wwPDB X-ray Structure Validation Summary Report (i)

Nov 16, 2023 – 04:14 AM JST

PDB ID	:	6KOE
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	:	3.75 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 (i) 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 (i)) were used in the production of this report:

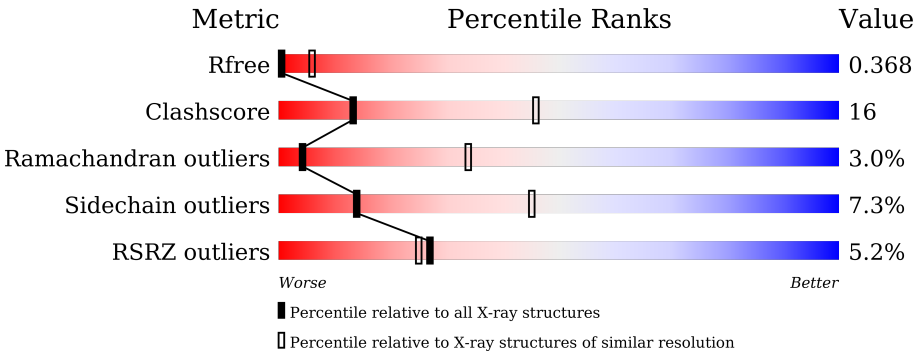
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.75 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	1039 (3.94-3.58)
Clashscore	141614	1051 (3.92-3.60)
Ramachandran outliers	138981	1015 (3.92-3.60)
Sidechain outliers	138945	1011 (3.92-3.60)
RSRZ outliers	127900	1050 (3.96-3.56)

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 <=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	2% 56% 32% · 7%
1	E	655	3% 57% 32% · 7%
2	B	296	10% 47% 33% 6% 14%
2	F	296	7% 51% 29% 7% 14%
3	C	204	4% 61% 24% · 13%
3	G	204	6% 64% 20% · 13%

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Mol	Chain	Length	Quality of chain
4	D	124	5% 39% 16% 44%
4	H	124	40% 16% 44%

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
5	HEA	A	1002	-	-	-	X
5	HEA	E	1001	-	-	-	X
5	HEA	E	1002	-	-	-	X

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 17910 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
1	A	607	Total	C	N	O	S	0	0	0
			4855	3270	752	792	41			
1	E	607	Total	C	N	O	S	0	0	0
			4855	3270	752	792	41			

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
2	B	256	Total	C	N	O	S	0	0	0
			2073	1348	328	390	7			
2	F	256	Total	C	N	O	S	0	0	0
			2073	1348	328	390	7			

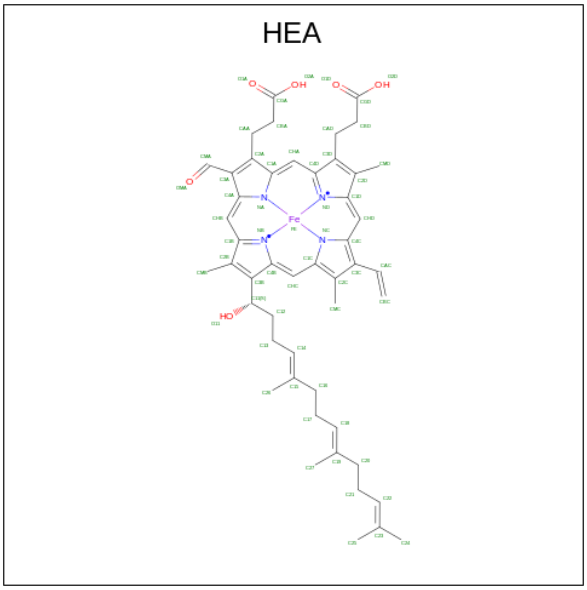
- Molecule 3 is a protein called AA3-600 quinol oxidase subunit IIII.

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

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

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

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

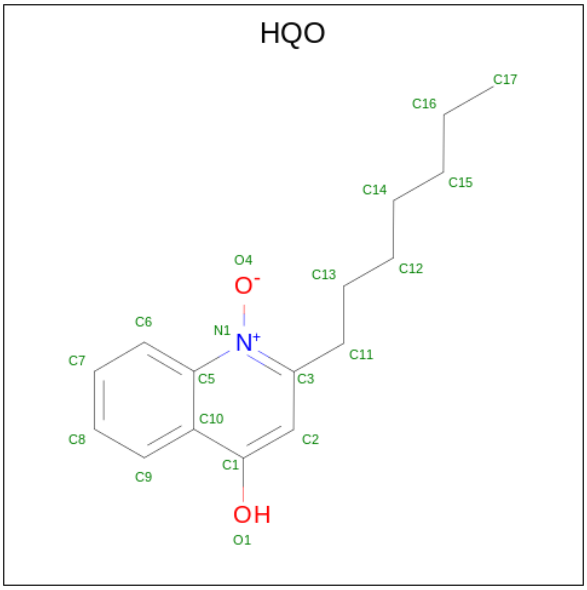


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
5	A	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
5	E	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
5	E	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		

- 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 2-HEPTYL-4-HYDROXY QUINOLINE N-OXIDE (three-letter code: HQO) (formula: $C_{16}H_{21}NO_2$).



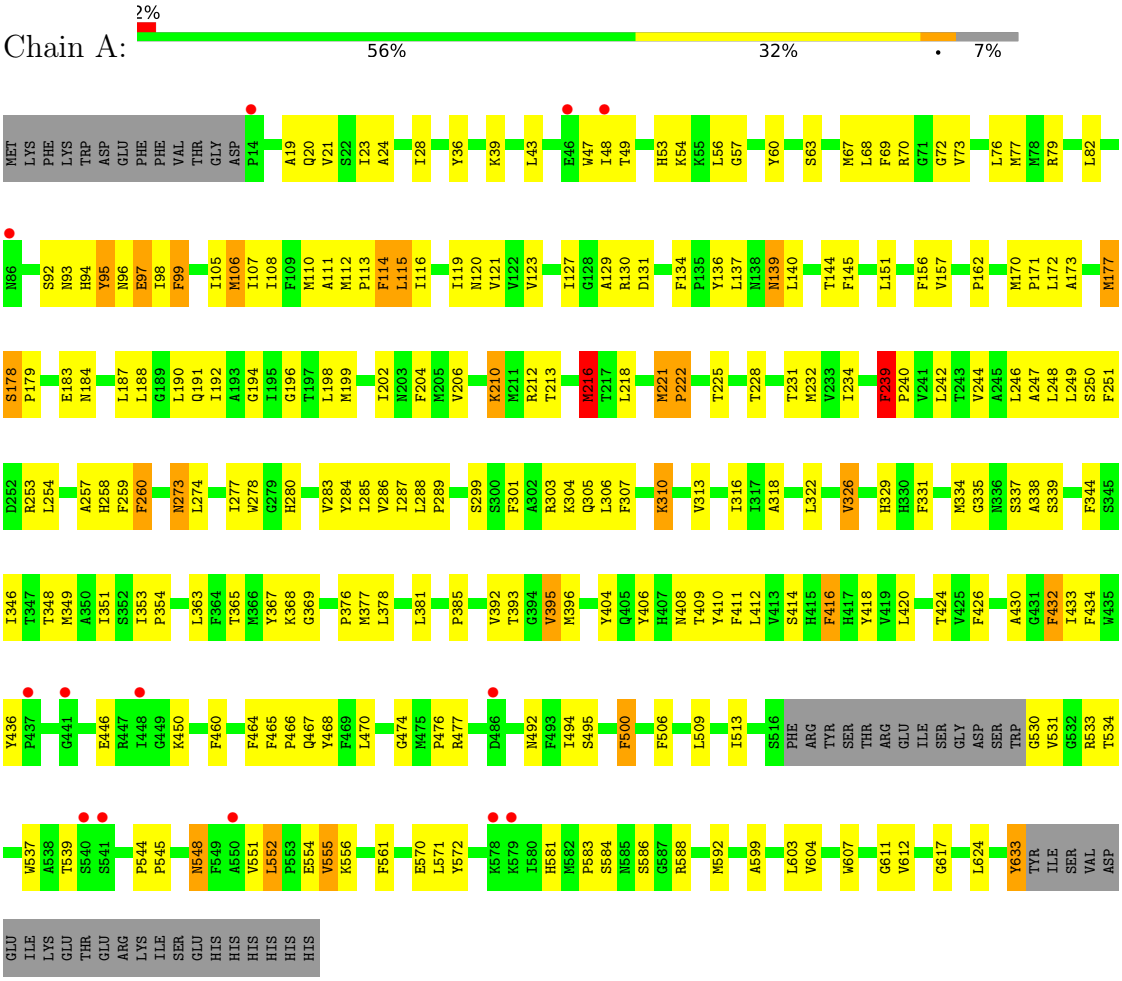
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C N O 13 10 1 2	0	0
7	E	1	Total C N O 13 10 1 2	0	0

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 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.

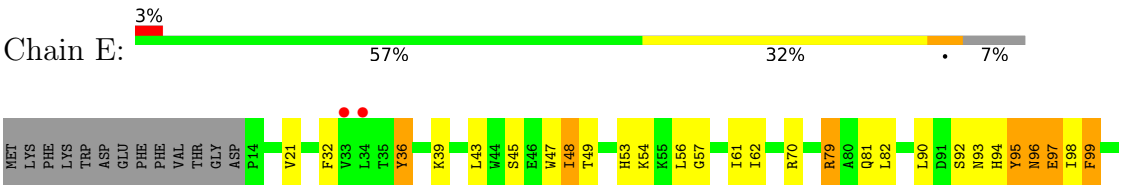
• Molecule 1: AA3-600 quinol oxidase subunit I

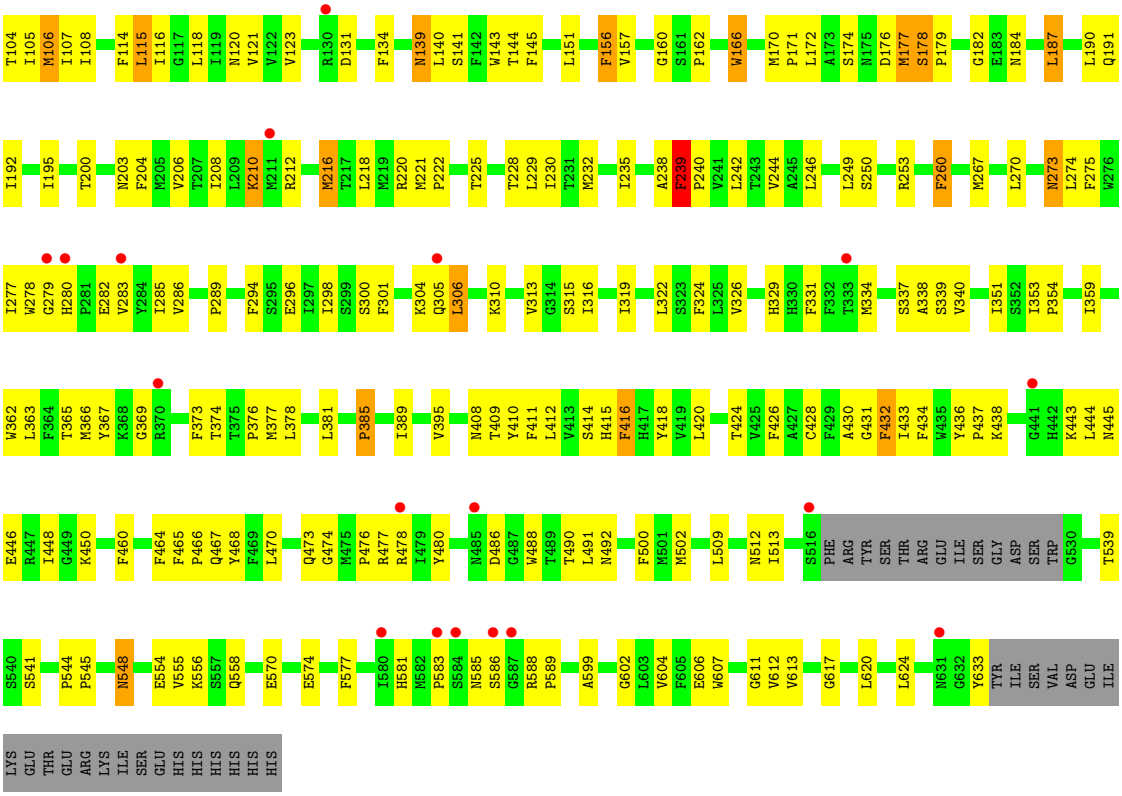
Chain A:



• Molecule 1: AA3-600 quinol oxidase subunit I

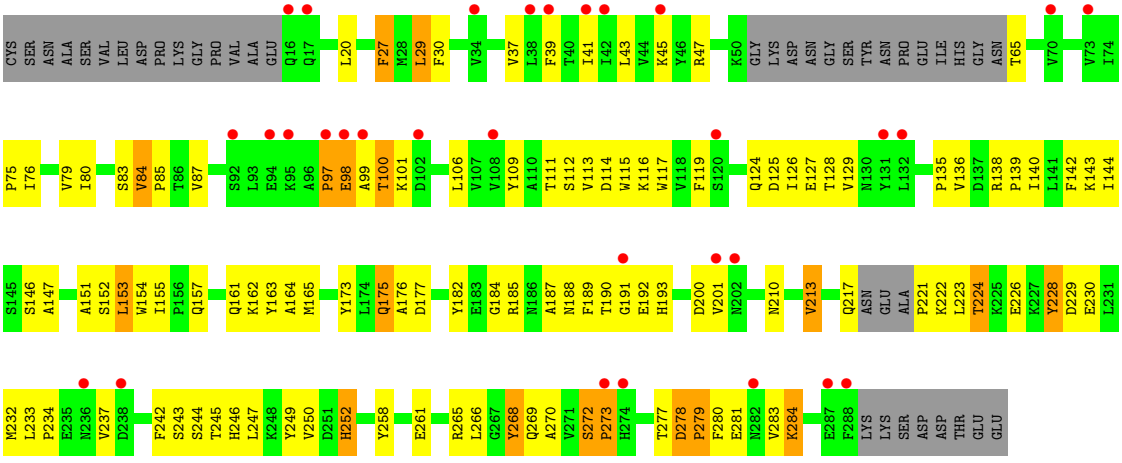
Chain E:





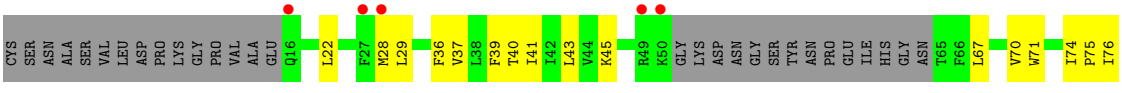
• Molecule 2: Quinol oxidase subunit 2

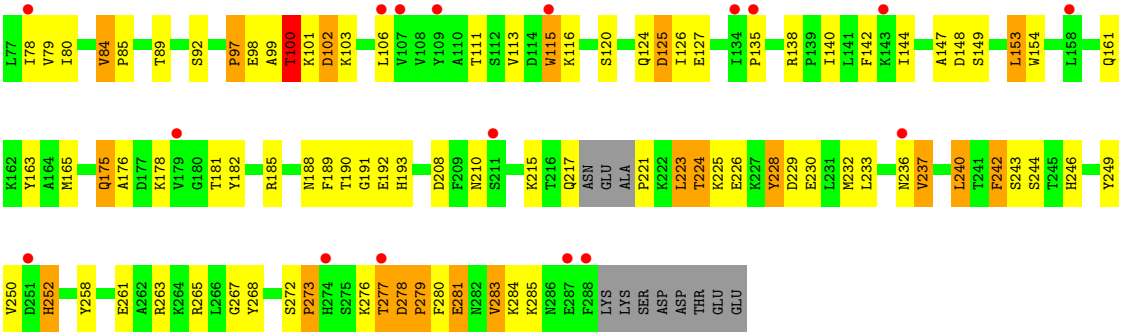
Chain B:



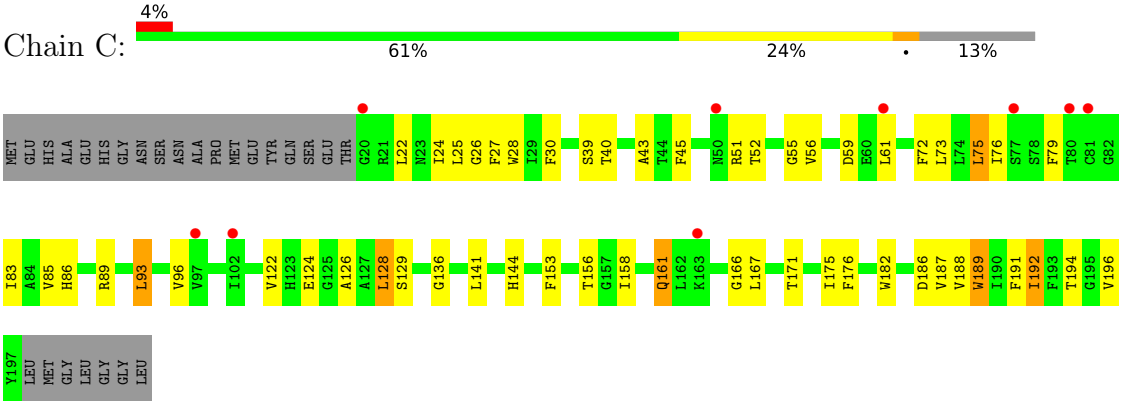
• Molecule 2: Quinol oxidase subunit 2

Chain F:

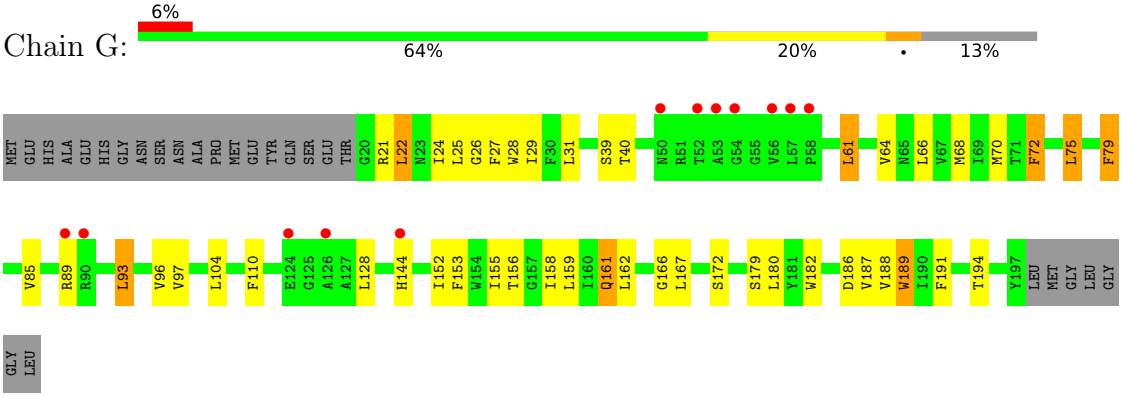




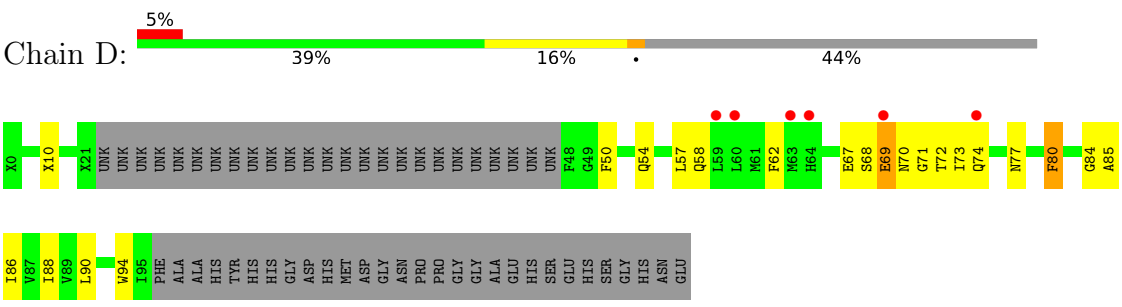
• Molecule 3: AA3-600 quinol oxidase subunit IIII



• Molecule 3: AA3-600 quinol oxidase subunit IIII

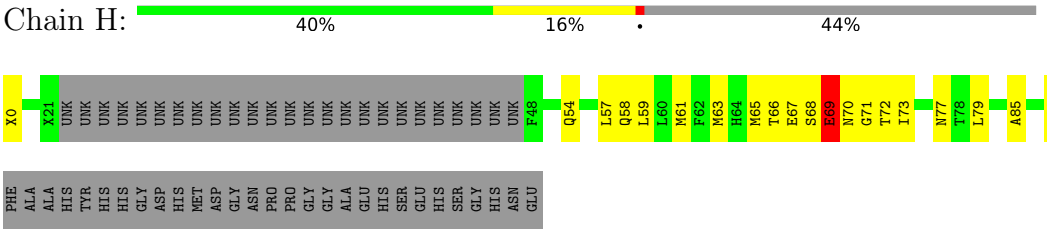


• Molecule 4: AA3-600 quinol oxidase subunit IV



• Molecule 4: AA3-600 quinol oxidase subunit IV

Chain H:


40%
16%
44%
X0 X21 UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK F48 Q54 L57 Q58 L59 L60 M61 F62 M63 H64 M65 T66 E67 S68 E69 N70 G71 T72 I73 N77 T78 L79 A85 I88 W94 I95
PHE ALA ALA HIS TYR HIS HIS GLY ASP HIS MET ASP GLY ASN PRO PRO GLY GLY ALA GLU HIS SER GLU HIS SER GLY HIS ASN GLU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	112.99Å 162.11Å 149.51Å 90.00° 109.02° 90.00°	Depositor
Resolution (Å)	49.25 – 3.75 49.25 – 3.75	Depositor EDS
% Data completeness (in resolution range)	99.5 (49.25-3.75) 99.1 (49.25-3.75)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.30 (at 3.77Å)	Xtriage
Refinement program	PHENIX 1.14_3235	Depositor
R, R_{free}	0.347 , 0.368 0.347 , 0.368	Depositor DCC
R_{free} test set	1993 reflections (3.85%)	wwPDB-VP
Wilson B-factor (Å^2)	95.0	Xtriage
Anisotropy	0.746	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.18 , -1.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.78	EDS
Total number of atoms	17910	wwPDB-VP
Average B, all atoms (Å^2)	121.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.93% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CU, HQO, 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	0.28	0/5022	0.45	0/6827
1	E	0.29	0/5022	0.45	0/6827
2	B	0.27	0/2122	0.48	0/2879
2	F	0.28	0/2122	0.50	0/2879
3	C	0.27	0/1452	0.44	0/1974
3	G	0.26	0/1452	0.44	0/1974
4	D	0.30	0/381	0.45	0/514
4	H	0.29	0/381	0.44	0/514
All	All	0.28	0/17954	0.46	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

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	184	0
1	E	4855	0	4855	173	0
2	B	2073	0	2061	82	0
2	F	2073	0	2061	73	0
3	C	1411	0	1444	47	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	1411	0	1444	43	0
4	D	482	0	395	16	0
4	H	482	0	395	22	0
5	A	120	0	106	18	0
5	E	120	0	106	12	0
6	A	1	0	0	0	0
6	E	1	0	0	0	0
7	A	13	0	4	4	0
7	E	13	0	5	5	0
All	All	17910	0	17731	577	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 16.

The worst 5 of 577 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:170:MET:HG2	1:A:260:PHE:HB2	1.51	0.92
1:E:170:MET:HG2	1:E:260:PHE:HB2	1.56	0.88
1:E:108:ILE:HG21	1:E:190:LEU:HD22	1.61	0.83
1:A:187:LEU:HD21	1:A:249:LEU:HG	1.63	0.81
1:A:134:PHE:HZ	3:C:26:GLY:HA3	1.42	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	603/655 (92%)	509 (84%)	76 (13%)	18 (3%)	4 34
1	E	603/655 (92%)	510 (85%)	77 (13%)	16 (3%)	5 35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	B	250/296 (84%)	188 (75%)	49 (20%)	13 (5%)	2 23
2	F	250/296 (84%)	189 (76%)	48 (19%)	13 (5%)	2 23
3	C	176/204 (86%)	154 (88%)	21 (12%)	1 (1%)	25 61
3	G	176/204 (86%)	157 (89%)	19 (11%)	0	100 100
4	D	46/124 (37%)	37 (80%)	7 (15%)	2 (4%)	2 26
4	H	46/124 (37%)	37 (80%)	7 (15%)	2 (4%)	2 26
All	All	2150/2558 (84%)	1781 (83%)	304 (14%)	65 (3%)	4 34

5 of 65 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	98	GLU

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%)	481 (94%)	31 (6%)	18 51
1	E	512/558 (92%)	477 (93%)	35 (7%)	16 47
2	B	230/263 (88%)	210 (91%)	20 (9%)	10 39
2	F	230/263 (88%)	207 (90%)	23 (10%)	7 32
3	C	151/171 (88%)	139 (92%)	12 (8%)	12 43
3	G	151/171 (88%)	141 (93%)	10 (7%)	16 48
4	D	38/59 (64%)	35 (92%)	3 (8%)	12 43
4	H	38/59 (64%)	36 (95%)	2 (5%)	22 54
All	All	1862/2102 (89%)	1726 (93%)	136 (7%)	14 45

5 of 136 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	151	LEU
1	E	177	MET
1	E	416	PHE
2	B	272	SER
2	B	268	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
2	F	252	HIS
1	E	184	ASN
2	B	246	HIS
2	B	252	HIS
4	H	58	GLN

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	$\#\|Z\|>2$
5	HEA	A	1001	1	57,67,67	2.26	19 (33%)	61,103,103	2.29	23 (37%)
5	HEA	E	1002	1	57,67,67	2.16	17 (29%)	61,103,103	2.58	26 (42%)
5	HEA	A	1002	-	57,67,67	2.12	18 (31%)	61,103,103	2.58	26 (42%)
7	HQO	E	1004	-	14,14,20	3.20	3 (21%)	13,20,26	1.49	1 (7%)
7	HQO	A	1004	1	14,14,20	3.23	3 (21%)	13,20,26	1.43	1 (7%)
5	HEA	E	1001	1	57,67,67	2.29	19 (33%)	61,103,103	2.22	21 (34%)

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
5	HEA	A	1001	1	-	7/32/76/76	-
5	HEA	E	1002	1	-	7/32/76/76	-
5	HEA	A	1002	-	-	7/32/76/76	-
7	HQO	E	1004	-	-	-	0/2/2/2
7	HQO	A	1004	1	-	-	0/2/2/2
5	HEA	E	1001	1	-	7/32/76/76	-

The worst 5 of 79 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1004	HQO	O4-N1	-10.62	1.24	1.38
7	E	1004	HQO	O4-N1	-10.52	1.24	1.38
5	E	1001	HEA	C3A-C2A	6.56	1.49	1.40
5	A	1001	HEA	C3A-C2A	6.18	1.49	1.40
5	E	1001	HEA	C3B-C2B	5.82	1.47	1.34

The worst 5 of 98 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	1002	HEA	C3D-C4D-ND	7.11	117.24	110.36
5	A	1002	HEA	C3D-C4D-ND	6.85	116.99	110.36
5	E	1002	HEA	C2B-C1B-NB	6.18	117.28	109.88
5	A	1002	HEA	C2B-C1B-NB	6.00	117.07	109.88
5	E	1001	HEA	CHA-C4D-ND	-5.86	118.06	124.43

There are no chirality outliers.

5 of 28 torsion outliers are listed below:

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

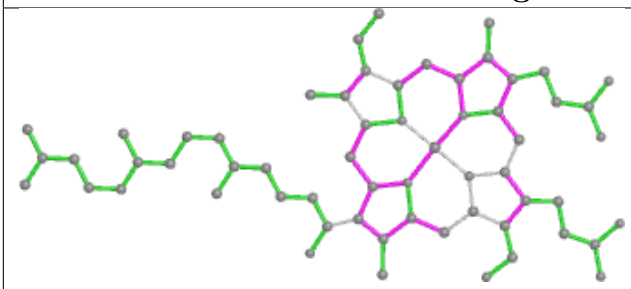
There are no ring outliers.

6 monomers are involved in 39 short contacts:

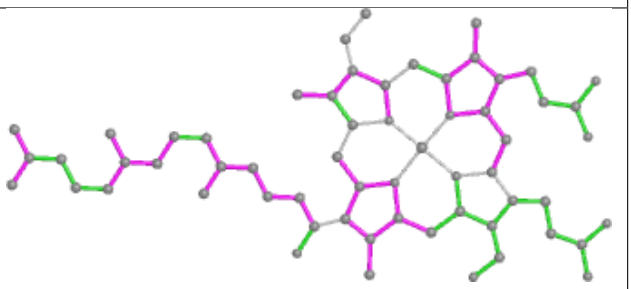
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1001	HEA	11	0
5	E	1002	HEA	7	0
5	A	1002	HEA	7	0
7	E	1004	HQO	5	0
7	A	1004	HQO	4	0
5	E	1001	HEA	5	0

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 then 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.

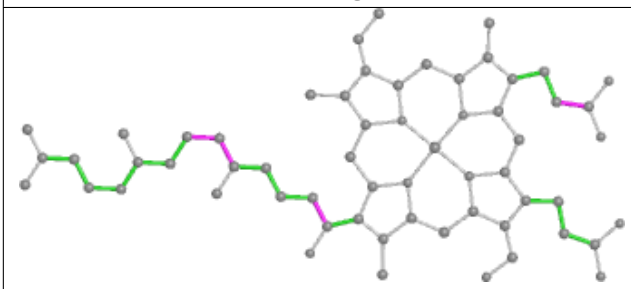
Ligand HEA A 1001



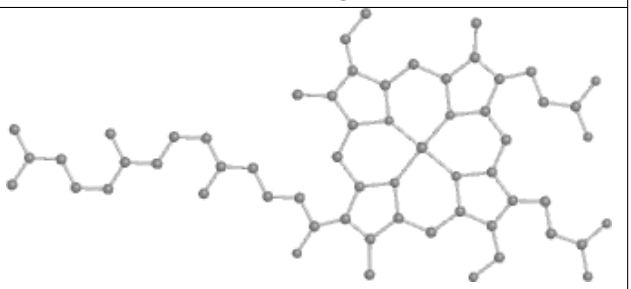
Bond lengths



Bond angles

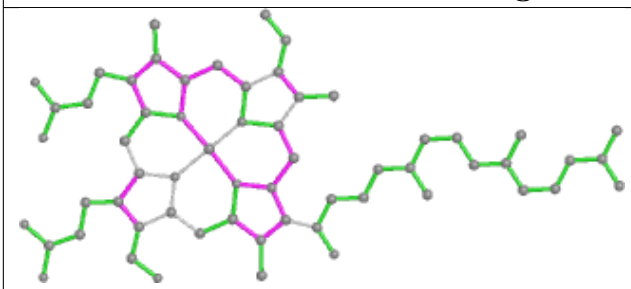


Torsions

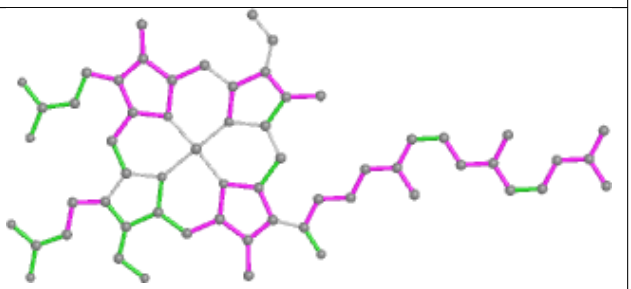


Rings

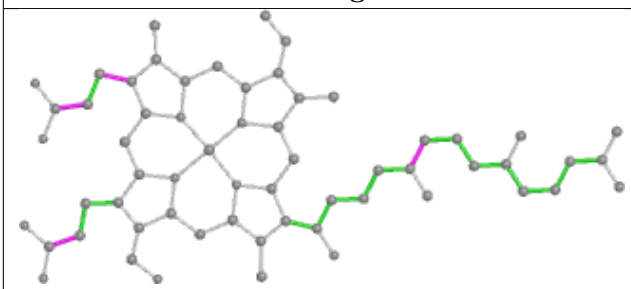
Ligand HEA E 1002



Bond lengths



Bond angles



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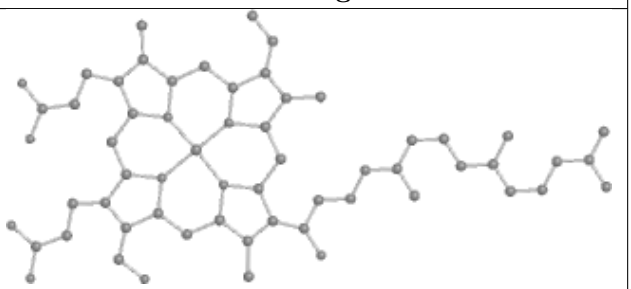
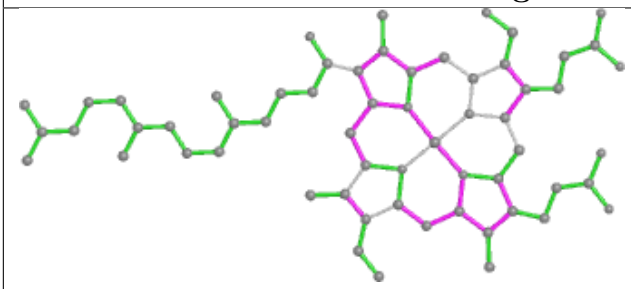
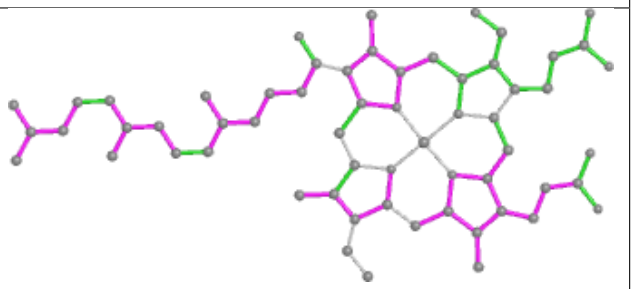


Rings

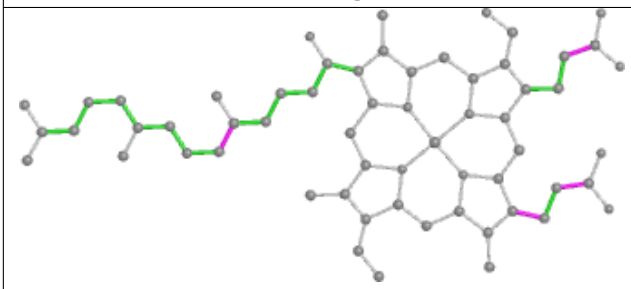
Ligand HEA A 1002



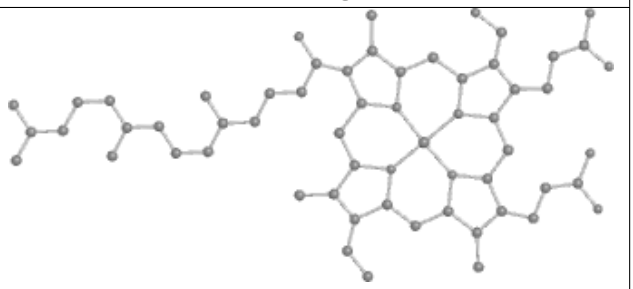
Bond lengths



Bond angles

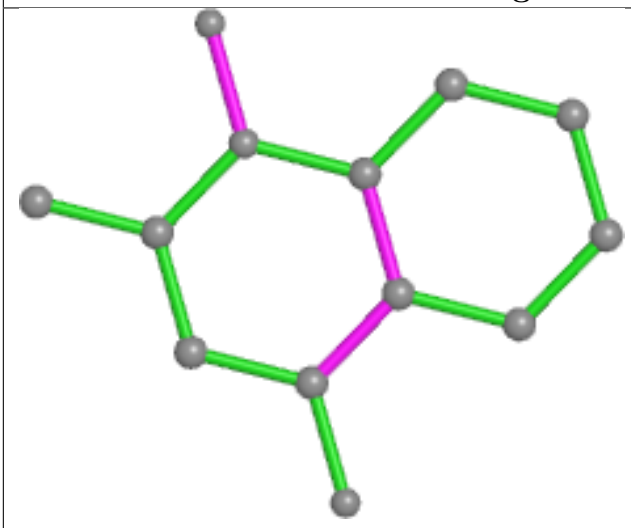


Torsions

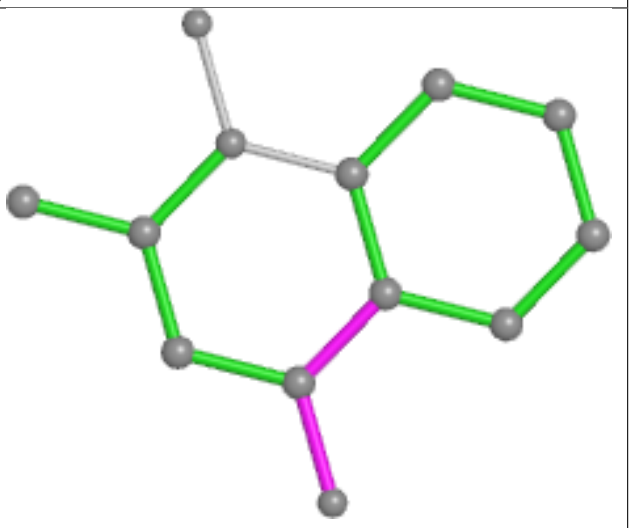


Rings

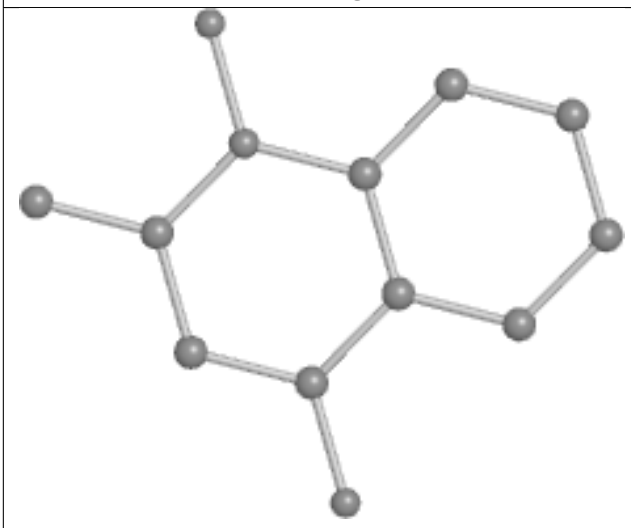
Ligand HQO E 1004



Bond lengths



Bond angles



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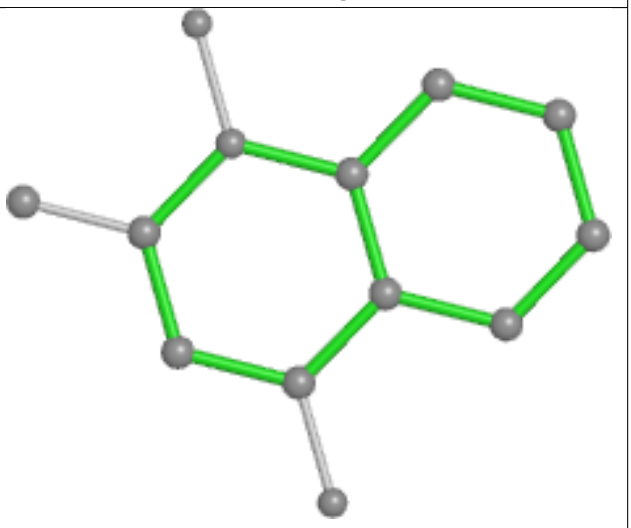
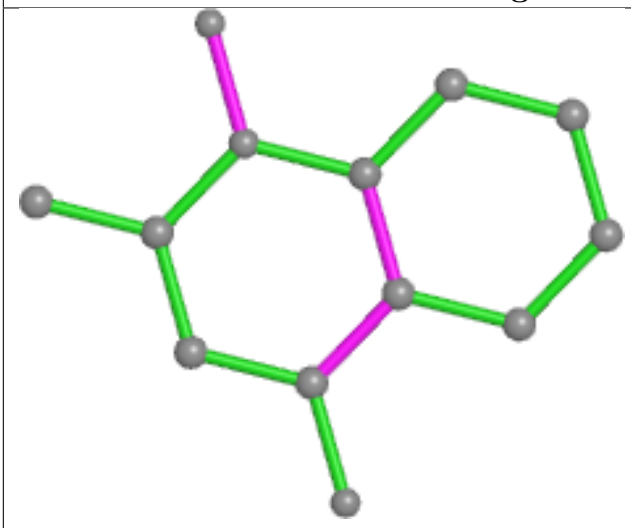


Rings

Ligand HQO A 1004



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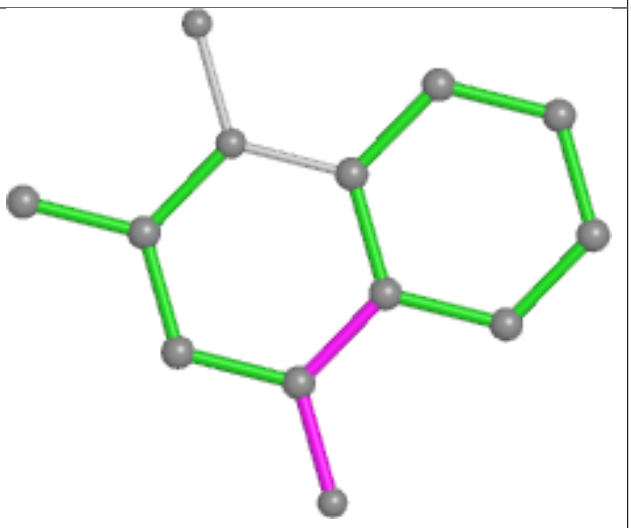
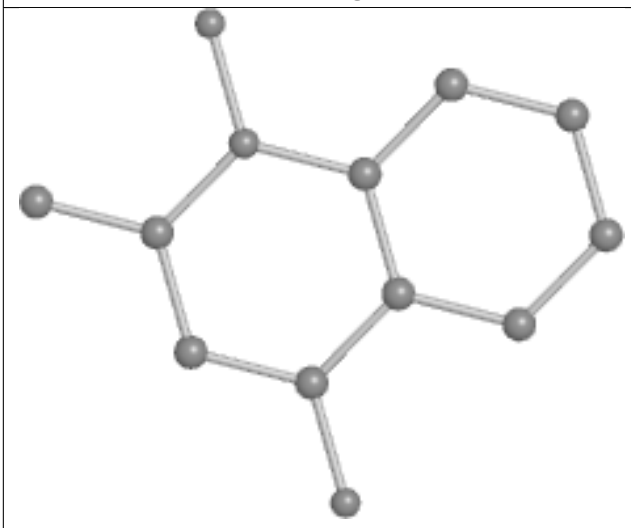


Bond angles



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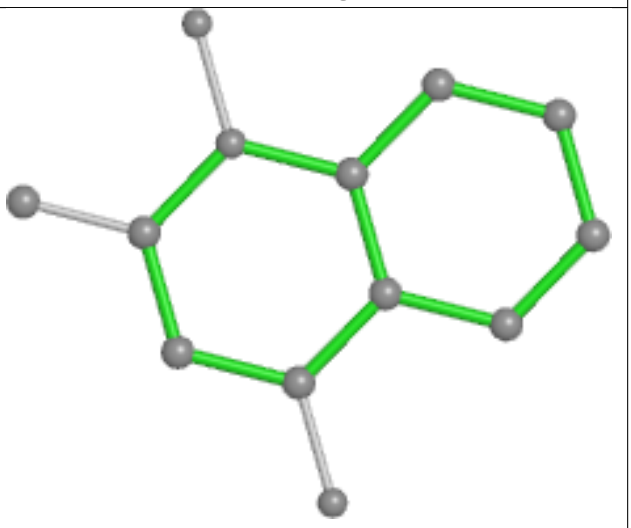
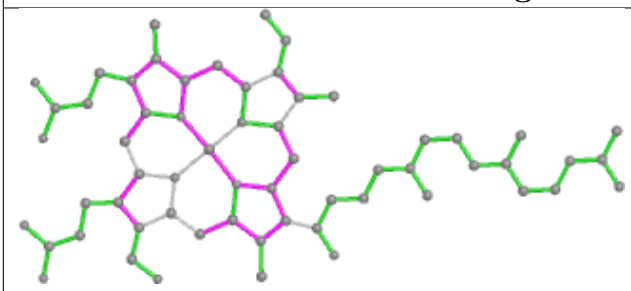
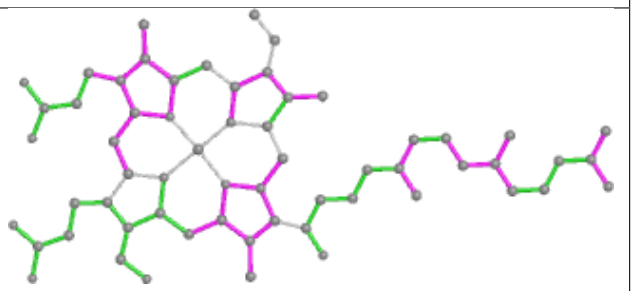


Rings

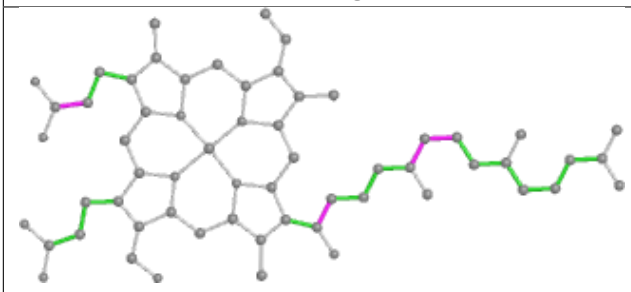
Ligand HEA E 1001



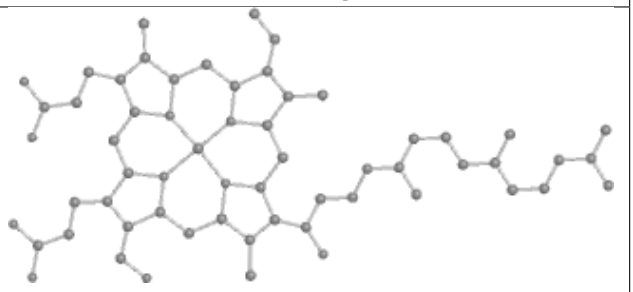
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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^{th} 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^2)	Q<0.9
1	A	607/655 (92%)	0.02	13 (2%) 63 58	68, 108, 149, 180	0
1	E	607/655 (92%)	0.03	20 (3%) 46 40	66, 111, 155, 191	0
2	B	256/296 (86%)	0.44	31 (12%) 4 4	90, 139, 195, 223	0
2	F	256/296 (86%)	0.41	22 (8%) 10 9	79, 134, 197, 235	0
3	C	178/204 (87%)	-0.03	9 (5%) 28 25	79, 115, 191, 235	0
3	G	178/204 (87%)	0.03	12 (6%) 17 14	72, 124, 187, 200	0
4	D	48/124 (38%)	0.43	6 (12%) 3 4	81, 115, 158, 166	0
4	H	48/124 (38%)	-0.37	0 100 100	72, 109, 152, 160	0
All	All	2178/2558 (85%)	0.11	113 (5%) 27 25	66, 117, 179, 235	0

The worst 5 of 113 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	274	HIS	7.3
4	D	60	LEU	7.0
3	G	53	ALA	6.9
2	F	106	LEU	6.4
2	B	42	ILE	5.7

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands (i)

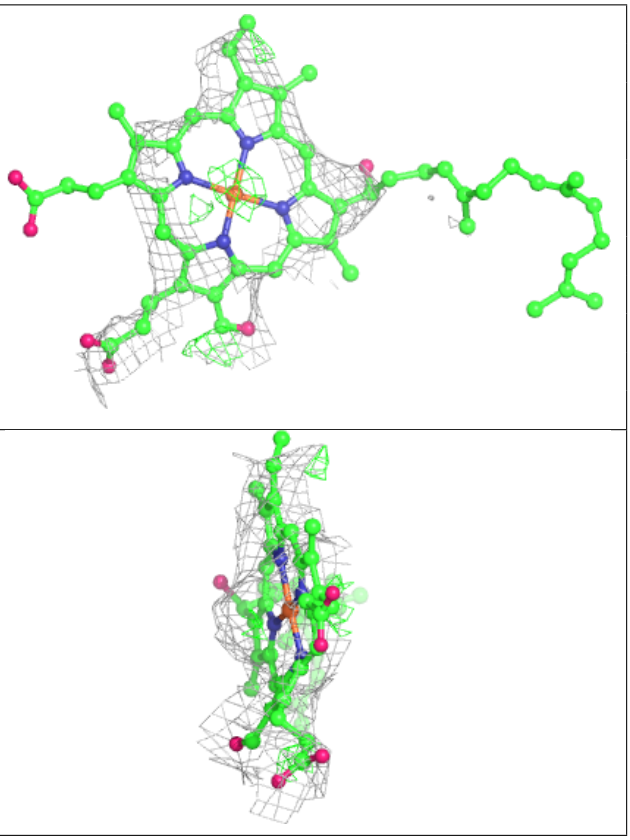
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	HEA	A	1002	60/60	0.73	0.48	96,118,163,168	0
5	HEA	E	1002	60/60	0.73	0.47	92,117,141,142	0
5	HEA	E	1001	60/60	0.78	0.50	88,109,131,135	0
6	CU	E	1003	1/1	0.79	0.29	104,104,104,104	0
5	HEA	A	1001	60/60	0.84	0.41	91,112,132,134	0
7	HQO	E	1004	13/19	0.84	0.22	102,107,111,114	0
6	CU	A	1003	1/1	0.85	0.20	109,109,109,109	0
7	HQO	A	1004	13/19	0.89	0.17	95,102,107,110	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.

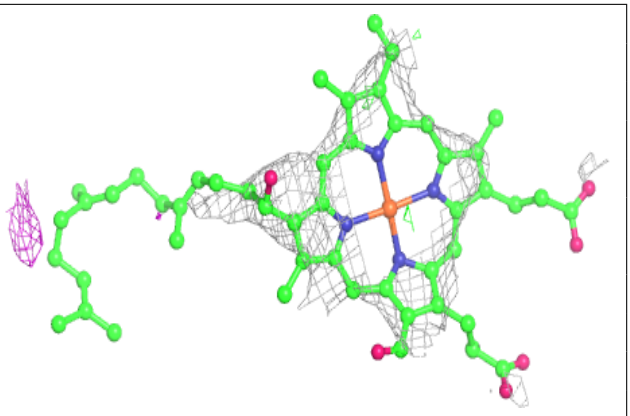
Electron density around HEA A 1002:

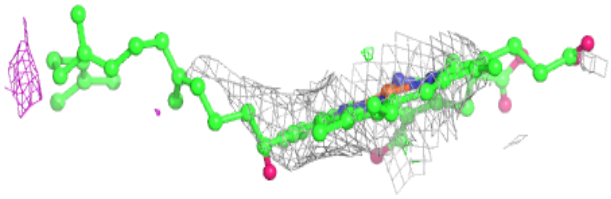
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

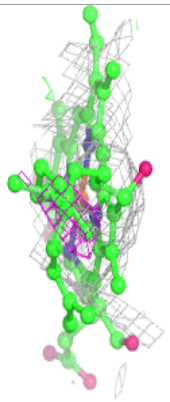


Electron density around HEA E 1002:

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

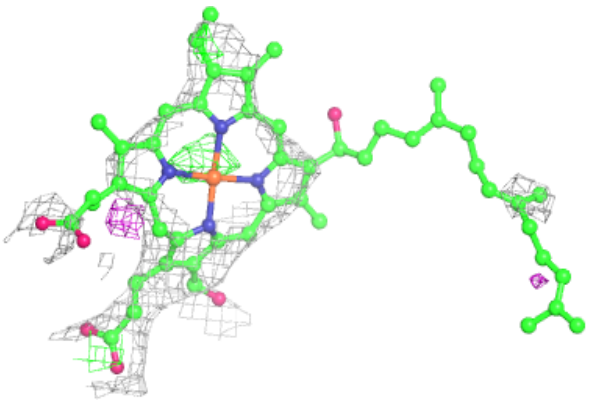


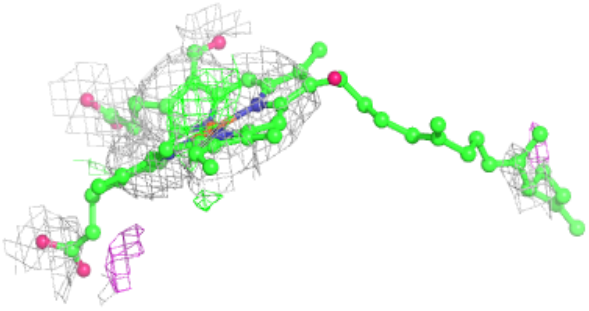


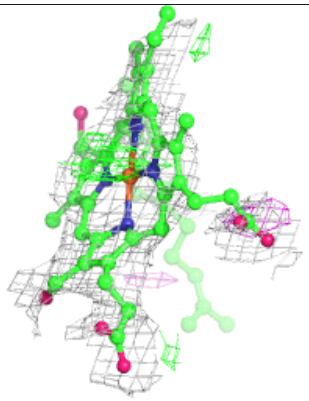


Electron density around HEA E 1001:

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

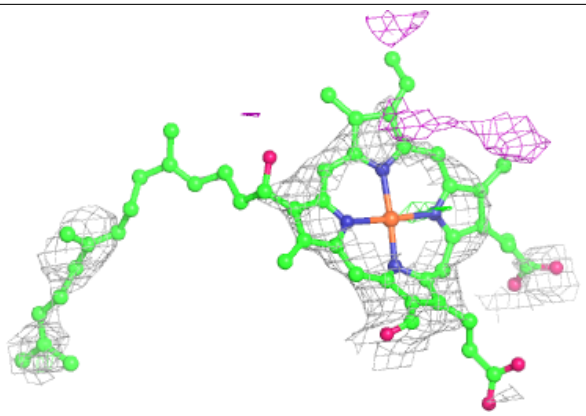


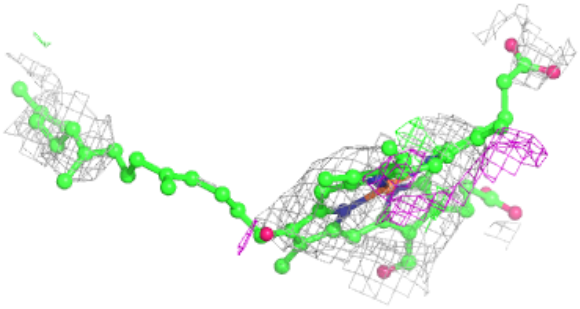


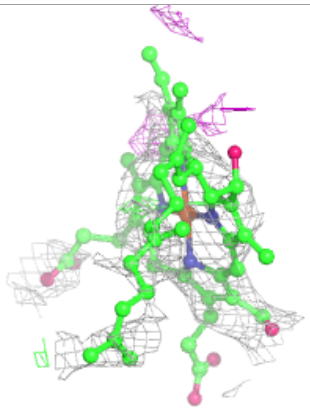


Electron density around HEA A 1001:

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

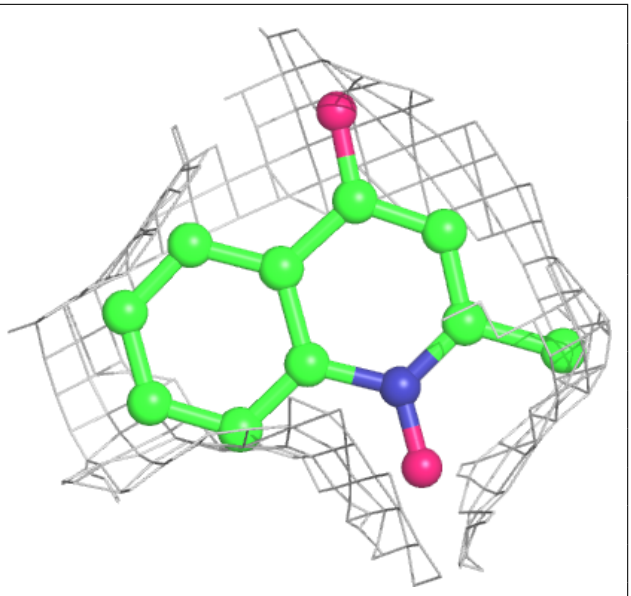


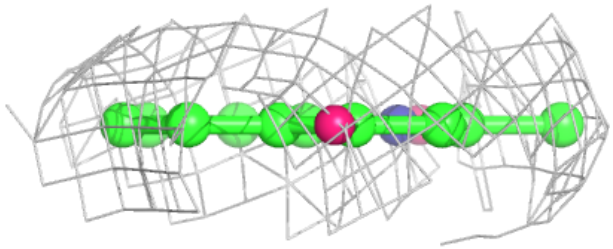


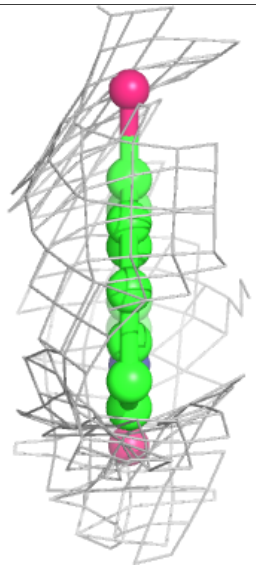


Electron density around HQO E 1004:

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

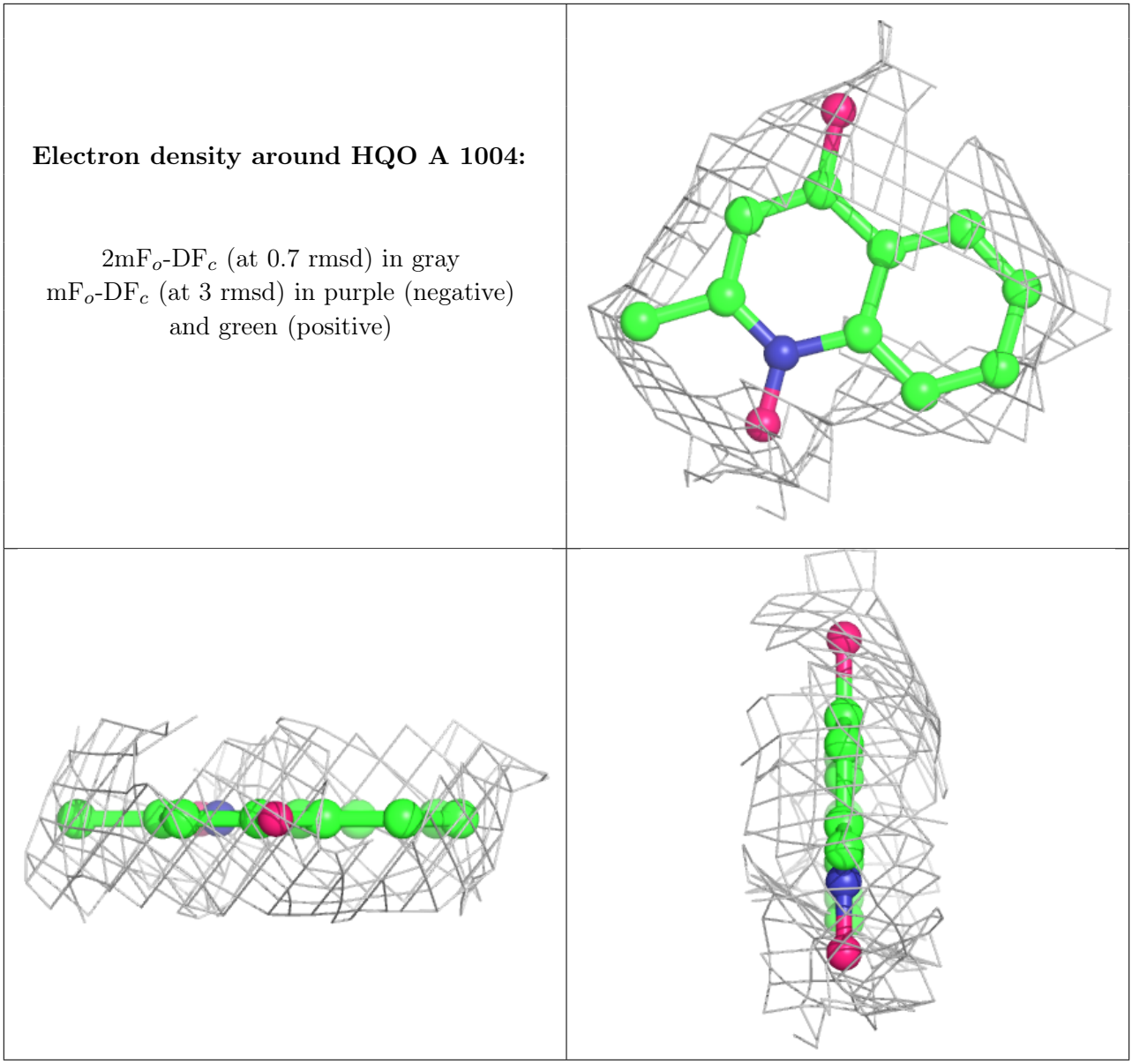






Electron density around HQO A 1004:

$2mF_o$-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.