

### wwPDB EM Validation Summary Report (i)

Dec 7, 2022 – 10:39 AM JST

PDB ID	:	5XTH
EMDB ID	:	EMD-6775
Title	:	Cryo-EM structure of human respiratory supercomplex I1III2IV1
Authors	:	Gu, J.; Wu, M.; Yang, M.
Deposited on	:	2017-06-19
Resolution	:	3.90  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 types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

EMDB validation analysis	:	0.0.1. dev 43
Mogul	:	1.8.5 (274361), 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)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

#### 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 3.90 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.



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	431	98%	·
2	В	176	99%	•
3	С	156	97%	•
4	Е	113	97%	•
5	F	83	100%	
6	G	85	46%	•
6	Х	85	95%	5%
7	Н	112	96%	•
8	Ι	110	5%           81%	14%



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Chain Length Quality of chain Mol 9 J 337 97% • 12% 10 Κ 33 91% 9% 9% 11  $\mathbf{L}$ 11897% • 12М 687 96% • i 13Ν 14395% 5% 14Ο 21297% • Р 1520895% 5% 6% Q 430• 1698%  $\mathbf{S}$ 701797% • Т 1895• 96% U 1983 99% • V 20140. 98% i 21W 138• 96% 22Υ 5975% 24% Ζ 80 23100% 24138 $\mathbf{a}$ 96% • 25124b 90% 10% • 26153 $\mathbf{c}$ 5% 95% <u>.</u> 27 $\mathbf{d}$ 1715%• 95% 6% • 2897е 97% 9% • f 294798% 30 119g 95% 5% i 10431 h 94% 6% i . 32i 34798% 5% 33 j 11597% .



Mol	Chain	Length	Quality of chain	
24	,	0 -	6%	
34	k	97	93%	6% •
35	1	603		50/
- 55	1	005	94%	5%
36	m	174	94%	6%
37	n	56	96%	•
		100	•	
38	0	128	97%	•
39	n	172	0.9%	
	Р	112	9070	• 
40	r	459	98%	•
			·	
41	S	318	97%	•
49		160		
42	u	109	97%	•
43	v	122	86%	5% 9%
				576 576
44	W	320	97%	•
			60%	
45	X	514	92%	8%
46	V	227	/ 6%	1.00/
40	у	221	46%	10%
47	Z	261	90%	10%
			92%	
48	0	144	94%	6%
10	1	100	83%	
49	1	109	94%	6%
50	2	98	0.10/	70/
		50	70%	/ 70 •
51	3	84	74%	25%
			57%	
52	4	75	87%	13%
50	F	79	97%	
- 33	G	13	93%	7%
54	6	56	88%	9%
			96%	
55	7	49	96%	•
			79%	
56	8	47	96%	•
	0	40	91%	
57	9	43	93%	7%
58	ΔΔ	81	00%	100/
00	1111		20.00	10.20



Mol	Chain	Length	Quality of chain	
50	AN	91	20%	
- 38	AN	01	99% 75%	•
59	AB	57	93%	7%
50		57	86%	120/
- 59	AU		20%	12%
60	AC	196	97%	•
60	AP	196	98%	
61	AD	62	16%	
			19%	
61	AQ	62	100%	
62	AE	74	96%	
62	AR	74	18%	
			10%	
63	AF	106	87%	13%
63	AS	106	100%	
64	AG	51	16%	
64	AT	51	96%	
65	AH	241	99%	•
65	AU	241	99%	•
66	AJ	378	98%	·
66	AV	378	96%	
67	AK	419	98%	
67	AW	<u>4</u> 19	16%	
	1100	713	96%	•
68	AL	446	99%	·
68	AY	446	97%	•

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
79	HEA	Х	603	Х	-	-	-
79	HEA	Х	604	Х	-	-	-



## 2 Entry composition (i)

There are 82 unique types of molecules in this entry. The entry contains 115642 atoms, of which 0 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 NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues		At	AltConf	Trace			
1	А	431	Total 3322	C 2096	N 594	0 612	S 20	0	0

• Molecule 2 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

Mol	Chain	Residues		A	toms		AltConf	Trace	
2	В	176	Total 1420	C 893	N 243	0 271	S 13	0	0

• Molecule 3 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

Mol	Chain	Residues		A	toms	AltConf	Trace		
3	С	156	Total 1249	C 794	N 227	0 214	S 14	0	0

• Molecule 4 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

Mol	Chain	Residues		At	oms	AltConf	Trace		
4	Е	113	Total 968	C 623	N 178	O 162	${ m S}{ m 5}$	0	0

• Molecule 5 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

Mol	Chain	Residues		At	oms		AltConf	Trace	
5	F	83	Total 670	C 422	N 124	0 122	$\begin{array}{c} \mathrm{S} \\ \mathrm{2} \end{array}$	0	0

• Molecule 6 is a protein called Acyl carrier protein, mitochondrial.



Mol	Chain	Residues		At	oms		AltConf	Trace	
6	6 G	85	Total	С	Ν	0	$\mathbf{S}$	0	0
	G	85	672	434	99	134	5		0
6	6 X	85	Total	С	Ν	0	$\mathbf{S}$	0	0
0			686	442	101	138	5	0	0

• Molecule 7 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5.

Mol	Chain	Residues		At	oms	AltConf	Trace		
7	Н	112	Total 922	$\begin{array}{c} \mathrm{C} \\ 593 \end{array}$	N 157	O 169	${ m S} { m 3}$	0	0

• Molecule 8 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues		At	oms			AltConf	Trace
8	Ι	95	Total 769	C 483	N 146	0 138	${ m S} { m 2}$	0	0

• Molecule 9 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial.

Mol	Chain	Residues		Ate	AltConf	Trace			
9	J	337	Total 2712	C 1759	N 482	0 463	S 8	0	0

• Molecule 10 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

Mol	Chain	Residues		Atc	$\mathbf{ms}$	AltConf	Trace		
10	K	33	Total	С	Ν	Ο	$\mathbf{S}$	0	0
10	17	55	274	173	47	53	1	0	0

• Molecule 11 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues		At	oms	AltConf	Trace		
11	L	118	Total 964	C 608	N 173	0 179	${S \atop 4}$	0	0

• Molecule 12 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.



	Siducs		$\mathbf{A}$	AltConf	Trace			
12 M	687	Total 5274	C 3310	N 017	O 1009	S 38	0	0

• Molecule 13 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues		At	AltConf	Trace			
13	Ν	143	Total 1195	C 770	N 210	0 212	$\frac{S}{3}$	0	0

• Molecule 14 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

Mol	Chain	Residues		At	AltConf	Trace			
14	О	212	Total 1643	C 1047	N 276	0 310	S 10	0	0

• Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial.

Mol	Chain	Residues		Ate	AltConf	Trace			
15	Р	208	Total 1730	C 1117	N 297	0 313	${ m S} { m 3}$	0	0

• Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

Mol	Chain	Residues		At	AltConf	Trace			
16	Q	430	Total 3460	C 2214	N 599	0 624	S 23	0	0

• Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1.

Mol	Chain	Residues		Ate	oms			AltConf	Trace
17	S	70	Total 568	C 367	N 101	O 96	${S \atop 4}$	0	0

• Molecule 18 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.



Mol	Chain	Residues		At	oms			AltConf	Trace
18	Т	95	Total 742	$\begin{array}{c} \mathrm{C} \\ 459 \end{array}$	N 138	0 142	${ m S} { m 3}$	0	0

• Molecule 19 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

Mol	Chain	Residues		At	oms	AltConf	Trace		
19	U	83	Total 647	C 427	N 105	0 113	${ m S} { m 2}$	0	0

• Molecule 20 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

Mol	Chain	Residues		At	oms	AltConf	Trace		
20	V	140	Total 1038	C 668	N 178	O 187	${ m S}{ m 5}$	0	0

• Molecule 21 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

Mol	Chain	Residues		At	oms		AltConf	Trace	
21	W	138	Total 1135	C 727	N 202	O 200	S 6	0	0

• Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial.

Mol	Chain	Residues		Ato	$\mathbf{ms}$	AltConf	Trace		
22	v	50	Total	С	Ν	0	S	0	0
	1		533	354	87	91	1	0	0

• Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

Mol	Chain	Residues		At	$\mathbf{oms}$			AltConf	Trace
23	Ζ	80	Total 648	C 426	N 110	0 110	${ m S} { m 2}$	0	0

• Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.



Mol	Chain	Residues		At	oms	AltConf	Trace		
24	a	138	Total 1174	С 771	N 199	O 202	${ m S} { m 2}$	0	0

• Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

Mol	Chain	Residues		At	oms	AltConf	Trace		
25	h	194	Total	С	Ν	0	$\mathbf{S}$	0	0
2.0	U	124	1059	697	181	176	5	0	0

• Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues		At	toms			AltConf	Trace
26	с	153	Total 1236	C 795	N 208	0 222	S 11	0	0

• Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

Mol	Chain	Residues		A	toms	AltConf	Trace		
27	d	171	Total 1418	C 885	N 262	O 259	S 12	0	0

• Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

Mol	Chain	Residues		At	oms	AltConf	Trace		
28	е	97	Total 810	C 522	N 132	0 152	${S \over 4}$	0	0

• Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

Mol	Chain	Residues		Aton	ns	AltConf	Trace	
29	f	47	Total 405	C 269	N 69	O 67	0	0

• Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues		At	oms	AltConf	Trace		
30	g	119	Total 1004	C 658	N 173	0 169	$\begin{array}{c} \mathrm{S} \\ 4 \end{array}$	0	0



• Molecule 31 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

Mol	Chain	Residues		At	oms			AltConf	Trace
31	h	104	Total 863	C 546	N 161	O 150	S 6	0	0

• Molecule 32 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues		At	oms			AltConf	Trace
32	i	347	Total 2735	C 1819	N 421	0 470	${ m S}\ 25$	0	0

• Molecule 33 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	j	115	Total 919	C 626	N 132	0 152	${ m S} 9$	0	0

• Molecule 34 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues		A	AltConf	Trace			
34	k	97	Total 740	C 487	N 113	0 127	S 13	0	0

• Molecule 35 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues		At	oms			AltConf	Trace
35	1	603	Total 4717	C 3119	N 742	0 823	S 33	0	0

• Molecule 36 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues		$\mathbf{A}^{\dagger}$	toms			AltConf	Trace
36	m	174	Total 1313	C 879	N 194	O 229	S 11	0	0

• Molecule 37 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1.

Mol	Chain	Residues		Ato	$\mathbf{ms}$	AltConf	Trace		
37	n	56	Total 473	C 305	N 85	O 80	${ m S} { m 3}$	0	0

• Molecule 38 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit



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Mol	Chain	Residues		At	$\mathbf{oms}$	AltConf	Trace		
38	О	128	Total 1066	C 685	N 192	0 187	${ m S} { m 2}$	0	0

• Molecule 39 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

Mol	Chain	Residues		At	oms			AltConf	Trace
39	р	172	Total 1495	C 961	N 265	O 261	S 8	0	0

• Molecule 40 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues		At		AltConf	Trace		
40	r	459	Total 3629	C 2411	N 569	O 619	S 30	0	0

• Molecule 41 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues		At		AltConf	Trace		
41	S	318	Total 2509	C 1678	N 380	0 435	S 16	0	0

• Molecule 42 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues		At	oms			AltConf	Trace
42	u	169	Total 1394	C 886	N 247	0 252	S 9	0	0

• Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues		At	$\mathbf{oms}$			AltConf	Trace
43	v	111	Total 921	C 569	N 187	0 156	S 9	0	0

• Molecule 44 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.



Mol	Chain	Residues		At	oms			AltConf	Trace
44	W	320	Total 2474	C 1573	N 429	O 464	S 8	0	0

• Molecule 45 is a protein called Cytochrome c oxidase subunit 1.

Mol	Chain	Residues		At	AltConf	Trace			
45	x	514	Total 4025	C 2690	N 623	O 677	${ m S}\ 35$	0	0

• Molecule 46 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues		At	AltConf	Trace			
46	У	227	Total 1822	C 1184	N 281	O 339	S 18	0	0

• Molecule 47 is a protein called Cytochrome c oxidase subunit 3.

Mol	Chain	Residues		At	oms			AltConf	Trace
47	Z	261	Total 2124	C 1420	N 338	O 353	S 13	0	0

• Molecule 48 is a protein called Cytochrome c oxidase subunit 4 isoform 1, mitochondrial.

Mol	Chain	Residues		At	oms			AltConf	Trace
48	0	144	Total 1195	C 777	N 196	0 218	$\begin{array}{c} \mathrm{S} \\ 4 \end{array}$	0	0

• Molecule 49 is a protein called Cytochrome c oxidase subunit 5A, mitochondrial.

Mol	Chain	Residues		At	oms			AltConf	Trace
49	1	109	Total 878	C 558	N 150	0 168	${S \over 2}$	0	0

• Molecule 50 is a protein called Cytochrome c oxidase subunit 5B, mitochondrial.

Mol	Chain	Residues		At	oms			AltConf	Trace
50	2	98	Total 748	C 464	N 134	0 145	${f S}{5}$	0	0

• Molecule 51 is a protein called Cytochrome c oxidase subunit 6A2, mitochondrial.



Mol	Chain	Residues		At	oms			AltConf	Trace
51	3	84	Total 672	C 431	N 129	0 111	S 1	0	0

• Molecule 52 is a protein called Cytochrome c oxidase subunit 6B1.

Mol	Chain	Residues		At	oms	AltConf	Trace		
52	4	75	Total 628	C 395	N 114	0 114	${ m S}{ m 5}$	0	0

• Molecule 53 is a protein called Cytochrome c oxidase subunit 6C.

Mol	Chain	Residues		Ate	oms	AltConf	Trace		
53	5	73	Total 598	C 388	N 107	O 99	${S \atop 4}$	0	0

• Molecule 54 is a protein called Cytochrome c oxidase subunit 7A1, mitochondrial.

Mol	Chain	Residues		Ato	$\mathbf{ms}$			AltConf	Trace
54	6	56	Total	C 285	N 73	0 80	S 3	0	0
			441	200	15	80	3		

• Molecule 55 is a protein called Cytochrome c oxidase subunit 7B, mitochondrial.

Mol	Chain	Residues		Atc	$\mathbf{ms}$	AltConf	Trace		
55	7	49	Total 384	C 250	N 65	O 67	$\begin{array}{c} \mathrm{S} \\ \mathrm{2} \end{array}$	0	0

• Molecule 56 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

Mol	Chain	Residues		Ato	$\mathbf{ms}$	AltConf	Trace		
56	8	47	Total	С	Ν	0	$\mathbf{S}$	0	0
	0	11	386	257	65	62	2		0

• Molecule 57 is a protein called Cytochrome c oxidase subunit 8B, mitochondrial.

Mol	Chain	Residues		Aton	ıs	AltConf	Trace	
57	9	43	Total 335	C 223	N 53	O 59	0	0

• Molecule 58 is a protein called Cytochrome b-c1 complex subunit 8.



Mol	Chain	Residues		At	oms		AltConf	Trace	
58	ΔΔ	81	Total	С	Ν	0	S	0	0
- 50	50 AA	01	694	450	126	117	1	0	0
58	ΔN	81	Total	С	Ν	0	S	0	0
50	AN	01	687	444	126	116	1	0	0

• Molecule 59 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues		Atc	$\mathbf{ms}$		AltConf	Trace	
50	٨B	57	Total	С	Ν	Ο	S	0	0
59 AD	AD	51	413	261	75	76	1	0	0
50	10	57	Total	С	Ν	Ο	S	0	0
- 39	AU	57	409	259	74	75	1	0	0

• Molecule 60 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues		At	oms	AltConf	Trace		
60	AC	196	Total 1521	C 960	N 264	O 290	${f S}{7}$	0	0
60	AP	196	Total 1521	C 960	N 264	O 290	${ m S} 7$	0	0

• Molecule 61 is a protein called Cytochrome b-c1 complex subunit 9.

Mol	Chain	Residues		Ato	$\mathbf{ms}$		AltConf	Trace	
61		62	Total	С	Ν	Ο	$\mathbf{S}$	0	0
01 AD	AD	02	509	332	87	89	1	0	0
61	10	62	Total	С	Ν	Ο	S	0	0
	лQ	02	509	332	87	89	1	0	U

• Molecule 62 is a protein called Cytochrome b-c1 complex subunit 6, mitochondrial.

Mol	Chain	Residues		At	oms		AltConf	Trace	
62	٨F	74	Total	С	Ν	0	S	0	0
02	02 AL	14	580	351	108	116	5	0	0
62	٨D	74	Total	С	Ν	0	S	0	0
02	AN	14	580	351	108	116	5		

• Molecule 63 is a protein called Cytochrome b-c1 complex subunit 7.

Mol	Chain	Residues		At	oms	AltConf	Trace		
63	AF	106	Total 921	C 589	N 162	0 168	$\begin{array}{c} \mathrm{S} \\ \mathrm{2} \end{array}$	0	0



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Mol	Chain	Residues		At	$\mathbf{oms}$	AltConf	Trace		
63	AS	106	Total 921	C 589	N 162	0 168	S 2	0	0

• Molecule 64 is a protein called Cytochrome b-c1 complex subunit 10.

Mol	Chain	Residues		Aton	ıs		AltConf	Trace
64	AG	51	Total 425	C 287	N 72	O 66	0	0
64	AT	51	Total 425	C 287	N 72	O 66	0	0

• Molecule 65 is a protein called Cytochrome c1, heme protein, mitochondrial.

Mol	Chain	Residues		At		AltConf	Trace		
65	۸Ц	241	Total	С	Ν	0	S	0	0
05 AII	241	1924	1231	329	349	15	0		
65	ATT	241	Total	С	Ν	0	S	0	0
05	AU	241	1924	1231	329	349	15	0	0

• Molecule 66 is a protein called Cytochrome b.

Mol	Chain	Residues		At	oms			AltConf	Trace
66	ΔΤ	378	Total	С	Ν	Ο	$\mathbf{S}$	0	0
00	ЛJ	510	3009	2017	467	509	16	0	0
66	AV	278	Total	С	Ν	Ο	$\mathbf{S}$	0	0
00	AV	510	3009	2017	467	509	16	0	0

• Molecule 67 is a protein called Cytochrome b-c1 complex subunit 2, mitochondrial.

Mol	Chain	Residues		At	oms			AltConf	Trace
67	AK	419	Total	С	Ν	0	$\mathbf{S}$	0	0
01	1111	415	3159	1986	553	610	10	0	0
67	AW	410	Total	С	Ν	Ο	$\mathbf{S}$	0	0
07	Ανν	419	3162	1989	553	610	10	0	0

• Molecule 68 is a protein called Cytochrome b-c1 complex subunit 1, mitochondrial.

Mol	Chain	Residues		At	oms			AltConf	Trace
68	ΔŢ	446	Total	С	Ν	0	$\mathbf{S}$	0	0
00	ΛL	440	3453	2169	603	661	20	0	0
68	۸V	446	Total	С	Ν	0	$\mathbf{S}$	0	0
00		440	3453	2169	603	661	20	0	0



• Molecule 69 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula:  $Fe_4S_4$ ).



Mol	Chain	Residues	Atoms	AltConf
69	А	1	Total Fe S 8 4 4	0
69	В	1	Total Fe S 16 8 8	0
69	В	1	TotalFeS1688	0
69	С	1	TotalFeS844	0
69	М	1	TotalFeS1688	0
69	М	1	TotalFeS1688	0

• Molecule 70 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula:  $C_{17}H_{21}N_4O_9P$ ).





Mol	Chain	Residues		Atoms					
70	А	1	Total	С	Ν	0	Р	0	
		_	31	17	4	9	1	Ŭ	

• Molecule 71 is (9R,11S)-9-({[(1S)-1-HYDROXYHEXADECYL]OXY}METHYL)-2,2-DIME THYL-5,7,10-TRIOXA-2LAMBDA 5 -AZA-6LAMBDA 5 -PHOSPHAOCTACOSANE-6,6, 11-TRIOL (three-letter code: PLX) (formula: C<sub>42</sub>H<sub>89</sub>NO<sub>8</sub>P).



Mol	Chain	Residues	Atoms	AltConf
71	В	1	Total C N O P	0
(1	D	1	52 $42$ $1$ $8$ $1$	0
71	II	1	Total C N O P	0
(1	U	1	52  42  1  8  1	0



Mol	Chain	Residues	_	Ato	$\mathbf{ms}$			AltConf
71	V	1	Total	С	Ν	Ο	Р	0
11	v	1	52	42	1	8	1	0
71	h	1	Total	С	Ν	Ο	Р	0
11	D	1	52	42	1	8	1	0
71	ď	1	Total	С	Ν	Ο	Р	0
11	8	1	156	126	3	24	3	0
71	ď	1	Total	С	Ν	Ο	Р	0
11	g	1	156	126	3	24	3	0
71	ď	1	Total	С	Ν	Ο	Р	0
	5	I	156	126	3	24	3	0
71	r	1	Total	С	Ν	Ο	Р	0
	1	1	104	84	2	16	2	0
71	r	1	Total	С	Ν	Ο	Р	0
	1	Ŧ	104	84	2	16	2	0
71	AT.	1	Total	С	Ν	Ο	Р	0
		Ŧ	52	42	1	8	1	0
71	AQ	1	Total	С	Ν	Ο	Р	0
	11%	1	52	42	1	8	1	
71	АТ	1	Total	С	Ν	Ο	Р	0
11	111	1	52	42	1	8	1	

• Molecule 72 is S-[2-({N-[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alan yl}amino)ethyl] dodecanethioate (three-letter code: 8Q1) (formula:  $C_{23}H_{45}N_2O_8PS$ ).



Mol	Chain	Residues		Atoms						
79	Б	1	Total	С	Ν	Ο	Р	$\mathbf{S}$	0	
12	E	1	35	23	2	8	1	1	0	



Mol	Chain	Residues		Atoms						
79	n	1	Total	С	Ν	Ο	Р	S	0	
12	р	1	35	23	2	8	1	1	0	

• Molecule 73 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula:  $C_{21}H_{30}N_7O_{17}P_3$ ).



Mol	Chain	Residues		Atoms					
73	т	1	Total	С	Ν	Ο	Р	0	
10	J	1	48	21	7	17	3	U	

• Molecule 74 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula:  $Fe_2S_2$ ).





Mol	Chain	Residues	Atoms	AltConf
74	М	1	Total Fe S 4 2 2	0
74	О	1	TotalFeS422	0
74	AC	1	TotalFeS422	0
74	AP	1	TotalFeS422	0

 $\bullet\,$  Molecule 75 is CARDIOLIPIN (three-letter code: CDL) (formula:  $C_{81}H_{156}O_{17}P_2).$ 



Mol	Chain	Residues	I	4ton	ns		AltConf
75	V	1	Total	С	0	Р	0
10	v	1	63	44	17	2	0
75	i	1	Total	С	Ο	Р	0
10	1	1	64	45	17	2	0
75	1	1	Total	С	Ο	Р	0
10	1	1	128	90	34	4	0
75	1	1	Total	С	Ο	Р	0
10	1	1	128	90	34	4	0
75	n	1	Total	С	0	Р	0
10	11	1	64	45	17	2	0
75	٨٨	1	Total	С	0	Р	0
10	AA	1	64	45	17	2	0
75		1	Total	С	Ο	Р	0
10	AG		64	45	17	2	
75	۸Ц	1	Total	С	Ο	Р	0
10	AII	1	64	45	17	2	



Mol	Chain	Residues	Atoms	AltConf
75	ΔΤ	1	Total C O P	0
10	AJ	1	128  90  34  4	0
75	ΔΤ	1	Total C O P	0
10	AJ	1	128  90  34  4	0
75	ΔT	1	Total C O P	0
10	AL	1	64  45  17  2	0
75	ΛN	1	Total C O P	0
10	AN	1	64  45  17  2	0
75	ATT	1	Total C O P	0
10	AU	1	64  45  17  2	0
75	۸V	1	Total C O P	0
10	AI		64  45  17  2	

Continued from previous page...

• Molecule 76 is 1,2-Dioleoyl-sn-glycero-3-phosphoethanolamine (three-letter code: PEE) (formula:  $C_{41}H_{78}NO_8P$ ).



Mol	Chain	Residues	Atoms	AltConf
76	V	1	Total C N O P	0
10	v	T	51 $41$ $1$ $8$ $1$	0
76	W	1	Total C N O P	0
10	vv	L	51 $41$ $1$ $8$ $1$	0
76	1	1	Total C N O P	0
10	1	1	100  80  2  16  2	0
76	1	1	Total C N O P	0
10	1	L	100  80  2  16  2	0
76	۸Ц	1	Total C N O P	0
70	АП	L	49  39  1  8  1	U



Mol	Chain	Residues	Atoms	AltConf
76	ΔŢ	1	Total C N O P	Ο
10	ЛJ	I	49  39  1  8  1	0
76	ΔT	1	Total C N O P	0
10		T	49  39  1  8  1	0
76	ΔIJ	1	Total C N O P	0
10	ло	T	41  31  1  8  1	0
76	ΔV	1	Total C N O P	0
10	ΛV	T	49  39  1  8  1	0
76	ΔV	1	Total C N O P	0
70	AI	L	49  39  1  8  1	0

• Molecule 77 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms	AltConf
77	х	1	Total Cu 1 1	0
77	У	2	Total Cu 2 2	0

• Molecule 78 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
78	х	1	Total Mg 1 1	0

• Molecule 79 is HEME-A (three-letter code: HEA) (formula:  $C_{49}H_{56}FeN_4O_6$ ).





Mol	Chain	Residues			AltConf			
70	v	1	Total	С	Fe	Ν	0	0
19	л	T	120	98	2	8	12	0
79	37	1	Total	С	Fe	Ν	0	0
	X	1	120	98	2	8	12	0

• Molecule 80 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
80	2	1	Total Z 1 1	n 0

• Molecule 81 is HEME C (three-letter code: HEC) (formula:  $C_{34}H_{34}FeN_4O_4$ ).



Mol	Chain	Residues		AltConf				
81	AH	1	Total 43	С 34	Fe 1	N 4	0 4	0
81	AU	1	Total 43	С 34	Fe 1	N 4	0 4	0

• Molecule 82 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).





Mol	Chain	Residues			AltConf			
82	ΔΤ	1	Total	С	Fe	Ν	Ο	0
02	AJ	1	86	68	2	8	8	0
89	ΛΤ	1	Total	С	Fe	Ν	Ο	0
02	ЛJ	T	86	68	2	8	8	0
89	ΔV	1	Total	С	Fe	Ν	Ο	0
02	Av	1	86	68	2	8	8	0
89	ΔV	1	Total	С	Fe	Ν	Ο	0
02	AV	1	86	68	2	8	8	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: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



• Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial



• Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial













• Molecule 12: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

Chain M:								96% •																				
N3O	D37	E44	T47	1130	T174	<mark>q178</mark>	I210	<mark>\$250</mark>	D255	1281	E310	E320	A322	D347	A350	E369	G376 A377	E396	D426	P435	G446	0482 R483	N484	G505		8 CCH	F546 L547 L548	G553
K562	V575	L653	D658	A662	N663	0667 0	N676 Q677	Dego	L689	T715	E716																	
•	Mo	leci	ule	13	8: I	١A	DH	I d	ehy	dro	oge	nas	e [ı	ıbio	quii	non	le] 1	alp	oha	su	bc	om	ple	x s	ubi	uni	it 12	

Chain N: 95% 5%

• Molecule 14: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial



• Molecule 15: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial



• Molecule 16: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial



• Molecule 17: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

Chain S: 97% ·



#### M1 K36 Y60 D70

• Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

Chain T:	96%	•
C22 V30 N31 P34 C44 C44 C44 C53 C53 C52 C52 C52 C52 C52 C52 C52 C52 C52 C52		

• Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

Chain U:	99%	·
A2 Q71 L84		

• Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

Chain V:	98%	
A2 R7 L34 E51 V135		

• Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

Chain W:	96%	•
K7 M10 P11 P11 C10 C20 C20 C33 C33 C33 C33 C33 C33 C33 C33 C33 C3	<b>11</b> <b>14</b>	

 $\bullet$  Molecule 22: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial

Chain Y:	75%	24% •
H39 P42 P43 Y44 T51 F73 H75 H75	E78 E79 1810 1811 1832 1835 1835 1835 1835 1835 1932 197	

• Molecule 23: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

Chain Z: 100%

There are no outlier residues recorded for this chain.

• Molecule 24: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial



Chain a:



• Molecule 25: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

96%

Cha	in ł	):													g	90%	6			10%	•
G3 R21	P36	038 038	G41	N53	K101	F105	T109	I110	L111 E112	-	E115	V116	I117	P118	F123	P124	C717	Q126			

 $\bullet$  Molecule 26: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



• Molecule 27: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

C	Ch	ıa	ir	1 (	d:												95%	5%•
M1	P2	-	R54	Y55	Y56 ve7	2	R60	Q61	2	<b>q113</b>	N114	Y115	Q116	A167	A1 70	T171		

 $\bullet$  Molecule 28: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



• Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial



 $\bullet$  Molecule 30: NADH dehydrogenase [ubiquinone] 1 subunit C2

Chain g: 95% 5%





• Molecule 31: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



• Molecule 32: NADH-ubiquinone oxidoreductase chain 2

С	hai	n i						98%	·
M1	K47	T87	N91 Q92	N150	ocuti		L347		

• Molecule 33: NADH-ubiquinone oxidoreductase chain 3

Chain j:	5%					97%	·
M1 N2 L13	P26 Q26 L27	S34	E68	L98	E115		

• Molecule 34: NADH-ubiquinone oxidoreductase chain 4L

Chain k:	6%	•				93%	6%	•
M1 P2 L3 I8	H52	N83	L87	N92	L95			

• Molecule 35: NADH-ubiquinone oxidoreductase chain 5



• Molecule 36: NADH-ubiquinone oxidoreductase chain 6







• Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1





• Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

Chain p:		98%	
	•		



N38 A20 G20 G20 A2:

 $\bullet$  Molecule 40: NADH-ubiquinone oxidore<br/>ductase chain 4

Chain r:	98% •									
M1 145 152 145 145 145 1250 1250 1250 1250 1251 1260 1251 1260 1251 1260 1261 1421 1421 1421										
$\bullet$ Molecule 41: NADH-ubiquinone oxidoreductase chain 1										
Chain s: 97% ·										
•• • •										

• Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain u: 97% .

• Molecule 43: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7





• Molecule 44: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial







#### 

• Molecule 47: Cytochrome c oxidase subunit 3



# S261

• Molecule 48: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial



• Molecule 49: Cytochrome c oxidase subunit 5A, mitochondrial







• Molecule 54: Cytochrome c oxidase subunit 7A1, mitochondrial








• Molecule 60: Cytochrome b-c1 complex subunit Rieske, mitochondrial

~ <b>1</b> .		_		20	%																									_							
Chain	AC	:											9	)7%	'														•	-							
	<b>1</b> 2	<mark>6 4</mark>	22	56	80	1	36	- 80	5	om	1	2	22	90		00	1	92	33	94		)4 -	م م	-2	_	0	21	22	8	80	60	0	22	22	يو دو	2 10	80
S75 D96 S95	A14	E16 I 18	K1!	L15 S15	D18	E16	A16 F16	K16	617	T16	Q18	K18	E18	Q18	410		E19	L19	S19	010	D2(	R2(	V2V K2C	K2(	Сп	L21	G23	C23	V25	A23	G25	D23	P2	T2(	F26 T26	S26	D2(
																																_					

D269 M270 G274

• Molecule 60: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain AP:	15% 									
S79 K84 L97 D98 S99 T100	K101	S141 1152 <b>+</b> P160 <b>+</b>	A166 F167 K168 K182	A189	R204 V205 N206 1220 0221 0221	2330	F265 T266 S267 D268 D269 C274			

• Molecule 61: Cytochrome b-c1 complex subunit 9

Chain AD: 100% 2 2 2 5 5 5 5 5 5 • Molecule 61: Cytochrome b-c1 complex subunit 9 19% Chain AQ: 100%



• Molecule 62: Cytochrome b-c1 complex subunit 6, mitochondrial



• Molecule 62: Cytochrome b-c1 complex subunit 6, mitochondrial





• Molecule 66:	Cytochrome b	
Chain AJ:	98%	
12 11 124 1153 1153 1153	dibr 1268 1268 1298 1298 1298 1298 1298 1300 1301 ₩379	
• Molecule 66:	Cytochrome b	
Chain AV:	96% •	
12 R5 145 N85 A122	T147       L149       L149       L149       L154       P154       P154       P154       P154       P154       P154       P154       P154       P154       P1556       D228       A229       P266       D254       P266       P266       P266       P346       P346       P346       P346       P346       P346       P346	
• Molecule 67:	Cytochrome b-c1 complex subunit 2, mitochondrial	
Chain AK:	98%	•
P36 149 N176 C198 ▲ R241	12244     1226     256     7302     1315     1317     1317     1317     1317     1317     1317     1317     1317     1317     1317     1317     1317     1317     1317     1317     1317     1318     1317     1318     1318     1318     1318     1318     1318     1318     1318     1318     1318     1317     1318     1317     1318 <td></td>	
• Molecule 67:	Cytochrome b-c1 complex subunit 2, mitochondrial	
Chain AW:	98%	•
P35 036 037 142 143 P44 P44	A50 A50 A50 A50 A105	F237 L238 N239 N240 R241 C243 C243 C243 C243 C243 C243 C243 C245 C245 C245 C248
A249 K250 R254 R261 A278 G279	A225 E282 A2295 P297 P297 P297 P297 P297 P297 P297 P297	6434 ← T447 P448 D451 E452 L453 L453
• Molecule 68:	Cytochrome b-c1 complex subunit 1, mitochondrial	
Chain AL:	99%	I
T35       4         Q40       4         R180       4         Q193       2         D279       2	G312     H313     Y314     Y315     Y316     T317     Y316     T317     Y316     T317     Y316     T317     Y316     T317     Y316     T317     Y318     G319     G321     Y322     H323     L324     S321     P463     P463     P463     P463     P463	
• Molecule 68:	Cytochrome b-c1 complex subunit 1, mitochondrial	
Chain AY:	.2% 97% .	I.
T35 A36 F37 F38 A39 A41 L42 L42	Q4:3     B47     B47     B47     B47     D54     D54     C03     P22     P33     P32     P176     A177     A177     A177     A177     A177     A177     A177     A256     A256     A256     P260     A251     V355     P260     A256     P260     A256     P260     P260     P260     P261     V355     P260     P261     P262     P263     P264     P264     P265     P265     P265  P	1266







# 4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	167761	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{\AA}^2)$	1.25	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.385	Depositor
Minimum map value	-0.091	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.0354	Depositor
Map size (Å)	519.83997, 519.83997, 519.83997	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.083, 1.083, 1.083	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: HEA, SF4, ZN, CDL, PEE, MG, NDP, 8Q1, FMN, CU, PLX, HEM, HEC, FES

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	B	ond lengths	E	Sond angles		
	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5		
1	А	0.30	0/3398	0.49	0/4590		
2	В	0.50	0/1452	0.57	0/1964		
3	С	0.58	0/1280	0.57	0/1732		
4	Е	0.34	0/993	0.53	0/1335		
5	F	0.28	0/682	0.53	0/922		
6	G	0.33	0/684	0.53	0/926		
6	Х	0.57	0/698	0.61	0/942		
7	Н	0.34	0/941	0.59	0/1275		
8	Ι	0.29	0/788	0.54	0/1066		
9	J	0.35	0/2785	0.52	0/3771		
10	Κ	0.27	0/282	0.47	0/381		
11	L	0.33	0/987	0.53	0/1331		
12	М	0.32	0/5362	0.53	0/7266		
13	Ν	0.37	0/1236	0.55	0/1681		
14	0	0.29	0/1682	0.51	0/2289		
15	Р	0.38	0/1780	0.59	0/2424		
16	Q	0.43	0/3552	0.59	1/4815~(0.0%)		
17	S	0.60	0/583	0.64	0/785		
18	Т	0.32	0/755	0.47	0/1017		
19	U	0.52	0/670	0.63	0/920		
20	V	0.51	0/1065	0.61	0/1450		
21	W	0.57	0/1166	0.68	1/1579~(0.1%)		
22	Y	0.52	0/559	0.73	3/763~(0.4%)		
23	Ζ	0.45	0/669	0.53	0/899		
24	а	0.68	0/1209	0.65	0/1639		
25	b	0.59	1/1095~(0.1%)	0.69	4/1480~(0.3%)		
26	с	0.59	0/1287	0.58	0/1761		
27	d	0.63	0/1445	0.65	1/1945~(0.1%)		
28	е	0.61	0/835	0.62	0/1134		
29	f	0.48	0/418	0.58	0/566		
30	g	0.64	0/1035	0.63	0/1398		
31	h	0.62	0/884	0.65	0/1182		



Mol	Chain	B	ond lengths	B	Sond angles
	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5
32	i	0.67	0/2808	0.77	2/3843~(0.1%)
33	j	0.55	0/945	0.69	1/1292~(0.1%)
34	k	0.68	1/751~(0.1%)	0.79	1/1019~(0.1%)
35	1	0.61	2/4840~(0.0%)	0.70	3/6611~(0.0%)
36	m	0.68	0/1346	0.67	0/1832
37	n	0.49	0/484	0.62	0/652
38	0	0.54	0/1093	0.61	0/1479
39	р	0.59	0/1549	0.59	0/2098
40	r	0.70	0/3723	0.76	2/5089~(0.0%)
41	s	0.62	0/2580	0.73	0/3539
42	u	0.57	0/1433	0.61	0/1937
43	V	0.49	0/934	0.67	3/1241~(0.2%)
44	W	0.44	0/2533	0.56	0/3440
45	Х	0.60	0/4164	0.76	1/5688~(0.0%)
46	у	0.58	0/1868	0.80	0/2544
47	Z	0.56	0/2211	0.69	0/3023
48	0	0.57	0/1229	0.65	1/1658~(0.1%)
49	1	0.50	0/898	0.66	0/1218
50	2	0.56	0/765	0.81	0/1038
51	3	0.55	0/699	0.73	1/950~(0.1%)
52	4	0.55	0/648	0.73	0/877
53	5	0.60	0/611	0.65	0/810
54	6	0.60	0/451	0.71	0/610
55	7	0.58	0/398	0.66	0/546
56	8	0.63	0/399	0.62	0/534
57	9	0.51	0/345	0.65	0/470
58	AA	0.31	0/715	0.48	0/964
58	AN	0.27	0/707	0.49	0/953
59	AB	0.23	0/421	0.60	1/574~(0.2%)
59	AO	0.25	0/417	0.61	1/569~(0.2%)
60	AC	0.24	0/1554	0.43	0/2104
60	AP	0.23	0/1554	0.42	0/2104
61	AD	0.26	0/521	0.42	0/699
61	AQ	0.27	0/521	0.43	0/699
62	AE	0.35	0/587	0.54	1/789~(0.1%)
62	AR	0.27	0/587	0.46	0/789
63	AF	0.42	1/942~(0.1%)	0.52	1/1263~(0.1%)
63	AS	0.27	0/942	0.44	0/1263
64	AG	0.27	0/442	0.48	0/608
64	AT	0.28	0/442	0.49	0/608
65	AH	0.26	0/1983	0.46	0/2691
65	AU	0.27	0/1983	0.45	0/2691
66	AJ	0.31	1/3108~(0.0%)	0.52	1/4254~(0.0%)



Mal	Chain	B	ond lengths	Bond angles			
	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5		
66	AV	0.34	2/3108~(0.1%)	0.54	2/4254~(0.0%)		
67	AK	0.27	0/3217	0.49	0/4361		
67	AW	0.29	1/3220~(0.0%)	0.48	1/4365~(0.0%)		
68	AL	0.27	0/3527	0.47	0/4788		
68	AY	0.29	1/3527~(0.0%)	0.50	2/4788~(0.0%)		
All	All	0.47	10/115987~(0.0%)	0.60	35/157444~(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
44	W	0	1

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\operatorname{Ideal}(\operatorname{\AA})$
67	AW	448	PRO	N-CD	5.34	1.55	1.47
66	AJ	154	PRO	N-CD	5.22	1.55	1.47
66	AV	154	PRO	N-CD	5.22	1.55	1.47
34	k	2	PRO	N-CD	5.17	1.55	1.47
25	b	118	PRO	N-CD	5.17	1.55	1.47

The worst 5 of 35 bond angle outliers are listed below:

Mol	Chain Res		Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
32	i	323	THR	C-N-CD	-7.38	104.37	120.60
21	W	31	SER	N-CA-C	-7.00	92.09	111.00
22	Y	92	TRP	N-CA-C	-6.99	92.12	111.00
27	d	2	PRO	N-CA-CB	6.77	111.43	103.30
22	Y	87	PRO	CA-N-CD	-6.56	102.31	111.50

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
44	W	338	LYS	Peptide



## 5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

## 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	Pe	Percentiles			
1	А	429/431~(100%)	396 (92%)	24 (6%)	9 (2%)		7	39		
2	В	174/176~(99%)	163 (94%)	10 (6%)	1 (1%)	6	25	63		
3	С	154/156~(99%)	136 (88%)	13 (8%)	5 (3%)		4	32		
4	Е	111/113~(98%)	101 (91%)	8 (7%)	2 (2%)		8	42		
5	F	81/83~(98%)	74 (91%)	7 (9%)	0	10	00	100		
6	G	83/85~(98%)	78 (94%)	3 (4%)	2 (2%)		6	37		
6	Х	83/85~(98%)	73 (88%)	6 (7%)	4 (5%)		2	24		
7	Н	110/112~(98%)	100 (91%)	5 (4%)	5 (4%)		2	25		
8	Ι	91/110 (83%)	79 (87%)	6 (7%)	6 (7%)		1	19		
9	J	335/337~(99%)	314 (94%)	14 (4%)	7 (2%)		7	39		
10	K	31/33~(94%)	27 (87%)	1 (3%)	3 (10%)		0	11		
11	L	116/118~(98%)	104 (90%)	8 (7%)	4 (3%)		3	31		
12	М	685/687~(100%)	608 (89%)	54 (8%)	23 (3%)		3	31		
13	N	141/143~(99%)	119 (84%)	15 (11%)	7 (5%)		2	23		
14	0	210/212 (99%)	188 (90%)	15 (7%)	7 (3%)		4	31		
15	Р	206/208~(99%)	173 (84%)	22 (11%)	11 (5%)		2	22		
16	Q	428/430 (100%)	398 (93%)	23 (5%)	7 (2%)		9	44		
17	S	68/70~(97%)	61 (90%)	5 (7%)	2 (3%)		4	33		
18	Т	93/95~(98%)	87 (94%)	2 (2%)	4 (4%)		2	26		
19	U	81/83~(98%)	76 (94%)	4 (5%)	1 (1%)		13	49		
20	V	138/140~(99%)	129 (94%)	6 (4%)	3 (2%)		6	38		



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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	entiles
21	W	136/138~(99%)	127 (93%)	4(3%)	5 (4%)	3	29
22	Y	57/59~(97%)	50 (88%)	1 (2%)	6 (10%)	0	9
23	Z	78/80~(98%)	73 (94%)	5(6%)	0	100	100
24	a	136/138~(99%)	121 (89%)	12 (9%)	3 (2%)	6	38
25	b	122/124~(98%)	107 (88%)	10 (8%)	5 (4%)	3	27
26	с	151/153~(99%)	129 (85%)	15 (10%)	7 (5%)	2	25
27	d	169/171~(99%)	165 (98%)	3 (2%)	1 (1%)	25	63
28	e	95/97~(98%)	83 (87%)	9 (10%)	3 (3%)	4	32
29	f	45/47~(96%)	43 (96%)	1 (2%)	1 (2%)	6	38
30	g	117/119~(98%)	105 (90%)	6 (5%)	6 (5%)	2	23
31	h	102/104~(98%)	86 (84%)	10 (10%)	6 (6%)	1	20
32	i	345/347~(99%)	324 (94%)	15 (4%)	6 (2%)	9	43
33	j	113/115~(98%)	103 (91%)	7 (6%)	3 (3%)	5	35
34	k	95/97~(98%)	88 (93%)	4 (4%)	3 (3%)	4	32
35	1	601/603~(100%)	553 (92%)	38 (6%)	10 (2%)	9	43
36	m	172/174~(99%)	150 (87%)	12 (7%)	10 (6%)	1	21
37	n	54/56~(96%)	50 (93%)	2 (4%)	2 (4%)	3	29
38	0	126/128~(98%)	113 (90%)	9 (7%)	4 (3%)	4	32
39	р	170/172~(99%)	158 (93%)	9 (5%)	3 (2%)	8	42
40	r	457/459~(100%)	420 (92%)	28 (6%)	9 (2%)	7	40
41	s	316/318~(99%)	285 (90%)	22 (7%)	9 (3%)	5	34
42	u	167/169~(99%)	152 (91%)	10 (6%)	5 (3%)	4	33
43	v	107/122~(88%)	90 (84%)	14 (13%)	3 (3%)	5	34
44	W	318/320~(99%)	281 (88%)	28 (9%)	9 (3%)	5	34
45	x	512/514~(100%)	479 (94%)	29 (6%)	4 (1%)	19	57
46	У	225/227~(99%)	203 (90%)	19 (8%)	3 (1%)	12	48
47	Z	259/261~(99%)	249 (96%)	10 (4%)	0	100	100
48	0	142/144~(99%)	135 (95%)	7(5%)	0	100	100
49	1	107/109~(98%)	104 (97%)	3 (3%)	0	100	100
50	2	$96/\overline{98}~(98\%)$	86 (90%)	6 (6%)	4 (4%)	3	26
51	3	$82/\overline{84}\ (98\%)$	67 (82%)	10 (12%)	5(6%)	1	20



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	entiles
52	4	73/75~(97%)	64~(88%)	8 (11%)	1 (1%)	11	46
53	5	71/73~(97%)	65~(92%)	6 (8%)	0	100	100
54	6	54/56~(96%)	47 (87%)	5~(9%)	2~(4%)	3	29
55	7	47/49~(96%)	41 (87%)	6 (13%)	0	100	100
56	8	45/47~(96%)	42 (93%)	3 (7%)	0	100	100
57	9	41/43~(95%)	39~(95%)	2(5%)	0	100	100
58	AA	79/81~(98%)	71 (90%)	6 (8%)	2 (2%)	5	36
58	AN	79/81~(98%)	74~(94%)	4 (5%)	1 (1%)	12	48
59	AB	55/57~(96%)	41 (74%)	11 (20%)	3~(6%)	2	22
59	AO	55/57~(96%)	43 (78%)	6 (11%)	6 (11%)	0	8
60	AC	194/196~(99%)	179~(92%)	10 (5%)	5 (3%)	5	35
60	AP	194/196~(99%)	178 (92%)	13 (7%)	3 (2%)	10	45
61	AD	60/62~(97%)	57~(95%)	3~(5%)	0	100	100
61	AQ	60/62~(97%)	55~(92%)	5 (8%)	0	100	100
62	AE	72/74~(97%)	65~(90%)	5(7%)	2(3%)	5	34
62	AR	72/74~(97%)	69~(96%)	2(3%)	1 (1%)	11	46
63	AF	104/106~(98%)	100~(96%)	3~(3%)	1 (1%)	15	52
63	AS	104/106~(98%)	102~(98%)	2(2%)	0	100	100
64	AG	49/51~(96%)	48~(98%)	1 (2%)	0	100	100
64	AT	49/51~(96%)	47~(96%)	2(4%)	0	100	100
65	AH	239/241~(99%)	225~(94%)	12 (5%)	2(1%)	19	57
65	AU	239/241~(99%)	230~(96%)	7(3%)	2(1%)	19	57
66	AJ	376/378~(100%)	363~(96%)	10 (3%)	3 (1%)	19	57
66	AV	376/378~(100%)	359~(96%)	14 (4%)	3~(1%)	19	57
67	AK	417/419~(100%)	390~(94%)	22~(5%)	5 (1%)	13	49
67	AW	417/419~(100%)	397~(95%)	15 (4%)	5 (1%)	13	49
68	AL	444/446~(100%)	405 (91%)	33 (7%)	6 (1%)	11	46
68	AY	444/446~(100%)	413 (93%)	24 (5%)	7 (2%)	9	44
All	All	$14029/14\overline{219}\ (99\%)$	12872 (92%)	849 (6%)	308 (2%)	10	38

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 $5~{\rm of}~308$  Ramachandran outliers are listed below:



Mol	Chain	Res	Type
1	А	63	TYR
1	А	73	PRO
1	А	379	CYS
2	В	62	THR
12	М	37	ASP

#### 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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	А	346/346~(100%)	346 (100%)	0	100 100	)
2	В	151/151~(100%)	151 (100%)	0	100 100	)
3	С	132/132~(100%)	132 (100%)	0	100 100	)
4	Ε	106/106~(100%)	105 (99%)	1 (1%)	78 87	
5	F	74/74~(100%)	74 (100%)	0	100 100	)
6	G	74/79~(94%)	74 (100%)	0	100 100	)
6	Х	78/79~(99%)	78 (100%)	0	100 100	)
7	Η	100/100~(100%)	100 (100%)	0	100 100	)
8	Ι	87/96~(91%)	87 (100%)	0	100 100	)
9	J	292/292~(100%)	288~(99%)	4 (1%)	67 81	
10	Κ	32/32~(100%)	32~(100%)	0	100 100	)
11	L	107/107~(100%)	107~(100%)	0	100 100	)
12	М	576/577~(100%)	574 (100%)	2 (0%)	92 95	
13	Ν	129/129~(100%)	129 (100%)	0	100 100	)
14	Ο	181/181~(100%)	181 (100%)	0	100 100	)
15	Р	190/190~(100%)	190 (100%)	0	100 100	)
16	Q	$37\overline{1/371}~(100\%)$	369~(100%)	2 (0%)	88 93	
17	S	$59/59~\overline{(100\%)}$	59~(100%)	0	100 100	)
18	Т	79/79~(100%)	79~(100%)	0	100 100	)
19	U	$7\overline{2/72}\ (100\%)$	72 (100%)	0	100 100	)



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Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
20	V	102/102~(100%)	102 (100%)	0	100	100
21	W	119/119~(100%)	119 (100%)	0	100	100
22	Y	57/57~(100%)	49 (86%)	8 (14%)	3	21
23	Ζ	62/63~(98%)	62 (100%)	0	100	100
24	a	124/124~(100%)	122 (98%)	2 (2%)	62	79
25	b	118/118~(100%)	114 (97%)	4 (3%)	37	62
26	с	124/137~(90%)	124 (100%)	0	100	100
27	d	145/154~(94%)	137 (94%)	8 (6%)	21	51
28	е	90/90~(100%)	90 (100%)	0	100	100
29	f	43/43 (100%)	43 (100%)	0	100	100
30	g	105/105~(100%)	105 (100%)	0	100	100
31	h	90/90~(100%)	90 (100%)	0	100	100
32	i	314/314~(100%)	314 (100%)	0	100	100
33	j	102/103~(99%)	102 (100%)	0	100	100
34	k	85/85~(100%)	82 (96%)	3 (4%)	36	62
35	1	531/532~(100%)	510 (96%)	21 (4%)	31	58
36	m	137/137~(100%)	137 (100%)	0	100	100
37	n	53/53~(100%)	53 (100%)	0	100	100
38	0	114/114~(100%)	114 (100%)	0	100	100
39	р	157/157~(100%)	156 (99%)	1 (1%)	86	91
40	r	416/416 (100%)	416 (100%)	0	100	100
41	s	278/278~(100%)	278 (100%)	0	100	100
42	u	153/153~(100%)	153 (100%)	0	100	100
43	V	89/111 (80%)	89 (100%)	0	100	100
44	W	249/288~(86%)	249 (100%)	0	100	100
45	х	427/427~(100%)	389 (91%)	38 (9%)	9	36
46	У	211/211~(100%)	191 (90%)	20 (10%)	8	33
47	Z	226/226~(100%)	199 (88%)	27 (12%)	5	25
48	0	128/128 (100%)	120 (94%)	8 (6%)	18	47
49	1	95/95~(100%)	89 (94%)	6 (6%)	18	47
50	2	81/81 (100%)	76 (94%)	5 (6%)	18	48



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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles		
51	3	68/68~(100%)	50 (74%)	18 (26%)	0 4		
52	4	67/67~(100%)	58~(87%)	9~(13%)	4 22		
53	5	58/58~(100%)	53~(91%)	5 (9%)	10 38		
54	6	47/47~(100%)	40 (85%)	7 (15%)	3 18		
55	7	39/39~(100%)	37~(95%)	2(5%)	24 53		
56	8	40/40~(100%)	38~(95%)	2(5%)	24 53		
57	9	37/37~(100%)	34 (92%)	3 (8%)	11 40		
58	AA	74/74~(100%)	68~(92%)	6 (8%)	11 40		
58	AN	73/74~(99%)	73 (100%)	0	100 100		
59	AB	46/46 (100%)	46 (100%)	0	100 100		
59	AO	45/46~(98%)	45 (100%)	0	100 100		
60	AC	166/166~(100%)	166 (100%)	0	100 100		
60	AP	166/166~(100%)	166 (100%)	0	100 100		
61	AD	52/52~(100%)	52 (100%)	0	100 100		
61	AQ	52/52~(100%)	52 (100%)	0	100 100		
62	AE	61/71~(86%)	59~(97%)	2 (3%)	38 63		
62	AR	61/71~(86%)	59~(97%)	2 (3%)	38 63		
63	AF	95/95~(100%)	84 (88%)	11 (12%)	5 26		
63	AS	95/95~(100%)	95 (100%)	0	100 100		
64	AG	42/42~(100%)	42 (100%)	0	100 100		
64	AT	42/42~(100%)	40 (95%)	2(5%)	25 54		
65	AH	207/207~(100%)	207 (100%)	0	100 100		
65	AU	207/207~(100%)	206 (100%)	1 (0%)	88 93		
66	AJ	330/330~(100%)	327~(99%)	3 (1%)	78 87		
66	AV	330/330~(100%)	322 (98%)	8 (2%)	49 69		
67	AK	334/335~(100%)	331 (99%)	3 (1%)	78 87		
67	AW	335/335~(100%)	332~(99%)	3 (1%)	78 87		
68	AL	367/367~(100%)	367 (100%)	0	100 100		
68	AY	367/367~(100%)	361 (98%)	6 (2%)	62 79		
All	All	12164/12289~(99%)	11911 (98%)	253 (2%)	56 73		

5 of 253 residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
47	Z	11	VAL
63	AF	49	ARG
48	0	40	LEU
63	AF	40	GLU
66	AV	147	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 234 such sidechains are listed below:

Mol	Chain	Res	Type
37	n	40	ASN
67	AW	212	HIS
45	Х	11	ASN
67	AW	155	GLN
68	AL	87	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)

Of 63 ligands modelled in this entry, 5 are monoatomic - leaving 58 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	Trung	Chain	Dec	Timle	Bo	ond leng	ths	Bo	ond angl	es
IVIOI	Tybe	Chain	Res	LINK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z  > 2
74	FES	М	803	-	0,4,4	-	-	-		
75	CDL	n	101	-	$63,\!63,\!99$	1.24	5 (7%)	$69,\!75,\!111$	1.07	4 (5%)
75	CDL	AJ	404	-	63,63,99	1.24	5 (7%)	69,75,111	1.03	4 (5%)
75	CDL	AY	501	-	63,63,99	1.24	5 (7%)	69,75,111	1.01	4 (5%)
69	SF4	М	802	12	0,12,12	-	-	-		
71	PLX	g	203	-	$51,\!51,\!51$	0.78	1 (1%)	$55,\!59,\!59$	0.58	1 (1%)
74	FES	AC	301	60	0,4,4	-	-	-		
82	HEM	AV	401	66	41,50,50	1.97	5 (12%)	45,82,82	1.55	<mark>5 (11%)</mark>
69	SF4	А	501	1	0,12,12	-	-	-		
76	PEE	AU	401	-	40,40,50	1.46	4 (10%)	$43,\!45,\!55$	0.95	3 (6%)
75	CDL	AG	101	-	$63,\!63,\!99$	1.15	4 (6%)	69,75,111	1.16	6 (8%)
69	SF4	С	301	3	0,12,12	-	-	-		
76	PEE	AV	403	-	48,48,50	1.34	4 (8%)	$51,\!53,\!55$	1.04	2 (3%)
75	CDL	AN	101	-	63,63,99	1.24	5 (7%)	69,75,111	1.02	4 (5%)
71	PLX	U	101	-	51,51,51	0.74	1 (1%)	$55,\!59,\!59$	0.72	2 (3%)
76	PEE	V	202	-	50,50,50	1.16	6 (12%)	$53,\!55,\!55$	0.91	2 (3%)
69	SF4	В	301	2	0,12,12	-	-	-		
76	PEE	AH	401	-	48,48,50	1.35	4 (8%)	$51,\!53,\!55$	0.95	2(3%)
76	PEE	1	702	-	50,50,50	1.16	6 (12%)	$53,\!55,\!55$	0.99	2 (3%)
74	FES	0	301	14	0,4,4	-	-	-		
74	FES	AP	301	60	0,4,4	-	-	-		
79	HEA	Х	604	45	57,67,67	1.47	6 (10%)	61,103,103	1.47	12 (19%)
71	PLX	g	201	-	$51,\!51,\!51$	0.82	1 (1%)	$55,\!59,\!59$	0.69	1 (1%)
76	PEE	AY	502	-	48,48,50	1.39	4 (8%)	$51,\!53,\!55$	0.96	2 (3%)
71	PLX	r	502	-	51,51,51	0.64	0	$55,\!59,\!59$	0.67	1 (1%)
75	CDL	AJ	405	-	63,63,99	1.13	4 (6%)	69,75,111	1.22	5 (7%)
75	CDL	1	704	-	63,63,99	1.26	5 (7%)	69,75,111	1.01	4 (5%)
71	PLX	V	203	-	51,51,51	0.78	1 (1%)	55, 59, 59	0.60	1 (1%)
72	8Q1	Е	201	-	31,34,34	1.64	6 (19%)	40,43,43	1.39	7 (17%)
75	CDL	AU	403	-	63,63,99	1.24	6 (9%)	69,75,111	1.04	4 (5%)
75	CDL	1	703	-	63,63,99	1.21	5 (7%)	69,75,111	1.07	4 (5%)
71	PLX	AT	101	-	51,51,51	0.75	1 (1%)	$55,\!59,\!59$	0.60	1 (1%)
76	PEE	AJ	403	-	48,48,50	1.33	4 (8%)	51,53,55	0.99	2 (3%)
76	PEE	1	701	-	48,48,50	1.34	4 (8%)	$51,\!53,\!55$	0.96	2 (3%)
75	CDL	AL	502	-	63,63,99	1.24	5 (7%)	69,75,111	1.05	4 (5%)
79	HEA	х	603	45	57,67,67	1.23	6 (10%)	61,103,103	1.47	10 (16%)



Mol	Tuno	Chain	Bos       Link       Bond lengths       E		Bo	ond angles				
	туре	Ullain	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
82	HEM	AJ	401	66	41,50,50	1.92	6 (14%)	45,82,82	1.60	5 (11%)
82	HEM	AJ	402	66	41,50,50	1.89	6 (14%)	45,82,82	1.57	9 (20%)
81	HEC	AU	402	65	32,50,50	2.28	3 (9%)	24,82,82	1.40	2 (8%)
76	PEE	W	201	-	50,50,50	1.14	6 (12%)	53,55,55	0.97	2 (3%)
75	CDL	AH	403	-	63,63,99	1.25	5 (7%)	69,75,111	1.03	4 (5%)
81	HEC	AH	402	65	32,50,50	2.22	3 (9%)	24,82,82	1.35	1 (4%)
71	PLX	В	303	-	51,51,51	0.77	1 (1%)	55,59,59	0.68	1 (1%)
69	SF4	В	302	2	0,12,12	-	-	-		
72	8Q1	р	201	-	31,34,34	1.67	5 (16%)	40,43,43	1.57	5 (12%)
82	HEM	AV	402	66	41,50,50	1.90	6 (14%)	45,82,82	1.60	8 (17%)
71	PLX	g	202	-	51,51,51	0.74	1 (1%)	55, 59, 59	0.61	1 (1%)
75	CDL	i	401	-	63,63,99	1.21	5 (7%)	69,75,111	1.04	5 (7%)
70	FMN	А	502	-	33,33,33	1.39	6 (18%)	48,50,50	1.34	8 (16%)
71	PLX	r	501	-	51,51,51	0.74	1 (1%)	55,59,59	0.65	1 (1%)
75	CDL	AA	101	-	63,63,99	1.24	5 (7%)	69,75,111	1.07	4 (5%)
71	PLX	b	201	-	51,51,51	0.57	0	55,59,59	0.64	0
75	CDL	V	201	-	61,61,99	1.21	5 (8%)	64,71,111	0.94	3 (4%)
71	PLX	AL	501	-	51,51,51	0.77	1 (1%)	55,59,59	0.63	1 (1%)
73	NDP	J	401	-	45,52,52	0.96	2 (4%)	53,80,80	1.32	4 (7%)
69	SF4	М	801	12	0,12,12	-	-	-		
71	PLX	AQ	101	-	51,51,51	0.77	1 (1%)	55,59,59	0.61	2 (3%)
76	PEE	AL	503	-	48,48,50	1.38	4 (8%)	51,53,55	0.92	2 (3%)

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
74	FES	М	803	-	-	-	0/1/1/1
75	CDL	n	101	-	-	33/74/74/110	-
75	CDL	AJ	404	-	-	33/74/74/110	-
75	CDL	AY	501	-	-	36/74/74/110	-
69	SF4	М	802	12	-	-	0/6/5/5
71	PLX	g	203	-	-	24/55/55/55	-
74	FES	AC	301	60	-	-	0/1/1/1
82	HEM	AV	401	66	-	3/12/54/54	-



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
69	SF4	А	501	1	-	-	0/6/5/5
76	PEE	AU	401	-	-	17/44/44/54	-
75	CDL	AG	101	-	-	38/74/74/110	-
69	SF4	С	301	3	-	-	0/6/5/5
76	PEE	AV	403	-	-	30/52/52/54	-
75	CDL	AN	101	-	-	40/74/74/110	-
71	PLX	U	101	-	-	22/55/55/55	-
76	PEE	V	202	-	-	27/54/54/54	-
76	PEE	AH	401	-	-	27/52/52/54	-
69	SF4	В	301	2	-	-	0/6/5/5
76	PEE	1	702	-	-	27/54/54/54	-
74	FES	0	301	14	-	-	0/1/1/1
74	FES	AP	301	60	-	-	0/1/1/1
79	HEA	x	604	45	3/3/7/16	5/32/76/76	-
71	PLX	g	201	-	-	25/55/55/55	-
76	PEE	AY	502	-	-	20/52/52/54	-
71	PLX	r	502	-	-	36/55/55/55	-
75	CDL	AJ	405	-	-	28/74/74/110	-
75	CDL	1	704	-	-	44/74/74/110	-
71	PLX	V	203	-	-	26/55/55/55	-
72	8Q1	Е	201	-	-	18/41/41/41	-
75	CDL	AU	403	-	-	48/74/74/110	-
75	CDL	1	703	-	-	38/74/74/110	-
71	PLX	AT	101	-	-	23/55/55/55	-
76	PEE	AJ	403	-	-	20/52/52/54	-
76	PEE	1	701	-	-	32/52/52/54	-
79	HEA	x	603	45	3/3/7/16	7/32/76/76	-
75	CDL	AL	502	-	-	43/74/74/110	-
82	HEM	AJ	401	66	-	1/12/54/54	-
82	HEM	AJ	402	66	-	2/12/54/54	-
81	HEC	AU	402	65	-	0/10/54/54	-
76	PEE	W	201	-	-	32/54/54/54	-
75	CDL	AH	403	-	-	42/74/74/110	-
81	HEC	AH	402	65	-	2/10/54/54	-
71	PLX	В	303	_	_	21/55/55/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
72	8Q1	р	201	-	-	19/41/41/41	-
82	HEM	AV	402	66	-	4/12/54/54	-
69	SF4	В	302	2	-	-	0/6/5/5
71	PLX	g	202	-	-	25/55/55/55	-
75	CDL	i	401	-	-	39/74/74/110	-
70	FMN	А	502	-	-	7/18/18/18	0/3/3/3
71	PLX	r	501	-	-	28/55/55/55	-
75	CDL	AA	101	-	-	35/74/74/110	-
71	PLX	b	201	-	-	27/55/55/55	-
75	CDL	V	201	-	-	41/69/69/110	-
71	PLX	AL	501	-	-	23/55/55/55	-
73	NDP	J	401	-	-	15/30/77/77	0/5/5/5
69	SF4	М	801	12	-	-	0/6/5/5
71	PLX	AQ	101	-	-	25/55/55/55	-
76	PEE	AL	503	-	-	22/52/52/54	-

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The worst 5 of 185 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	AJ	401	HEM	C3D-C2D	7.85	1.53	1.36
82	AV	402	HEM	C3D-C2D	7.85	1.53	1.36
82	AJ	402	HEM	C3D-C2D	7.80	1.53	1.36
82	AV	401	HEM	C3D-C2D	7.75	1.53	1.36
81	AU	402	HEC	C3C-C2C	-6.96	1.33	1.40

The worst 5 of 169 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
82	AV	402	HEM	C4D-ND-C1D	6.20	111.47	105.07
82	AJ	401	HEM	C4D-ND-C1D	6.12	111.39	105.07
82	AJ	402	HEM	C4D-ND-C1D	6.02	111.30	105.07
72	р	201	8Q1	C6-C1-S44	6.02	120.47	113.46
82	AV	401	HEM	C4D-ND-C1D	5.32	110.57	105.07

5 of 6 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
79	Х	603	HEA	NB
79	Х	603	HEA	NA
	a		1	1



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Mol	Chain	Res	Type	Atom
79	Х	603	HEA	ND
79	Х	604	HEA	NB
79	Х	604	HEA	NA

5 of 1180 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
70	А	502	FMN	C1'-C2'-C3'-O3'
70	А	502	FMN	C1'-C2'-C3'-C4'
70	А	502	FMN	C3'-C4'-C5'-O5'
70	А	502	FMN	O4'-C4'-C5'-O5'
71	В	303	PLX	C2-O1-P1-O2

There are no ring outliers.

No monomer is involved in short contacts.

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.























































![](_page_69_Picture_4.jpeg)

![](_page_70_Figure_3.jpeg)

![](_page_70_Picture_4.jpeg)

![](_page_71_Figure_3.jpeg)

![](_page_71_Picture_4.jpeg)






















## 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-6775. 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.

#### Orthogonal projections (i) 6.1

#### 6.1.1Primary map



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

#### 6.2Central slices (i)

#### 6.2.1Primary map



X Index: 240

Y Index: 240



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: 194

Y Index: 261

Z Index: 214

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 0.0354. 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 1319  $\rm nm^3;$  this corresponds to an approximate mass of 1191 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)



\*Reported resolution corresponds to spatial frequency of 0.256  $\text{\AA}^{-1}$ 



# 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-6775 and PDB model 5XTH. Per-residue inclusion information can be found in section 3 on page 26.

## 9.1 Map-model overlay (i)



The images above show the 3D surface view of the map at the recommended contour level 0.0354 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 Q-score mapped to coordinate model (i)



The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

### 9.3 Atom inclusion mapped to coordinate model (i)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0354).



## 9.4 Atom inclusion (i)



At the recommended contour level, 86% of all backbone atoms, 73% of all non-hydrogen atoms, are inside the map.



1.0

0.0 <0.0

## 9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.0354) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	$\mathbf{Q} extsf{-score}$
All	0.7318	0.2930
0	0.1288	0.0250
1	0.1760	0.0530
2	0.4301	0.0700
3	0.2680	0.0410
4	0.3498	0.0370
5	0.0948	0.0310
6	0.3418	0.0880
7	0.1040	0.0240
8	0.2816	0.0120
9	0.1355	0.0240
А	0.7826	0.2470
AA	0.7186	0.3250
AB	0.2283	0.0740
AC	0.6506	0.2070
AD	0.6413	0.2820
AE	0.7306	0.2250
AF	0.7022	0.2830
AG	0.6364	0.2600
AH	0.7733	0.2990
AJ	0.7417	0.3490
AK	0.8260	0.2600
AL	0.7964	0.3320
AN	0.6846	0.1970
AO	0.1153	-0.0360
AP	0.6975	0.1840
AQ	0.6497	0.1980
AR	0.7165	0.1870
AS	0.7787	0.2640
AT	0.6443	0.1700
AU	0.7818	0.2360
AV	0.7582	0.3070
AW	0.6953	0.1790
AY	0.7272	0.1890
B	0.8840	0.4270

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Chain	Atom inclusion	Q-score
С	0.9007	0.4360
Е	0.6869	0.2550
F	0.7819	0.1840
G	0.4550	0.1620
Н	0.7204	0.2130
Ι	0.7933	0.3150
J	0.8074	0.2950
K	0.7537	0.2440
L	0.7279	0.3180
М	0.7950	0.2910
N	0.8212	0.3440
0	0.8015	0.2630
Р	0.7981	0.3200
Q	0.8197	0.3830
S	0.9091	0.4250
Т	0.7845	0.3430
U	0.8795	0.4120
V	0.7819	0.4030
W	0.8903	0.4140
Х	0.8662	0.3870
Y	0.8900	0.3530
Z	0.8515	0.3550
a	0.9173	0.4530
b	0.8369	0.3440
С	0.8957	0.4430
d	0.8905	0.4060
e	0.8316	0.4170
f	0.7970	0.3270
g	0.8480	0.4350
h	0.8829	0.4310
i	0.8498	0.4610
j	0.7549	0.3810
k	0.7916	0.4260
1	0.8172	0.4190
m	0.7978	0.4080
n	0.8531	0.3850
0	0.8560	0.4240
р	0.8950	0.4010
r	0.8721	0.4660
S	0.8480	0.4340
u	0.9118	0.4080
V	0.8314	0.3020

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Chain	Atom inclusion	Q-score
W	0.8349	0.3410
X	0.3690	0.0410
У	0.2578	0.0090
Z	0.4567	0.0910

