

wwPDB EM Validation Summary Report (i)

Apr 1, 2023 – 10:22 am BST

PDB ID	:	8B6F
EMDB ID	:	EMD-15865
Title	:	Cryo-EM structure of NADH:ubiquinone oxidoreductase (complex-I) from res- piratory supercomplex of Tetrahymena thermophila
Authors	:	Muhleip, A.; Kock Flygaard, R.; Amunts, A.
Deposited on	:	2022-09-27
Resolution	:	2.80 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.dev50
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)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.2

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 2.80 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.



Matria	Whole archive	EM structures		
Metric	$(\# {\rm Entries})$	$(\# { m Entries})$		
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	A0	516	9%89%	7% ••
2	A1	362	89%	• 7%
3	A2	317	7% 89	6 15%
4	A3	333	79%	8% 13%
5	A4	311	18%	5%
6	A5	282	90%	10%
7	A6	251	83%	9% 8%
8	A7	238	• 50% 6% 44%	



Mol	Chain	Length	Quality of chain	
9	A8	217	93%	7%
10	A9	231	<u>6%</u> 95%	5%
11	AA	750	84%	11% 5%
12	AB	718	<mark>6%</mark>	10% •
13	AC	505	90%	10%
14	AD	474	82%	10% 7%
15	AE	442	• 87%	12%
16	AF	360	• 89%	11%
17	AG	346	• 96%	
18	AH	284	• 89%	11%
19	AI	274	16%	7% 16%
20	AJ	255	93%	7%
21	AK	257	€ 82%	8% 11%
22	AL	236	•	14% 8%
23	AM	233	80%	0%
20	ΔN	206	700/	240/
24		108	· · · · · · · · · · · · · · · · · · ·	2470
20		190	87%	13%
20		194	89%	9% •
27	AQ	189	94%	5% •
28	AR	185	94%	••
29	AS	172	92%	7% •
30	AT	162	81%	17% ••
31	AU	150	94%	5%•
32	AV	138	78%	• 19%
33	AW	133	68% 5%	26%



Mol	Chain	Length	Quality of chain
34	AX	121	
35	AY	116	88% 12%
36	AZ	103	85% 6% 9%
37	B0	94	89% 10% •
38	B1	93	<u>97%</u>
39	B2	94	9% 90% 9% •
40	B3	83	7% 83% 5% 12%
41	B4	73	96% •
42	B5	71	• 76% 24%
43	B6	59	78% 22%
44	BA	212	86% 8% 6%
45	BB	214	10% 72% 6% 22%
46	BC	207	
47	BD	205	8% 66% 5% 28%
48	BE	189	7% 84% 5% 11%
49	BF	188	5% 81% 13% 6%
50	BG	175	8 2% 9% 9%
51	BH	178	9 1% 9%
52	BI	172	• 78% 8% 13%
53	BJ	166	8 3% • 13%
54	BK	144	6% 74% • 24%
55	BL	143	6%
56	BM	135	84% 10% 5%
57	BN	135	7% 90% 9% •
58	во	136	96%



Mol	Chain	Length		Quality of chain		
59	BP	129	• 50%	5%	44%	
60	BQ	127		%	5%	20%
61	BR	132	6 8%	• 33	1%	
62	BS	126	6%	92%		• 5%
63	BT	125	-	86%		13% •
64	BU	134	26%	89%		11%
65	BV	125		98%		•
66	BW	120	7%	94%		
67	BX	113	.	80%	5%	15%
68	BY	100	•	88%		12%
69	ΒZ	102	6%	96%		·

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
78	FES	AI	301	-	-	Х	-
79	SF4	AB	803	-	-	Х	-
79	SF4	AL	302	-	-	Х	-



2 Entry composition (i)

There are 82 unique types of molecules in this entry. The entry contains 234355 atoms, of which 117595 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 Lipid-A-disaccharide synthase.

Mol	Chain	Residues			AltConf	Trace				
1	A0	503	Total 8090	C 2609	H 4019	N 699	O 750	S 13	0	0

• Molecule 2 is a protein called NAD-dependent epimerase/dehydratase family protein.

Mol	Chain	Residues			AltConf	Trace				
2	A1	338	Total 5368	C 1737	Н 2650	N 475	0 494	S 12	0	0

• Molecule 3 is a protein called DnaJ domain protein.

Mol	Chain	Residues			AltConf	Trace				
3	A2	269	Total 4362	C 1392	Н 2163	N 408	O 396	${ m S} { m 3}$	0	0

• Molecule 4 is a protein called Acyl-CoA synthetase (AMP-forming)/AMP-acid ligase II.

Mol	Chain	Residues		Atoms						Trace
4	A3	291	Total 4523	C 1438	Н 2260	N 390	0 434	S 1	0	0

• Molecule 5 is a protein called RNase III domain-containing protein.

Mol	Chain	Residues			Atoms	5			AltConf	Trace
5	A4	311	Total 4985	C 1583	Н 2491	N 434	0 469	S 8	0	0

• Molecule 6 is a protein called 37S ribosomal protein S25, mitochondrial.

Mol	Chain	Residues			Atoms	5			AltConf	Trace
6	A5	282	Total 4596	C 1478	Н 2249	N 413	O 453	${ m S} { m 3}$	0	0



• Molecule 7 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues			Atoms	5			AltConf	Trace
7	A6	230	Total 3770	C 1241	Н 1862	N 322	0 340	${f S}{5}$	0	0

• Molecule 8 is a protein called CX9C domain-containing protein.

Mol	Chain	Residues			Atom	ıs			AltConf	Trace
8	A7	133	Total	C	H	N 100	0	S	0	0
			2124	682	1040	182	209	11		

• Molecule 9 is a protein called NDUTT15.

Mol	Chain	Residues			Atoms	5			AltConf	Trace
9	A8	217	Total 3597	C 1153	Н 1803	N 305	0 328	S 8	0	0

• Molecule 10 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues			Atoms	5			AltConf	Trace
10	A9	231	Total 3697	C 1219	Н 1818	N 317	O 336	S 7	0	0

• Molecule 11 is a protein called NADH dehydrogenase subunit 5.

Mol	Chain	Residues			Atom	ıs			AltConf	Trace
11	AA	713	Total 11919	C 4066	Н 5978	N 855	O 1004	S 16	0	0

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

Mol	Chain	Residues			Atom	ıs			AltConf	Trace
12	AB	688	Total 10762	C 3410	Н 5359	N 935	O 1030	S 28	0	0

• Molecule 13 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues			Atom	s			AltConf	Trace
13	AC	505	Total 8393	C 2859	Н 4223	N 601	O 692	S 18	0	0

• Molecule 14 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.



Mol	Chain	Residues			Atom	s			AltConf	Trace
14	AD	441	Total	С	Н	Ν	0	S	0	0
			6744	2140	3345	596	639	24	Ŭ	Ŭ

• Molecule 15 is a protein called NADH dehydrogenase subunit 7.

Mol	Chain	Residues			Atom	.s			AltConf	Trace
15	AE	441	Total	C	H 2520	N 620	0	S 24	0	0
_			7126	2285	3539	620	658	24	_	-

• Molecule 16 is a protein called Ymf65.

Mol	Chain	Residues			Atoms	5			AltConf	Trace
16	AF	359	Total 6216	C 2132	Н 3148	N 435	O 494	${ m S} 7$	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AF	208	VAL	GLY	conflict	UNP Q951A3

• Molecule 17 is a protein called Transcription factor apfi protein, putative.

Mol	Chain	Residues			Atoms	5			AltConf	Trace
17	AG	346	Total 5531	C 1766	Н 2727	N 481	0 549	S 8	0	0

• Molecule 18 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues			Atom	.S			AltConf	Trace
18	AH	283	Total 4656	C 1581	Н 2350	N 334	0 379	S 12	0	0

• Molecule 19 is a protein called NADH-ubiquinone oxidoreductase 24 kDa subunit.

Mol	Chain	Residues			Atom	s			AltConf	Trace
19	AI	231	Total 3710	C 1173	Н 1848	N 321	O 358	S 10	0	0

• Molecule 20 is a protein called Ymf62.



Mol	Chain	Residues			Atom	5			AltConf	Trace
20	ΔΤ	254	Total	С	Η	Ν	0	\mathbf{S}	0	0
20	лJ	204	4316	1478	2156	305	373	4	0	0

• Molecule 21 is a protein called Gamma-carbonic anhydrase.

Mol	Chain	Residues			AltConf	Trace				
21	AK	230	Total 3519	C 1117	Н 1740	N 306	0 351	${ m S}{ m 5}$	0	0

• Molecule 22 is a protein called NADH-ubiquinone oxidoreductase 1, chain, putative.

Mol	Chain	Residues			AltConf	Trace				
22	AL	218	Total 3501	C 1155	H 1689	N 299	0 347	S 11	0	0

• Molecule 23 is a protein called Gamma-carbonic anhydrase.

Mol	Chain	Residues			Atoms	5			AltConf	Trace
23	AM	231	Total 3558	C 1112	H 1788	N 316	O 335	S 7	0	0

• Molecule 24 is a protein called ETC complex I subunit motif protein.

Mol	Chain	Residues			Atom	S			AltConf	Trace
24	AN	157	Total 2651	C 846	Н 1329	N 221	O 249	S 6	0	0

• Molecule 25 is a protein called NADH dehydrogenase subunit 9.

Mol	Chain	Residues			Atoms	5			AltConf	Trace
25	AO	198	Total 3363	C 1097	Н 1680	N 268	O 312	S 6	0	0

• Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues			Atom	s			AltConf	Trace
26	AP	191	Total 3104	C 1013	Н 1505	N 301	O 280	${f S}{5}$	0	0

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



Mol	Chain	Residues			Atom	5			AltConf	Trace
27	AQ	187	Total	C	Н	N	0	S	0	0
	~		3084	1027	1496	254	303	4		

• Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues			Atom	IS			AltConf	Trace
28	AR	181	Total 2937	C 948	Н 1445	N 267	O 269	S 8	0	0

• Molecule 29 is a protein called NADH dehydrogenase, putative.

Mol	Chain	Residues			Atom	IS			AltConf	Trace
29	AS	172	Total 2802	C 903	Н 1382	N 253	O 256	S 8	0	0

• Molecule 30 is a protein called NADH dehydrogenase subunit 10.

Mol	Chain	Residues			AltConf	Trace				
30	AT	161	Total 2549	C 822	Н 1272	N 220	О 225	S 10	0	0

• Molecule 31 is a protein called NADH-ubiquinone oxidoreductase complex I, 21 kDa subunit.

Mol	Chain	Residues		A	toms			AltConf	Trace
31	AU	149	Total 2436	C 800	Н 1209	N 213	O 214	0	0

• Molecule 32 is a protein called Acyl carrier protein.

Mol	Chain	Residues		Α	toms			AltConf	Trace
32	AV	112	Total 1829	C 586	Н 904	N 158	0 181	0	0

• Molecule 33 is a protein called Acyl carrier protein.

Mol	Chain	Residues			Aton	ns			AltConf	Trace
33	AW	98	Total 1584	C 512	Н 781	N 133	0 157	S 1	0	0

• Molecule 34 is a protein called NADH-ubiquinone oxidoreductase chain 3.



Mol	Chain	Residues			Atom	S			AltConf	Trace
34	AX	121	Total 2047	C 710	Н 1020	N 143	O 170	$\frac{S}{4}$	0	0

• Molecule 35 is a protein called Ymf58.

Mol	Chain	Residues			Atom	ıs			AltConf	Trace
35	AY	116	Total 1944	C 648	Н 987	N 142	0 163	${S \over 4}$	0	0

• Molecule 36 is a protein called Ribosomal protein L51/S25/CI-B8 domain protein.

Mol	Chain	Residues			Aton	ns			AltConf	Trace
36	AZ	94	Total 1552	C 491	Н 775	N 140	0 144	${ m S} { m 2}$	0	0

• Molecule 37 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues		Α	toms			AltConf	Trace
37	B0	93	Total 1607	C 531	H 802	N 139	O 135	0	0

• Molecule 38 is a protein called ATP synthase subunit e, mitochondrial.

Mol	Chain	Residues			Aton	ns			AltConf	Trace
38	B1	92	Total 1536	C 497	Н 746	N 146	O 146	S 1	0	0

• Molecule 39 is a protein called GRAM domain protein.

Mol	Chain	Residues			Aton	ns			AltConf	Trace
39	B2	93	Total 1485	C 480	Н 728	N 129	0 142	S 6	0	0

• Molecule 40 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues			Aton	ns			AltConf	Trace
40	B3	73	Total 1251	C 414	H 618	N 113	0 105	S 1	0	0

• Molecule 41 is a protein called Transmembrane protein, putative.



Mol	Chain	Residues			Aton	ns			AltConf	Trace
41	Β4	73	Total 1247	C 408	Н 623	N 111	O 104	S 1	0	0

• Molecule 42 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues		A	Atom	s			AltConf	Trace
42	B5	54	Total 917	C 305	Н 464	N 71	O 75	${ m S} { m 2}$	0	0

• Molecule 43 is a protein called ND1b.

Mol	Chain	Residues		ŀ	Atom	s			AltConf	Trace
43	B6	59	Total 1043	C 362	Н 528	N 78	0 72	${ m S} { m 3}$	0	0

• Molecule 44 is a protein called Transmembrane protein.

Mol	Chain	Residues			Atoms	5			AltConf	Trace
44	BA	199	Total 3289	C 1071	Н 1638	N 285	O 292	${ m S} { m 3}$	0	0

• Molecule 45 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues			Atom	S			AltConf	Trace
45	BB	167	Total 2626	C 848	Н 1280	N 228	O 265	${ m S}{ m 5}$	0	0

• Molecule 46 is a protein called NDUB8.

Mol	Chain	Residues			Atom	IS			AltConf	Trace
46	BC	173	Total 2848	C 928	Н 1406	N 244	0 264	S 6	0	0

• Molecule 47 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues			Atom	IS			AltConf	Trace
47	BD	148	Total 2414	C 764	Н 1223	N 211	0 214	$\begin{array}{c} \mathrm{S} \\ \mathrm{2} \end{array}$	0	0

• Molecule 48 is a protein called NDUPH2.



Mol	Chain	Residues			Atom	S			AltConf	Trace
48	BE	168	Total 2807	C 930	Н 1385	N 227	O 260	${ m S}{ m 5}$	0	0

• Molecule 49 is a protein called NDUB10.

Mol	Chain	Residues			Atom	.s			AltConf	Trace
49	BF	177	Total 2961	C 934	Н 1486	N 267	O 270	$\frac{S}{4}$	0	0

• Molecule 50 is a protein called NDUA13.

Mol	Chain	Residues			Atom	.S			AltConf	Trace
50	BG	160	Total 2725	C 858	Н 1376	N 256	O 227	S 8	0	0

• Molecule 51 is a protein called NADH dehydrogenase subunit 2.

Mol	Chain	Residues			Atoms	5			AltConf	Trace
51	BH	178	Total 3036	C 1015	Н 1554	N 215	0 247	${ m S}{ m 5}$	0	0

• Molecule 52 is a protein called 2 iron, 2 sulfur cluster-binding protein.

Mol	Chain	Residues			Atom	ıs			AltConf	Trace
52	BI	149	Total 2318	С 731	Н 1139	N 211	O 227	S 10	0	0

• Molecule 53 is a protein called Thioredoxin.

Mol	Chain	Residues			Atom	IS		Atoms						
53	BJ	144	Total 2361	C 767	Н 1156	N 205	O 226	${ m S} 7$	0	0				

• Molecule 54 is a protein called COX assembly mitochondrial protein.

Mol	Chain	Residues		Atoms						Trace
54	BK	109	Total 1757	C 562	Н 854	N 161	0 174	S 6	0	0

• Molecule 55 is a protein called Transmembrane protein, putative.



Mol	Chain	Residues			Atom	IS			AltConf	Trace
55	BL	142	Total 2325	C 770	Н 1138	N 202	O 209	S 6	0	0

• Molecule 56 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues			AltConf	Trace				
56	BM	128	Total 2074	C 695	Н 1002	N 194	O 180	${ m S} { m 3}$	0	0

• Molecule 57 is a protein called PH domain-containing protein.

Mol	Chain	Residues		A	toms			AltConf	Trace
57	BN	133	Total 2229	C 716	Н 1126	N 196	O 191	0	0

• Molecule 58 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues			AltConf	Trace				
58	BO	136	Total 2156	C 690	Н 1058	N 190	O 208	S 10	0	0

• Molecule 59 is a protein called NDUB6.

Mol	Chain	Residues			Atom			AltConf	Trace	
59	BP	72	Total	C 404	H	N 100	0	S 4	0	0
			1194	404	590	100	90	4		

• Molecule 60 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

Mol	Chain	Residues			Aton	ns			AltConf	Trace
60	BQ	101	Total 1674	С 547	Н 829	N 140	O 153	${ m S}{ m 5}$	0	0

• Molecule 61 is a protein called Zinc-finger protein.

Mol	Chain	Residues			Aton	AltConf	Trace			
61	BR	91	Total 1449	C 460	Н 719	N 129	0 137	$\frac{S}{4}$	0	0

• Molecule 62 is a protein called NDUB4.



Mol	Chain	Residues			Aton	ns			AltConf	Trace
62	BS	120	Total 1907	C 621	Н 941	N 167	O 175	${ m S} { m 3}$	0	0

• Molecule 63 is a protein called NDUB15.

Mol	Chain	Residues			Aton	ıs			AltConf	Trace
63	BT	125	Total 2016	C 696	Н 953	N 172	O 190	${f S}{5}$	0	0

• Molecule 64 is a protein called NDUTT16.

Mol	Chain	Residues			AltConf	Trace				
64	BU	134	Total 2176	C 683	Н 1094	N 194	O 204	S 1	0	0

• Molecule 65 is a protein called NDUTT17.

Mol	Chain	Residues			AltConf	Trace				
65	BV	125	Total 2001	C 632	Н 1014	N 177	0 177	S 1	0	0

• Molecule 66 is a protein called CHCH domain-containing protein.

Mol	Chain	Residues			AltConf	Trace				
66	BW	118	Total 1848	C 603	Н 893	N 167	O 179	${ m S}{ m 6}$	0	0

• Molecule 67 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues		Α	AltConf	Trace			
67	BX	96	Total 1552	C 512	Н 755	N 139	O 146	0	0

• Molecule 68 is a protein called Ymf57.

Mol	Chain	Residues			AltConf	Trace				
68	BY	100	Total 1806	C 620	Н 917	N 128	0 138	${ m S} { m 3}$	0	0

• Molecule 69 is a protein called Complex I-MNLL.



Mol	Chain	Residues			AltConf	Trace				
69	BZ	102	Total 1690	C 553	Н 840	N 139	O 150	S 8	0	0

• Molecule 70 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
70	10	1	Total C H O P	0
10	AU	1	256 81 156 17 2	0
70	4.0	1	Total C H O P	0
10	AU	1	256 81 156 17 2	0
70	Δ 1	1	Total C H O P	0
10	ΛI	1	256 81 156 17 2	0
70	ΛΛ	1	Total C H O P	0
10	лл	1	256 81 156 17 2	0
70	ΔΔ	1	Total C H O P	0
10	ΠΠ	I	256 81 156 17 2	0
70	AC	1	Total C H O P	0
10	ΛU	I	256 81 156 17 2	0
70	AC	1	Total C H O P	0
10	ΛU	I	256 81 156 17 2	0
70	ΔF	1	Total C H O P	0
10		I	256 81 156 17 2	0
70	ΔF	1	Total C H O P	0
10		1	256 81 156 17 2	0
70	ΔM	1	Total C H O P	0
10		1	256 81 156 17 2	0



Mol	Chain	Residues		At	oms			AltConf
70	٨D	1	Total	С	Н	Ο	Р	0
10	AP	1	256	81	156	17	2	0
70	DO	1	Total	С	Η	Ο	Р	0
10	D0	1	256	81	156	17	2	0
70	D0	1	Total	С	Η	Ο	Р	0
10	D0	1	256	81	156	17	2	0
70	D1	1	Total	С	Η	Ο	Р	0
10	DI	1	256	81	156	17	2	0
70	BC	1	Total	С	Η	Ο	Р	0
10	DU	1	256	81	156	17	2	0
70	BC	1	Total	С	Η	Ο	Р	0
10	DC	1	256	81	156	17	2	0
70	BE	1	Total	С	Η	Ο	Р	0
10	DĽ	1	256	81	156	17	2	0
70	BC	1	Total	С	Η	Ο	Р	0
10	DG	1	256	81	156	17	2	0
70	BL.	1	Total	С	Η	Ο	Р	0
10	DL	1	256	81	156	17	2	0
70	вт	1	Total	\mathbf{C}	Η	Ο	Р	0
10	DI	I	256	81	156	17	2	0
70	BV	1	Total	\mathbf{C}	Η	Ο	Р	0
		L	256	81	156	17	2	0
70	BY	1	Total	\mathbf{C}	Η	Ο	Р	0
10		T	256	81	156	17	2	

• Molecule 71 is URIDINE-5'-DIPHOSPHATE (three-letter code: UDP) (formula: $C_9H_{14}N_2O_{12}P_2$) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues		AltConf					
71	10	1	Total	С	Η	Ν	0	Р	0
(1	AU	L	36	9	11	2	12	2	0

• Molecule 72 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
72	A0	1	Total Mg 1 1	0
72	A8	1	Total Mg 1 1	0

• Molecule 73 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: $C_{44}H_{88}NO_8P$).



Mol	Chain	Residues		A	tom	ıs			AltConf
73	4.0	1	Total	С	Η	Ν	0	Р	0
10	AU	T	142	44	88	1	8	1	0
72	Δ.1	1	Total	С	Η	Ν	0	Р	0
10	AI	L	142	44	88	1	8	1	0
73	Δ.1	1	Total	С	Η	Ν	0	Р	0
10		T	142	44	88	1	8	1	0
73	12	1	Total	С	Η	Ν	0	Р	0
10	ΛL	T	142	44	88	1	8	1	0
73	16	1	Total	С	Η	Ν	0	Р	0
10	AU	T	142	44	88	1	8	1	0
73	46	1	Total	С	Η	N	0	Р	0
10	ЛО	L	142	44	88	1	8	1	U



Continued from previous page...

Mol	Chain	Residues		A	tom	IS			AltConf
72	10	1	Total	С	Н	Ν	0	Р	0
13	A9	1	142	44	88	1	8	1	0
79	10	1	Total	С	Η	Ν	Ο	Р	0
10	A9	1	142	44	88	1	8	1	0
73	ΛΛ	1	Total	С	Η	Ν	0	Р	0
15	ЛЛ	I	142	44	88	1	8	1	0
73	ΔΔ	1	Total	\mathbf{C}	Η	Ν	Ο	Р	0
10		1	142	44	88	1	8	1	0
73	АА	1	Total	С	Η	Ν	Ο	Р	0
		1	142	44	88	1	8	1	Ŭ
73	AA	1	Total	С	Η	Ν	Ο	Р	0
		-	142	44	88	1	8	1	Ŭ
73	AA	1	Total	С	Н	Ν	0	Р	0
		_	142	44	88	1	8	1	
73	AH	1	Total	С	Н	Ν	0	Р	0
			142	44	88	1	8	1	
73	AJ	1	Total	С	Н	Ν	0	Р	0
			142	44	88	1	8	<u> </u>	
73	AL	1	Total	С	Н	N	Ô	Р	0
			142	44	88		8	<u> </u>	
73	AM	1	Total	C	H	N 1	0	P	0
			142	44	88	1	8	1 	
73	AQ	1	1 Iotal	C	H	IN 1	0	Р 1	0
			142 Tetal	$\frac{44}{C}$	88	1 	8		
73	AU	1	10tai		П 00	1N 1	0	Г 1	0
			Total	$\frac{44}{C}$	оо Ц	I N	0	1 D	
73	AU	1	100a1		11 88	1 I	8	1	0
			Total	$\frac{44}{C}$	<u>00</u> Н	I N	0	 р	
73	B1	1	1/12		88	1	8	1	0
			Total	-11 C	H	N	0	P	
73	B1	1	142	44	88	1	8	1	0
			Total	$\frac{\Gamma}{C}$	H	N	$\frac{0}{0}$	P	
73	BQ	1	142	44	88	1	8	1	0
			Total	$\frac{\Gamma}{C}$	H	N	$\overline{0}$	P	
73	BS	1	142	44	88	1	8	1	0
			Total	C	H	N	0	- P	
73	BS	1	142	44	88	1	8	1	0
			Total	C	Н	N	0	Р	
73	BT	1	142	44	88	1	8	1	0
		_	Total	C	Н	N	0	Р	
73	BY	1	142	44	88	1	8	1	0



• Molecule 74 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf	
74	Δ.1	1	Total	С	Η	Ν	Ο	Р	0
14	AI	1	74	21	26	7	17	3	0

• Molecule 75 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: $C_{41}H_{82}NO_8P$).





Mol	Chain	Residues		A	tom	ıs			AltConf		
75	1.9	1	Total	С	Η	Ν	Ο	Р	0		
15	A2	1	133	41	82	1	8	1	0		
75	10	1	Total	С	Η	Ν	Ο	Р	0		
15	A9	A9	A9	A9 1	133	41	82	1	8	1	0
75	4.0	1	Total	С	Η	Ν	0	Р	0		
15	A9	1	133	41	82	1	8	1	0		
75	ΔΤ	1	Total	С	Η	Ν	0	Р	0		
15	$\Lambda 0$	T	133	41	82	1	8	1	0		
75	BΔ	1	Total	С	Η	Ν	Ο	Р	0		
15	DA	1	133	41	82	1	8	1	0		
75	BĐ	1	Total	С	Η	N	Ō	Р	0		
10		1	133	41	82	1	8	1	0		

• Molecule 76 is 2-(HEXADECANOYLOXY)-1-[(PHOSPHONOOXY)METHYL]ETHYL HEXADECANOATE (three-letter code: LPP) (formula: C₃₅H₆₉O₈P).



Mol	Chain	Residues	Atoms					AltConf
76	16	1	Total	С	Η	Ο	Р	0
10	A0	L	111	35	67	8	1	0
76	ΛΛ	1	Total	С	Η	0	Р	0
10	10 AA	T	111	35	67	8	1	0
76	ΔT	1	Total	С	Η	Ο	Р	0
10	AL	L	111	35	67	8	1	0
76 DN	1	Total	С	Η	Ο	Р	0	
10	DN	L	111	35	67	8	1	0

• Molecule 77 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms					AltConf	
77	٨٩	1	Total	С	Η	Ν	Ο	Р	0
	1	39	10	12	5	10	2	0	
77	40	1	Total	С	Η	Ν	Ο	Р	0
((лQ		39	10	12	5	10	2	0

• Molecule 78 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
78	AB	1	TotalFeS422	0



Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
79	ΔŢ	1	Total Fe S	0
10	AI	1	4 2 2	0
79	BI	1	Total Fe S	0
10	DI	1	4 2 2	0

• Molecule 79 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
79	AB	1	Total Fe S 8 4 4	0
79	AB	1	TotalFeS844	0
79	AD	1	TotalFeS844	0
79	AL	1	TotalFeS844	0
79	AL	1	TotalFeS844	0
79	AT	1	TotalFeS844	0

• Molecule 80 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms						AltConf
80		1	Total	С	Η	Ν	0	Р	0
80	AD	1	49	17	18	4	9	1	0

• Molecule 81 is S-[2-({N-[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta -alanyl}amino)ethyl] dodecanethioate (three-letter code: 8Q1) (formula: $C_{23}H_{45}N_2O_8PS$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf		
Q1	٨S	1	Total	С	Η	Ν	0	Р	\mathbf{S}	0
01	AS	T	77	23	43	2	7	1	1	0

• Molecule 82 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of



Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
82	BR	1	Total Zn 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: Lipid-A-disaccharide synthase









F604 N380 T615 N380 T61 Y385 T62 Y41 T14 A11 A23 A411 A23 A425 T144 H426 T144 H426 T144 H426 T144 H43 F44 H43 F476 F











 \bullet Molecule 19: NADH-ubiquinone oxidore
ductase 24 kDa subunit



• Molecule 23: Gamma-carbonic anhydrase









Chain AY:	88%		12%
M1 I5 86 W8 I11	114 118 118 129 129 183 183 184 183 184 184 184 184 184		
• Molecule 3	6: Ribosomal protein $L51/S25/CI-B8$ domain protein		
Chain AZ:	85%	6%	9%
MET SER SER TRP Q5 K6 L7	H 11 E 14 E 23 R 30 R 31 R 41 R 41 R 44 R 64 R 65 R 7 R 7 R 7 R 7 R 7 R 7 R 7 R 7		
• Molecule 3	7: Transmembrane protein, putative		
Chain B0:	89%		10% •
MET V2 K11 112 113 V21	V25 D43 R51 R51 R87 R89 R89		
• Molecule 3	8: ATP synthase subunit e, mitochondrial		
Chain B1:	97%		
MET V2 E48 H55			
• Molecule 3	9: GRAM domain protein		
Chain B2:	9%90%		9% •
MET 82 M35 T40 L44 L44	K50 E76 M78 M78 H91 192 F93 Q94 Q94		
• Molecule 4	0: Transmembrane protein, putative		
Chain B3:	7%	%	12%
MET ASN SER PRO GLN CJN CJN ALA GLN GLN	AL1 N47 T48 D80 H82 H83 H83		
• Molecule 4	1: Transmembrane protein, putative		
Chain B4:	96%		·
M1 N2 R38 P45 F46	D553 P564 A 23 C 33 C 32 C 32		



• Molecule 42: Transm	embrane protein, putative	e	
Chain B5:	76%	24	%
MET ASP ASP TYR TYR TLE GLN GLN GLN GLN CYS SER FHE SER TLEU	18 11 11		
• Molecule 43: ND1b			
Chain B6:	78%	2	2%
M1 P2 P2 P2 P2 P2 P2 P2 P2 P2 P2	12 15 15 15 15 15 15 15 15 15 15 15 15 15		
• Molecule 44: Transm	embrane protein		
Chain BA:	86%		8% 6%
MET GLY GLY ASP ASP HIS HIS ASP ASP ASP ASP ASP ASP ASP ASP ASP AS	D17 E20 E20 M25 K27 K27 B34 H35 H35 H35 H50 H50 L51	L52 E53 E54 K55 H57 H57 A58 K59 K59 K59 N61 N61	Fes D66 Q67 K68 K70 E71 E71 E75 E75 C77 C77 C77 C78 C77 C78 C78 C78 C78 C78
A85 139 139 139 139 139 139 139 139 139 139	A177 K178 C185 C185 C185 C185 C185 C185 C185 C191 C192 N194 N194	E200 H201 L202 R203 H204 Y212	
• Molecule 45: Transm	embrane protein, putative	е	
Chain BB:	72%	6% 2	2%
MET ASIN PRO ARG ARG ASIN TILE PHE LEU ALLA ALLA ALLA ASIN ASIN ASIN	SER TILE TILE TILE CALM GLN PHHE CLY ALA ALA ALA ALA ALA ALA ALA ALA ALA A	Hask HIS HIS ASP ASP ASP ASP ASP G17 G12 G12 G12 G12 G12 G12 G12 G12 G12 G12	VS1 HIS2 CE9 D77 D77 D80
H81 H82 H83 H83 H84 B85 E86 M120 L144 L165 L165	P170 A171 B172 B125 R192 R192 L198 D196 C198 C198 C198 C198 C109 R201	E208	
• Molecule 46: NDUB8	3		
Chain BC:	79%		16%
MET ALA ALA ARG ARG ARG ARG CLIN CLU ARU CLIS ASN CLIS ASN CLIS CLIS CLIS CLIS CLIS	GLN ALA GLN ALA ALA ALA ALA ALA ALA ALA ALA ALA A	C C C C C C C C C C C C C C C C C C C	A161 K156 N165 C17 G17 A1A
THR GLN SER HIS HIS			
• Molecule 47: Transm	embrane protein, putative	e	
Chain BD:	66%	5% 28%	










• Molecule 60: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4





M1 K9 L10 E11 D15 M34 K22 K22 K22 K22 K22 K22 K22 K22 K22 K2	D54 V75 D82 R83 184 A105 A125	
• Molecule 66: CHCH d	lomain-containing protein	
Chain BW:	94%	
MET MET GLY GLY H4 E9 E9 E22 E22 E9 K70 K70 K98	A99 A101 A101 G103 L119 N120	
• Molecule 67: Transme	embrane protein, putative	
Chain BX:	80%	5% 15%
MET PHE TRP ARG ARG VAL VAL VAL VAL VAL CSS CSS CSS CSS CSS CSS CSS CSS CSS CS	1113 1113 1113 1113	
• Molecule 68: Ymf57		
Chain BY:	88%	12%
M1 115 142 142 142 142 143 143 144 144 144 144	154 100 1100 1100	
• Molecule 69: Complex	x I-MNLL	
Chain BZ:	96%	
M 82 82 82 84 86 86 86 86 86 86 86 86 86 86 86 86 86		



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	138746	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 $(e^-/\text{\AA}^2)$	25.66	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM $(4k \ge 4k)$	Depositor
Maximum map value	5.836	Depositor
Minimum map value	-2.721	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.179	Depositor
Recommended contour level	0.9	Depositor
Map size (Å)	600.0, 600.0, 600.0	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	$1.25, 1.25, \overline{1.25}$	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: CDL, 8Q1, SF4, 3PE, PC1, LPP, UDP, NDP, MG, ZN, FMN, ADP, 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		Bond lengths		Bond angles		
		RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A0	0.26	0/4166	0.44	0/5634	
2	A1	0.26	0/2789	0.47	0/3777	
3	A2	0.25	0/2248	0.48	0/3027	
4	A3	0.25	0/2308	0.45	0/3134	
5	A4	0.25	0/2542	0.43	0/3441	
6	A5	0.24	0/2408	0.46	0/3269	
7	A6	0.26	0/1963	0.47	0/2658	
8	A7	0.26	0/1108	0.41	0/1488	
9	A8	0.24	0/1833	0.44	0/2479	
10	A9	0.26	0/1935	0.44	0/2616	
11	AA	0.27	0/6132	0.40	0/8343	
12	AB	0.26	0/5511	0.50	0/7465	
13	AC	0.27	0/4303	0.40	0/5844	
14	AD	0.26	0/3474	0.49	0/4699	
15	AE	0.27	0/3669	0.48	0/4955	
16	AF	0.27	0/3168	0.38	0/4307	
17	AG	0.25	0/2865	0.47	0/3877	
18	AH	0.27	0/2377	0.41	0/3234	
19	AI	0.26	0/1899	0.46	0/2563	
20	AJ	0.27	0/2224	0.39	0/3025	
21	AK	0.26	0/1816	0.47	0/2475	
22	AL	0.29	0/1867	0.55	0/2538	
23	AM	0.26	0/1801	0.50	0/2449	
24	AN	0.25	0/1351	0.44	0/1817	
25	AO	0.25	0/1720	0.45	0/2322	
26	AP	0.25	0/1654	0.49	0/2240	
27	AQ	0.27	0/1636	0.43	0/2214	
28	AR	0.26	0/1535	0.48	0/2077	
29	AS	0.25	0/1458	0.47	0/1965	
30	AT	0.28	0/1310	0.54	0/1779	
31	AU	0.26	0/1261	0.47	0/1698	
32	AV	0.25	0/941	0.43	0/1272	



Mal	Chain	Bond lengths Bond		angles	
	Unain	RMSZ	# Z > 5	RMSZ	# Z > 5
33	AW	0.25	0/819	0.47	0/1110
34	AX	0.26	0/1061	0.39	0/1441
35	AY	0.25	0/982	0.40	0/1335
36	AZ	0.25	0/790	0.47	0/1066
37	B0	0.27	0/833	0.50	0/1132
38	B1	0.25	0/812	0.44	0/1093
39	B2	0.26	0/776	0.44	0/1048
40	B3	0.25	0/654	0.45	0/884
41	B4	0.26	0/642	0.47	0/865
42	B5	0.27	0/466	0.41	0/630
43	B6	0.28	0/535	0.43	0/727
44	BA	0.25	0/1696	0.41	0/2292
45	BB	0.25	0/1376	0.42	0/1862
46	BC	0.26	0/1479	0.47	0/1996
47	BD	0.25	0/1216	0.44	0/1643
48	BE	0.26	0/1462	0.43	0/1981
49	BF	0.25	0/1503	0.49	0/2018
50	BG	0.25	0/1379	0.49	0/1841
51	BH	0.27	0/1519	0.39	0/2058
52	BI	0.25	0/1203	0.48	0/1630
53	BJ	0.26	0/1234	0.44	0/1662
54	BK	0.26	0/923	0.43	0/1239
55	BL	0.26	0/1223	0.45	0/1648
56	BM	0.26	0/1110	0.46	0/1502
57	BN	0.25	0/1132	0.44	0/1534
58	BO	0.26	0/1120	0.46	0/1500
59	BP	0.30	0/631	0.42	0/860
60	BQ	0.26	0/868	0.43	0/1170
61	BR	0.25	0/747	0.45	0/1011
62	BS	0.26	0/991	0.42	0/1333
63	BT	0.28	0/1106	0.41	0/1504
64	BU	0.24	0/1102	0.45	0/1486
65	BV	0.25	0/1003	0.46	0/1353
66	BW	0.26	0/983	0.40	0/1327
67	BX	0.27	0/821	0.46	0/1111
68	BY	0.28	0/916	0.41	0/1224
69	BZ	0.26	0/873	0.43	0/1175
All	All	0.26	0/115258	0.45	0/155972

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	A0	4071	4019	4018	28	0
2	A1	2718	2650	2649	9	0
3	A2	2199	2163	2160	13	0
4	A3	2263	2260	2260	15	0
5	A4	2494	2491	2491	10	0
6	A5	2347	2249	2249	22	0
7	A6	1908	1862	1861	14	0
8	A7	1084	1040	1039	12	0
9	A8	1794	1803	1800	11	0
10	A9	1879	1818	1818	6	0
11	AA	5941	5978	5977	47	0
12	AB	5403	5359	5358	49	0
13	AC	4170	4223	4223	33	0
14	AD	3399	3345	3345	33	0
15	AE	3587	3539	3539	37	0
16	AF	3068	3148	3147	31	0
17	AG	2804	2727	2727	13	0
18	AH	2306	2350	2349	21	0
19	AI	1862	1848	1847	14	0
20	AJ	2160	2156	2155	13	0
21	AK	1779	1740	1739	15	0
22	AL	1812	1689	1688	27	0
23	AM	1770	1788	1788	15	0
24	AN	1322	1329	1328	10	0
25	AO	1683	1680	1680	17	0
26	AP	1599	1505	1504	13	0
27	AQ	1588	1496	1495	6	0
28	AR	1492	1445	1445	5	0
29	AS	1420	1382	1382	6	0
30	AT	1277	1272	1271	19	0
31	AU	1227	1209	1208	5	0
32	AV	925	904	903	4	0
33	AW	803	781	780	5	0
34	AX	1027	1020	1020	13	0



Conti	Continuea from previous page						
Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes	
35	AY	957	987	987	13	0	
36	AZ	777	775	774	3	0	
37	B0	805	802	801	6	0	
38	B1	790	746	745	1	0	
39	B2	757	728	727	7	0	
40	B3	633	618	617	4	0	
41	B4	624	623	623	3	0	
42	B5	453	464	463	0	0	
43	B6	515	528	528	11	0	
44	BA	1651	1638	1637	12	0	
45	BB	1346	1280	1279	10	0	
46	BC	1442	1406	1405	7	0	
47	BD	1191	1223	1222	12	0	
48	BE	1422	1385	1384	5	0	
49	BF	1475	1486	1485	20	0	
50	BG	1349	1376	1375	13	0	
51	BH	1482	1554	1554	15	0	
52	BI	1179	1139	1134	10	0	
53	BJ	1205	1156	1155	3	0	
54	BK	903	854	853	2	0	
55	BL	1187	1138	1137	9	0	
56	BM	1072	1002	1001	10	0	
57	BN	1103	1126	1125	10	0	
58	BO	1098	1058	1058	3	0	
59	BP	604	590	589	7	0	
60	BQ	845	829	828	7	0	
61	BR	730	719	718	1	0	
62	BS	966	941	940	5	0	
63	BT	1063	953	950	9	0	
64	BU	1082	1094	1094	9	0	
65	BV	987	1014	1014	1	0	
66	BW	955	893	892	4	0	
67	BX	797	755	754	6	0	
68	BY	889	917	917	10	0	
69	BZ	850	840	840	4	0	
70	A0	200	312	312	1	0	
70	A1	100	156	156	0	0	
70	AA	200	312	312	3	0	
70	AC	200	312	312	0	0	
70	AF	200	312	312	0	0	
70	AM	100	156	156	0	0	
70	AP	100	156	156	3	0	



Conti	nuea fron	<i>i previous</i>	page			
Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
70	B0	200	312	312	1	0
70	B1	100	156	156	0	0
70	BC	200	312	312	1	0
70	BE	100	156	156	1	0
70	BG	100	156	156	0	0
70	BL	100	156	156	1	0
70	BT	100	156	156	0	0
70	BV	100	156	156	0	0
70	BY	100	156	156	0	0
71	A0	25	11	11	2	0
72	A0	1	0	0	0	0
72	A8	1	0	0	0	0
73	A0	54	88	88	0	0
73	A1	108	176	176	0	0
73	A2	54	88	88	0	0
73	A6	108	176	176	2	0
73	A9	108	176	176	0	0
73	AA	270	440	440	0	0
73	AH	54	88	88	0	0
73	AJ	54	88	88	0	0
73	AL	54	88	88	2	0
73	AM	54	88	88	0	0
73	AQ	54	88	88	0	0
73	AU	108	176	176	0	0
73	B1	108	176	176	0	0
73	BQ	54	88	88	0	0
73	BS	108	176	176	1	0
73	BT	54	88	88	1	0
73	BY	54	88	88	0	0
74	A1	48	26	25	0	0
75	A2	51	82	82	0	0
75	A9	102	164	164	1	0
75	AJ	51	82	82	0	0
75	BA	51	82	82	1	0
75	BP	51	82	82	0	0
76	A6	44	67	67	0	0
76	AA	44	67	67	1	0
76	AL	44	67	67	2	0
76	BN	44	67	67	0	0
77	A8	27	12	12	0	0
77	AQ	27	12	12	0	0
78	AB	4	0	0	1	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
78	AI	4	0	0	2	0
78	BI	4	0	0	1	0
79	AB	16	0	0	3	0
79	AD	8	0	0	1	0
79	AL	16	0	0	6	0
79	AT	8	0	0	0	0
80	AD	31	18	19	0	0
81	AS	34	43	0	2	0
82	BR	1	0	0	0	0
All	All	116760	117595	117495	670	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

The worst 5 of 670 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} \text{Interatomic} \\ \text{distance} \ (\text{\AA}) \end{array}$	Clash overlap (Å)
26:AP:3:LEU:N	70:AP:301:CDL:OA3	1.70	1.23
17:AG:54:ARG:O	23:AM:225:GLN:NE2	2.11	0.82
24:AN:105:LYS:NZ	25:AO:52:GLU:OE2	2.14	0.80
14:AD:40:ARG:NH1	14:AD:290:GLU:O	2.16	0.79
70:AP:301:CDL:OA4	70:AP:301:CDL:O1	2.00	0.79

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	A0	501/516~(97%)	486 (97%)	15 (3%)	0	100	100
2	A1	336/362~(93%)	329(98%)	7 (2%)	0	100	100



~	0		
Continued	trom	nreminus	naae
Continucu	110110	pretious	page

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
3	A2	263/317~(83%)	260 (99%)	3 (1%)	0	100	100
4	A3	289/333~(87%)	285 (99%)	4 (1%)	0	100	100
5	A4	309/311~(99%)	302 (98%)	7 (2%)	0	100	100
6	A5	280/282~(99%)	279 (100%)	1 (0%)	0	100	100
7	A6	228/251~(91%)	224 (98%)	4 (2%)	0	100	100
8	A7	131/238~(55%)	129 (98%)	2 (2%)	0	100	100
9	A8	215/217~(99%)	209 (97%)	6 (3%)	0	100	100
10	A9	229/231~(99%)	227 (99%)	2 (1%)	0	100	100
11	AA	711/750~(95%)	691 (97%)	19 (3%)	1 (0%)	51	81
12	AB	686/718~(96%)	671 (98%)	15 (2%)	0	100	100
13	AC	503/505~(100%)	490 (97%)	13 (3%)	0	100	100
14	AD	439/474~(93%)	425 (97%)	14 (3%)	0	100	100
15	AE	439/442~(99%)	430 (98%)	9 (2%)	0	100	100
16	AF	357/360~(99%)	348 (98%)	9 (2%)	0	100	100
17	AG	344/346~(99%)	339 (98%)	5 (2%)	0	100	100
18	AH	281/284~(99%)	273 (97%)	8 (3%)	0	100	100
19	AI	229/274~(84%)	228 (100%)	1 (0%)	0	100	100
20	AJ	252/255~(99%)	246 (98%)	6 (2%)	0	100	100
21	AK	228/257~(89%)	220 (96%)	8 (4%)	0	100	100
22	AL	216/236~(92%)	209 (97%)	7 (3%)	0	100	100
23	AM	229/233~(98%)	220 (96%)	8 (4%)	1 (0%)	34	66
24	AN	155/206~(75%)	155 (100%)	0	0	100	100
25	AO	196/198~(99%)	192 (98%)	4 (2%)	0	100	100
26	AP	189/194~(97%)	183 (97%)	6 (3%)	0	100	100
27	AQ	185/189~(98%)	182 (98%)	3 (2%)	0	100	100
28	AR	179/185~(97%)	177 (99%)	2 (1%)	0	100	100
29	AS	170/172~(99%)	169 (99%)	1 (1%)	0	100	100
30	AT	$\overline{159/162} \ (98\%)$	152 (96%)	7 (4%)	0	100	100
31	AU	147/150 (98%)	145 (99%)	2 (1%)	0	100	100
32	AV	110/138 (80%)	109 (99%)	1 (1%)	0	100	100
33	AW	96/133~(72%)	94 (98%)	2 (2%)	0	100	100



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
34	AX	119/121~(98%)	115 (97%)	4 (3%)	0	100	100
35	AY	114/116~(98%)	114 (100%)	0	0	100	100
36	AZ	92/103~(89%)	89 (97%)	3 (3%)	0	100	100
37	B0	91/94~(97%)	91 (100%)	0	0	100	100
38	B1	90/93~(97%)	89 (99%)	1 (1%)	0	100	100
39	B2	91/94~(97%)	89 (98%)	2 (2%)	0	100	100
40	B3	71/83~(86%)	68 (96%)	3 (4%)	0	100	100
41	B4	71/73~(97%)	71 (100%)	0	0	100	100
42	B5	52/71~(73%)	52 (100%)	0	0	100	100
43	B6	57/59~(97%)	54 (95%)	3 (5%)	0	100	100
44	BA	197/212~(93%)	194 (98%)	3 (2%)	0	100	100
45	BB	165/214~(77%)	164 (99%)	1 (1%)	0	100	100
46	BC	171/207~(83%)	170 (99%)	1 (1%)	0	100	100
47	BD	146/205~(71%)	145 (99%)	1 (1%)	0	100	100
48	BE	166/189~(88%)	160 (96%)	6 (4%)	0	100	100
49	BF	175/188~(93%)	167 (95%)	8 (5%)	0	100	100
50	BG	158/175~(90%)	154 (98%)	4 (2%)	0	100	100
51	BH	176/178~(99%)	172 (98%)	4 (2%)	0	100	100
52	BI	147/172~(86%)	145~(99%)	2 (1%)	0	100	100
53	BJ	142/166~(86%)	142 (100%)	0	0	100	100
54	BK	107/144~(74%)	106 (99%)	1 (1%)	0	100	100
55	BL	140/143~(98%)	137 (98%)	3 (2%)	0	100	100
56	BM	126/135~(93%)	119 (94%)	7 (6%)	0	100	100
57	BN	131/135~(97%)	128 (98%)	3 (2%)	0	100	100
58	BO	134/136~(98%)	133~(99%)	1 (1%)	0	100	100
59	BP	70/129~(54%)	69 (99%)	1 (1%)	0	100	100
60	BQ	99/127~(78%)	97 (98%)	2 (2%)	0	100	100
61	BR	$89/132~(\overline{67\%})$	88 (99%)	1 (1%)	0	100	100
62	BS	118/126~(94%)	115 (98%)	3 (2%)	0	100	100
63	BT	$123/125~(\overline{98\%})$	123 (100%)	0	0	100	100
64	BU	132/134~(98%)	131 (99%)	1 (1%)	0	100	100



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
65	BV	123/125~(98%)	120 (98%)	3(2%)	0	100	100
66	BW	116/120~(97%)	111 (96%)	5 (4%)	0	100	100
67	BX	94/113~(83%)	93~(99%)	1 (1%)	0	100	100
68	BY	98/100~(98%)	93~(95%)	5(5%)	0	100	100
69	ΒZ	100/102~(98%)	100 (100%)	0	0	100	100
All	All	13572/14758~(92%)	13286 (98%)	284 (2%)	2(0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	AA	119	GLU
23	AM	51	PRO

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	Percentiles
1	A0	441/454~(97%)	433~(98%)	8 (2%)	59 86
2	A1	288/311~(93%)	287~(100%)	1 (0%)	92 98
3	A2	225/270~(83%)	222~(99%)	3 (1%)	69 91
4	A3	244/280~(87%)	242~(99%)	2(1%)	81 94
5	A4	275/275~(100%)	273~(99%)	2 (1%)	84 95
6	A5	257/257~(100%)	257~(100%)	0	100 100
7	A6	207/223~(93%)	206 (100%)	1 (0%)	88 96
8	A7	122/224~(54%)	122 (100%)	0	100 100
9	A8	195/195~(100%)	194 (100%)	1 (0%)	88 96
10	A9	199/199~(100%)	195~(98%)	4 (2%)	55 84
11	AA	657/694~(95%)	644~(98%)	13~(2%)	55 84
12	AB	589/617~(96%)	586 (100%)	3 (0%)	88 96
13	AC	$46\overline{3}/463~(100\%)$	458 (99%)	5 (1%)	73 92



α i 1	ſ	• • • • •	
Continuea	Jrom	previous	page

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	AD	361/392~(92%)	359~(99%)	2(1%)	86	96
15	AE	398/399~(100%)	389~(98%)	9 (2%)	50	82
16	AF	346/347~(100%)	346 (100%)	0	100	100
17	AG	309/309~(100%)	307~(99%)	2 (1%)	86	96
18	AH	249/250~(100%)	245 (98%)	4 (2%)	62	88
19	AI	206/236~(87%)	205 (100%)	1 (0%)	88	96
20	AJ	243/244~(100%)	242 (100%)	1 (0%)	91	97
21	AK	196/218~(90%)	194 (99%)	2 (1%)	76	93
22	AL	197/215~(92%)	194 (98%)	3 (2%)	65	89
23	AM	196/197~(100%)	193 (98%)	3 (2%)	65	89
24	AN	146/186~(78%)	146 (100%)	0	100	100
25	AO	191/191~(100%)	191 (100%)	0	100	100
26	AP	168/170~(99%)	168 (100%)	0	100	100
27	AQ	170/172~(99%)	168 (99%)	2 (1%)	71	92
28	AR	159/163~(98%)	158 (99%)	1 (1%)	86	96
29	AS	154/154~(100%)	152 (99%)	2 (1%)	69	91
30	AT	136/137~(99%)	131 (96%)	5 (4%)	34	68
31	AU	132/133~(99%)	131 (99%)	1 (1%)	81	94
32	AV	104/129~(81%)	104 (100%)	0	100	100
33	AW	87/119 (73%)	87 (100%)	0	100	100
34	AX	112/112~(100%)	109 (97%)	3 (3%)	44	78
35	AY	108/108~(100%)	108 (100%)	0	100	100
36	AZ	84/93~(90%)	84 (100%)	0	100	100
37	B0	88/89~(99%)	88 (100%)	0	100	100
38	B1	83/84~(99%)	82 (99%)	1 (1%)	71	92
39	B2	82/83~(99%)	82 (100%)	0	100	100
40	B3	66/74~(89%)	66 (100%)	0	100	100
41	B4	65/65~(100%)	65 (100%)	0	100	100
42	B5	48/63~(76%)	48 (100%)	0	100	100
43	B6	55/55~(100%)	54 (98%)	1 (2%)	59	86
44	BA	179/190~(94%)	178 (99%)	1 (1%)	86	96



Mol	Chain	Analysed	Rotameric	otameric Outliers		Percentiles		
45	BB	145/182~(80%)	145 (100%)	0	100	100		
46	BC	155/180~(86%)	154 (99%)	1 (1%)	86	96		
47	BD	124/179~(69%)	123 (99%)	1 (1%)	81	94		
48	BE	159/178~(89%)	157~(99%)	2 (1%)	69	91		
49	BF	161/172~(94%)	161 (100%)	0	100	100		
50	BG	142/156~(91%)	141 (99%)	1 (1%)	84	95		
51	BH	170/170~(100%)	170 (100%)	0	100	100		
52	BI	131/152~(86%)	130 (99%)	1 (1%)	81	94		
53	BJ	128/147~(87%)	127 (99%)	1 (1%)	81	94		
54	BK	97/131 (74%)	97 (100%)	0	100	100		
55	BL	124/125~(99%)	123 (99%)	1 (1%)	81	94		
56	BM	108/114~(95%)	107 (99%)	1 (1%)	78	94		
57	BN	120/122~(98%)	120 (100%)	0	100	100		
58	BO	122/122~(100%)	122 (100%)	0	100	100		
59	BP	64/117~(55%)	64 (100%)	0	100	100		
60	BQ	93/117~(80%)	93 (100%)	0	100	100		
61	BR	81/116 (70%)	80 (99%)	1 (1%)	71	92		
62	BS	103/109~(94%)	103 (100%)	0	100	100		
63	BT	110/110 (100%)	103 (94%)	7 (6%)	17	45		
64	BU	121/121~(100%)	120 (99%)	1 (1%)	81	94		
65	BV	102/102~(100%)	102 (100%)	0	100	100		
66	BW	98/99~(99%)	98 (100%)	0	100	100		
67	BX	81/97~(84%)	81 (100%)	0	100	100		
68	BY	98/98~(100%)	98 (100%)	0	100	100		
69	ΒZ	89/89~(100%)	89 (100%)	0	100	100		
All	All	12206/13144~(93%)	12101 (99%)	105 (1%)	79	94		

5 of 105 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
18	AH	167	LEU
27	AQ	22	TYR
63	BT	52	VAL



 $Continued \ from \ previous \ page...$

Mol	Chain	Res	Type
18	AH	245	TYR
22	AL	155	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
11	AA	168	ASN
27	AQ	63	ASN
61	BR	109	HIS
1	A0	452	ASN
1	A0	450	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 77 ligands modelled in this entry, 3 are monoatomic - leaving 74 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with |Z| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol Type	Type	Type Chain	Dog	Link	B	ond leng	gths	Bo	nd angle	es
WIOI	туре	Ullalli	n Res Link		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
70	CDL	A1	402	-	99,99,99	1.20	7 (7%)	105,111,111	0.68	2 (1%)



Mol	Type	Chain	Dog	Link	В	ond leng	gths	Bo	nd angle	es
	Type	Ullalli	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
70	CDL	AF	401	-	99,99,99	1.19	8 (8%)	105,111,111	0.74	1 (0%)
73	PC1	A6	303	-	53,53,53	1.07	3 (5%)	59,61,61	0.60	1 (1%)
73	PC1	AQ	202	-	$53,\!53,\!53$	1.09	3(5%)	59,61,61	0.63	1 (1%)
75	3PE	BA	301	-	50,50,50	1.06	5 (10%)	$53,\!55,\!55$	0.58	0
70	CDL	AC	802	-	99,99,99	1.18	7 (7%)	105,111,111	0.67	0
70	CDL	BC	302	-	99,99,99	1.19	7 (7%)	105,111,111	0.73	1 (0%)
70	CDL	BY	201	-	99,99,99	1.20	8 (8%)	105,111,111	0.73	2 (1%)
71	UDP	A0	603	72	24,26,26	3.62	14 (58%)	37,40,40	1.49	5 (13%)
73	PC1	A9	604	-	53,53,53	1.05	3 (5%)	59,61,61	0.63	0
74	NDP	A1	401	-	45,52,52	4.23	20 (44%)	53,80,80	1.66	5 (9%)
70	CDL	BC	301	-	99,99,99	1.18	7 (7%)	105,111,111	0.74	1 (0%)
70	CDL	AM	301	-	99,99,99	1.21	9 (9%)	105,111,111	0.69	2 (1%)
70	CDL	B0	101	-	99,99,99	1.19	7 (7%)	105,111,111	0.72	2 (1%)
70	CDL	BT	201	-	99,99,99	1.21	8 (8%)	105,111,111	0.67	2 (1%)
73	PC1	A0	605	-	53,53,53	1.07	3 (5%)	59,61,61	0.59	0
76	LPP	AA	902	-	43,43,43	0.91	3 (6%)	47,48,48	0.71	1 (2%)
73	PC1	AU	201	-	53,53,53	1.06	3 (5%)	59,61,61	0.58	0
73	PC1	BY	202	-	53,53,53	1.06	3 (5%)	59,61,61	0.61	1 (1%)
75	3PE	A2	401	-	50,50,50	1.07	5 (10%)	53,55,55	0.65	1 (1%)
81	8Q1	AS	200	-	27,33,34	1.59	4 (14%)	32,40,43	1.53	6 (18%)
76	LPP	A6	301	-	43,43,43	0.90	3 (6%)	47,48,48	0.93	1 (2%)
73	PC1	BS	1301	-	53,53,53	1.04	3 (5%)	59,61,61	0.66	2(3%)
75	3PE	A9	603	-	50,50,50	1.07	5 (10%)	53,55,55	0.66	1 (1%)
73	PC1	AA	904	-	53,53,53	1.04	3 (5%)	59,61,61	0.72	1 (1%)
73	PC1	B1	403	-	53,53,53	1.07	3 (5%)	59,61,61	0.54	0
70	CDL	BV	201	-	99,99,99	1.17	7 (7%)	105,111,111	0.66	0
77	ADP	A8	401	72	24,29,29	3.56	10 (41%)	29,45,45	<mark>3.39</mark>	6 (20%)
79	SF4	AL	301	22	0,12,12	-	-	-		
70	CDL	B0	102	-	99,99,99	1.19	7 (7%)	105,111,111	0.68	2 (1%)
70	CDL	BL	301	-	99,99,99	1.18	7 (7%)	105,111,111	0.72	2 (1%)
70	CDL	AC	801	-	99,99,99	1.15	7 (7%)	105,111,111	0.74	2 (1%)
73	PC1	A2	402	-	53,53,53	1.05	3 (5%)	59,61,61	0.62	0
73	PC1	BT	202	-	53,53,53	1.06	3 (5%)	59,61,61	0.71	2 (3%)
73	PC1	AA	905	-	53,53,53	1.06	3 (5%)	59,61,61	0.58	0
73	PC1	AM	302	-	53,53,53	1.06	3 (5%)	59,61,61	0.62	1 (1%)



Mal	Turne	Chain	Dec	Tink	В	Bond lengths		Bond angles		
	Type	Chain	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
78	FES	BI	201	52	0,4,4	-	-	-		
76	LPP	BN	301	-	43,43,43	0.90	3 (6%)	47,48,48	0.73	1 (2%)
79	SF4	AD	501	14	0,12,12	-	-	-		
70	CDL	AF	402	-	99,99,99	1.19	7 (7%)	105,111,111	0.70	2 (1%)
73	PC1	BS	1302	-	$53,\!53,\!53$	1.06	3 (5%)	59,61,61	0.60	1 (1%)
79	SF4	AB	802	12	0,12,12	-	-	-		
73	PC1	AU	202	-	$53,\!53,\!53$	1.06	3 (5%)	59,61,61	0.62	0
70	CDL	AP	301	-	99,99,99	1.17	6 (6%)	105,111,111	0.75	0
70	CDL	BG	201	-	99,99,99	1.19	7 (7%)	105,111,111	0.73	3 (2%)
79	SF4	AT	201	30	0,12,12	-	-	_		
73	PC1	A1	404	-	$53,\!53,\!53$	1.06	3 (5%)	59,61,61	0.75	2 (3%)
77	ADP	AQ	201	-	24,29,29	3.55	9 (37%)	29,45,45	3.43	7 (24%)
80	FMN	AD	502	-	33,33,33	0.72	0	48,50,50	0.78	0
78	FES	AB	801	12	0,4,4	-	-	-		
73	PC1	A9	601	-	$53,\!53,\!53$	1.07	3 (5%)	59,61,61	0.58	1 (1%)
73	PC1	BQ	401	-	$53,\!53,\!53$	1.06	3 (5%)	59,61,61	0.58	0
73	PC1	AA	903	-	53,53,53	1.06	3 (5%)	59,61,61	0.64	1 (1%)
70	CDL	AA	908	-	99,99,99	1.16	6 (6%)	105,111,111	0.68	1 (0%)
76	LPP	AL	304	-	43,43,43	0.90	3 (6%)	47,48,48	0.68	1 (2%)
73	PC1	A1	403	-	53,53,53	1.09	3 (5%)	59,61,61	0.62	1 (1%)
79	SF4	AL	302	22	0,12,12	-	-	-		I
73	PC1	AH	301	-	$53,\!53,\!53$	1.07	3 (5%)	59,61,61	0.60	0
78	FES	AI	301	19	0,4,4	-	-	-		
70	CDL	BE	201	-	99,99,99	1.19	8 (8%)	105,111,111	0.74	2 (1%)
73	PC1	AA	907	-	53,53,53	1.07	3 (5%)	59,61,61	0.56	1 (1%)
73	PC1	AJ	501	-	53,53,53	1.06	3 (5%)	59,61,61	0.64	1 (1%)
73	PC1	AL	303	-	53,53,53	1.06	3 (5%)	59,61,61	0.72	1 (1%)
70	CDL	A0	601	-	99,99,99	1.17	7 (7%)	105,111,111	0.77	1 (0%)
70	CDL	AA	901	_	99,99,99	1.19	7 (7%)	105,111,111	0.74	2 (1%)
73	PC1	B1	401	-	53,53,53	1.07	3 (5%)	59,61,61	0.68	1 (1%)
70	CDL	B1	402	_	99,99,99	1.19	7 (7%)	105,111,111	0.64	1 (0%)
73	PC1	A6	302	-	53,53,53	1.08	3 (5%)	59,61,61	0.66	1 (1%)
79	SF4	AB	803	12	0,12,12	-	_	-		
73	PC1	AA	906	-	53,53,53	1.06	3 (5%)	59,61,61	0.68	1 (1%)
70	CDL	A0	602	-	99,99,99	1.19	8 (8%)	105,111,111	0.75	2 (1%)
75	3PE	AJ	502	-	50,50,50	1.05	5 (10%)	53,55,55	0.71	1 (1%)



Mal	I Toma Chain Dag Linh		Bond lengths			Bond angles				
NIOI	туре	Chain	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
75	3PE	A9	602	-	$50,\!50,\!50$	1.09	5 (10%)	$53,\!55,\!55$	1.01	5 (9%)
75	3PE	BP	201	-	50,50,50	1.07	5 (10%)	$53,\!55,\!55$	0.71	1 (1%)

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
70	CDL	A1	402	-	-	33/110/110/110	-
70	CDL	AF	401	-	-	20/110/110/110	-
73	PC1	A6	303	-	-	9/57/57/57	-
73	PC1	AQ	202	-	-	18/57/57/57	-
75	3PE	BA	301	-	-	19/54/54/54	-
70	CDL	AC	802	-	-	26/110/110/110	-
70	CDL	BC	302	-	-	23/110/110/110	-
70	CDL	BY	201	-	-	21/110/110/110	-
71	UDP	A0	603	72	-	7/16/32/32	0/2/2/2
73	PC1	A9	604	-	-	20/57/57/57	-
74	NDP	A1	401	-	-	7/30/77/77	0/5/5/5
70	CDL	BC	301	-	-	19/110/110/110	-
70	CDL	AM	301	-	-	26/110/110/110	-
70	CDL	B0	101	-	-	30/110/110/110	-
70	CDL	BT	201	-	-	21/110/110/110	-
73	PC1	A0	605	-	-	14/57/57/57	-
76	LPP	AA	902	-	-	10/45/45/45	-
73	PC1	AU	201	-	-	12/57/57/57	-
73	PC1	BY	202	-	-	12/57/57/57	-
75	3PE	A2	401	-	-	8/54/54/54	-
81	8Q1	AS	200	-	-	10/38/40/41	-
76	LPP	A6	301	-	-	9/45/45/45	-
73	PC1	BS	1301	-	-	16/57/57/57	-
75	3PE	A9	603	-	-	7/54/54/54	-
73	PC1	AA	904	_	-	15/57/57/57	-
73	PC1	B1	403	-	-	15/57/57/57	-
70	CDL	BV	201	-	-	18/110/110/110	-



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
77	ADP	A8	401	72	-	0/12/32/32	0/3/3/3
79	SF4	AL	301	22	-	-	0/6/5/5
70	CDL	B0	102	-	-	21/110/110/110	-
70	CDL	BL	301	-	-	17/110/110/110	-
70	CDL	AC	801	-	-	25/110/110/110	-
73	PC1	A2	402	-	-	8/57/57/57	-
73	PC1	BT	202	-	-	13/57/57/57	-
73	PC1	AA	905	-	-	17/57/57/57	-
73	PC1	AM	302	-	-	17/57/57/57	-
78	FES	BI	201	52	-	-	0/1/1/1
76	LPP	BN	301	-	-	7/45/45/45	-
79	SF4	AD	501	14	-	-	0/6/5/5
70	CDL	AF	402	-	-	27/110/110/110	-
73	PC1	BS	1302	_	-	10/57/57/57	_
79	SF4	AB	802	12	-	-	0/6/5/5
73	PC1	AU	202	-	-	13/57/57/57	-
70	CDL	AP	301	-	-	24/110/110/110	-
70	CDL	BG	201	-	-	36/110/110/110	-
79	SF4	AT	201	30	-	-	0/6/5/5
73	PC1	A1	404	-	-	13/57/57/57	-
77	ADP	AQ	201	-	-	1/12/32/32	0/3/3/3
80	FMN	AD	502	-	-	7/18/18/18	0/3/3/3
78	FES	AB	801	12	-	-	0/1/1/1
73	PC1	A9	601	-	-	15/57/57/57	-
73	PC1	BQ	401	-	-	21/57/57/57	-
73	PC1	AA	903	-	-	14/57/57/57	_
70	CDL	AA	908	-	-	31/110/110/110	-
76	LPP	AL	304	-	-	4/45/45/45	-
73	PC1	A1	403	-	-	6/57/57/57	-
79	SF4	AL	302	22	-	-	0/6/5/5
73	PC1	AH	301	-	-	8/57/57/57	-
78	FES	AI	301	19	-	-	0/1/1/1
70	CDL	BE	201	-	-	31/110/110/110	-
73	PC1	AA	907	-	-	21/57/57/57	-
73	PC1	AJ	501	-	-	17/57/57/57	-
73	PC1	AL	303	-	-	9/57/57/57	-



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
70	CDL	A0	601	-	-	21/110/110/110	-
70	CDL	AA	901	-	-	23/110/110/110	-
73	PC1	B1	401	-	-	18/57/57/57	-
70	CDL	B1	402	-	-	26/110/110/110	-
73	PC1	A6	302	-	-	11/57/57/57	-
79	SF4	AB	803	12	-	-	0/6/5/5
73	PC1	AA	906	-	-	20/57/57/57	-
70	CDL	A0	602	-	-	25/110/110/110	-
75	3PE	AJ	502	-	-	12/54/54/54	-
75	3PE	A9	602	-	-	16/54/54/54	-
75	3PE	BP	201	-	-	13/54/54/54	-

The worst 5 of 339 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
74	A1	401	NDP	O4B-C1B	14.77	1.61	1.41
74	A1	401	NDP	C6N-C5N	12.07	1.54	1.33
77	AQ	201	ADP	C2'-C3'	-11.05	1.23	1.53
77	A8	401	ADP	C2'-C3'	-10.99	1.23	1.53
74	A1	401	NDP	C2D-C3D	-10.66	1.24	1.53

The worst 5 of 96 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms		$Observed(^{o})$	$Ideal(^{o})$
77	AQ	201	ADP	C1'-N9-C4	10.73	145.50	126.64
77	A8	401	ADP	C1'-N9-C4	10.72	145.48	126.64
77	A8	401	ADP	C5-C6-N6	10.44	136.21	120.35
77	AQ	201	ADP	C5-C6-N6	10.28	135.98	120.35
74	A1	401	NDP	C5A-C6A-N6A	7.25	131.37	120.35

There are no chirality outliers.

5 of 1063 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
70	A0	601	CDL	C11-CA5-OA6-CA4
70	A0	601	CDL	CB3-OB5-PB2-OB4
70	A0	601	CDL	C51-CB5-OB6-CB4
70	A0	602	CDL	C1-CB2-OB2-PB2
70	A0	602	CDL	OB5-CB3-CB4-OB6



There are no ring outliers.

26 monomers are involved in 40 short contacts	::
-----------------------------------------------	----

Mol	Chain	Res	Type	Clashes	Symm-Clashes
73	A6	303	PC1	2	0
75	BA	301	3PE	1	0
70	BC	302	CDL	1	0
71	A0	603	UDP	2	0
76	AA	902	LPP	1	0
81	AS	200	8Q1	2	0
73	BS	1301	PC1	1	0
79	AL	301	SF4	1	0
70	B0	102	CDL	1	0
70	BL	301	CDL	1	0
73	BT	202	PC1	1	0
78	BI	201	FES	1	0
79	AD	501	SF4	1	0
79	AB	802	SF4	1	0
70	AP	301	CDL	3	0
78	AB	801	FES	1	0
70	AA	908	CDL	1	0
76	AL	304	LPP	2	0
79	AL	302	SF4	5	0
78	AI	301	FES	2	0
70	BE	201	CDL	1	0
73	AL	303	PC1	2	0
70	AA	901	CDL	2	0
79	AB	803	SF4	2	0
70	A0	602	CDL	1	0
75	A9	602	3PE	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 sufficient 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-15865. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

6.1.1 Primary map



6.1.2 Raw map



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



6.2 Central slices (i)

6.2.1 Primary map



X Index: 240



Y Index: 240



Z Index: 240

6.2.2 Raw 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: 243



Y Index: 278



Z Index: 177

6.3.2 Raw map



X Index: 244

Y Index: 278



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



6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map



6.4.2 Raw map



The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.



6.5 Orthogonal surface views (i)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.9. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.



Mask visualisation (i) 6.6

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

$emd_{15865}msk_{1.map}$ (i) 6.6.1





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 843 $\rm nm^3;$ this corresponds to an approximate mass of 762 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 0.357 \AA^{-1}



8 Fourier-Shell correlation (i)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.357 ${\rm \AA^{-1}}$



8.2 Resolution estimates (i)

$\mathbf{Bosolution} \text{ ostimato } (\mathbf{\hat{\lambda}})$	Estimation criterion (FSC cut-off)		
Resolution estimate (A)	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	2.76	3.23	2.80
Unmasked-calculated*	4.06	8.35	4.19

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.06 differs from the reported value 2.8 by more than 10 %



9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-15865 and PDB model 8B6F. 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 0.9 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 (0.9).



9.4 Atom inclusion (i)



At the recommended contour level, 68% of all backbone atoms, 68% of all non-hydrogen atoms, are inside the map.



9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.9) and Q-score for the entire model and for each chain.

\mathbf{Chain}	Atom inclusion	$\mathbf{Q} extsf{-score}$
All	0.6850	0.4630
A0	0.6510	0.4540
A1	0.7180	0.4840
A2	0.6830	0.4610
A3	0.5250	0.4510
A4	0.5720	0.3870
A5	0.7200	0.4890
A6	0.6880	0.4230
A7	0.7030	0.4540
A8	0.7050	0.5010
A9	0.6710	0.4470
AA	0.6540	0.4260
AB	0.6810	0.4860
AC	0.7300	0.4560
AD	0.6030	0.4830
AE	0.7770	0.5050
AF	0.7440	0.4730
AG	0.7320	0.4920
AH	0.7330	0.4880
AI	0.5940	0.4700
AJ	0.7320	0.4760
AK	0.7860	0.4980
AL	0.7750	0.5100
AM	0.7110	0.4730
AN	0.7220	0.5010
AO	0.7760	0.5070
AP	0.7300	0.4960
AQ	0.7220	0.4490
AR	0.7110	0.5000
AS	0.7760	0.4920
AT	0.7850	0.5010
AU	0.6610	0.4630
AV	0.7020	0.4770
AW	0.7040	0.4570
AX	0.7480	0.4870

0.0 <.00

1.0

Continued on next page...



Continued from previous page...

Chain	Atom inclusion	Q-score
AY	0.7590	0.4970
AZ	0.6130	0.4490
B0	0.6870	0.4590
B1	0.6490	0.4560
B2	0.6810	0.4490
B3	0.7020	0.4380
B4	0.6300	0.4390
B5	0.6950	0.4610
B6	0.7880	0.5130
BA	0.5750	0.3710
BB	0.6560	0.4170
BC	0.6560	0.4260
BD	0.6600	0.4210
BE	0.6510	0.4250
BF	0.7190	0.4340
BG	0.7080	0.4670
BH	0.7700	0.4720
BI	0.7840	0.4840
BJ	0.7350	0.4660
BK	0.6760	0.4410
BL	0.6770	0.4640
BM	0.7490	0.4790
BN	0.6820	0.4520
BO	0.6460	0.4250
BP	0.7360	0.4550
BQ	0.6620	0.4510
BR	0.7480	0.5090
BS	0.6650	0.4120
BT	0.6930	0.4480
BU	0.5560	0.4140
BV	0.6830	0.4420
BW	0.6900	0.4210
BX	0.7190	0.4580
BY	0.7080	0.4600
BZ	0.7220	0.4640

