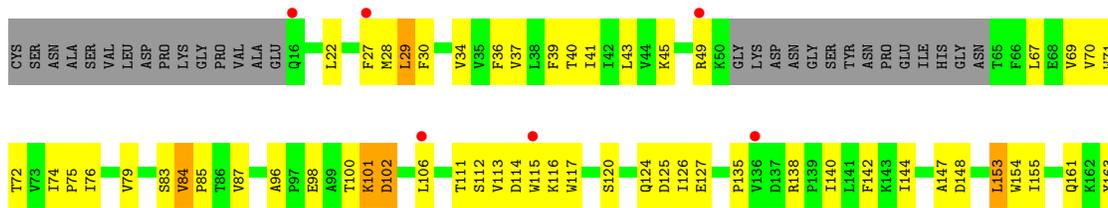




• Molecule 2: Quinol oxidase subunit 2

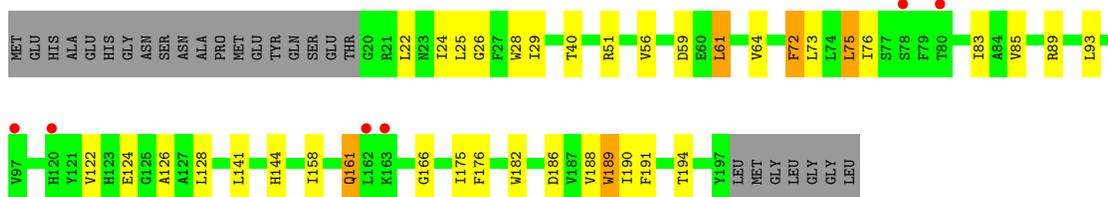


• Molecule 2: Quinol oxidase subunit 2

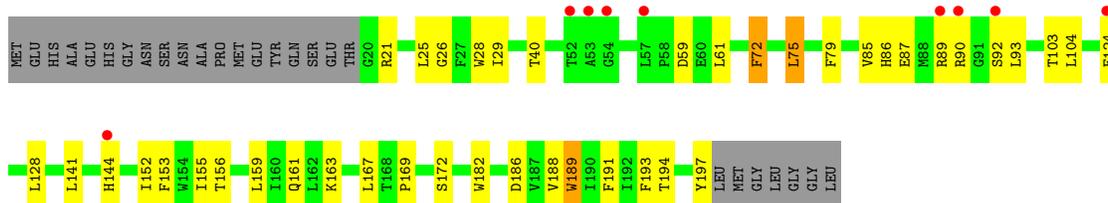




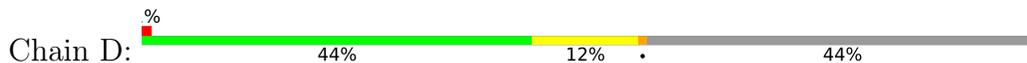
● Molecule 3: AA3-600 quinol oxidase subunit IIII



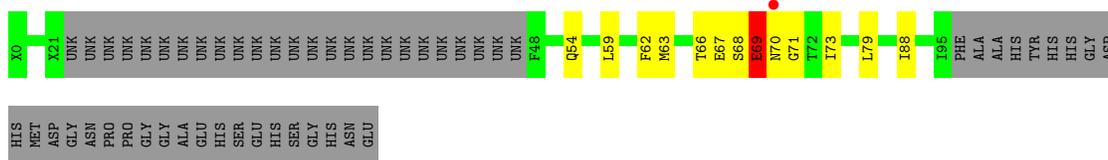
● Molecule 3: AA3-600 quinol oxidase subunit IIII



● Molecule 4: AA3-600 quinol oxidase subunit IV,Quinol oxidase subunit 4



● Molecule 4: AA3-600 quinol oxidase subunit IV,Quinol oxidase subunit 4



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	110.89Å 158.07Å 147.01Å 90.00° 107.47° 90.00°	Depositor
Resolution (Å)	50.06 – 3.60 50.06 – 3.61	Depositor EDS
% Data completeness (in resolution range)	98.6 (50.06-3.60) 99.5 (50.06-3.61)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.20 (at 3.57Å)	Xtrriage
Refinement program	PHENIX 1.14_3235, PHENIX 1.14_3235	Depositor
R, $R_{free}$	0.321 , 0.350 0.312 , 0.350	Depositor DCC
$R_{free}$ test set	1723 reflections (3.10%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	109.7	Xtrriage
Anisotropy	0.553	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.21 , 41.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.39$ , $\langle L^2 \rangle = 0.22$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.82	EDS
Total number of atoms	17944	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	134.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.44% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 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: HEA, CU, MQ7

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	0.25	0/5022	0.40	0/6827
1	E	0.25	0/5022	0.40	0/6827
2	B	0.26	0/2122	0.47	0/2879
2	F	0.25	0/2122	0.48	0/2879
3	C	0.24	0/1452	0.40	0/1974
3	G	0.24	0/1452	0.39	0/1974
4	D	0.26	0/381	0.40	0/514
4	H	0.25	0/381	0.40	0/514
All	All	0.25	0/17954	0.42	0/24388

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	4855	0	4855	138	0
1	E	4855	0	4855	144	0
2	B	2073	0	2061	63	0
2	F	2073	0	2061	69	0
3	C	1411	0	1444	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	1411	0	1444	27	0
4	D	482	0	395	9	0
4	H	482	0	395	10	0
5	A	120	0	107	15	0
5	E	120	0	107	15	0
6	A	1	0	0	0	0
6	E	1	0	0	0	0
7	A	30	0	33	1	0
7	E	30	0	33	1	0
All	All	17944	0	17790	455	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 13.

The worst 5 of 455 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:E:170:MET:HG2	1:E:260:PHE:HB2	1.61	0.82
1:A:170:MET:HG2	1:A:260:PHE:HB2	1.63	0.79
2:B:261:GLU:O	2:B:265:ARG:NH2	2.18	0.77
1:A:39:LYS:HE3	1:A:43:LEU:HB2	1.69	0.75
1:E:409:THR:HA	1:E:476:PRO:HA	1.69	0.74

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	603/655 (92%)	512 (85%)	76 (13%)	15 (2%)	<b>5</b> 36
1	E	603/655 (92%)	511 (85%)	75 (12%)	17 (3%)	<b>5</b> 34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	250/296 (84%)	188 (75%)	51 (20%)	11 (4%)	2	23
2	F	250/296 (84%)	191 (76%)	48 (19%)	11 (4%)	2	23
3	C	176/204 (86%)	158 (90%)	17 (10%)	1 (1%)	25	64
3	G	176/204 (86%)	159 (90%)	16 (9%)	1 (1%)	25	64
4	D	46/124 (37%)	39 (85%)	6 (13%)	1 (2%)	6	39
4	H	46/124 (37%)	39 (85%)	6 (13%)	1 (2%)	6	39
All	All	2150/2558 (84%)	1797 (84%)	295 (14%)	58 (3%)	5	35

5 of 58 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	178	SER
1	A	222	PRO
1	A	239	PHE
1	A	548	ASN
2	B	279	PRO

### 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	512/558 (92%)	483 (94%)	29 (6%)	20	55
1	E	512/558 (92%)	487 (95%)	25 (5%)	25	59
2	B	230/263 (88%)	211 (92%)	19 (8%)	11	42
2	F	230/263 (88%)	207 (90%)	23 (10%)	7	35
3	C	151/171 (88%)	142 (94%)	9 (6%)	19	54
3	G	151/171 (88%)	144 (95%)	7 (5%)	27	61
4	D	38/59 (64%)	34 (90%)	4 (10%)	7	33
4	H	38/59 (64%)	35 (92%)	3 (8%)	12	44
All	All	1862/2102 (89%)	1743 (94%)	119 (6%)	17	52

5 of 119 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	D	62	PHE
1	E	273	ASN
2	F	22	LEU
1	E	260	PHE
1	E	633	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	HIS
2	B	246	HIS
2	B	252	HIS
2	F	252	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 8 ligands modelled in this entry, 2 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
7	MQ7	A	1004	-	31,31,49	1.74	2 (6%)	38,41,63	1.44	8 (21%)
5	HEA	E	1002	-	57,67,67	2.11	17 (29%)	61,103,103	2.52	25 (40%)
7	MQ7	E	1004	-	31,31,49	1.74	2 (6%)	38,41,63	1.47	8 (21%)
5	HEA	A	1002	-	57,67,67	2.12	17 (29%)	61,103,103	2.54	25 (40%)
5	HEA	E	1001	1	57,67,67	2.21	19 (33%)	61,103,103	2.36	23 (37%)
5	HEA	A	1001	1	57,67,67	2.22	19 (33%)	61,103,103	2.36	23 (37%)

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
7	MQ7	A	1004	-	-	6/20/40/61	0/2/2/2
5	HEA	E	1002	-	-	7/32/76/76	-
7	MQ7	E	1004	-	-	6/20/40/61	0/2/2/2
5	HEA	A	1002	-	-	7/32/76/76	-
5	HEA	E	1001	1	-	11/32/76/76	-
5	HEA	A	1001	1	-	11/32/76/76	-

The worst 5 of 76 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1004	MQ7	C3-C2	7.82	1.49	1.35
7	E	1004	MQ7	C3-C2	7.81	1.49	1.35
5	A	1001	HEA	C3A-C2A	6.02	1.48	1.40
5	E	1001	HEA	C3A-C2A	5.96	1.48	1.40
5	A	1001	HEA	C3B-C2B	5.66	1.47	1.34

The worst 5 of 112 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1002	HEA	C3D-C4D-ND	7.06	117.19	110.36
5	E	1002	HEA	C3D-C4D-ND	7.02	117.15	110.36
5	A	1001	HEA	C3D-C4D-ND	5.99	116.16	110.36
5	E	1001	HEA	C3D-C4D-ND	5.99	116.15	110.36
5	A	1002	HEA	C2B-C1B-NB	5.74	116.76	109.88

There are no chirality outliers.

5 of 48 torsion outliers are listed below:

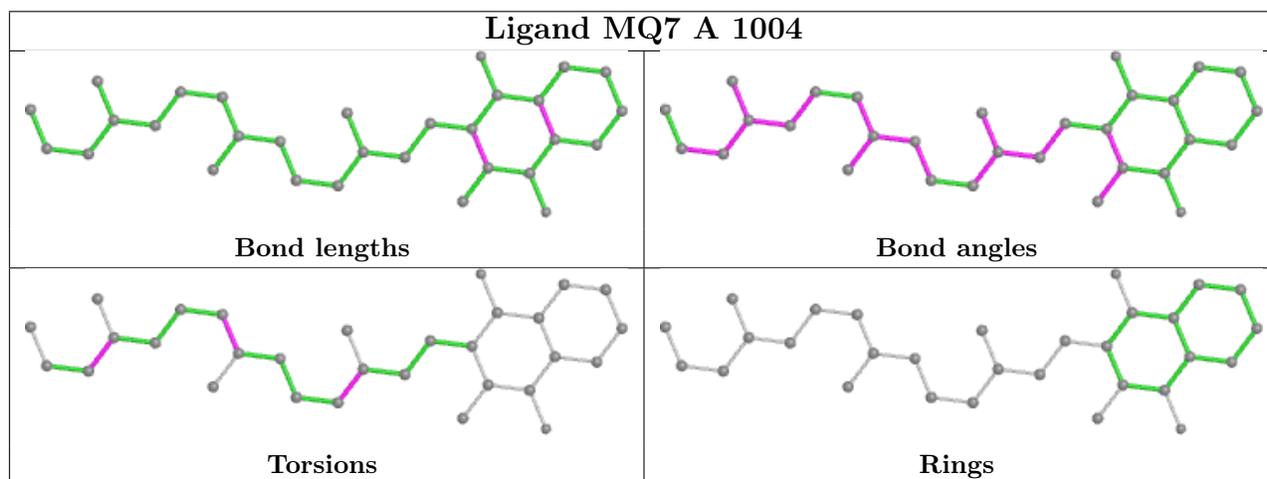
Mol	Chain	Res	Type	Atoms
5	A	1001	HEA	C3B-C11-C12-C13
5	A	1001	HEA	O11-C11-C12-C13
5	E	1001	HEA	C3B-C11-C12-C13
5	E	1001	HEA	O11-C11-C12-C13
5	A	1001	HEA	C15-C16-C17-C18

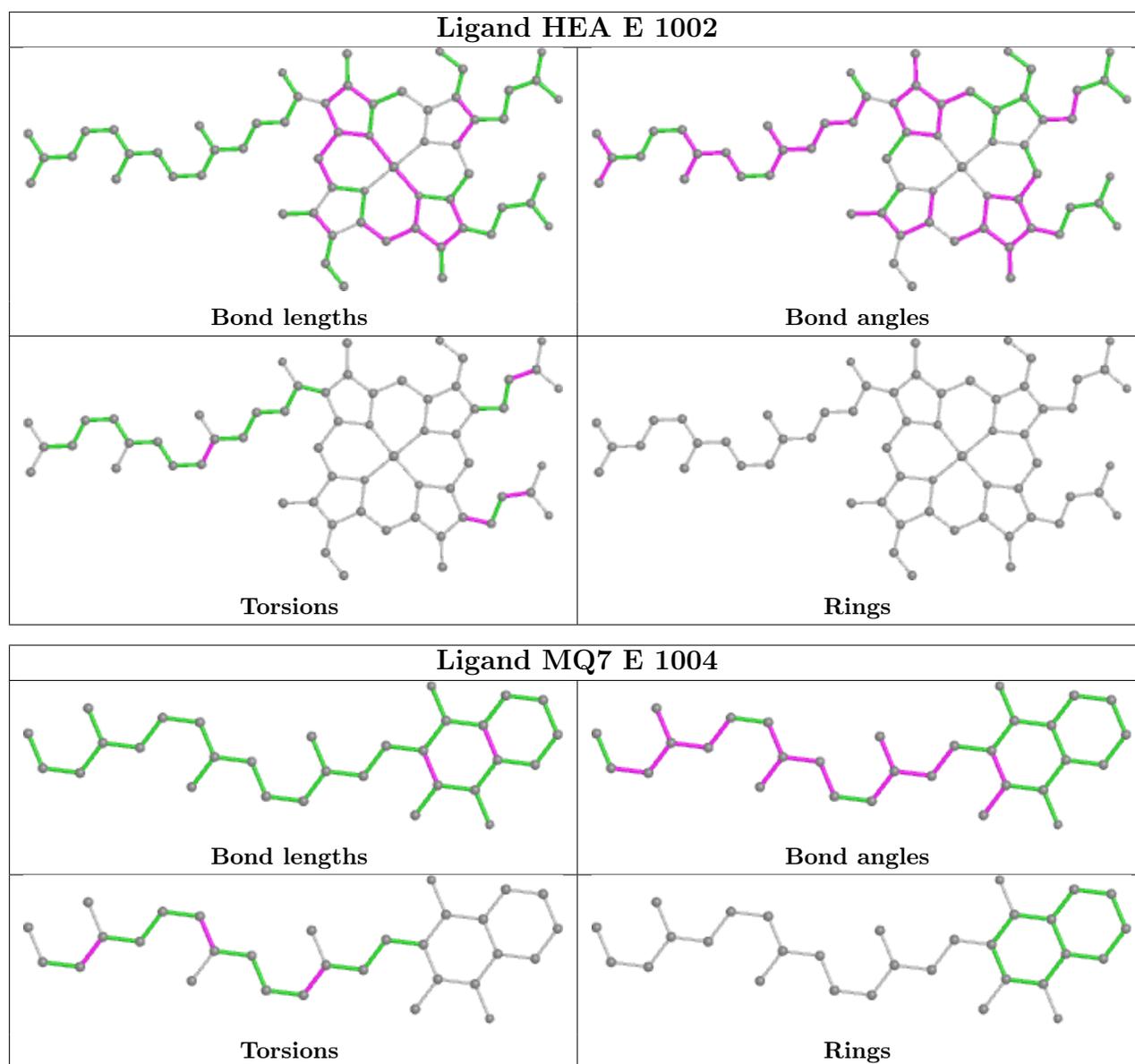
There are no ring outliers.

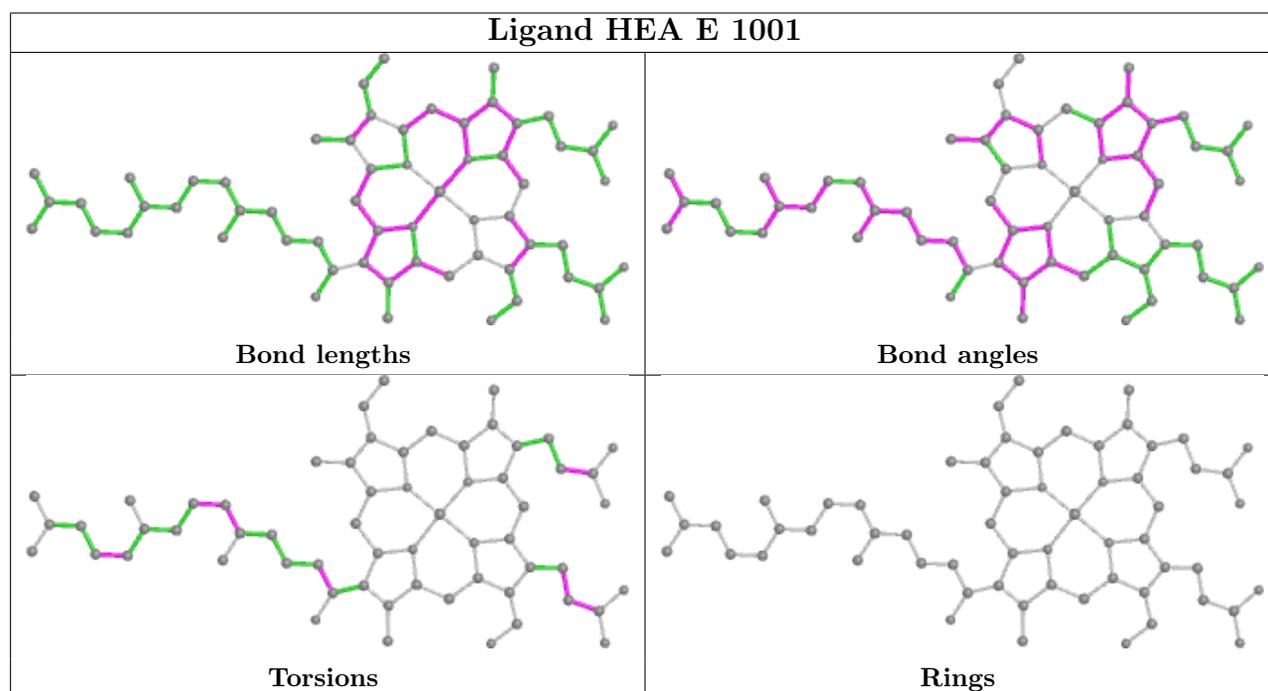
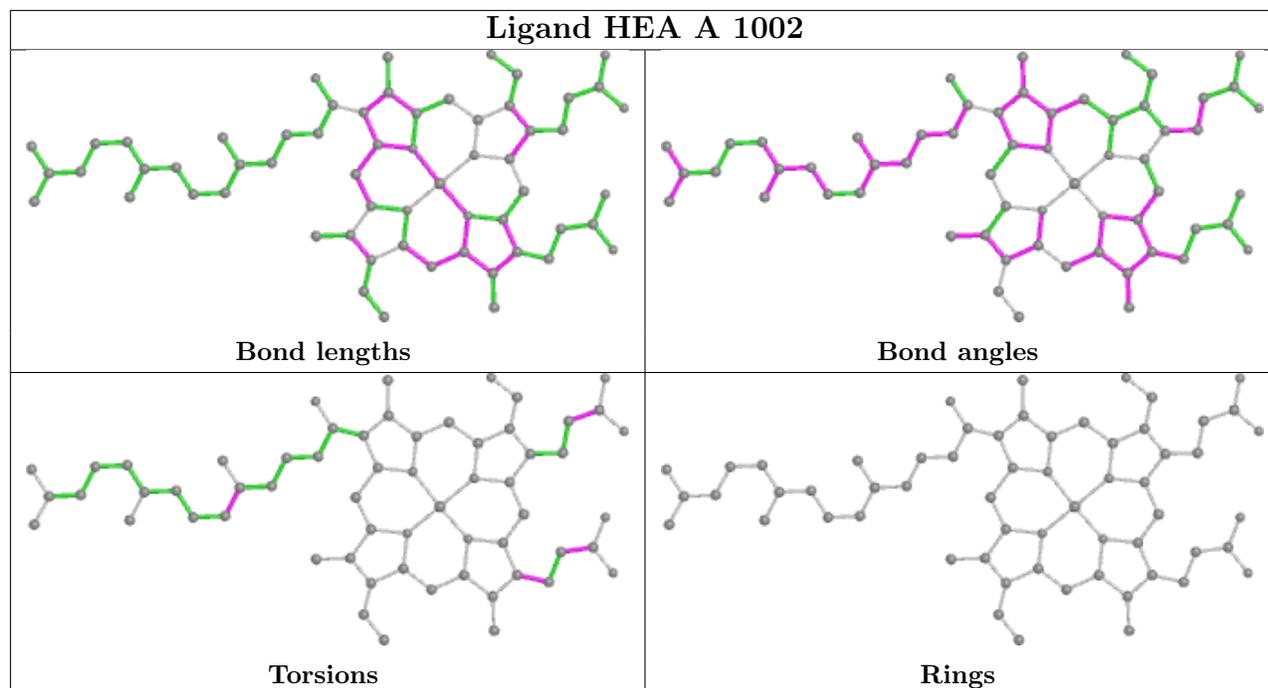
6 monomers are involved in 32 short contacts:

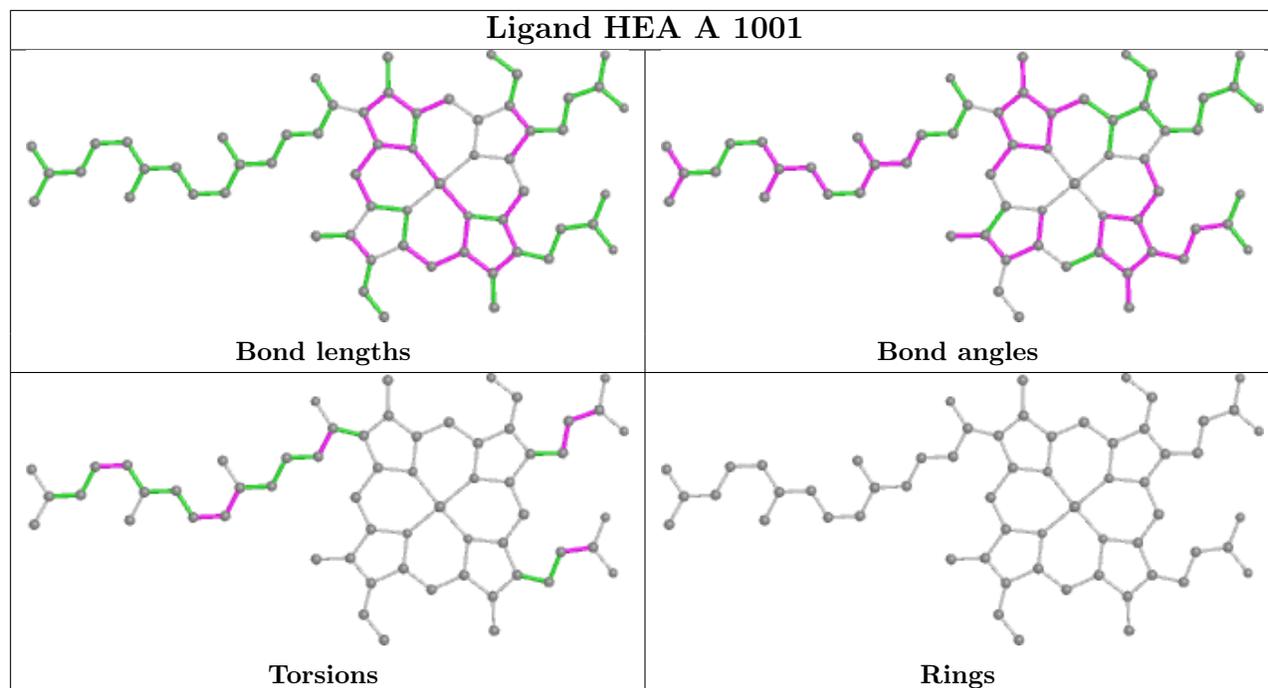
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1004	MQ7	1	0
5	E	1002	HEA	9	0
7	E	1004	MQ7	1	0
5	A	1002	HEA	9	0
5	E	1001	HEA	6	0
5	A	1001	HEA	6	0

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](#)

There are no chain breaks in this entry.

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

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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	607/655 (92%)	-0.19	7 (1%) 79 66	56, 118, 176, 223	0
1	E	607/655 (92%)	0.02	22 (3%) 42 28	68, 127, 201, 269	0
2	B	256/296 (86%)	0.16	15 (5%) 22 13	72, 151, 205, 238	0
2	F	256/296 (86%)	0.07	8 (3%) 49 33	70, 147, 210, 258	0
3	C	178/204 (87%)	-0.05	6 (3%) 45 30	72, 125, 188, 237	0
3	G	178/204 (87%)	-0.10	9 (5%) 28 17	75, 134, 203, 230	0
4	D	48/124 (38%)	-0.20	1 (2%) 63 48	84, 126, 172, 190	0
4	H	48/124 (38%)	-0.34	1 (2%) 63 48	73, 122, 174, 191	0
All	All	2178/2558 (85%)	-0.05	69 (3%) 47 32	56, 130, 199, 269	0

The worst 5 of 69 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	486	ASP	10.9
3	G	53	ALA	7.8
1	E	441	GLY	4.8
1	E	487	GLY	4.7
2	B	274	HIS	4.5

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

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

### 6.3 Carbohydrates [i](#)

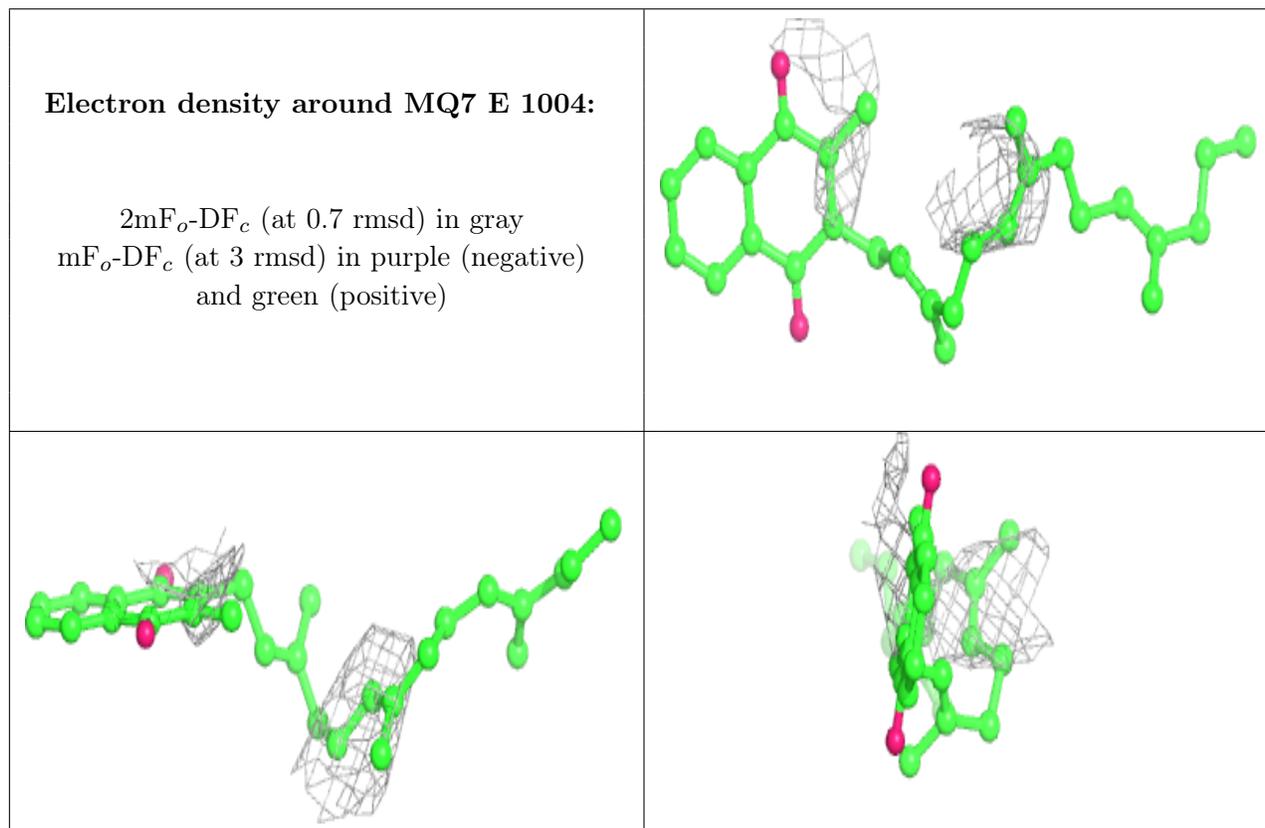
There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

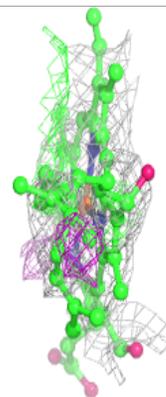
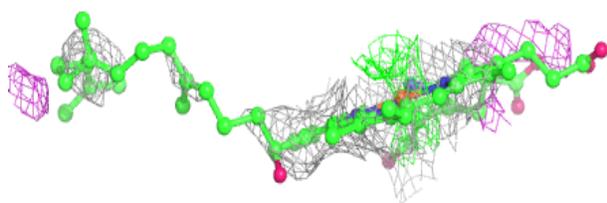
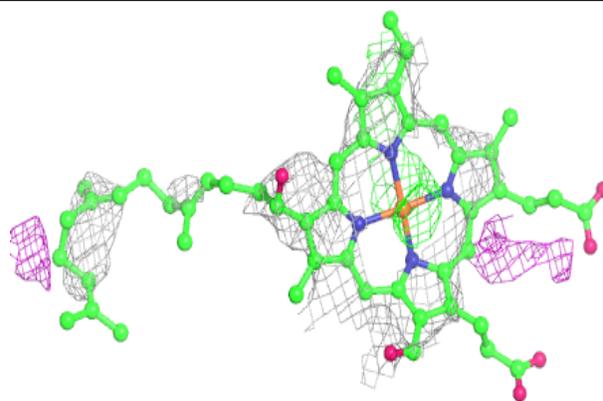
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
7	MQ7	E	1004	30/48	0.65	0.88	176,203,224,225	0
6	CU	A	1003	1/1	0.72	0.18	169,169,169,169	0
5	HEA	E	1002	60/60	0.80	0.40	97,140,157,163	0
5	HEA	E	1001	60/60	0.83	0.43	66,114,186,214	0
5	HEA	A	1002	60/60	0.83	0.42	68,147,209,219	0
7	MQ7	A	1004	30/48	0.85	0.26	121,147,178,189	0
6	CU	E	1003	1/1	0.86	0.36	122,122,122,122	0
5	HEA	A	1001	60/60	0.88	0.37	74,125,158,169	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

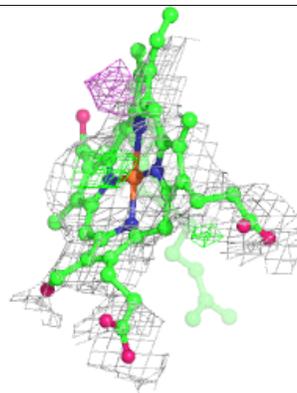
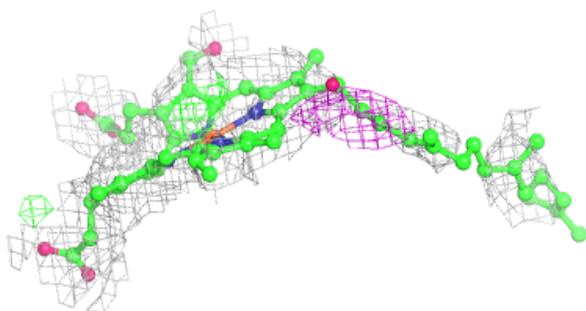
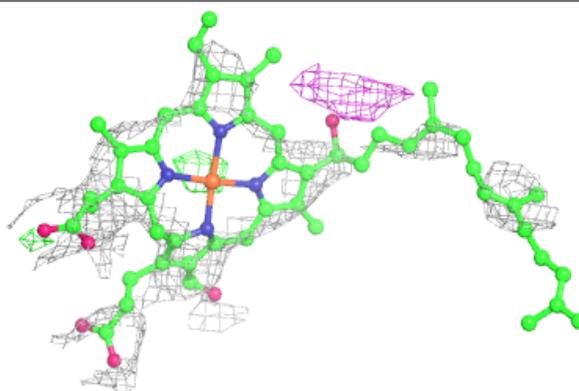


**Electron density around HEA E 1002:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

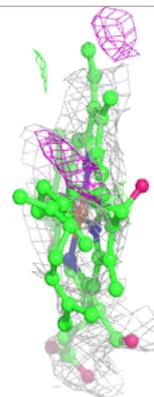
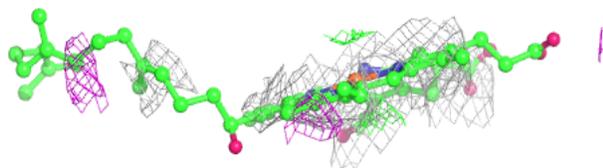
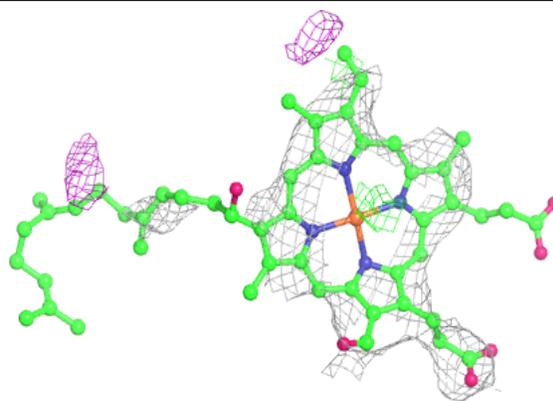
**Electron density around HEA E 1001:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

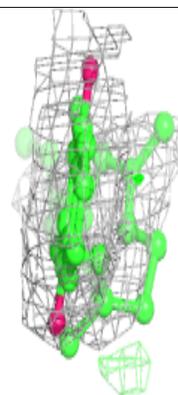
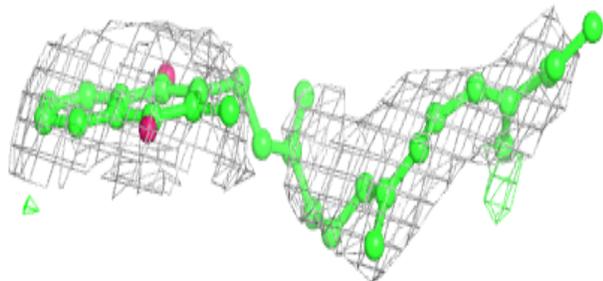
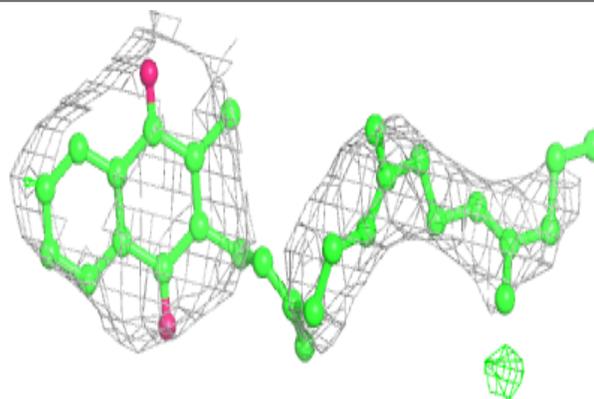


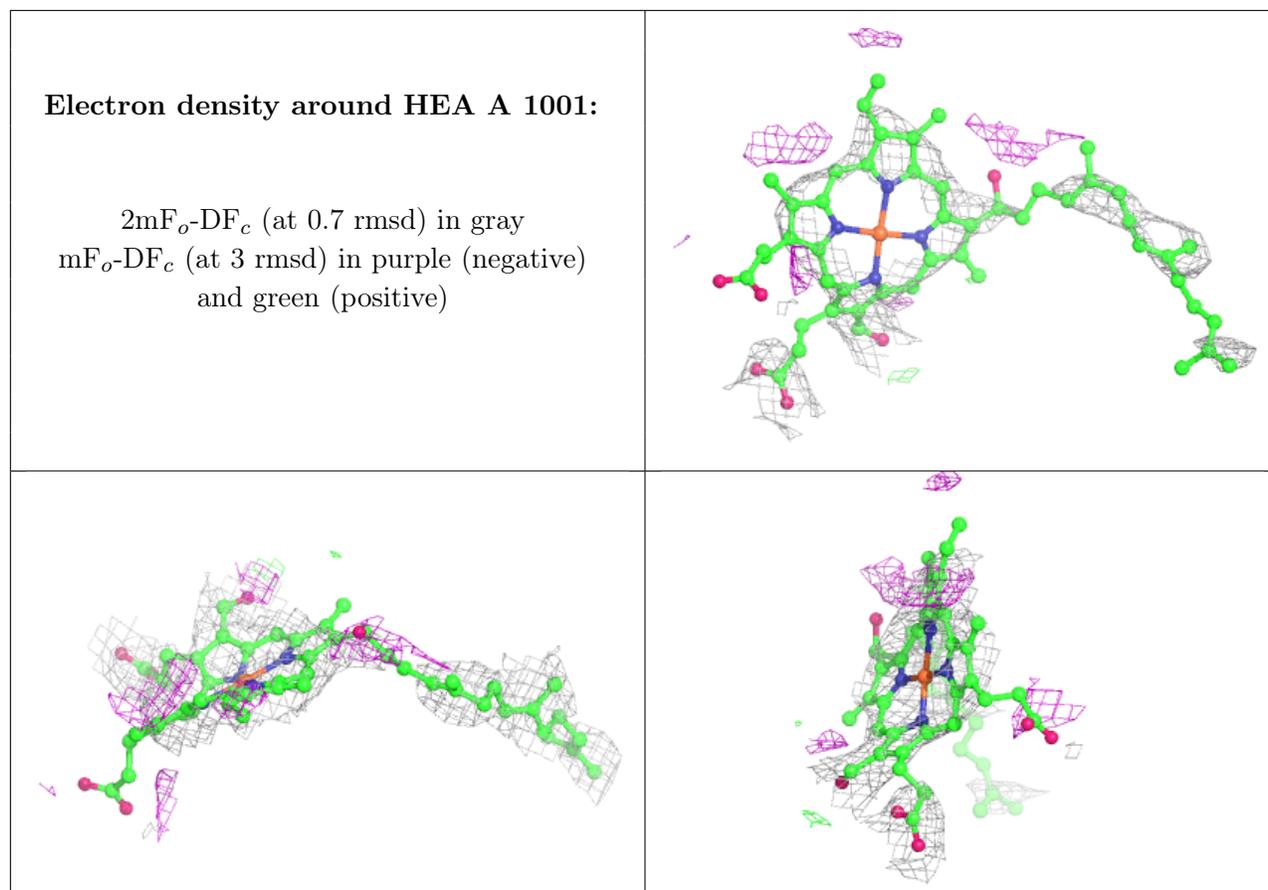
**Electron density around HEA A 1002:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around MQ7 A 1004:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.