

wwPDB X-ray Structure Validation Summary Report (i)

Nov 6, 2023 – 04:20 PM JST

PDB ID : 8K6Y

Title: Serial femtosecond crystallography structure of photo dissociated CO from

ba3- type cytochrome c oxidase determined by extrapolation method

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Deposited on : 2023-07-25

Resolution : 2.00 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)

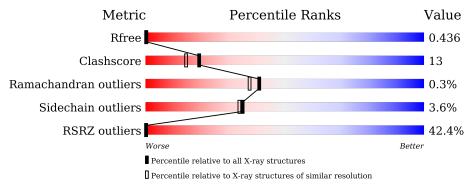
Validation Pipeline (wwPDB-VP) : 2.36

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 2.00 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	$\begin{array}{c} \textbf{Whole archive} \\ (\#\text{Entries}) \end{array}$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries},{\rm resolution\ range}({\rm \AA})) \end{array}$
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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		
			44%		
1	A	569	70%	26%	
			33%		
2	В	168	76%	22%	• •
			35%		
3	С	34	85%		9%

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 crite-



ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	HAS	A	603	X	-	-	-
7	OLC	A	607	-	-	-	X
7	OLC	A	610	-	-	-	X
7	OLC	С	101	_	-	-	X



2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 6474 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 subunit 1.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	A	554	Total 4368	C 2963	N 698	O 691	S 16	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	MET	-	initiating methionine	UNP Q5SJ79
A	-5	HIS	-	expression tag	UNP Q5SJ79
A	-4	HIS	-	expression tag	UNP Q5SJ79
A	-3	HIS	-	expression tag	UNP Q5SJ79
A	-2	HIS	-	expression tag	UNP Q5SJ79
A	-1	HIS	-	expression tag	UNP Q5SJ79
A	0	HIS	-	expression tag	UNP Q5SJ79
A	1	HIS	-	expression tag	UNP Q5SJ79

• Molecule 2 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
2	В	167	Total 1301	C 846	N 216	O 235	S 4	0	0	0

• Molecule 3 is a protein called Cytochrome c oxidase polypeptide 2A.

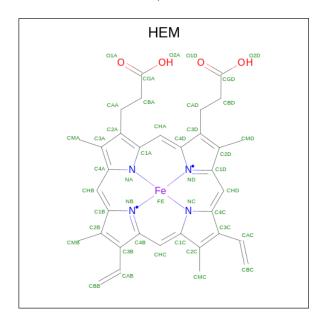
Mol	Chain	Residues		Aton	ns		ZeroOcc	AltConf	Trace
3	С	31	Total 241	C 169		O 35	0	0	0

• Molecule 4 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Cu 1 1	0	0

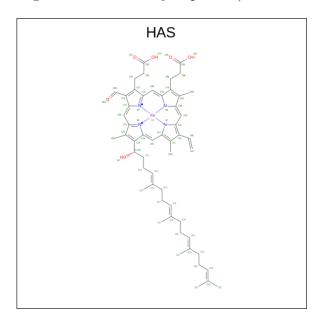


• Molecule 5 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues		Ato	oms			ZeroOcc	AltConf
5	A	1	Total	С	Fe	N	O	0	0
			43	34	1	4	4		

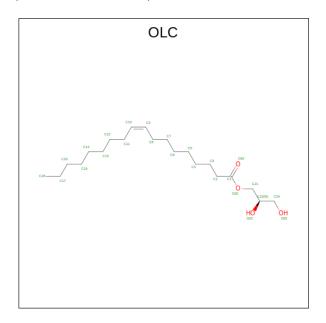
• Molecule 6 is HEME-AS (three-letter code: HAS) (formula: $C_{54}H_{64}FeN_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues		Ato	oms			ZeroOcc	AltConf
6	A	1	Total 65	C 54	Fe 1	N 4	O 6	0	0



 \bullet Molecule 7 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (three-letter code: OLC) (formula: $C_{21}H_{40}O_4).$



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 23 19 4	0	0
7	A	1	Total C O 18 14 4	0	0
7	A	1	Total C O 17 13 4	0	0
7	A	1	Total C O 15 11 4	0	0
7	A	1	Total C O 18 14 4	0	0
7	A	1	Total C O 15 11 4	0	0
7	A	1	Total C O 20 16 4	0	0
7	A	1	Total C O 21 17 4	0	0
7	A	1	Total C O 20 18 2	0	0
7	A	1	Total C 9 9	0	0
7	A	1	Total C 9 9	0	0
7	A	1	Total C O 15 11 4	0	0

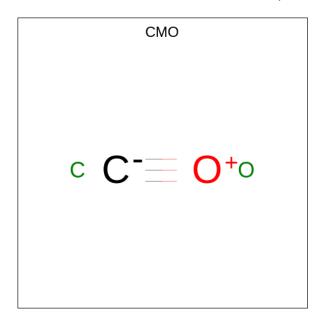
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	В	1	Total C O 25 21 4	0	0
7	В	1	Total C O 24 20 4	0	0
7	С	1	Total C O 24 20 4	0	0

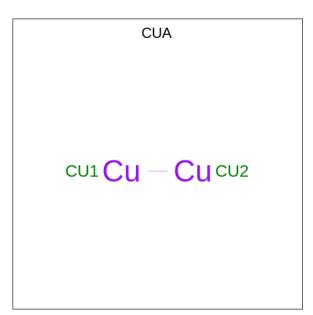
• Molecule 8 is CARBON MONOXIDE (three-letter code: CMO) (formula: CO).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O 2 1 1	0	0

• Molecule 9 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu₂).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	В	1	Total Cu 2 2	0	0

• Molecule 10 is water.

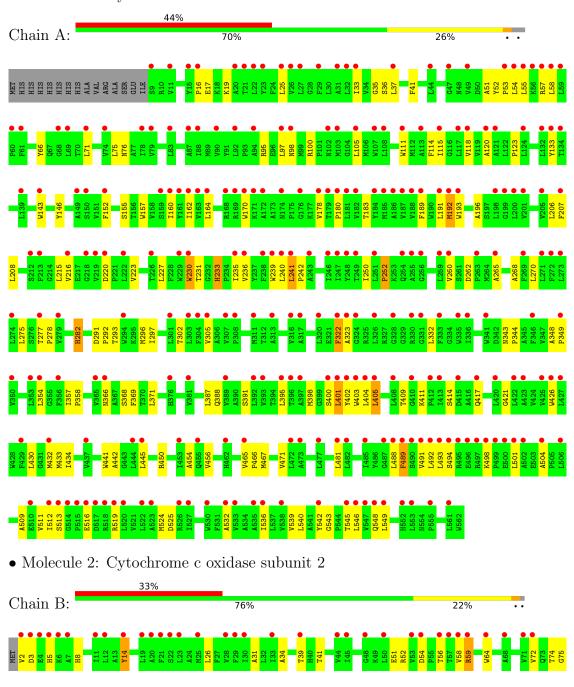
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	97	Total O 97 97	0	0
10	В	76	Total O 76 76	0	0
10	С	5	Total O 5 5	0	0

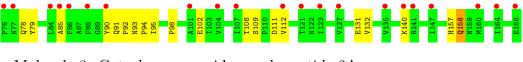


3 Residue-property plots (i)

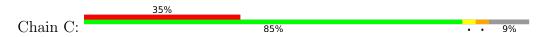
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Cytochrome c oxidase subunit 1





 \bullet Molecule 3: Cytochrome c oxidase polypeptide 2A







4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants	145.85Å 100.32Å 96.62Å	Donositor
a, b, c, α , β , γ	90.00° 126.76° 90.00°	Depositor
Resolution (Å)	37.15 - 2.00	Depositor
rtesolution (A)	37.15 - 2.00	EDS
% Data completeness	94.8 (37.15-2.00)	Depositor
(in resolution range)	94.8 (37.15-2.00)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	0.48 (at 2.00Å)	Xtriage
Refinement program	REFMAC v8.0	Depositor
D D.	0.396 , 0.435	Depositor
R, R_{free}	0.405 , 0.436	DCC
R_{free} test set	1877 reflections (2.63%)	wwPDB-VP
Wilson B-factor (Å ²)	26.3	Xtriage
Anisotropy	0.119	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.32, 79.3	EDS
L-test for twinning ²	$ < L >=0.58, < L^2>=0.43$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.81	EDS
Total number of atoms	6474	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 6.19% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities estimated from amplitudes.

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: OLC, CU, CUA, HEM, CMO, HAS

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	
IVIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5
1	A	0.43	0/4525	0.84	$2/6213 \ (0.0\%)$
2	В	0.43	0/1338	0.88	1/1828 (0.1%)
3	С	0.43	0/247	0.79	0/335
All	All	0.43	0/6110	0.84	3/8376 (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
2	В	0	1
All	All	0	2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^o)$	$Ideal(^{o})$
1	A	233	HIS	CA-CB-CG	-6.99	101.71	113.60
1	A	489	PHE	CB-CA-C	6.44	123.28	110.40
2	В	14	TYR	CB-CA-C	5.36	121.13	110.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	100	ARG	Sidechain
2	В	59	ARG	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	4368	0	4467	129	0
2	В	1301	0	1278	30	0
3	С	241	0	267	2	0
4	A	1	0	0	0	0
5	A	43	0	30	3	0
6	A	65	0	62	11	0
7	A	200	0	276	8	0
7	В	49	0	75	3	0
7	С	24	0	35	2	0
8	A	2	0	0	1	0
9	В	2	0	0	0	0
10	A	97	0	0	6	0
10	В	76	0	0	7	1
10	С	5	0	0	0	0
All	All	6474	0	6490	165	1

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 165 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	${ m distance} ({ m \AA})$	overlap (Å)
7:A:610:OLC:C13	7:A:610:OLC:C12	1.87	1.51
1:A:414:SER:OG	1:A:417:GLN:HG3	1.52	1.07
5:A:602:HEM:HMC2	5:A:602:HEM:HBC2	1.49	0.95
6:A:603:HAS:HMC1	6:A:603:HAS:HBC1	1.55	0.88
1:A:387:LEU:CD2	1:A:433:MET:CE	2.53	0.85

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1 Atom-2		$\begin{array}{c} \text{Interatomic} \\ \text{distance (Å)} \end{array}$	Clash overlap (Å)
10:B:359:HOH:O	10:B:365:HOH:O[2_556]	1.95	0.25



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	Perce	ntiles
1	A	552/569 (97%)	515 (93%)	36 (6%)	1 (0%)	47	44
2	В	165/168 (98%)	155 (94%)	9 (6%)	1 (1%)	25	19
3	С	29/34 (85%)	27 (93%)	2 (7%)	0	100	100
All	All	746/771 (97%)	697 (93%)	47 (6%)	2 (0%)	41	37

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	В	3	ASP
1	A	322	PHE

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	Percent	iles
1	A	447/463 (96%)	430 (96%)	17 (4%)	33 3	1
2	В	136/138 (99%)	132 (97%)	4 (3%)	42 4	:3
3	С	24/27 (89%)	23 (96%)	1 (4%)	30 2	27
All	All	607/628 (97%)	585 (96%)	22 (4%)	35 3	4

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	513	SER

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Mol	Chain	Res	Type
2	В	26	LEU
1	A	548	GLN
2	В	108	THR
1	A	252	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
2	В	158	GLN
2	В	99	GLN
1	A	548	GLN
1	A	455	GLN
2	В	60	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 20 ligands modelled in this entry, 1 is monoatomic - leaving 19 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	В	ond leng	$_{ m gths}$	Во	ond angl	les
MIOI	Type	Chain	nes	Lilik	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
7	OLC	A	616	-	14,14,24	0.75	1 (7%)	15,15,25	0.67	0
7	OLC	A	610	_	19,19,24	1.09	1 (5%)	20,20,25	0.34	0
7	OLC	A	604	-	22,22,24	0.24	0	23,23,25	0.43	0
7	OLC	С	101	-	23,23,24	0.44	0	24,24,25	0.33	0
7	OLC	В	202	-	24,24,24	0.32	0	25,25,25	0.32	0
6	HAS	A	603	1	69,72,72	2.67	25 (36%)	73,109,109	3.13	39 (53%)
7	OLC	A	608	-	17,17,24	0.31	0	18,18,25	0.38	0
8	CMO	A	615	4	0,1,1	-	-	-		
7	OLC	A	614	-	8,8,24	0.17	0	7,7,25	0.14	0
7	OLC	A	605	_	17,17,24	0.24	0	18,18,25	0.31	0
7	OLC	A	606	-	16,16,24	0.27	0	17,17,25	0.35	0
7	OLC	A	609	_	14,14,24	0.21	0	15,15,25	0.29	0
7	OLC	A	613	_	8,8,24	0.18	0	7,7,25	0.16	0
5	HEM	A	602	1	41,50,50	1.49	6 (14%)	45,82,82	1.96	16 (35%)
7	OLC	A	611	_	20,20,24	0.69	0	21,21,25	0.56	0
7	OLC	A	612	-	19,19,24	0.27	0	19,19,25	0.26	0
7	OLC	В	203	-	23,23,24	0.26	0	24,24,25	0.22	0
9	CUA	В	201	2	0,1,1	_	_	_		
7	OLC	A	607	-	14,14,24	0.23	0	15,15,25	0.33	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	OLC	A	605	-	-	10/17/17/24	-
7	OLC	A	606	-	-	8/16/16/24	-
7	OLC	A	609	-	-	8/14/14/24	-
7	OLC	A	616	-	-	2/14/14/24	-
7	OLC	A	610	-	-	11/19/19/24	-
7	OLC	A	604	-	-	10/22/22/24	-
7	OLC	С	101	-	-	16/23/23/24	-
7	OLC	A	613	-	-	5/6/6/24	-
7	OLC	A	612	-	-	9/18/18/24	-
7	OLC	В	202	-	-	11/24/24/24	-
6	HAS	A	603	1	1/1/8/18	8/40/82/82	-
7	OLC	A	608	-	-	10/17/17/24	-
7	OLC	В	203	-	-	9/23/23/24	_

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	OLC	A	611	-	-	8/20/20/24	_
7	OLC	A	614	-	-	3/6/6/24	_
5	HEM	A	602	1	-	1/12/54/54	-
7	OLC	A	607	-	-	3/14/14/24	_

The worst 5 of 33 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\text{\AA})$	$Ideal(\AA)$
6	A	603	HAS	CHD-C4A	10.31	1.49	1.35
6	A	603	HAS	C3B-C2B	6.29	1.48	1.34
6	A	603	HAS	CHA-C1A	5.13	1.48	1.38
6	A	603	HAS	C3C-C2C	4.99	1.47	1.40
6	A	603	HAS	FE-NA	4.88	2.14	1.95

The worst 5 of 55 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(^o)$	$Ideal(^{o})$
6	A	603	HAS	C2D-C3D-C4D	-11.60	98.22	106.49
6	A	603	HAS	CAD-C3D-C4D	6.73	136.42	124.66
6	A	603	HAS	C3D-C4D-ND	6.19	116.35	110.36
6	A	603	HAS	C2B-C1B-NB	5.70	116.71	109.88
6	A	603	HAS	C3B-C4B-NB	5.69	116.58	109.84

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	A	603	HAS	NA

5 of 132 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	603	HAS	C1D-C2D-CMD-OMD
6	A	603	HAS	C3D-C2D-CMD-OMD
6	A	603	HAS	C23-C24-C28-C29
7	A	604	OLC	C21-C22-C24-O25
7	A	608	OLC	C21-C22-C24-O25

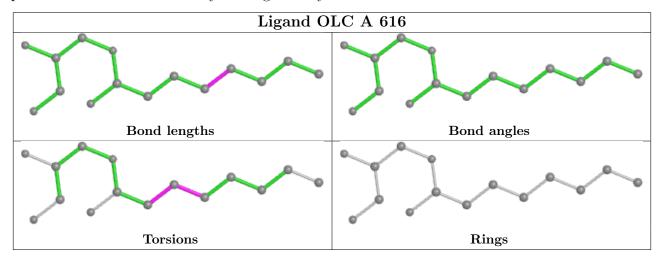
There are no ring outliers.

11 monomers are involved in 26 short contacts:

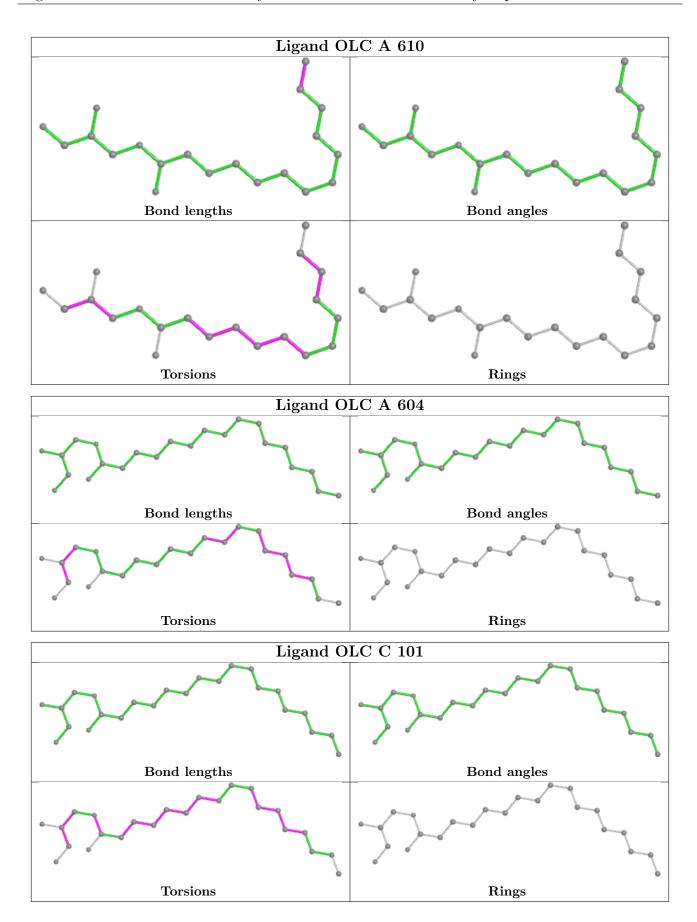


Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	616	OLC	2	0
7	A	610	OLC	2	0
7	A	604	OLC	1	0
7	С	101	OLC	2	0
6	A	603	HAS	11	0
8	A	615	CMO	1	0
7	A	605	OLC	1	0
7	A	606	OLC	1	0
5	A	602	HEM	3	0
7	A	612	OLC	1	0
7	В	203	OLC	3	0

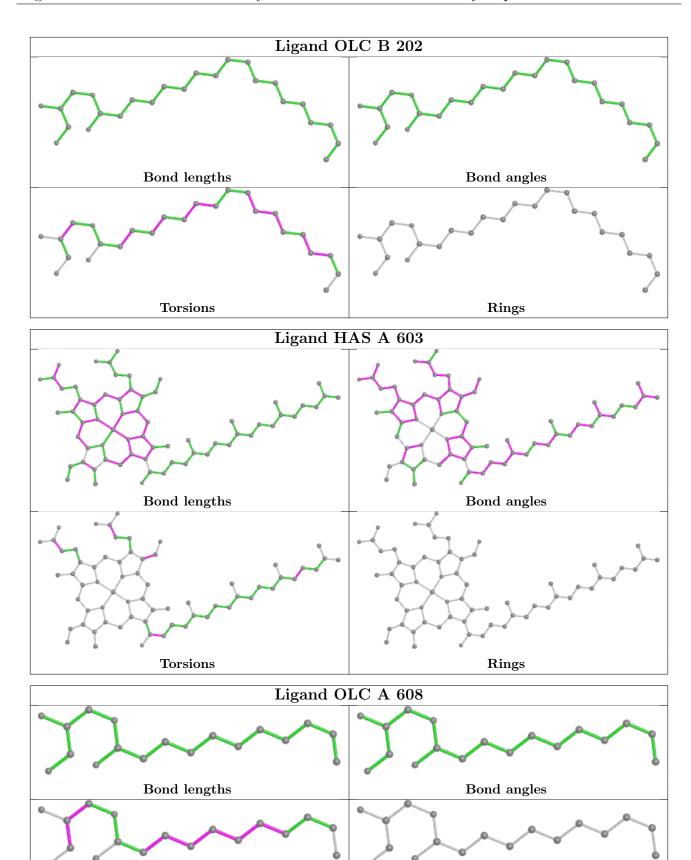
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.







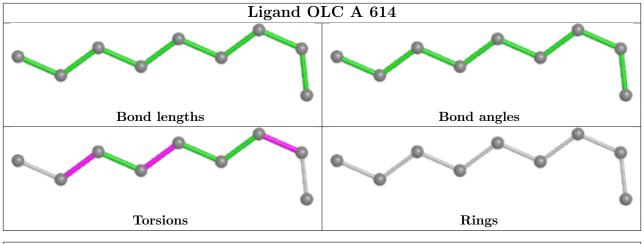


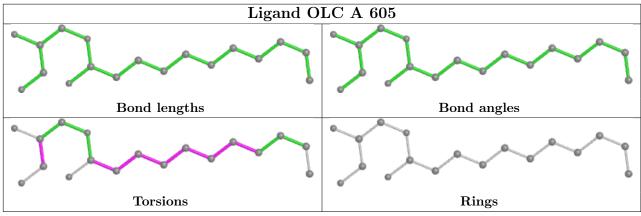


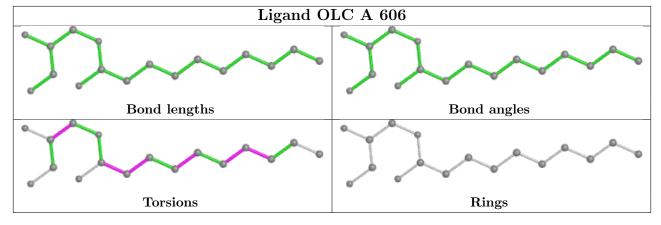


Rings

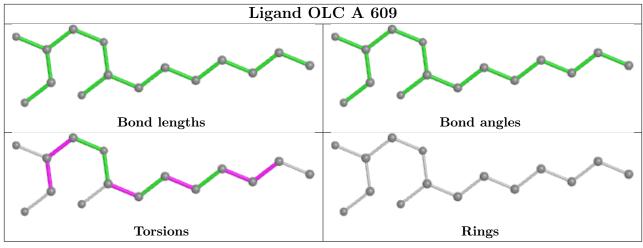
Torsions

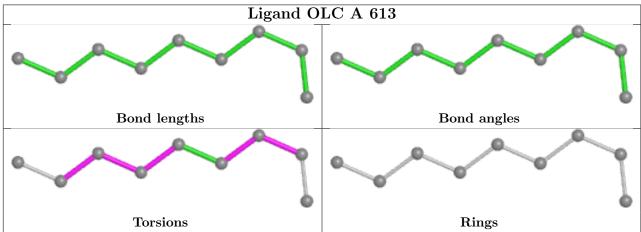




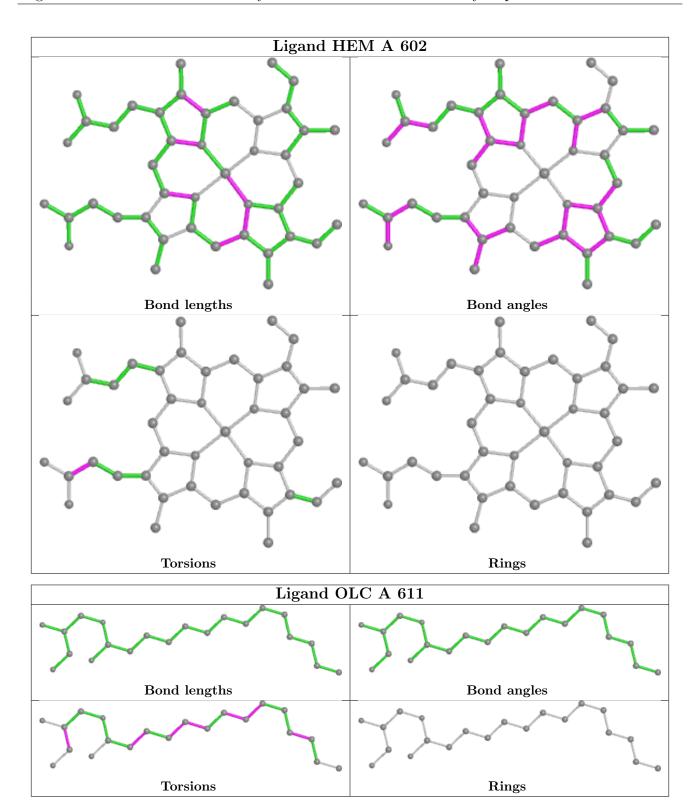




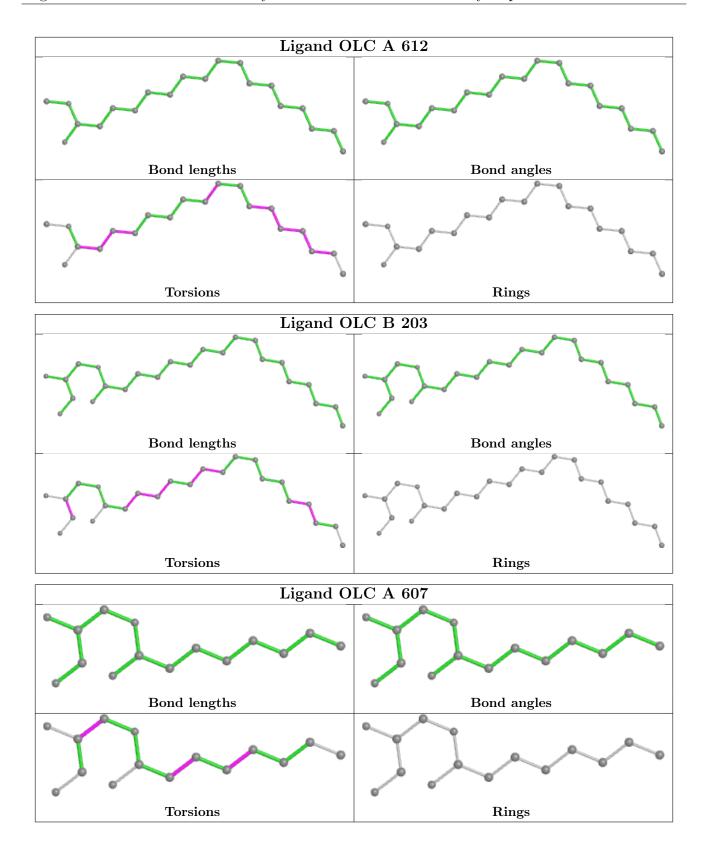












5.7 Other polymers (i)

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^{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	$\langle { m RSRZ} \rangle$	# RSRZ > 2		$OWAB(Å^2)$	Q<0.9	
1	A	554/569~(97%)	2.07	252 (45%)	0	0	21, 32, 59, 91	0
2	В	167/168 (99%)	1.70	55 (32%)	0	0	22, 32, 57, 104	0
3	С	31/34 (91%)	1.86	12 (38%)	0	0	27, 34, 42, 66	0
All	All	752/771 (97%)	1.98	319 (42%)	0	0	21, 32, 59, 104	0

The worst 5 of 319 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	В	2	VAL	11.8
1	A	331	GLY	7.7
1	A	496	GLU	7.2
1	A	495	ARG	7.1
1	A	494	SER	6.6

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^{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.



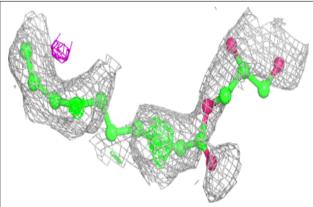
Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\operatorname{B-factors}({ ext{\AA}}^2)$	Q<0.9
7	OLC	A	606	17/25	0.18	0.38	70,73,88,91	0
7	OLC	A	616	15/25	0.21	0.36	67,74,89,92	0
7	OLC	В	202	25/25	0.26	0.38	64,68,86,101	0
7	OLC	A	609	15/25	0.27	0.39	80,94,101,102	0
7	OLC	A	610	20/25	0.28	0.42	70,80,96,100	0
7	OLC	A	607	15/25	0.32	0.49	67,84,97,99	0
7	OLC	С	101	24/25	0.38	0.41	54,66,98,101	0
7	OLC	A	614	9/25	0.44	0.31	56,59,75,76	0
7	OLC	В	203	24/25	0.47	0.33	68,80,93,103	0
7	OLC	A	612	20/25	0.47	0.34	69,77,86,97	0
7	OLC	A	608	18/25	0.48	0.36	62,79,91,92	0
7	OLC	A	611	21/25	0.49	0.34	56,77,94,105	0
7	OLC	A	613	9/25	0.56	0.31	64,69,74,77	0
7	OLC	A	605	18/25	0.57	0.35	61,77,95,102	0
7	OLC	A	604	23/25	0.63	0.28	42,60,91,94	0
6	HAS	A	603	65/65	0.75	0.25	20,26,44,59	0
5	HEM	A	602	43/43	0.79	0.23	20,23,27,36	0
8	CMO	A	615	2/2	0.97	0.14	20,20,20,26	0
9	CUA	В	201	2/2	0.98	0.05	25,25,25,26	0
4	CU	A	601	1/1	0.99	0.08	29,29,29,29	0

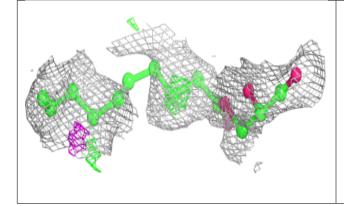
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

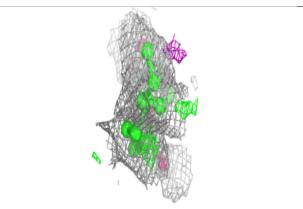


Electron density around OLC A 606:

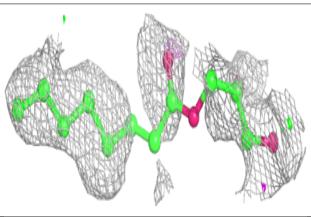
 $2 {
m mF}_o {
m -DF}_c$ (at 0.7 rmsd) in gray ${
m mF}_o {
m -DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)

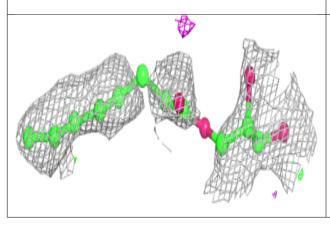


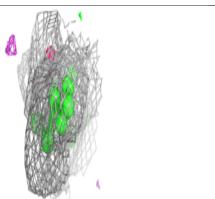




Electron density around OLC A 616:



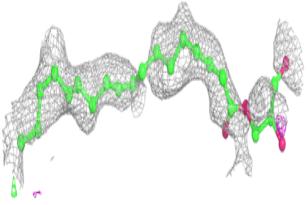


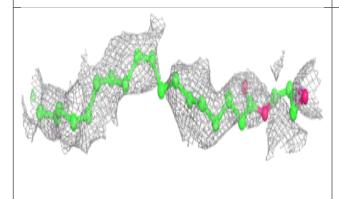


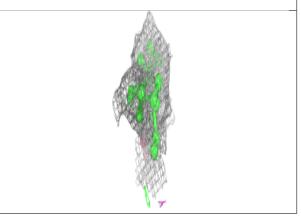


Electron density around OLC B 202:

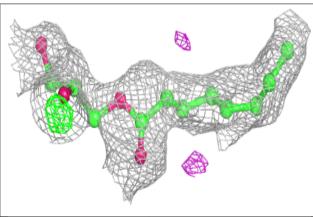
 $2 {\rm mF}_o\text{-}{\rm DF}_c$ (at 0.7 rmsd) in gray ${\rm mF}_o\text{-}{\rm DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)

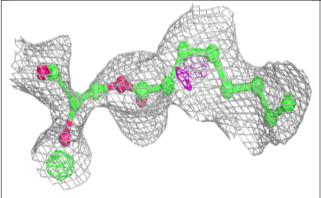


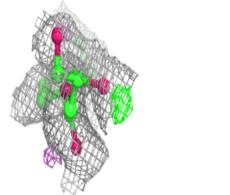




Electron density around OLC A 609:



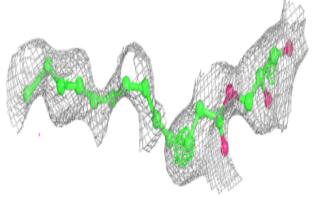


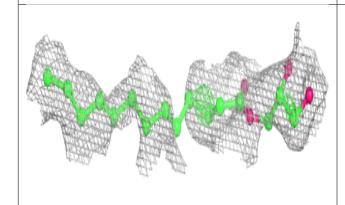


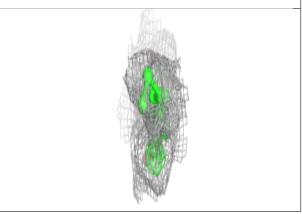


Electron density around OLC A 610:

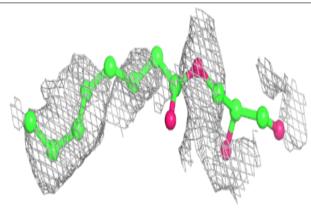
 $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray $\mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)

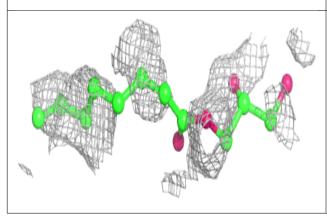


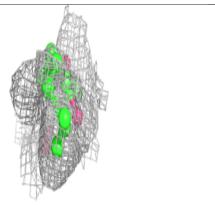




Electron density around OLC A 607:



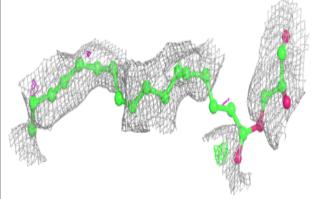


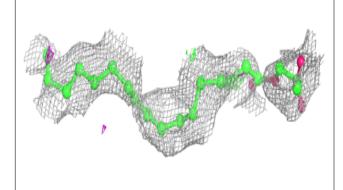


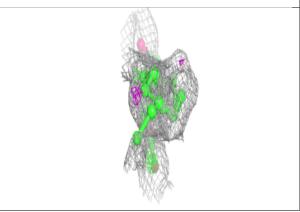


Electron density around OLC C 101:

 $2 {\rm mF}_o\text{-}{\rm DF}_c$ (at 0.7 rmsd) in gray ${\rm mF}_o\text{-}{\rm DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)

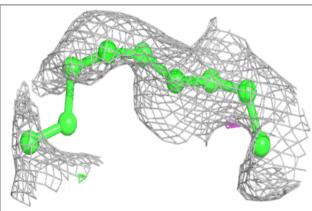


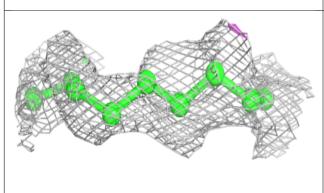


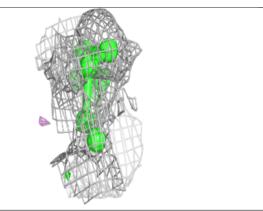


Electron density around OLC A 614:

 $2 \text{mF}_o\text{-DF}_c$ (at 0.7 rmsd) in gray $\text{mF}_o\text{-DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)

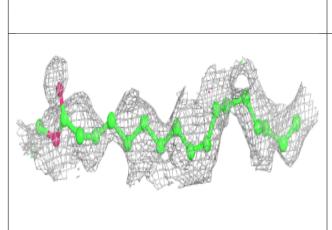


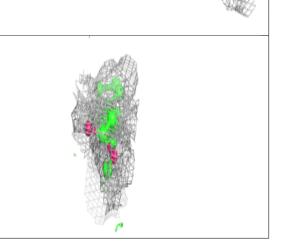






Electron density around OLC B 203: $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray ${ m mF}_o{ m -DF}_c$ (at 3 rmsd) in purple (negative) and green (positive) Electron density around OLC A 612: $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray mF_o -DF_c (at 3 rmsd) in purple (negative) and green (positive)

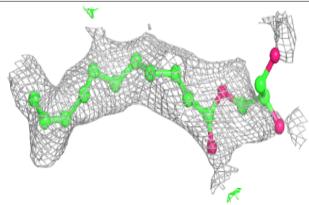


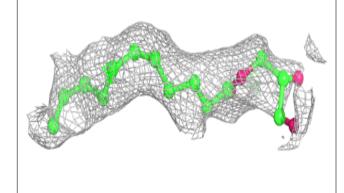


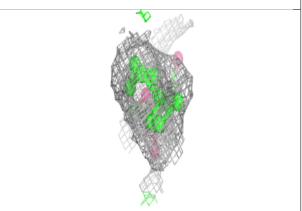


Electron density around OLC A 608:

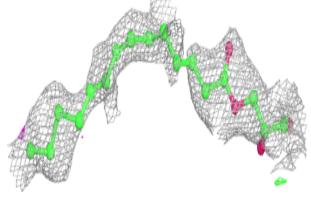
 $2 {\rm mF}_o\text{-}{\rm DF}_c$ (at 0.7 rmsd) in gray ${\rm mF}_o\text{-}{\rm DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)

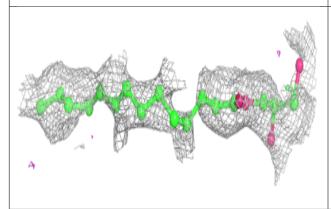


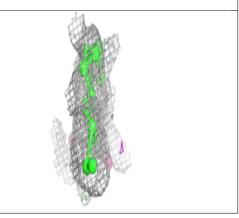




Electron density around OLC A 611:



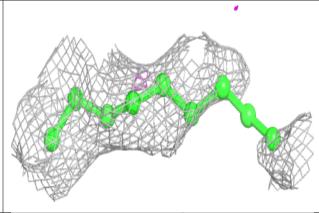


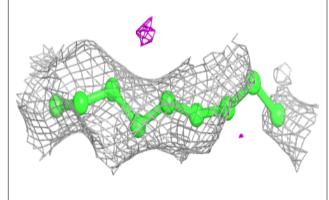


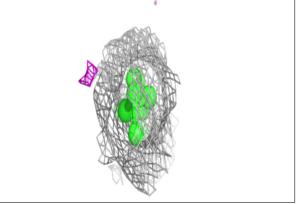


Electron density around OLC A 613:

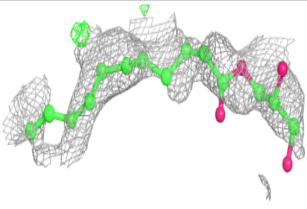
 $2 {\rm mF}_o\text{-}{\rm DF}_c$ (at 0.7 rmsd) in gray ${\rm mF}_o\text{-}{\rm DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)

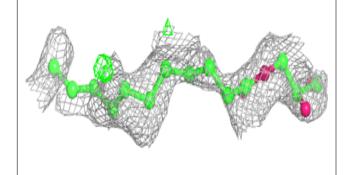


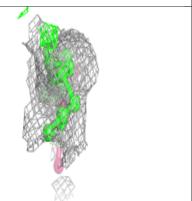




Electron density around OLC A 605:



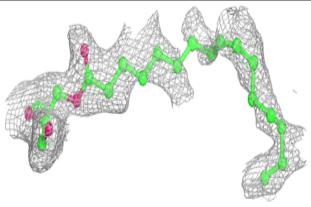


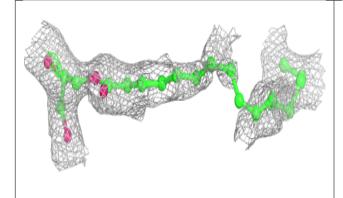


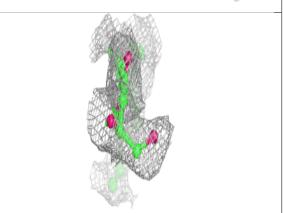


Electron density around OLC A 604:

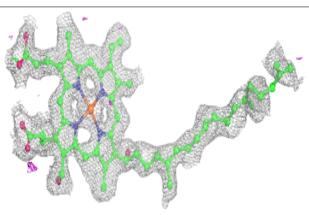
 $2 {\rm mF}_o\text{-}{\rm DF}_c$ (at 0.7 rmsd) in gray ${\rm mF}_o\text{-}{\rm DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)

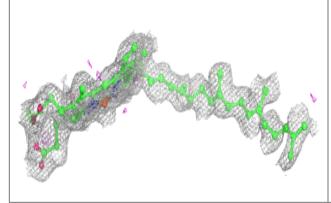


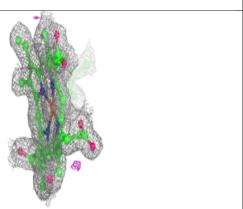




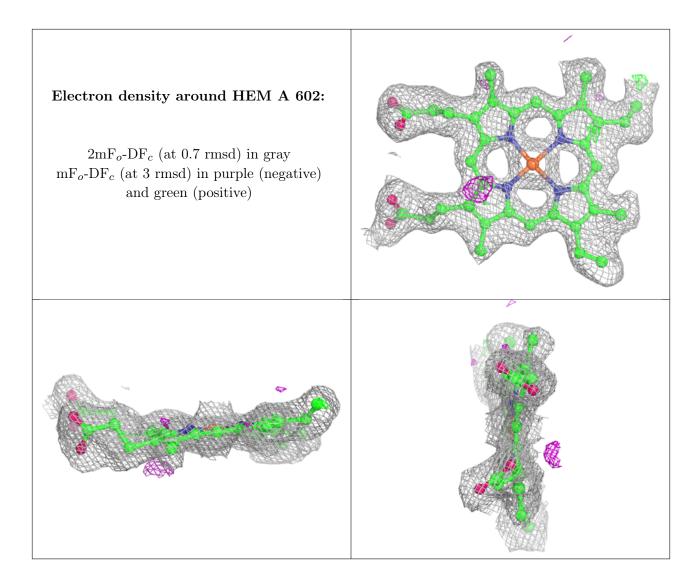
Electron density around HAS A 603:











6.5 Other polymers (i)

There are no such residues in this entry.

