

wwPDB EM Validation Summary Report (i)

May 10, 2022 - 01:32 pm BST

PDB ID	:	7QHO
EMDB ID	:	EMD-13977
Title	:	Cytochrome bcc-aa3 supercomplex (respiratory supercomplex III2/IV2) from
		Corynebacterium glutamicum (as isolated)
Authors	:	Kao, WC.; Hunte, C.
Deposited on	:	2021-12-13
Resolution	:	3.10 Å(reported)

This is a wwPDB EM 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/EMValidationReportHelp with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (i)) were used in the production of this report:

EMDB validation analysis	:	0.0.1. dev 8
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7(2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.28.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $ELECTRON\ MICROSCOPY$

The reported resolution of this entry is 3.10 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.



Motric	Whole archive	EM structures
	$(\# {\rm Entries})$	$(\# { m Entries})$
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain	
1	А	408	92%	7% •
1	Ν	408	91%	7% •
2	В	539	92%	7% •
2	0	539	91%	8% •
3	С	283	78% ••	18%
3	Р	283	78%	18%
4	D	594	91%	6% ·
4	Q	594	90%	6% •



Mol	Chain	Length	Quality of chain	
5	Е	331	8%	·
5	R	331	7% 	•
6	F	205	89%	• 7%
6	S	205	88%	• 7%
7	G	143	94%	6%
7	Т	143	<u>6%</u> 92%	8%
8	Н	163	5% 91%	• 6%
8	U	163	91%	• 6%
9	Ι	147	9%	• 12%
9	V	147	86%	• 12%
10	J	112	86%	• 11%
10	W	112	85%	• 11%
11	K	73	8% 74% •	22%
11	Х	73	73% 5%	22%
12	L	65	18%	• •
12	Y	65	95%	•••
13	М	168	12% • 85%	
13	Z	168	▲ 14% • 85%	

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2 Entry composition (i)

There are 33 unique types of molecules in this entry. The entry contains 95954 atoms, of which 47460 are hydrogens and 0 are deuteriums.

In the tables below, 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 bc1 complex Rieske iron-sulfur subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	Δ	402	Total	С	Η	Ν	0	\mathbf{S}	0	0
I A	402	6206	1998	3070	536	586	16	0	0	
1	N	402	Total	С	Η	Ν	0	S	0	0
	402	6206	1998	3070	536	586	16	0	0	

• Molecule 2 is a protein called Cytochrome bc1 complex cytochrome b subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	В	534	Total	С	Η	Ν	Ο	\mathbf{S}	5	0
	001	8491	2775	4268	707	719	22	0	0	
9	2 O	534	Total	С	Η	Ν	Ο	\mathbf{S}	5	0
2			8491	2775	4268	707	719	22	5	0

• Molecule 3 is a protein called Cytochrome bc1 complex cytochrome c subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	C	າງງ	Total	С	Η	Ν	0	\mathbf{S}	0	0
3 U	233	3418	1083	1680	302	343	10	0	0	
2	D	022	Total	С	Η	Ν	0	S	0	0
3 P	233	3418	1083	1680	302	343	10		U	

• Molecule 4 is a protein called Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
4		574	Total	С	Η	Ν	0	\mathbf{S}	0	Ο
4 D	014	8994	3023	4458	733	748	32	0	0	
4	4 0	Q 574	Total	С	Η	Ν	0	S	0	0
4 Q	Q		8994	3023	4458	733	748	32	0	0

There are 20 discrepancies between the modelled and reference sequences:

D 585 ALA - expression tag UNP Q79	sidue Modelled Actu	Reference
	585 ALA -	UNP Q79VD7



Chain	Residue	Modelled	Actual	Comment	Reference
D	586	ALA	-	expression tag	UNP Q79VD7
D	587	TRP	-	expression tag	UNP Q79VD7
D	588	SER	_	expression tag	UNP Q79VD7
D	589	HIS	-	expression tag	UNP Q79VD7
D	590	PRO	-	expression tag	UNP Q79VD7
D	591	GLN	-	expression tag	UNP Q79VD7
D	592	PHE	-	expression tag	UNP Q79VD7
D	593	GLU	-	expression tag	UNP Q79VD7
D	594	LYS	-	expression tag	UNP Q79VD7
Q	585	ALA	-	expression tag	UNP Q79VD7
Q	586	ALA	-	expression tag	UNP Q79VD7
Q	587	TRP	-	expression tag	UNP Q79VD7
Q	588	SER	-	expression tag	UNP Q79VD7
Q	589	HIS	-	expression tag	UNP Q79VD7
Q	590	PRO	-	expression tag	UNP Q79VD7
Q	591	GLN	-	expression tag	UNP Q79VD7
Q	592	PHE	-	expression tag	UNP Q79VD7
Q	593	GLU	-	expression tag	UNP Q79VD7
Q	594	LYS	-	expression tag	UNP Q79VD7

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• Molecule 5 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	F	221	Total	С	Η	Ν	0	S	0	0
9 E	551	5066	1660	2468	429	498	11	0	0	
5	D	221	Total	С	Η	Ν	0	S	0	0
0 h	331	5066	1660	2468	429	498	11	0	0	

• Molecule 6 is a protein called Cytochrome c oxidase subunit 3.

Mol	Chain	Residues		Atoms					AltConf	Trace
6	Б	100	Total	С	Η	Ν	0	S	0	0
0	Г	190	2981	992	1495	236	251	7	0	0
6	C	100	Total	С	Η	Ν	0	S	0	0
0	G	190	2981	992	1495	236	251	7	0	0

• Molecule 7 is a protein called Cytochrome c oxidase polypeptide 4.

Mol	Chain	Residues			Atom	.s			AltConf	Trace
7	G	143	Total 2201	C 728	Н 1106	N 167	0 191	S 9	0	0



Continued from previous page...

Mol	Chain	Residues			Atom	S			AltConf	Trace
7	Т	143	Total 2201	C 728	Н 1106	N 167	0 191	${ m S} 9$	0	0

• Molecule 8 is a protein called Uncharacterized protein Cgl2664/cg2949.

Mol	Chain	Residues		Atoms						Trace
8	Ц	154	Total	С	Η	Ν	0	\mathbf{S}	0	0
0	11	104	2182	686	1058	185	250	3	0	0
0	II	154	Total	С	Η	Ν	0	S	0	0
0	U	104	2182	686	1058	185	250	3	0	

• Molecule 9 is a protein called Uncharacterized membrane protein Cgl2017/cg2211.

Mol	Chain	Residues		Atoms						Trace
0	т	120	Total	С	Η	Ν	Ο	S	0	0
9	1	129	2059	664	1031	182	181	1	0	0
0	V	120	Total	С	Η	Ν	0	S	0	0
9	v	129	2059	664	1031	182	181	1	0	0

• Molecule 10 is a protein called Hypothetical membrane protein.

Mol	Chain	Residues		Atoms					AltConf	Trace
10	т	100	Total	С	Η	Ν	0	S	0	0
10	1	100	1547	498	780	132	134	3	0	0
10	W	100	Total	С	Η	Ν	0	S	0	0
10	vv	100	1547	498	780	132	134	3	0	0

• Molecule 11 is a protein called Actinobacterial supercomplex, subunit C (AscC).

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	57	Total 864	C 286	Н 413	N 78	0 87	0	0
11	Х	57	Total 864	C 286	Н 413	N 78	0 87	0	0

• Molecule 12 is a protein called Hypothetical membrane protein.

Mol	Chain	Residues		Atoms						Trace
19	т	63	Total	С	Н	Ν	0	S	0	0
12		05	915	294	470	70	78	3	0	0
19	V	63	Total	С	Н	Ν	0	S	0	0
	I	00	915	294	470	70	78	3	0	0



• Molecule 13 is a protein called Thiamine biosynthesis protein X.

Mol	Chain	Residues		Atoms					AltConf	Trace
13	М	25	Total	С	Η	Ν	Ο	\mathbf{S}	0	Ο
15	101	20	372	114	179	36	42	1	0	0
12	7	25	Total	С	Η	Ν	Ο	\mathbf{S}	0	0
10		20	372	114	179	36	42	1	0	0

• Molecule 14 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
14	А	1	Total Fe S 4 2 2	0
14	Ν	1	Total Fe S 4 2 2	0

• Molecule 15 is $[(2 \{R\})-3-[[(1 \{S\},2 \{R\},3 \{S\},4 \{S\},5 \{R\},6 \{R\})-2-[(2 \{R\},3 \{S\},4 \{S\},5 \{S\},6 \{R\})-6-[[(2 \{S\},3 \{S\},4 \{S\},5 \{S\},6 \{R\})-6-(hydroxymethyl)-3-[(2 \{R\},3 \{S\},4 \{S\},5 \{S\},6 \{R\})-6-(hydroxymethyl)-3,4,5-tris(oxidanyl)oxan-2-yl]oxy-4,5-bis(oxidanyl)oxan-2-yl]oxymethyl]-3,4,5-tris(oxidanyl)oxan-2-yl]oxymethyl]-3,4,5-tris(oxidanyl)oxan-2-yl]oxymethyl]-3,4,5-tris(oxidanyl)oxan-2-yl]oxy-3,4,5-tris(oxidanyl)-6-[(2 {R},3 {S},4 {S},5 {S},6 {R})-3,4,5-tris(oxidanyl)-6-(undecanoyloxymethyl)oxan-2-yl]oxy-cyclohexyl]oxy-oxidanyl-phosph oryl]oxy-2-undecanoyloxy-propyl] (10 {R})-10-methyldodecanoate (three-letter code: IZL) (formula: <math>C_{74}H_{133}O_{39}P$) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues		At		AltConf		
15	Δ	1	Total	С	Η	Ο	Р	0
10	A	1	212	63	109	39	1	0
15	N	1	Total	С	Н	Ο	Р	0
10	IN IN	1	212	63	109	39	1	

• Molecule 16 is (2R)-2-(hexadecanoyloxy)-3-{[(S)-hydroxy{[(1R,2R,3R,4R,5R,6S)-2,3,4,5,6-pentahydroxycyclohexyl]oxy}phosphoryl]oxy}propyl (9S)-9-methyloctadecan oate (three-letter code: 9YF) (formula: C₄₄H₈₅O₁₃P) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues		At	oms			AltConf
16	Δ	1	Total	С	Η	Ο	Р	0
10	A	1	66	22	30	13	1	0
16	D	1	Total	С	Η	0	Р	0
10	D	1	60	20	26	13	1	0
16	N	1	Total	С	Η	0	Р	0
10	IN	1	66	22	30	13	1	0
16	TT	1	Total	С	Η	0	Р	0
10	U	1	60	20	26	13	1	0

• Molecule 17 is MENAQUINONE-9 (three-letter code: MQ9) (formula: $C_{56}H_{80}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	1	Aton	ns		AltConf
17	Δ	1	Total	С	Η	Ο	0
11	A	L	52	24	26	2	0
17	В	1	Total	С	Η	Ο	0
11	D	L	92	42	46	4	0
17	р	1	Total	С	Η	Ο	0
11	D	L	92	42	46	4	0
17	N	1	Total	С	Η	Ο	0
11	IN	L	52	24	26	2	0
17	0	1	Total	С	Η	Ο	0
11	0	I	92	42	46	4	0
17	0	1	Total	С	Η	Ο	0
11	U		92	42	46	4	

• Molecule 18 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: $C_{41}H_{82}NO_8P$) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues		A	tom	ıs			AltConf
10	Λ	1	Total	С	Η	Ν	Ο	Р	0
10	A	1	66	28	28	1	8	1	0
10	Л	1	Total	С	Η	Ν	0	Р	0
10	D	1	57	21	26	1	8	1	0
10	F	1	Total	С	Η	Ν	0	Р	0
10	Ľ	1	57	21	26	1	8	1	0
18	F	1	Total	С	Η	Ν	0	Р	0
10	Г	1	54	22	22	1	8	1	0
18	Т	1	Total	С	Η	Ν	0	Р	0
10	J	1	111	37	64	1	8	1	0
18	Ν	1	Total	С	Η	Ν	0	Р	0
10	IN	I	66	28	28	1	8	1	0
18	0	1	Total	С	Η	Ν	Ο	Р	0
10	Q	T	57	21	26	1	8	1	0
18	В	1	Total	С	Η	Ν	0	Р	0
10	10	I	57	21	26	1	8	1	0
18	S	1	Total	С	Η	Ν	0	Р	0
10	U U	1	54	22	22	1	8	1	U
18	W	1	Total	С	Η	Ν	0	Р	0
10	vv		111	37	64	1	8	1	0

• Molecule 19 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues		Atoms					AltConf
10	В	1	Total	С	Fe	Η	Ν	Ο	0
19	D	1	146	68	2	60	8	8	0
10	В	1	Total	С	Fe	Η	Ν	Ο	0
19	D	1	146	68	2	60	8	8	0
10	0	1	Total	С	Fe	Η	Ν	Ο	0
19	0	1	146	68	2	60	8	8	0
10	0	1	Total	С	Fe	Η	Ν	Ο	0
19	U	1	146	68	2	60	8	8	

• Molecule 20 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms	AltConf
20	В	1	Total C H O P	0
20	D	1	72 26 27 17 2	0
20	С	1	Total C H O P	0
		-		Ŭ
20	D	1	Total C H O P	0
			289 102 149 34 4	
20	D	1	Total C H O P	0
			289 102 149 34 4	
20	F	1	Total C H O P	0
			94 38 37 17 2	
20	G	1	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	0
			$\begin{array}{cccccccccccccccccccccccccccccccccccc$	
20	Ι	1	107 38 50 17 2	0
			Total C H O P	
20	О	1	72 26 27 17 2	0
			Total C H O P	
20	Р	1	113 46 48 17 2	0
	0		Total C H O P	
20	Q	1	289 102 149 34 4	0
- 20	0	1	Total C H O P	0
20	Q	1	289 102 149 34 4	0
20	C	1	Total C H O P	0
20	G	I	198 81 79 34 4	0
20	S	1	Total C H O P	0
20	5	1	198 81 79 34 4	0
20	V	1	Total C H O P	0
	V	*	107 38 50 17 2	Ŭ

• Molecule 21 is LYCOPENE (three-letter code: LYC) (formula: $C_{40}H_{56}$) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms	AltConf
91	В	1	Total C H	0
21	D	1	96 40 56	0
91	0	1	Total C H	0
	0	1	96 40 56	0

• Molecule 22 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms				AltConf
22	В	1	Total	С	Η	0	0
	D	1	71	21	39	11	0



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Mol	Chain	Residues	1	AltConf			
22	О	1	Total 71	C 21	Н 39	0 11	0

• Molecule 23 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues		Atoms					AltConf
23	С	1	Total	С	Fe	Η	Ν	Ο	0
20	U	1	146	68	2	60	8	8	0
23	С	1	Total	С	Fe	Η	Ν	0	0
20	U	1	146	68	2	60	8	8	0
23	P	1	Total	С	Fe	Η	Ν	0	0
20	1	1	146	68	2	60	8	8	0
23	P	1	Total	С	Fe	Η	Ν	0	0
20	L	1	146	68	2	60	8	8	

• Molecule 24 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (three-letter code: 3PH) (formula: C₃₉H₇₇O₈P) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues		Ate	oms			AltConf
24	C	1	Total	С	Η	Ο	Р	0
24	U	L	90	29	52	8	1	0
24	Т	1	Total	С	Η	0	Р	0
24	L	L	90	29	52	8	1	0

• Molecule 25 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	Atoms					AltConf	
25	Л	1	Total	С	Fe	Η	Ν	0	0
20	D	1	254	108	2	124	8	12	0



	J	1	5						
Mol	Chain	Residues		Atoms					
25	Л	1	Total	С	Fe	Н	Ν	0	0
20	D	1	254	108	2	124	8	12	0
25	0	1	Total	С	Fe	Η	Ν	0	0
20	Q	1	254	108	2	124	8	12	0
25	0	1	Total	С	Fe	Н	Ν	0	0
20	Q	1	254	108	2	124	8	12	

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• Molecule 26 is COPPER (II) ION (three-letter code: CU) (formula: Cu) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
26	D	1	Total Cu 1 1	0
26	Q	1	Total Cu 1 1	0

• Molecule 27 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
27	D	1	Total Ca 1 1	0
27	Q	1	Total Ca 1 1	0

• Molecule 28 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
28	Е	1	Total Mn 1 1	0
28	R	1	Total Mn 1 1	0

• Molecule 29 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu₂) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms	AltConf
29	Е	1	Total Cu 2 2	0
29	Е	1	Total Cu 2 2	0
29	R	1	Total Cu 2 2	0
29	R	1	Total Cu 2 2	0

• Molecule 30 is DIACYL GLYCEROL (three-letter code: DGA) (formula: $C_{39}H_{76}O_5$) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms	AltConf
30	Е	1	Total C O	0
			20 16 4	
30	н	1	Total C O	0
	11	Ĩ	17 13 4	0
30	М	1	Total C O	0
50	101	1	22 18 4	0
30	В	1	Total C O	0
50	п	1	20 16 4	0
20	II	1	Total C O	0
- 50	U	1	17 13 4	0
20	7	1	Total C O	0
30	L	1	22 18 4	0

• Molecule 31 is PALMITIC ACID (three-letter code: PLM) (formula: $C_{16}H_{32}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
21	н	1	Total C H O	0
51	11	T	35 14 20 1	0
21	М	1	Total C H O	0
51	111	1	9 4 4 1	0
21	II	1	Total C H O	0
51	U	1	35 14 20 1	0
91	7	1	Total C H O	0
51	Z	1	9 4 4 1	0

• Molecule 32 is [(2 {R})-3-[[(1 {S},2 {R},3 {R},4 {S},5 {S},6 {R})-2-[(2 {R},3 {S},4 {S},5 {S},6 {R})-6-(hexadecanoyloxymethyl)-3,4,5-tris(oxidanyl)oxan-2-yl]oxy-6-[(2 {R},3 {S},4 {S},4 {S},5 {R})-6-(hexadecanoyloxymethyl)-3,4,5-tris(oxidanyl)oxan-2-yl]oxy-6-[(2 {R},3 {S},4 {S},4 {S},5 {R})-6-(hexadecanoyloxymethyl)-3,4,5-tris(oxidanyl)oxan-2-yl]oxy-6-[(2 {R},3 {S},4 {S},4 {S},5 {R})-6-(hexadecanoyloxymethyl)-3,4,5-tris(oxidanyl)oxan-2-yl]oxy-6-[(2 {R},3 {S},4 {S},5 {R})-6-(hexadecanoyloxymethyl)-3,4,5-tris(oxidanyl)oxan-2-yl]oxy-6-[(2 {R},3 {S},4 {S},5 {R})-6-(hexadecanoyloxymethyl)-3,4,5-tris(oxidanyl)oxan-2-yl]oxy-6-[(2 {R},3 {S},4 {S},4 {S})-6-(hexadecanoyloxymethyl)-3,4,5-tris(oxidanyl)oxan-2-yl]oxy-6-[(2 {R},3 {S},4 {S})-6-(hexadecanoyloxymethyl)-3,4-(hexadecanoyloxymethyl)-3,4-(hexadecanoyloxymethyl)-3,4-(hexadecanoyloxymethyl)-3,4-(hexadecanoyloxymethyl)-3,4-(hexadecanoyloxymethyl)-3,4-(hexadecanoyloxymethyl)-3,4-(hexadecanoyloxymethyl)-3,4-(hexadecanoyloxymethyl)-3,4-(hexadecanoyloxymethyl)-3,4-(hexadecanoyloxymethyl)-3,4-(hexadecanoyloxymethyl)-3,4-(hexadecanoyloxymethyl)-3,4-(hexadecanoyloxymethyl)-3,4-



S},5 {S},6 {R})-6-(hydroxymethyl)-3,4,5-tris(oxidanyl)oxan-2-yl]oxy-3,4,5-tris(oxidanyl)cy clohexyl]oxy-oxidanyl-phosphoryl]oxy-2-undecanoyloxy-propyl] (10 {S})-10-methylhenicos anoate (three-letter code: IX7) (formula: $C_{70}H_{131}O_{24}P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf	
30	Т	1	Total	С	Η	Ο	Р	0	
32	1	1	155	47	83	24	1	0	
20	D	1	Total	С	Η	0	Р	0	
32	К	1	155	47	83	24	1	0	

• Molecule 33 is water.

Mol	Chain	Residues	Atoms	AltConf
33	В	2	Total O 2 2	0
33	D	2	Total O 2 2	0
33	Е	1	Total O 1 1	0
33	О	2	Total O 2 2	0
33	Q	2	Total O 2 2	0
33	R	1	Total O 1 1	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 atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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 bc1 complex Rieske iron-sulfur subunit



• Molecule 1: Cytochrome bc1 complex Rieske iron-sulfur subunit





V271 M1 M1 Q293 WE M1 Q293 WE WE Q311 N3 M3 M311 N8 M1 A322 M1 N6 A322 M1 N6 A322 M1 N16 R431 113 N16 A421 114 N16 A473 N16 N16 A473 N16 N16 A473 N16 N16 A473 N14 1142 A473 N14 1142 A473 N14 1142 B48 M32 1142 A53 N14 1142 A54 M33 117 A54 M33 117 A53 M34 11

• Molecule 3: Cytochrome bc1 complex cytochrome c subunit

Chain C:	78%		18%			
MET ALA LYS PRO SER ALA LYS LYS VAL LYS ARSN ARSN	ARG LYS VAL ARG ARG ARG ARA ALA ALA ALA ALA ALA ALA ALA ALA ALA	PRD ASP ALA GLN VAL ALA ALA ALA	GLN ARG D51 D52	C67 D103	1104	

R117 N142 E143 D144 R156 P144 V156 P219 P219 V258 V258 V273 V273 V273

• Molecule 3: Cytochrome bc1 complex cytochrome c subunit

Chain P:	78%	• •		18%	-		
MET ALA LYS PRO SER ALA LYS LYS VAL	LYS ANG ANG ANG ANG ANG ANG ANA ANA ANA ANA	ALA THR	ALA GLN ARG	D51 D52	C67	P103 1104	A111 E112

• Molecule 4: Cytochrome c oxidase subunit 1



• Molecule 4: Cytochrome c oxidase subunit 1













LEU ASP ASP ASP ASP ALM ALA ALA ALA ALA ALA



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	51060	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE	Depositor
	CORRECTION	
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{\AA}^2)$	49.95	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	2.056	Depositor
Minimum map value	-0.798	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.093	Depositor
Recommended contour level	0.09	Depositor
Map size (Å)	232.20001, 249.48001, 162.0	wwPDB
Map dimensions	150, 231, 215	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	Depositor



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: 3PH, CDL, IZL, HEC, MN, CU, FES, PLM, HEM, LYC, LMT, CUA, 3PE, CA, DGA, 9YF, HAS, MQ9, IX7

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).

Mal	Chain	Bond	lengths	Bond	angles
	Ullalli	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.37	0/3216	0.63	0/4375
1	Ν	0.37	0/3216	0.63	0/4375
2	В	0.40	0/4361	0.61	0/5944
2	0	0.40	0/4361	0.61	0/5944
3	С	0.29	0/1770	0.58	0/2394
3	Р	0.29	0/1770	0.58	0/2394
4	D	0.31	0/4705	0.55	0/6419
4	Q	0.31	0/4705	0.55	0/6419
5	Е	0.30	0/2671	0.55	0/3642
5	R	0.30	0/2671	0.55	0/3642
6	F	0.30	0/1528	0.51	0/2081
6	S	0.30	0/1528	0.51	0/2081
7	G	0.31	0/1126	0.50	0/1529
7	Т	0.31	0/1126	0.50	0/1529
8	Н	0.29	0/1138	0.57	0/1558
8	U	0.29	0/1138	0.57	0/1558
9	Ι	0.27	0/1057	0.57	0/1444
9	V	0.27	0/1057	0.57	0/1444
10	J	0.27	0/786	0.56	0/1068
10	W	0.27	0/786	0.56	0/1068
11	Κ	0.32	0/468	0.54	0/640
11	Х	0.32	0/468	0.54	0/640
12	L	0.26	0/453	0.49	0/616
12	Y	0.26	0/453	0.49	0/616
13	М	0.27	0/197	0.57	0/271
13	Ζ	0.28	0/197	0.57	0/271
All	All	0.33	0/46952	0.57	0/63962

There are no bond length outliers.

There are no bond angle outliers.



There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	3136	3070	3070	35	0
1	Ν	3136	3070	3070	30	0
2	В	4223	4268	4252	35	0
2	0	4223	4268	4252	38	0
3	С	1738	1680	1680	11	0
3	Р	1738	1680	1680	12	0
4	D	4536	4458	4459	19	0
4	Q	4536	4458	4459	22	0
5	Е	2598	2468	2468	5	0
5	R	2598	2468	2468	5	0
6	F	1486	1495	1494	5	0
6	S	1486	1495	1494	6	0
7	G	1095	1106	1106	6	0
7	Т	1095	1106	1106	11	0
8	Н	1124	1058	1057	3	0
8	U	1124	1058	1057	3	0
9	Ι	1028	1031	1031	3	0
9	V	1028	1031	1031	2	0
10	J	767	780	780	2	0
10	W	767	780	780	4	0
11	Κ	451	413	413	3	0
11	Х	451	413	413	5	0
12	L	445	470	469	1	0
12	Y	445	470	469	1	0
13	М	193	179	179	2	0
13	Ζ	193	179	179	1	0
14	А	4	0	0	1	0
14	N	4	0	0	1	0
15	A	103	109	0	4	0
15	N	103	109	0	3	0
16	A	36	30	0	0	0
16	В	34	26	0	0	0
16	N	36	30	0	0	0



		i previous		TT(11 1)		a al i
Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	U	34	26	0	0	0
17	A	26	26	26	8	0
17	B	46	46	42	0	0
17	N	26	26	26	6	0
17	0	46	46	42	2	0
18	A	38	28	53	8	0
18	D	31	26	36	1	0
18	E	31	26	36	0	0
18	F	32	22	38	1	0
18	J	47	64	71	1	0
18	Ν	38	28	53	9	0
18	Q	31	26	36	1	0
18	R	31	26	36	0	0
18	S	32	22	38	1	0
18	W	47	64	71	1	0
19	В	86	60	60	1	0
19	0	86	60	60	1	0
20	В	45	27	34	1	0
20	С	65	48	74	2	0
20	D	140	149	171	0	0
20	F	57	37	58	0	0
20	G	62	42	68	3	0
20	Ι	57	50	61	0	0
20	0	45	27	34	1	0
20	Р	65	48	74	2	0
20	Q	140	149	171	1	0
20	S	119	79	126	2	0
20	V	57	50	61	0	0
21	В	40	56	56	2	0
21	0	40	56	56	2	0
22	В	32	39	37	3	0
22	0	32	39	37	3	0
23	С	86	60	60	7	0
23	Р	86	60	60	7	0
24	С	38	52	48	0	0
24	Т	38	52	48	0	0
25	D	130	124	124	5	0
25	Q	130	124	124	4	0
26	D	1	0	0	0	0
26	Q	1	0	0	0	0
27	D	1	0	0	0	0
27	Q	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	Е	1	0	0	0	0
28	R	1	0	0	0	0
29	Е	2	0	0	0	0
29	R	2	0	0	0	0
30	Е	20	0	21	1	0
30	Н	17	0	15	0	0
30	М	22	0	25	0	0
30	R	20	0	21	1	0
30	U	17	0	15	0	0
30	Ζ	22	0	25	1	0
31	Н	15	20	20	0	0
31	М	5	4	4	0	0
31	U	15	20	20	0	0
31	Ζ	5	4	4	0	0
32	Ι	72	83	0	2	0
32	R	72	83	0	1	0
33	В	2	0	0	0	0
33	D	2	0	0	0	0
33	Е	1	0	0	0	0
33	0	2	0	0	0	0
33	Q	2	0	0	0	0
33	R	1	0	0	0	0
All	All	48494	47460	47392	239	0

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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 2.

The worst 5 of 239 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)
17:A:504:MQ9:H5M1	2:O:50:THR:HG23	1.65	0.79
15:N:504:IZL:O30	15:N:504:IZL:O33	2.07	0.72
25:Q:601:HAS:HMC1	25:Q:601:HAS:HBC1	1.72	0.72
15:A:502:IZL:O30	15:A:502:IZL:O33	2.07	0.71
25:D:601:HAS:HMC1	25:D:601:HAS:HBC1	1.72	0.71

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 PDB entries followed by that with respect to all EM entries.

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	А	400/408~(98%)	376~(94%)	24~(6%)	0	100	100
1	Ν	400/408~(98%)	376~(94%)	24~(6%)	0	100	100
2	В	537/539~(100%)	525~(98%)	12 (2%)	0	100	100
2	Ο	537/539~(100%)	524 (98%)	13~(2%)	0	100	100
3	С	231/283~(82%)	219~(95%)	12~(5%)	0	100	100
3	Р	231/283~(82%)	219 (95%)	12 (5%)	0	100	100
4	D	572/594~(96%)	556 (97%)	16 (3%)	0	100	100
4	Q	572/594~(96%)	556 (97%)	16 (3%)	0	100	100
5	Е	329/331~(99%)	311 (94%)	17 (5%)	1 (0%)	41	73
5	R	329/331~(99%)	311 (94%)	17 (5%)	1 (0%)	41	73
6	F	188/205~(92%)	187 (100%)	1 (0%)	0	100	100
6	S	188/205~(92%)	187 (100%)	1 (0%)	0	100	100
7	G	141/143~(99%)	138 (98%)	3 (2%)	0	100	100
7	Т	141/143~(99%)	138 (98%)	3(2%)	0	100	100
8	Н	152/163~(93%)	148 (97%)	4 (3%)	0	100	100
8	U	152/163~(93%)	148 (97%)	4 (3%)	0	100	100
9	Ι	127/147~(86%)	120 (94%)	7 (6%)	0	100	100
9	V	127/147~(86%)	120 (94%)	7~(6%)	0	100	100
10	J	98/112 (88%)	96 (98%)	2(2%)	0	100	100
10	W	98/112~(88%)	96 (98%)	2(2%)	0	100	100
11	К	55/73~(75%)	54 (98%)	1 (2%)	0	100	100
11	X	55/73~(75%)	54 (98%)	1 (2%)	0	100	100
12	L	61/65~(94%)	59 (97%)	2(3%)	0	100	100
12	Y	61/65~(94%)	59 (97%)	2(3%)	0	100	100
13	М	23/168 (14%)	23 (100%)	0	0	100	100



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Mol	Chain	Analysed	Favoured	CavouredAllowed		Percentiles		
13	Z	23/168~(14%)	23 (100%)	0	0	100	100	
All	All	5828/6462 (90%)	5623 (96%)	203 (4%)	2~(0%)	100	100	

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	Е	242	VAL
5	R	242	VAL

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	Perce	ntiles
1	А	326/332~(98%)	325~(100%)	1 (0%)	92	96
1	Ν	326/332~(98%)	325 (100%)	1 (0%)	92	96
2	В	442/441~(100%)	437~(99%)	5 (1%)	73	89
2	Ο	442/441~(100%)	437~(99%)	5 (1%)	73	89
3	С	177/212~(84%)	175~(99%)	2(1%)	73	89
3	Р	177/212~(84%)	175~(99%)	2(1%)	73	89
4	D	472/488~(97%)	467~(99%)	5 (1%)	73	89
4	Q	472/488~(97%)	467~(99%)	5(1%)	73	89
5	Ε	274/274~(100%)	272~(99%)	2(1%)	84	93
5	R	274/274~(100%)	272~(99%)	2(1%)	84	93
6	F	156/166~(94%)	155~(99%)	1 (1%)	86	94
6	S	156/166~(94%)	155~(99%)	1 (1%)	86	94
7	G	114/114~(100%)	114 (100%)	0	100	100
7	Т	114/114~(100%)	114 (100%)	0	100	100
8	Н	$12\overline{7}/133~(96\%)$	127~(100%)	0	100	100
8	U	$12\overline{7}/133~(96\%)$	127 (100%)	0	100	100
9	Ι	$11\overline{1/125}~(89\%)$	110 (99%)	1 (1%)	78	91



Mol	Chain	Analysed	Rotameric	Outliers	Percentiles		
9	V	111/125~(89%)	110 (99%)	1 (1%)	78	91	
10	J	80/90~(89%)	79~(99%)	1 (1%)	69	87	
10	W	80/90~(89%)	79~(99%)	1 (1%)	69	87	
11	Κ	48/63~(76%)	48 (100%)	0	100	100	
11	Х	48/63~(76%)	48 (100%)	0	100	100	
12	L	43/45~(96%)	43 (100%)	0	100	100	
12	Υ	43/45~(96%)	43 (100%)	0	100	100	
13	М	25/135~(18%)	25~(100%)	0	100	100	
13	Z	25/135~(18%)	25~(100%)	0	100	100	
All	All	4790/5236 (92%)	4754 (99%)	36(1%)	84	92	

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5 of 36 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	Q	263	PHE
10	W	58	PHE
4	Q	314	HIS
5	R	132	GLN
4	D	462	TYR

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

Mol	Chain	Res	Type
1	А	232	HIS
1	А	287	HIS
1	Ν	232	HIS
1	Ν	287	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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



5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 78 ligands modelled in this entry, 6 are monoatomic and 4 are modelled with single atom - leaving 68 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).

Mal	Turne	Chain	Dec	Tiple	Boi	nd lengt	hs	Bo	nd angl	es
INIOI	туре	Unam	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
30	DGA	Н	201	-	16,16,43	0.29	0	18,18,45	0.20	0
20	CDL	F	302	-	56, 56, 99	0.38	0	62,68,111	0.33	0
25	HAS	Q	601	4	56,72,72	4.11	20 (35%)	50,109,109	3.49	23 (46%)
20	CDL	Р	301	-	64,64,99	0.37	0	70,76,111	0.36	0
20	CDL	D	605	-	76,76,99	0.35	0	82,88,111	0.50	1 (1%)
31	PLM	U	202	8	13,13,17	0.25	0	11,11,17	0.18	0
20	CDL	V	201	-	56,56,99	0.38	0	62,68,111	0.34	0
19	HEM	В	603	2	27,50,50	1.26	4 (14%)	17,82,82	1.51	3 (17%)
20	CDL	Q	605	-	76,76,99	0.35	0	82,88,111	0.50	1 (1%)
31	PLM	М	202	13	4,4,17	0.33	0	3,3,17	0.46	0
14	FES	N	503	1	0,4,4	-	-	-		
15	IZL	А	502	-	108,108,119	0.40	0	150,152,163	1.04	11 (7%)
18	3PE	R	405	-	30,30,50	0.38	0	33,35,55	0.35	0
15	IZL	Ν	504	-	108,108,119	0.40	0	150,152,163	1.04	11 (7%)
23	HEC	С	302	3	26,50,50	1.25	2 (7%)	18,82,82	1.95	6 (33%)
20	CDL	D	606	-	62,62,99	0.38	0	68,74,111	0.36	0
18	3PE	W	201	-	46,46,50	0.32	0	49,51,55	0.31	0
18	3PE	Q	607	-	30,30,50	0.38	0	33,35,55	0.33	0
18	3PE	J	201	-	46,46,50	0.32	0	49,51,55	0.31	0
23	HEC	С	303	3	$26,\!50,\!50$	1.46	2 (7%)	18,82,82	2.08	6 (33%)
18	3PE	S	301	-	31,31,50	0.40	0	34,36,55	0.68	1 (2%)
23	HEC	Р	302	3	26,50,50	1.24	2 (7%)	18,82,82	1.95	6 (33%)
16	9YF	А	503	-	36, 36, 58	0.35	0	46,48,71	0.51	0
20	CDL	Q	606	-	62,62,99	0.38	0	68,74,111	0.36	0



Mal	T	Chain	Dec	T : 1-	Bo	nd lengt	hs	Bo	nd angl	es
IVIOI	Type	Chain	Res	LINK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
32	IX7	I	202	-	74,74,97	0.30	0	97,99,123	0.83	6 (6%)
17	MQ9	В	601	-	24,24,59	0.44	0	30,33,75	0.61	1 (3%)
24	3PH	Т	201	-	36,36,47	0.28	0	39,40,52	0.55	1 (2%)
25	HAS	D	601	4	56,72,72	4.11	20 (35%)	50,109,109	3.49	23 (46%)
25	HAS	D	602	4	56,72,72	4.17	21 (37%)	50,109,109	3.92	24 (48%)
16	9YF	N	505	-	36,36,58	0.35	0	46,48,71	0.51	0
30	DGA	R	404	-	19,19,43	0.27	0	21,21,45	0.26	0
25	HAS	Q	602	4	56,72,72	4.17	21 (37%)	50,109,109	3.92	24 (48%)
31	PLM	Z	202	13	4,4,17	0.33	0	3,3,17	0.46	0
19	HEM	0	603	2	27,50,50	1.27	4 (14%)	17,82,82	1.44	5 (29%)
20	CDL	С	301	-	64,64,99	0.37	0	70,76,111	0.36	0
21	LYC	В	606	-	39,39,39	0.19	0	44,46,46	0.39	0
20	CDL	Ι	201	-	56, 56, 99	0.38	0	62,68,111	0.34	0
20	CDL	В	605	-	44,44,99	0.42	0	50,56,111	0.43	0
16	9YF	В	607	-	34,34,58	0.38	0	44,46,71	0.36	0
22	LMT	В	608	-	33,33,36	0.40	0	44,44,47	0.74	1 (2%)
17	MQ9	Ο	605	-	$24,\!24,\!59$	0.40	0	$30,\!33,\!75$	0.66	1 (3%)
21	LYC	0	607	-	39,39,39	0.20	0	44,46,46	0.39	0
16	9YF	U	203	-	$34,\!34,\!58$	0.38	0	44,46,71	0.37	0
31	PLM	Н	202	8	13,13,17	0.25	0	11,11,17	0.18	0
30	DGA	М	201	-	21,21,43	0.27	0	23,23,45	0.23	0
30	DGA	U	201	-	16,16,43	0.29	0	18,18,45	0.20	0
22	LMT	0	601	-	33,33,36	0.40	0	44,44,47	0.74	1 (2%)
24	3PH	C	304	-	36, 36, 47	0.28	0	$39,\!40,\!52$	0.55	1 (2%)
20	CDL	G	201	-	$61,\!61,\!99$	0.38	0	67,73,111	0.39	0
17	MQ9	В	604	-	$24,\!24,\!59$	0.40	0	$30,\!33,\!75$	0.67	1 (3%)
18	3PE	Ν	502	-	$37,\!37,\!50$	0.39	0	$40,\!42,\!55$	0.72	1 (2%)
20	CDL	S	303	-	61,61,99	0.38	0	67,73,111	0.39	0
30	DGA	E	404	-	19,19,43	0.27	0	21,21,45	0.26	0
17	MQ9	Ν	501	-	$27,\!27,\!59$	0.96	1 (3%)	$33,\!36,\!75$	1.72	2 (6%)
17	MQ9	А	504	-	$27,\!27,\!59$	0.96	1 (3%)	$33,\!36,\!75$	1.72	2 (6%)
20	CDL	S	302	-	56, 56, 99	0.38	0	62,68,111	0.33	0
18	3PE	F	301	-	31,31,50	0.40	0	34,36,55	0.68	1 (2%)
23	HEC	Р	303	3	$26,\!50,\!50$	1.46	2 (7%)	18,82,82	2.09	6 (33%)
30	DGA	Z	201	-	21,21,43	0.27	0	23,23,45	0.23	0
17	MQ9	0	602	-	24,24,59	0.44	0	30,33,75	0.61	1 (3%)
32	IX7	R	406	-	74,74,97	0.30	0	97,99,123	0.83	6 (6%)
18	3PE	D	607	-	30,30,50	0.38	0	33,35,55	0.33	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
19	HEM	Ο	604	2	$27,\!50,\!50$	1.26	4 (14%)	17,82,82	1.51	3 (17%)
18	3PE	А	505	-	37,37,50	0.39	0	40,42,55	0.72	1 (2%)
19	HEM	В	602	2	$27,\!50,\!50$	1.27	4 (14%)	17,82,82	1.44	5 (29%)
20	CDL	0	606	-	44,44,99	0.42	0	50,56,111	0.43	0
14	FES	А	501	1	$0,\!4,\!4$	-	-	-		
18	3PE	E	405	-	$30,\!30,\!50$	0.38	0	$33,\!35,\!55$	0.35	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
30	DGA	Н	201	-	-	1/17/17/45	-
20	CDL	F	302	-	-	19/67/67/110	-
25	HAS	Q	601	4	-	7/35/122/122	-
20	CDL	Р	301	-	-	16/75/75/110	-
20	CDL	D	605	-	-	27/87/87/110	-
31	PLM	U	202	8	-	0/8/9/15	-
20	CDL	V	201	-	-	19/67/67/110	-
19	HEM	В	603	2	-	0/6/54/54	-
20	CDL	Q	605	-	-	27/87/87/110	-
31	PLM	М	202	13	-	0/1/2/15	-
15	IZL	А	502	-	-	34/73/197/208	0/6/6/6
18	3PE	R	405	-	-	1/34/34/54	-
14	FES	N	503	1	-	-	0/1/1/1
15	IZL	Ν	504	-	-	34/73/197/208	0/6/6/6
23	HEC	С	302	3	-	0/6/54/54	-
20	CDL	D	606	-	-	21/73/73/110	-
18	3PE	W	201	-	-	8/50/50/54	-
18	3PE	Q	607	-	-	5/34/34/54	-
18	3PE	J	201	-	-	7/50/50/54	-
23	HEC	С	303	3	-	0/6/54/54	-
18	3PE	S	301	-	-	16/35/35/54	-
23	HEC	Р	302	3	-	0/6/54/54	-
16	9YF	А	503	-	-	6/31/55/78	0/1/1/1
20	CDL	Q	606	-	-	21/73/73/110	-
32	IX7	Ι	202	-	-	29/58/122/146	0/3/3/3


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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	MQ9	В	601	-	-	3/11/31/73	0/2/2/2
24	3PH	Т	201	-	-	8/37/37/49	-
25	HAS	D	601	4	-	7/35/122/122	-
25	HAS	D	602	4	-	9/35/122/122	-
16	9YF	Ν	505	-	-	6/31/55/78	0/1/1/1
30	DGA	R	404	-	-	0/20/20/45	-
25	HAS	Q	602	4	-	9/35/122/122	-
31	PLM	Ζ	202	13	-	0/1/2/15	-
19	HEM	0	603	2	-	1/6/54/54	-
20	CDL	С	301	-	-	16/75/75/110	-
21	LYC	В	606	-	-	3/43/43/43	-
20	CDL	Ι	201	-	-	19/67/67/110	-
20	CDL	В	605	-	-	7/54/54/110	-
16	9YF	В	607	-	-	5/29/53/78	0/1/1/1
31	PLM	Н	202	8	-	0/8/9/15	-
17	MQ9	0	605	-	-	0/11/31/73	0/2/2/2
21	LYC	0	607	-	-	3/43/43/43	-
16	9YF	U	203	-	-	5/29/53/78	0/1/1/1
14	FES	А	501	1	-	-	0/1/1/1
30	DGA	М	201	-	-	3/22/22/45	-
30	DGA	U	201	-	-	1/17/17/45	-
22	LMT	Ο	601	-	-	3/18/58/61	0/2/2/2
24	3PH	С	304	-	-	8/37/37/49	-
20	CDL	G	201	-	-	19/72/72/110	-
18	3PE	Ν	502	-	-	25/41/41/54	-
17	MQ9	В	604	-	-	0/11/31/73	0/2/2/2
20	CDL	S	303	-	-	19/72/72/110	-
30	DGA	Е	404	-	-	0/20/20/45	-
17	MQ9	Ν	501	-	-	6/15/35/73	0/2/2/2
17	MQ9	А	504	-	-	6/15/35/73	0/2/2/2
20	CDL	S	302	-	-	19/67/67/110	-
18	3PE	F	301	-	-	16/35/35/54	-
23	HEC	Р	303	3	-	0/6/54/54	-
30	DGA	Z	201	-	-	3/22/22/45	-
17	MQ9	О	602	-	-	3/11/31/73	0/2/2/2
32	IX7	R	406	-	-	29/58/122/146	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	3PE	D	607	-	-	5/34/34/54	-
19	HEM	0	604	2	-	0/6/54/54	-
18	3PE	А	505	-	-	25/41/41/54	-
19	HEM	В	602	2	-	1/6/54/54	-
20	CDL	Ο	606	-	-	7/54/54/110	-
22	LMT	В	608	-	-	3/18/58/61	0/2/2/2
18	3PE	E	405	_	-	1/34/34/54	-

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The worst 5 of 108 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	D	602	HAS	CHD-C4A	-12.38	1.38	1.51
25	Q	602	HAS	CHD-C4A	-12.36	1.38	1.51
25	Q	601	HAS	CHD-C4A	-12.30	1.38	1.51
25	D	601	HAS	CHD-C4A	-12.20	1.38	1.51
25	D	602	HAS	CHD-C4C	-12.05	1.38	1.51

The worst 5 of 186 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
25	D	601	HAS	CHB-C1B-NB	12.54	126.54	110.94
25	Q	601	HAS	CHB-C1B-NB	12.54	126.53	110.94
25	D	602	HAS	CAA-C2A-C1A	-12.20	118.72	127.30
25	Q	602	HAS	CAA-C2A-C1A	-12.20	118.73	127.30
25	Q	602	HAS	CHB-C1B-NB	11.92	125.76	110.94

There are no chirality outliers.

5 of 601 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	А	502	IZL	O34-C45-C46-O32
15	А	502	IZL	C61-C60-O34-C45
15	А	502	IZL	O35-C60-O34-C45
15	А	502	IZL	C44-O31-P-O28
15	N	504	IZL	O34-C45-C46-O32

There are no ring outliers.

41 monomers are involved in 99 short contacts:



Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	Q	601	HAS	1	0
20	Р	301	CDL	2	0
19	В	603	HEM	1	0
14	Ν	503	FES	1	0
15	А	502	IZL	4	0
15	Ν	504	IZL	3	0
23	С	302	HEC	5	0
18	W	201	3PE	1	0
18	Q	607	3PE	1	0
18	J	201	3PE	1	0
23	С	303	HEC	2	0
18	S	301	3PE	1	0
23	Р	302	HEC	5	0
20	Q	606	CDL	1	0
32	Ι	202	IX7	2	0
25	D	601	HAS	1	0
25	D	602	HAS	4	0
30	R	404	DGA	1	0
25	Q	602	HAS	3	0
20	С	301	CDL	2	0
21	В	606	LYC	2	0
20	В	605	CDL	1	0
22	В	608	LMT	3	0
21	0	607	LYC	2	0
22	0	601	LMT	3	0
20	G	201	CDL	3	0
18	Ν	502	3PE	9	0
20	S	303	CDL	2	0
30	Е	404	DGA	1	0
17	Ν	501	MQ9	6	0
17	А	504	MQ9	8	0
18	F	301	3PE	1	0
23	Р	303	HEC	2	0
30	Ζ	201	DGA	1	0
17	0	602	MQ9	2	0
32	R	406	IX7	1	0
18	D	607	3PE	1	0
19	0	604	HEM	1	0
18	А	505	3PE	8	0
20	0	606	CDL	1	0
14	А	501	FES	1	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.






















































































































































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 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-13977. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

6.1.1 Primary map



The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map



X Index: 107



Y Index: 115



Z Index: 75

The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 136



Y Index: 123



Z Index: 79

The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.09. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.



6.5 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.



7 Map analysis (i)

This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.



7.2 Volume estimate (i)



The volume at the recommended contour level is 359 nm^3 ; this corresponds to an approximate mass of 325 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.



8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.



9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-13977 and PDB model 7QHO. Per-residue inclusion information can be found in section 3 on page 20.

9.1 Map-model overlay (i)



The images above show the 3D surface view of the map at the recommended contour level 0.09 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.



9.2 Atom inclusion (i)



At the recommended contour level, 90% of all backbone atoms, 84% of all non-hydrogen atoms, are inside the map.

