



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 12, 2024 – 11:52 PM EDT

PDB ID : 3RKO  
Title : Crystal structure of the membrane domain of respiratory complex I from E. coli at 3.0 angstrom resolution  
Authors : Efremov, R.G.; Sazanov, L.A.  
Deposited on : 2011-04-18  
Resolution : 3.00 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](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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
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)	:	2.36.2

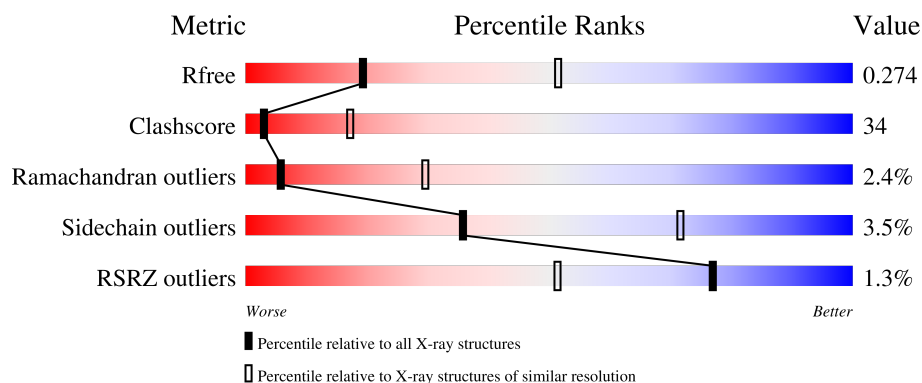
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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  $\geq 3$ , 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	B	613	<div> <div>47%</div> <div>50%</div> <div>.</div> </div>
1	L	613	<div> <div>47%</div> <div>50%</div> <div>.</div> </div>
2	C	509	<div> <div>44%</div> <div>50%</div> <div>5%</div> <div>.</div> </div>
2	M	509	<div> <div>44%</div> <div>50%</div> <div>5%</div> <div>.</div> </div>
3	D	485	<div> <div>38%</div> <div>54%</div> <div>5%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
3	N	485	
4	G	100	
4	K	100	
5	A	147	
5	E	147	
6	F	184	
6	J	184	

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 30310 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 NADH-QUINONE OXIDOREDUCTASE SUBUNIT L.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	612	Total	C	N	O	S	0	0	0
			4676	3108	749	787	32			
1	B	612	Total	C	N	O	S	0	0	0
			4676	3108	749	787	32			

- Molecule 2 is a protein called NADH-QUINONE OXIDOREDUCTASE SUBUNIT M.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	504	Total	C	N	O	S	0	0	0
			3953	2661	617	646	29			
2	C	504	Total	C	N	O	S	0	0	0
			3953	2661	617	646	29			

- Molecule 3 is a protein called NADH-QUINONE OXIDOREDUCTASE SUBUNIT N.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	N	473	Total	C	N	O	S	0	0	0
			3590	2399	566	606	19			
3	D	473	Total	C	N	O	S	0	0	0
			3590	2399	566	606	19			

- Molecule 4 is a protein called NADH-QUINONE OXIDOREDUCTASE SUBUNIT K.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	K	100	Total	C	N	O	S	0	0	0
			760	494	132	129	5			
4	G	100	Total	C	N	O	S	0	0	0
			760	494	132	129	5			

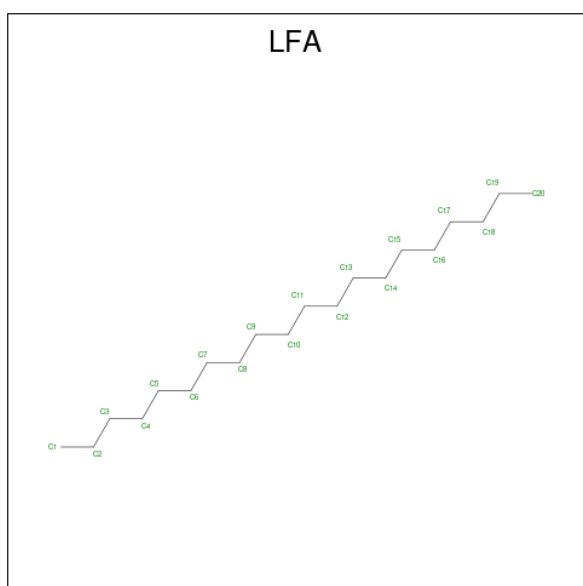
- Molecule 5 is a protein called NADH-QUINONE OXIDOREDUCTASE SUBUNIT A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	A	95	Total	C	N	O	S	0	0	0
			752	516	118	114	4			
5	E	95	Total	C	N	O	S	0	0	0
			752	516	118	114	4			

- Molecule 6 is a protein called NADH-QUINONE OXIDOREDUCTASE SUBUNIT J.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	J	168	Total	C	N	O	S	0	0	0
			1270	851	197	215	7			
6	F	168	Total	C	N	O	S	0	0	0
			1270	851	197	215	7			

- Molecule 7 is EICOSANE (three-letter code: LFA) (formula:  $C_{20}H_{42}$ ).



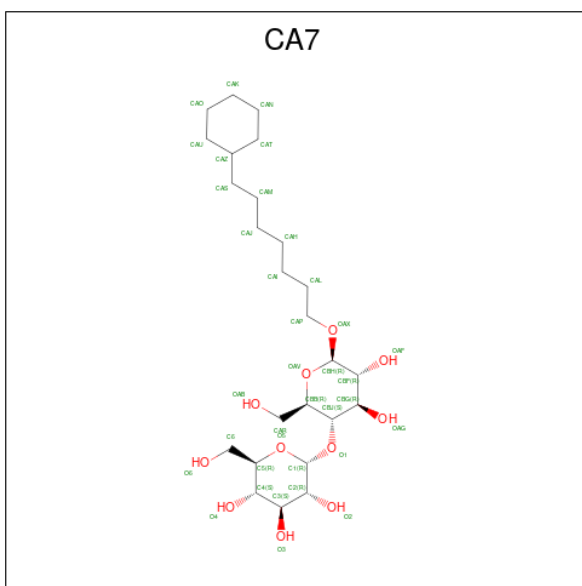
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	L	1	Total	C	0	0
			12	12		
7	L	1	Total	C	0	0
			14	14		
7	L	1	Total	C	0	0
			8	8		
7	M	1	Total	C	0	0
			14	14		
7	M	1	Total	C	0	0
			12	12		
7	N	1	Total	C	0	0
			12	12		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	N	1	Total C 14 14	0	0
7	N	1	Total C 12 12	0	0
7	N	1	Total C 12 12	0	0
7	B	1	Total C 12 12	0	0
7	B	1	Total C 14 14	0	0
7	B	1	Total C 8 8	0	0
7	C	1	Total C 14 14	0	0
7	C	1	Total C 12 12	0	0
7	C	1	Total C 12 12	0	0
7	D	1	Total C 14 14	0	0
7	D	1	Total C 12 12	0	0
7	D	1	Total C 12 12	0	0

- Molecule 8 is 7-cyclohexylheptyl 4-O-alpha-D-glucopyranosyl-beta-D-glucopyranoside (three-letter code: CA7) (formula: C<sub>25</sub>H<sub>46</sub>O<sub>11</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	M	1	Total	C	O	0	0
			36	25	11		
8	C	1	Total	C	O	0	0
			36	25	11		

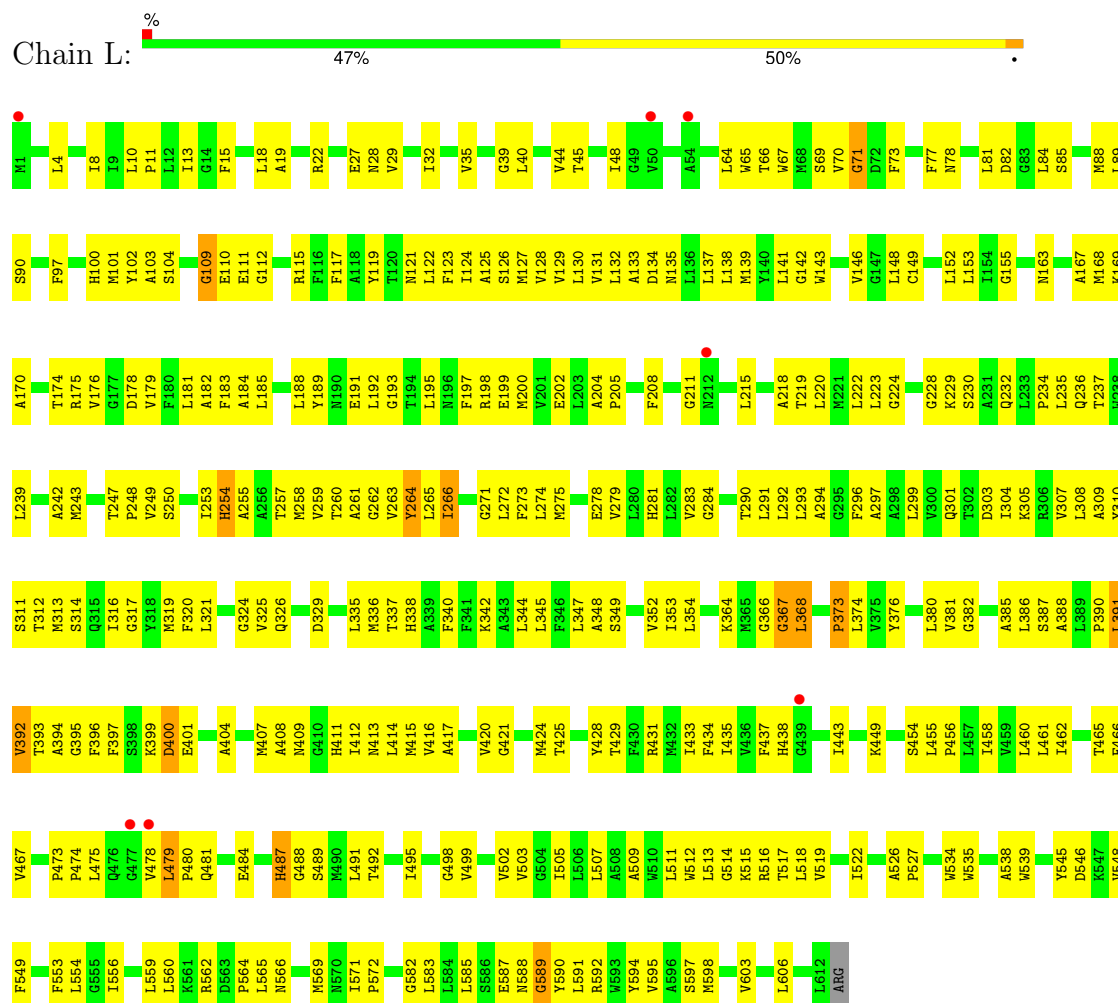
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	L	2	Total	O	0	0
			2	2		
9	M	2	Total	O	0	0
			2	2		
9	N	3	Total	O	0	0
			3	3		
9	K	1	Total	O	0	0
			1	1		
9	B	2	Total	O	0	0
			2	2		
9	C	2	Total	O	0	0
			2	2		
9	D	3	Total	O	0	0
			3	3		
9	G	1	Total	O	0	0
			1	1		

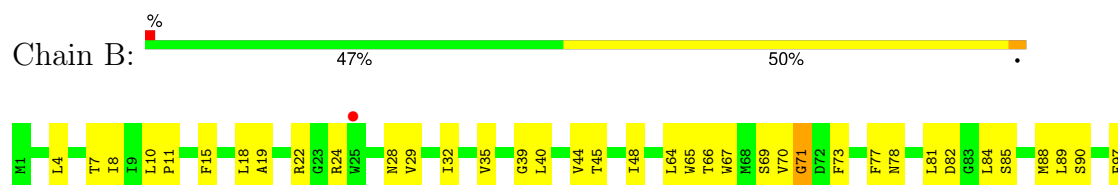
### 3 Residue-property plots [i](#)

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.

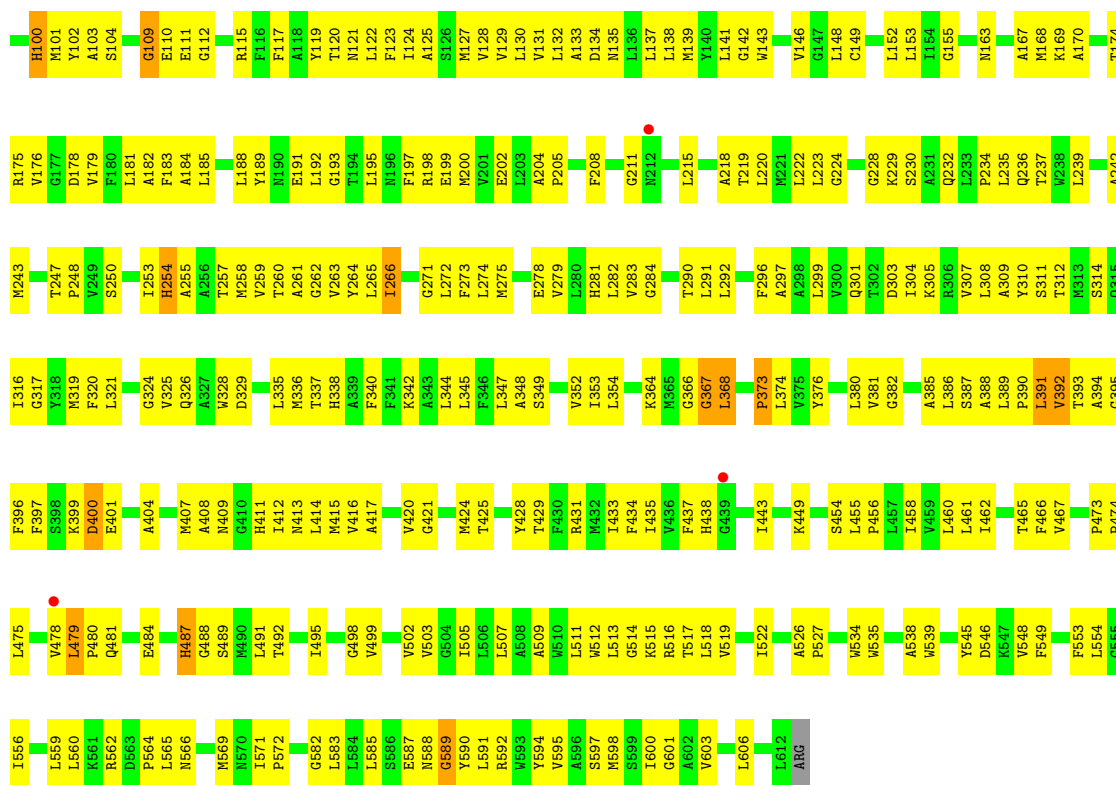
#### • Molecule 1: NADH-QUINONE OXIDOREDUCTASE SUBUNIT L



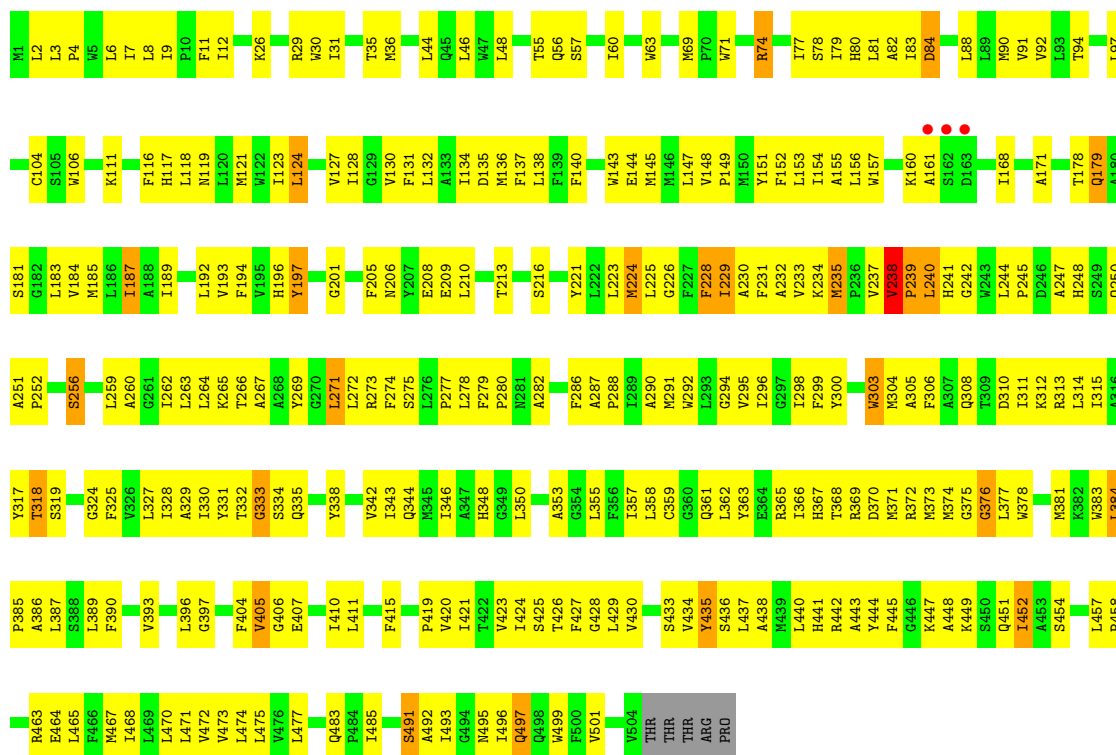
#### • Molecule 1: NADH-QUINONE OXIDOREDUCTASE SUBUNIT L



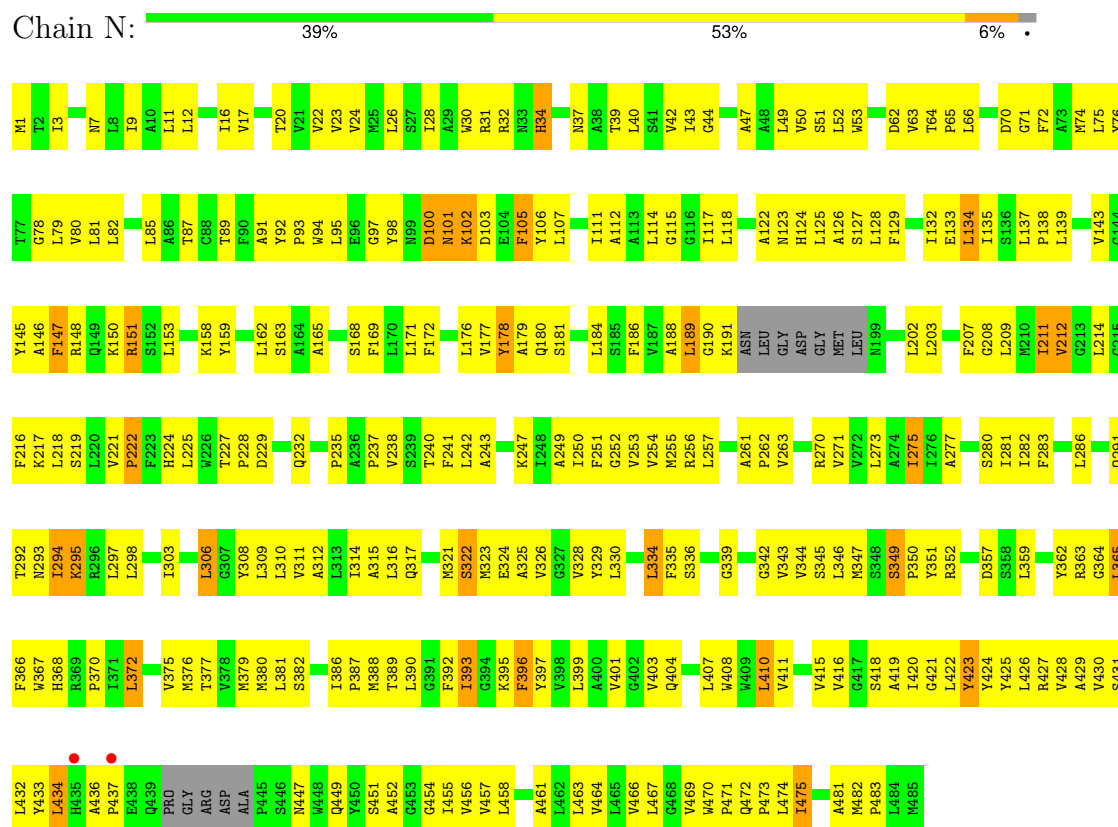
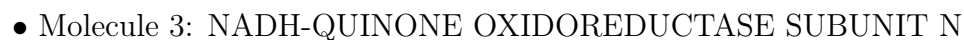




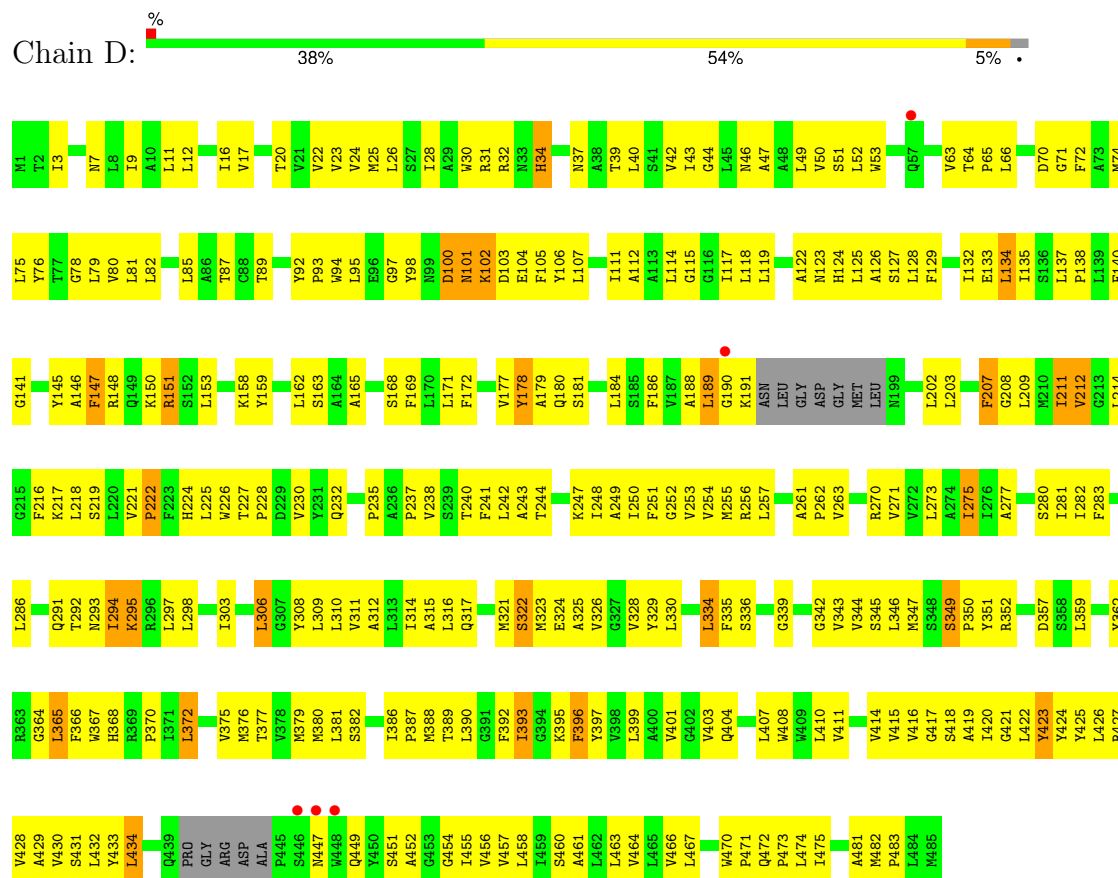
### • Molecule 2: NADH-QUINONE OXIDOREDUCTASE SUBUNIT M



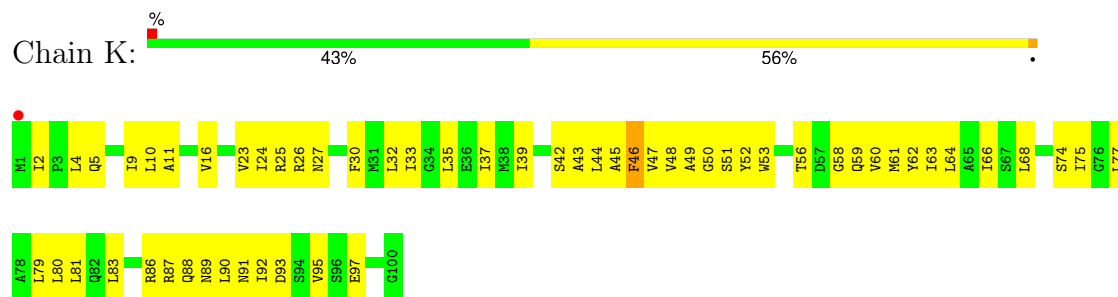
### • Molecule 2: NADH-QUINONE OXIDOREDUCTASE SUBUNIT M



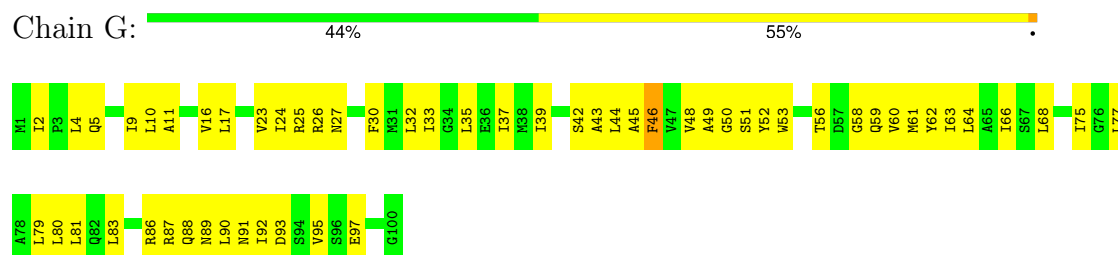
• Molecule 3: NADH-QUINONE OXIDOREDUCTASE SUBUNIT N



• Molecule 4: NADH-QUINONE OXIDOREDUCTASE SUBUNIT K

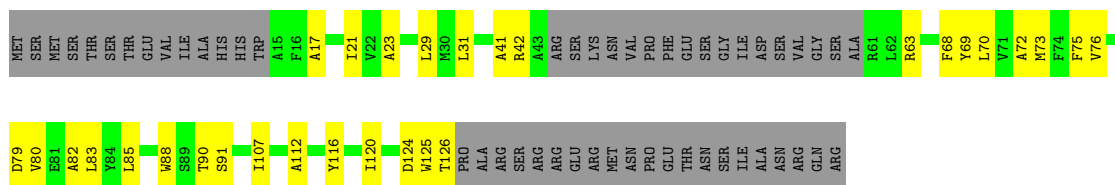


• Molecule 4: NADH-QUINONE OXIDOREDUCTASE SUBUNIT K




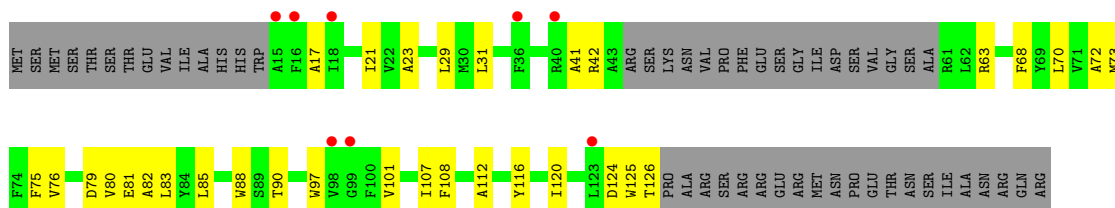
• Molecule 5: NADH-QUINONE OXIDOREDUCTASE SUBUNIT A

Chain A:  44% 20% 35%



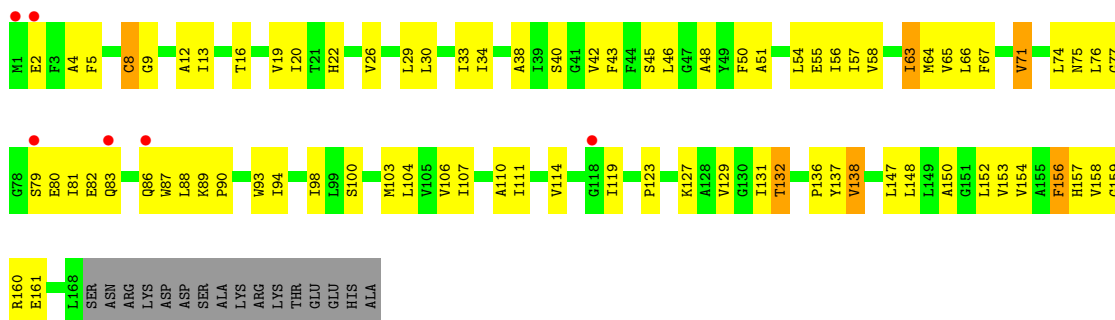
• Molecule 5: NADH-QUINONE OXIDOREDUCTASE SUBUNIT A

Chain E:  5% 43% 22% 35%



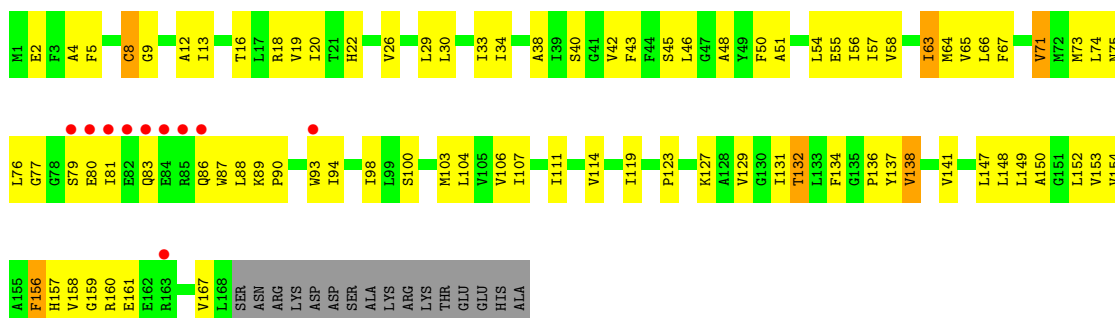
• Molecule 6: NADH-QUINONE OXIDOREDUCTASE SUBUNIT J

Chain J:  3% 47% 41% 9%



• Molecule 6: NADH-QUINONE OXIDOREDUCTASE SUBUNIT J

Chain F:  5% 45% 43% 9%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	94.98Å 116.57Å 191.37Å 98.51° 104.08° 108.51°	Depositor
Resolution (Å)	19.99 – 3.00 29.98 – 3.00	Depositor EDS
% Data completeness (in resolution range)	86.5 (19.99-3.00) 86.5 (29.98-3.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.17	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.65 (at 3.00Å)	Xtriage
Refinement program	PHENIX 1.6.4_486	Depositor
R, $R_{free}$	0.232 , 0.282 0.226 , 0.274	Depositor DCC
$R_{free}$ test set	2554 reflections (2.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	58.1	Xtriage
Anisotropy	0.035	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.25 , 71.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	30310	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.29% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LFA, CA7

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	B	0.31	0/4797	0.49	0/6538
1	L	0.31	0/4797	0.49	0/6538
2	C	0.39	0/4074	0.58	1/5546 (0.0%)
2	M	0.39	0/4074	0.58	1/5546 (0.0%)
3	D	0.37	0/3678	0.58	0/5018
3	N	0.37	0/3678	0.58	0/5018
4	G	0.31	0/769	0.49	0/1040
4	K	0.31	0/769	0.49	0/1040
5	A	0.30	0/772	0.45	0/1046
5	E	0.30	0/772	0.45	0/1046
6	F	0.29	0/1296	0.48	0/1767
6	J	0.29	0/1296	0.48	0/1767
All	All	0.34	0/30772	0.54	2/41910 (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
2	C	0	1
2	M	0	1
All	All	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	124	LEU	CA-CB-CG	5.68	128.36	115.30
2	C	124	LEU	CA-CB-CG	5.44	127.81	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	238	VAL	Peptide
2	M	238	VAL	Peptide

## 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	B	4676	0	4820	336	0
1	L	4676	0	4820	337	0
2	C	3953	0	4053	301	0
2	M	3953	0	4053	306	0
3	D	3590	0	3756	323	0
3	N	3590	0	3756	311	0
4	G	760	0	817	84	0
4	K	760	0	817	76	0
5	A	752	0	778	30	0
5	E	752	0	778	31	0
6	F	1270	0	1344	128	0
6	J	1270	0	1344	113	0
7	B	34	0	65	11	0
7	C	38	0	73	7	0
7	D	38	0	73	9	0
7	L	34	0	65	20	0
7	M	26	0	50	11	0
7	N	50	0	96	9	0
8	C	36	0	46	10	0
8	M	36	0	46	12	0
9	B	2	0	0	0	0
9	C	2	0	0	0	0
9	D	3	0	0	0	0
9	G	1	0	0	0	0
9	K	1	0	0	0	0
9	L	2	0	0	0	0
9	M	2	0	0	0	0
9	N	3	0	0	0	0
All	All	30310	0	31650	2117	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 34.

The worst 5 of 2117 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)
3:D:232:GLN:HA	3:D:295:LYS:HD3	1.38	1.05
3:N:232:GLN:HA	3:N:295:LYS:HD3	1.38	1.05
3:D:390:LEU:HD21	3:D:467:LEU:HB3	1.39	1.04
3:N:390:LEU:HD21	3:N:467:LEU:HB3	1.39	1.04
2:M:449:LYS:HD3	2:M:454:SER:HB2	1.39	1.02

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	B	610/613 (100%)	515 (84%)	85 (14%)	10 (2%)	9	40
1	L	610/613 (100%)	514 (84%)	86 (14%)	10 (2%)	9	40
2	C	502/509 (99%)	412 (82%)	77 (15%)	13 (3%)	5	27
2	M	502/509 (99%)	408 (81%)	80 (16%)	14 (3%)	5	25
3	D	467/485 (96%)	359 (77%)	90 (19%)	18 (4%)	3	17
3	N	467/485 (96%)	358 (77%)	90 (19%)	19 (4%)	3	16
4	G	98/100 (98%)	87 (89%)	10 (10%)	1 (1%)	15	53
4	K	98/100 (98%)	87 (89%)	9 (9%)	2 (2%)	7	34
5	A	91/147 (62%)	82 (90%)	9 (10%)	0	100	100
5	E	91/147 (62%)	82 (90%)	9 (10%)	0	100	100
6	F	166/184 (90%)	140 (84%)	23 (14%)	3 (2%)	8	37
6	J	166/184 (90%)	140 (84%)	23 (14%)	3 (2%)	8	37
All	All	3868/4076 (95%)	3184 (82%)	591 (15%)	93 (2%)	6	29



5 of 93 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	392	VAL
1	L	479	LEU
2	M	239	PRO
3	N	294	ILE
3	N	434	LEU

### 5.3.2 Protein sidechains ⓘ

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	B	485/486 (100%)	475 (98%)	10 (2%)	53	82
1	L	485/486 (100%)	474 (98%)	11 (2%)	50	80
2	C	413/418 (99%)	391 (95%)	22 (5%)	22	58
2	M	413/418 (99%)	391 (95%)	22 (5%)	22	58
3	D	377/385 (98%)	362 (96%)	15 (4%)	31	68
3	N	377/385 (98%)	362 (96%)	15 (4%)	31	68
4	G	79/79 (100%)	78 (99%)	1 (1%)	69	89
4	K	79/79 (100%)	77 (98%)	2 (2%)	47	79
5	A	73/119 (61%)	72 (99%)	1 (1%)	67	88
5	E	73/119 (61%)	72 (99%)	1 (1%)	67	88
6	F	132/146 (90%)	127 (96%)	5 (4%)	33	69
6	J	132/146 (90%)	127 (96%)	5 (4%)	33	69
All	All	3118/3266 (96%)	3008 (96%)	110 (4%)	36	71

5 of 110 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	163	ASN
2	C	179	GLN
6	F	156	PHE
3	D	352	ARG

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Mol	Chain	Res	Type
1	B	266	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	232	GLN
3	D	368	HIS
2	C	248	HIS
3	D	46	ASN
2	C	206	ASN

### 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](#)

20 ligands are modelled in this entry.

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	$\# Z  > 2$
8	CA7	M	510	-	38,38,38	0.98	1 (2%)	51,51,51	1.76	9 (17%)
7	LFA	M	511	-	13,13,19	0.41	0	12,12,18	0.65	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	LFA	N	486	-	11,11,19	0.54	0	10,10,18	0.59	0
7	LFA	L	614	-	11,11,19	0.50	0	10,10,18	0.54	0
7	LFA	D	486	-	13,13,19	0.41	0	12,12,18	0.53	0
7	LFA	B	616	-	7,7,19	0.56	0	6,6,18	0.32	0
7	LFA	N	489	-	11,11,19	0.37	0	10,10,18	0.68	0
7	LFA	C	512	-	11,11,19	0.51	0	10,10,18	0.63	0
7	LFA	B	614	-	11,11,19	0.47	0	10,10,18	0.55	0
8	CA7	C	510	-	38,38,38	0.88	3 (7%)	51,51,51	1.57	8 (15%)
7	LFA	B	615	-	13,13,19	0.43	0	12,12,18	0.62	0
7	LFA	C	513	-	11,11,19	0.36	0	10,10,18	0.70	0
7	LFA	D	488	-	11,11,19	0.41	0	10,10,18	0.73	0
7	LFA	M	512	-	11,11,19	0.34	0	10,10,18	0.73	0
7	LFA	L	616	-	7,7,19	0.50	0	6,6,18	0.36	0
7	LFA	L	615	-	13,13,19	0.43	0	12,12,18	0.58	0
7	LFA	N	488	-	11,11,19	0.47	0	10,10,18	0.58	0
7	LFA	D	487	-	11,11,19	0.46	0	10,10,18	0.57	0
7	LFA	C	511	-	13,13,19	0.39	0	12,12,18	0.72	0
7	LFA	N	487	-	13,13,19	0.38	0	12,12,18	0.56	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
8	CA7	M	510	-	-	4/19/67/67	0/3/3/3
7	LFA	M	511	-	-	0/11/11/17	-
7	LFA	N	486	-	-	0/9/9/17	-
7	LFA	L	614	-	-	0/9/9/17	-
7	LFA	D	486	-	-	0/11/11/17	-
7	LFA	B	616	-	-	0/5/5/17	-
7	LFA	N	489	-	-	0/9/9/17	-
7	LFA	C	512	-	-	0/9/9/17	-
7	LFA	B	614	-	-	0/9/9/17	-
8	CA7	C	510	-	-	3/19/67/67	0/3/3/3
7	LFA	B	615	-	-	0/11/11/17	-
7	LFA	C	513	-	-	0/9/9/17	-
7	LFA	D	488	-	-	0/9/9/17	-
7	LFA	M	512	-	-	0/9/9/17	-
7	LFA	L	616	-	-	0/5/5/17	-
7	LFA	L	615	-	-	0/11/11/17	-
7	LFA	N	488	-	-	0/9/9/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	LFA	D	487	-	-	0/9/9/17	-
7	LFA	C	511	-	-	0/11/11/17	-
7	LFA	N	487	-	-	0/11/11/17	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	M	510	CA7	OAX-CBH	3.60	1.46	1.40
8	C	510	CA7	OAX-CBH	2.41	1.44	1.40
8	C	510	CA7	CAT-CAZ	2.18	1.58	1.52
8	C	510	CA7	O5-C1	2.03	1.47	1.41

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	M	510	CA7	CAR-CBB-CBJ	-6.28	95.72	113.38
8	C	510	CA7	OAV-CBH-CBF	-5.24	99.61	110.37
8	M	510	CA7	OAV-CBB-CAR	-4.54	95.19	106.44
8	C	510	CA7	O5-C5-C6	3.97	116.27	106.44
8	C	510	CA7	O1-CBJ-CBG	3.93	117.22	107.23

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	C	510	CA7	CBG-CBJ-O1-C1
8	M	510	CA7	OAV-CBH-OAX-CAP
8	C	510	CA7	OAV-CBH-OAX-CAP
8	M	510	CA7	CBG-CBJ-O1-C1
8	M	510	CA7	CBF-CBH-OAX-CAP

There are no ring outliers.

16 monomers are involved in 83 short contacts:

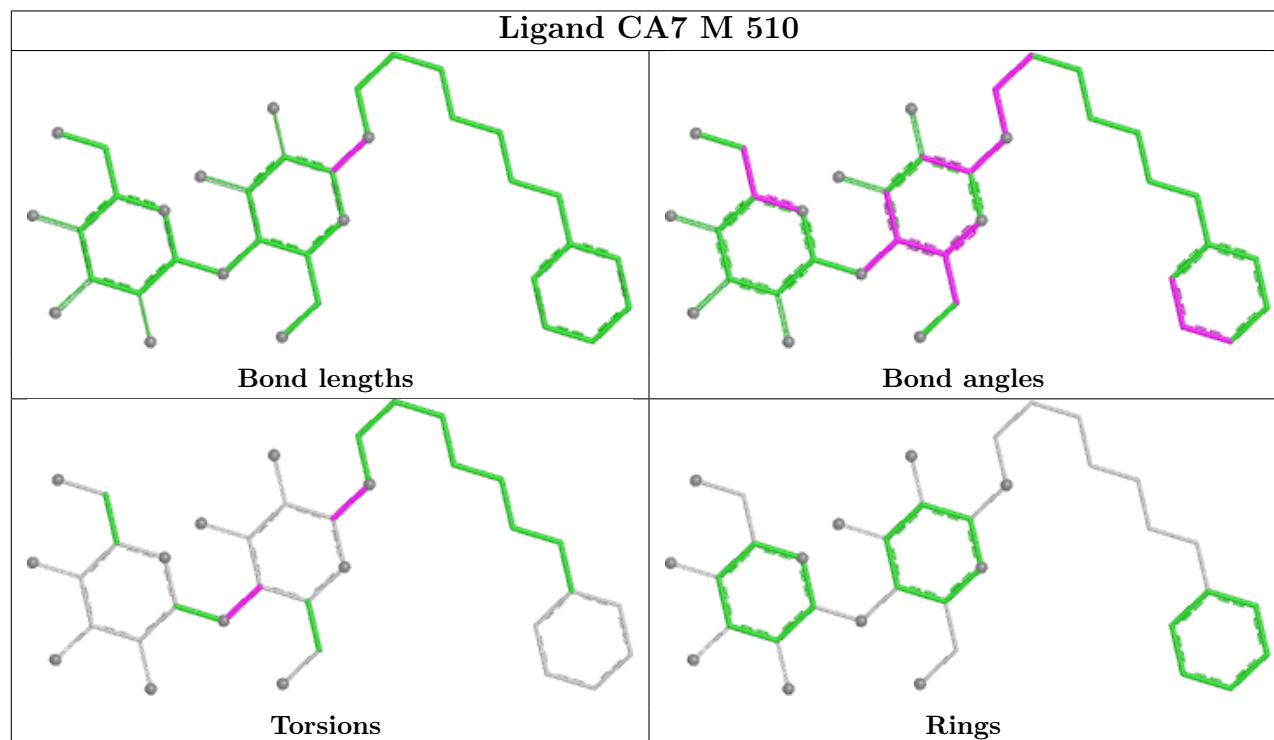
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	M	510	CA7	12	0
7	M	511	LFA	3	0
7	N	486	LFA	1	0
7	L	614	LFA	3	0
7	D	486	LFA	7	0
7	B	614	LFA	2	0

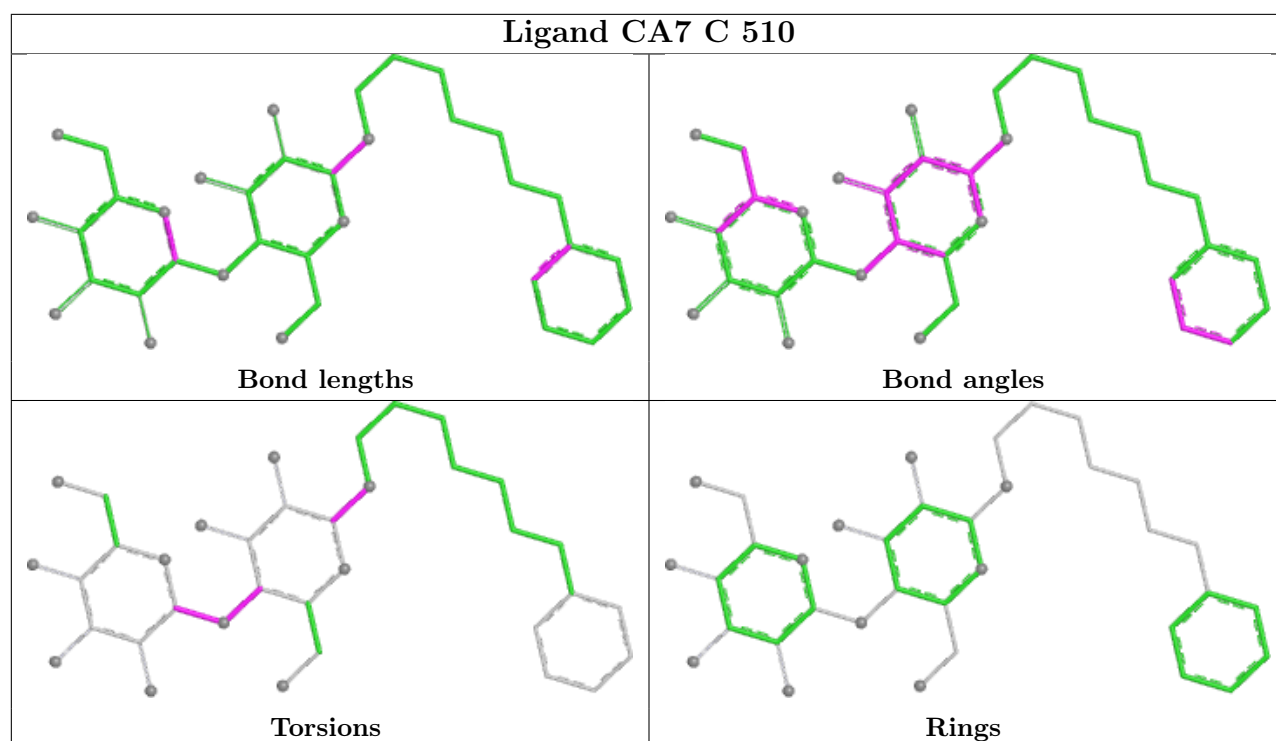
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	C	510	CA7	10	0
7	B	615	LFA	9	0
7	C	513	LFA	4	0
7	M	512	LFA	8	0
7	L	616	LFA	3	0
7	L	615	LFA	14	0
7	N	488	LFA	3	0
7	D	487	LFA	2	0
7	C	511	LFA	3	0
7	N	487	LFA	5	0

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 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	B	612/613 (99%)	-0.56	4 (0%) 87 69	35, 81, 131, 196	0
1	L	612/613 (99%)	-0.55	7 (1%) 80 56	35, 83, 131, 196	0
2	C	504/509 (99%)	-0.79	3 (0%) 89 72	16, 56, 106, 181	0
2	M	504/509 (99%)	-0.81	3 (0%) 89 72	14, 56, 107, 184	0
3	D	473/485 (97%)	-0.75	5 (1%) 80 56	17, 58, 113, 201	0
3	N	473/485 (97%)	-0.79	2 (0%) 92 79	15, 57, 111, 202	0
4	G	100/100 (100%)	-0.58	0 100 100	43, 80, 127, 166	0
4	K	100/100 (100%)	-0.50	1 (1%) 82 59	39, 79, 127, 166	0
5	A	95/147 (64%)	-0.33	0 100 100	53, 93, 152, 178	0
5	E	95/147 (64%)	-0.06	8 (8%) 11 3	57, 94, 153, 179	0
6	F	168/184 (91%)	-0.30	10 (5%) 21 7	49, 98, 165, 192	0
6	J	168/184 (91%)	-0.31	6 (3%) 42 17	51, 96, 160, 186	0
All	All	3904/4076 (95%)	-0.63	49 (1%) 77 51	14, 72, 133, 202	0

The worst 5 of 49 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	212	ASN	6.0
6	F	79	SER	5.4
1	L	212	ASN	5.0
6	J	79	SER	4.5
5	E	99	GLY	4.2

### 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 ⓘ

There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

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.

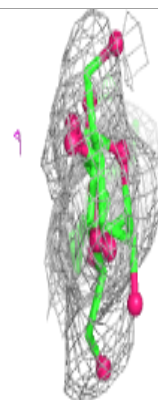
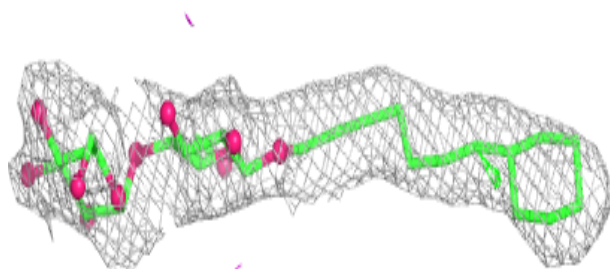
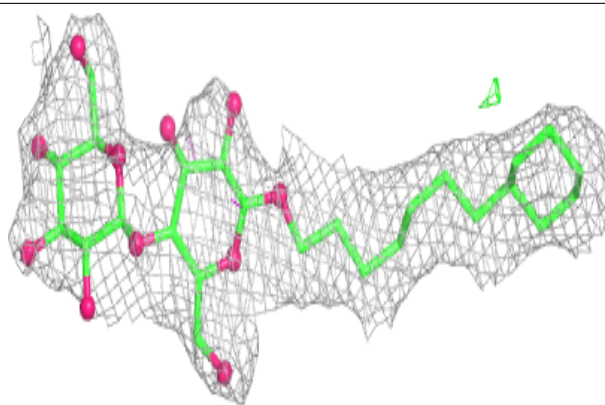
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
7	LFA	L	616	8/20	0.84	0.21	52,61,96,118	0
7	LFA	M	511	14/20	0.87	0.22	7,54,73,82	0
7	LFA	N	488	12/20	0.87	0.21	22,50,94,102	0
7	LFA	M	512	12/20	0.88	0.26	47,75,111,115	0
7	LFA	L	614	12/20	0.88	0.20	23,66,140,147	0
7	LFA	D	486	14/20	0.88	0.18	27,63,118,118	0
7	LFA	N	486	12/20	0.89	0.18	23,40,69,85	0
7	LFA	D	488	12/20	0.89	0.25	19,78,116,133	0
7	LFA	C	513	12/20	0.90	0.30	56,96,117,119	0
7	LFA	B	616	8/20	0.90	0.25	24,73,104,123	0
7	LFA	C	511	14/20	0.90	0.26	11,46,79,83	0
7	LFA	N	487	14/20	0.91	0.19	19,75,100,101	0
7	LFA	N	489	12/20	0.91	0.21	6,75,116,122	0
7	LFA	C	512	12/20	0.91	0.18	24,60,65,69	0
7	LFA	D	487	12/20	0.92	0.17	13,44,101,112	0
7	LFA	L	615	14/20	0.92	0.24	25,65,116,119	0
8	CA7	C	510	36/36	0.92	0.17	20,82,148,192	0
8	CA7	M	510	36/36	0.93	0.20	12,97,165,215	0
7	LFA	B	615	14/20	0.93	0.20	23,50,100,103	0
7	LFA	B	614	12/20	0.94	0.16	14,66,119,129	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.

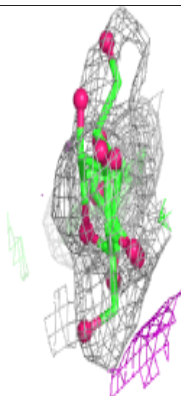
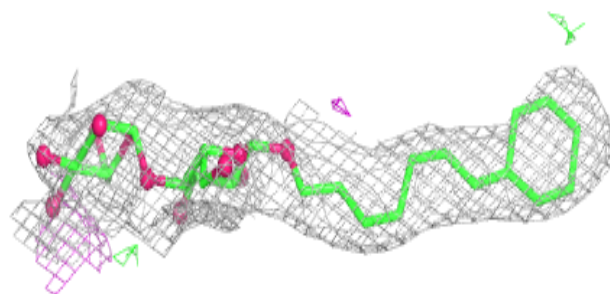
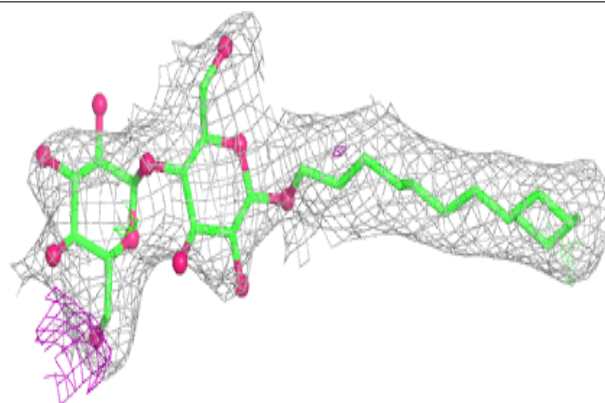


**Electron density around CA7 C 510:**

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

**Electron density around CA7 M 510:**

$2mF_o-DF_c$  (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.