wwPDB EM Validation Summary Report (i)

Sep 8, 2026 – 08:52 am BST

PDB ID	:	7ZDJ / pdb_00007zdj
EMDB ID	:	EMD-14651
Title	:	Complex I from Ovis aries at pH5.5, Open state
Authors	:	Petrova, O.; Sazanov, L.
Deposited on	:	2022-03-29
Resolution	:	3.25 Å(reported)
Based on initial model	:	6ZKE

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 (i)) were used in the production of this report:

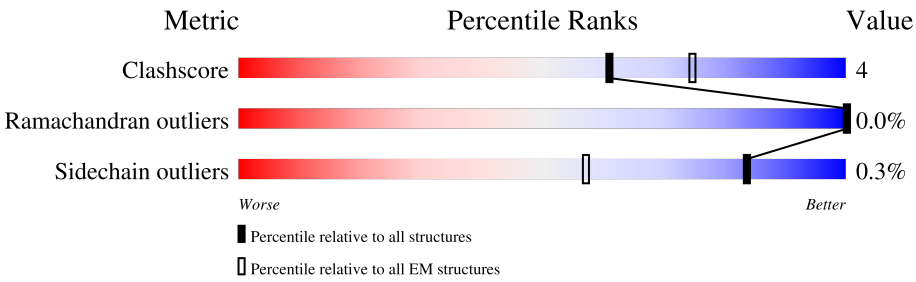
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

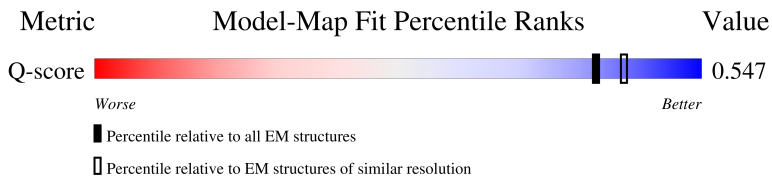
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.25 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.





Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14599 (2.75 - 3.75)

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	4	463	78% 13% 9%
2	A	115	9% 85% 10%
3	H	318	85% 14%
4	J	175	79% 17%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	K	98	89% 11%
6	L	606	86% 14%
7	M	459	87% 13%
8	N	347	86% 14%
9	V	140	94% 6%
10	W	139	89% 11%
11	X	157	41% 14% 45%
11	j	157	19% 46% 6% 48%
12	Y	171	89% 11%
13	Z	171	93% 7%
14	k	320	86% 14%
15	l	105	89% 11%
16	m	80	89% 11%
17	n	79	9% 86% 14%
18	o	120	88% 12%
19	p	128	6% 91% 9%
20	q	144	83% 13%
21	r	128	5% 64% 13% 23%
22	s	122	11% 89% 11%
23	t	177	8% 89% 11%
24	u	65	5% 86% 14%
25	v	155	89% 11%
26	w	101	6% 82% 18%
27	x	49	94% 6%
28	y	50	8% 86% 14%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
29	z	70	87% 13%
30	1	430	90% 10%
31	2	213	89% 11%
32	3	688	88% 12%
33	5	208	85% 15%
34	6	156	87% 13%
35	9	176	91% 9%
36	a	44	5% 82% 18%
37	b	95	6% 94% 6%
38	c	126	5% 91% 9%
39	d	380	6% 71% 7% 22%
40	e	86	7% 91% 9%
41	f	113	5% 89% 11%
42	g	114	7% 85% 15%
43	h	114	5% 78% 6% 16%
44	i	145	6% 91% 9%

2 Entry composition (i)

There are 53 unique types of molecules in this entry. The entry contains 65812 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 Complex I-49kD.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	4	421	3390	2165	581	619	25	0	0

- Molecule 2 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	A	110	880	593	128	153	6	0	0

- Molecule 3 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	H	314	2498	1685	380	414	19	0	0

- Molecule 4 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	J	169	1294	870	185	226	13	0	0

- Molecule 5 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	K	98	749	490	112	132	15	0	0

- Molecule 6 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	L	606	4806	3187	746	829	44	0	0

- Molecule 7 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	M	459	3647	2429	571	607	40	0	0

- Molecule 8 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	N	347	2723	1808	416	459	40	0	0

- Molecule 9 is a protein called Complex I-B14.7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	V	140	1028	656	175	191	6	0	0

- Molecule 10 is a protein called Complex I-SGDH.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	W	139	1155	761	194	198	2	0	0

- Molecule 11 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	X	87	701	451	103	142	5	0	0
11	j	82	660	425	98	132	5	0	0

- Molecule 12 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	Y	171	1403	889	253	251	10	0	0

- Molecule 13 is a protein called Complex I-PDSW.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	Z	171	1441	905	266	262	8	0	0

- Molecule 14 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	N	O	P	S		
14	k	320	2596	1659	432	494	1	10	0	0

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	l	105	874	551	164	153	6	0	0

- Molecule 16 is a protein called Complex I-B9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	m	80	626	411	103	110	2	0	0

- Molecule 17 is a protein called Complex I-B12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	n	79	634	415	106	111	2	0	0

- Molecule 18 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	o	120	1004	652	175	172	5	0	0

- Molecule 19 is a protein called NADH:ubiquinone oxidoreductase subunit B4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	p	128	1059	675	189	194	1	0	0

- Molecule 20 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	q	139	1142	733	200	200	9	0	0

- Molecule 21 is a protein called Mitochondrial complex I, B17 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	r	99	846	554	149	142	1	0	0

- Molecule 22 is a protein called Complex I-B18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	s	122	1047	653	199	186	9	0	0

- Molecule 23 is a protein called Complex I-B22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	t	177	1520	973	279	262	6	0	0

- Molecule 24 is a protein called Complex I-AGGG.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	u	65	563	372	93	97	1	0	0

- Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	v	155	1307	846	213	239	9	0	0

- Molecule 26 is a protein called Complex I-ESSS.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	w	101	846	542	140	160	4	0	0

- Molecule 27 is a protein called Complex I-KFYI.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
27	x	49	412	271	70	71	0	0

- Molecule 28 is a protein called Complex I-MNLL.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
28	y	50	436	287	77	72	0	0

- Molecule 29 is a protein called Complex I-MWFE.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	z	70	576	369	106	96	5	0	0

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	1	430	3312	2086	593	613	20	0	0

- Molecule 31 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	2	213	1655	1058	278	309	10	0	0

- Molecule 32 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	3	688	5275	3301	922	1011	41	0	0

- Molecule 33 is a protein called Complex I-30kD.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	5	208	1726	1112	296	315	3	0	0

- Molecule 34 is a protein called Complex I-20kD.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	6	156	1247	795	225	213	14	0	0

- Molecule 35 is a protein called Complex I-23kD.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	9	176	1414	889	243	270	12	0	0

- Molecule 36 is a protein called Complex I-9kD.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	a	44	371	233	66	71	1	0	0

- Molecule 37 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	b	95	737	451	139	144	3	0	0

- Molecule 38 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	c	126	1024	646	182	193	3	0	0

- Molecule 39 is a protein called NADH:ubiquinone oxidoreductase subunit A9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	d	297	2372	1516	432	419	5	0	0

- Molecule 40 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	e	86	691	434	129	126	2	0	0

- Molecule 41 is a protein called Complex I subunit B13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	f	113	917	595	153	167	2	0	0

- Molecule 42 is a protein called Complex I-B14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	g	114	969	619	180	166	4	0	0

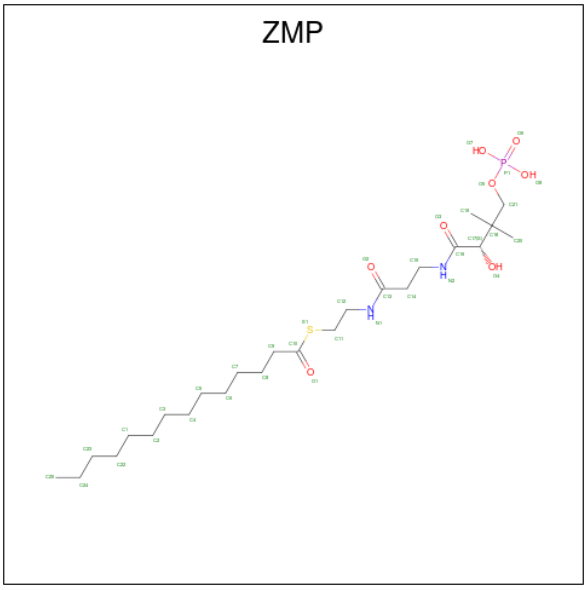
- Molecule 43 is a protein called Mitochondrial complex I, B14.5a subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	h	96	769	480	146	140	3	0	0

- Molecule 44 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

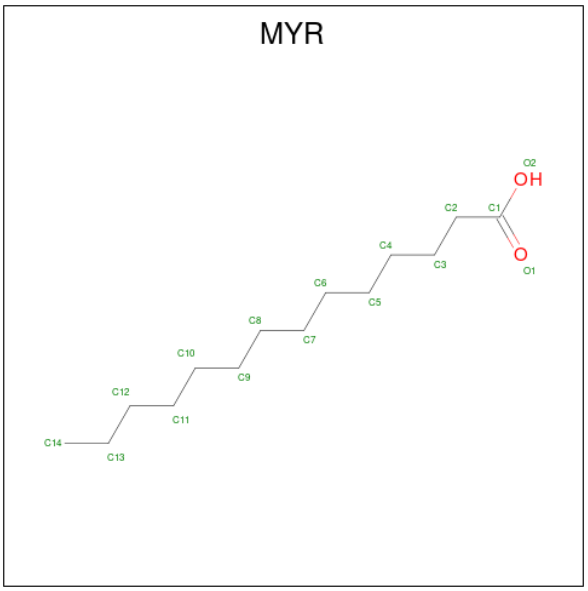
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	i	145	1209	778	216	210	5	0	0

- Molecule 45 is S-[2-({N-[(2S)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] tetradecanethioate (CCD ID: ZMP) (formula: $C_{25}H_{49}N_2O_8PS$).



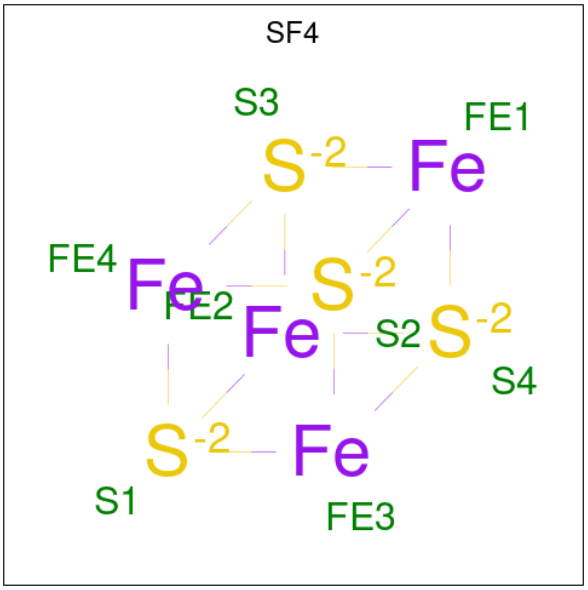
Mol	Chain	Residues	Atoms						AltConf
			Total	C	N	O	P	S	
45	X	1	31	20	2	7	1	1	0
			Total	C	N	O	P	S	
45	j	1	34	23	2	7	1	1	0

- Molecule 46 is MYRISTIC ACID (CCD ID: MYR) (formula: $C_{14}H_{28}O_2$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
46	s	1	15	14	1	0

- Molecule 47 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



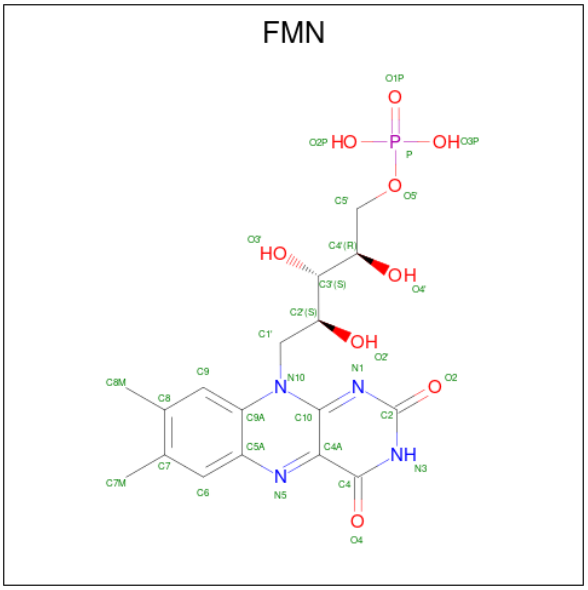
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
47	1	1	8	4	4	0
			Total	Fe	S	
47	3	1	8	4	4	0
			Total	Fe	S	
47	3	1	8	4	4	0

Continued on next page...

Continued from previous page...

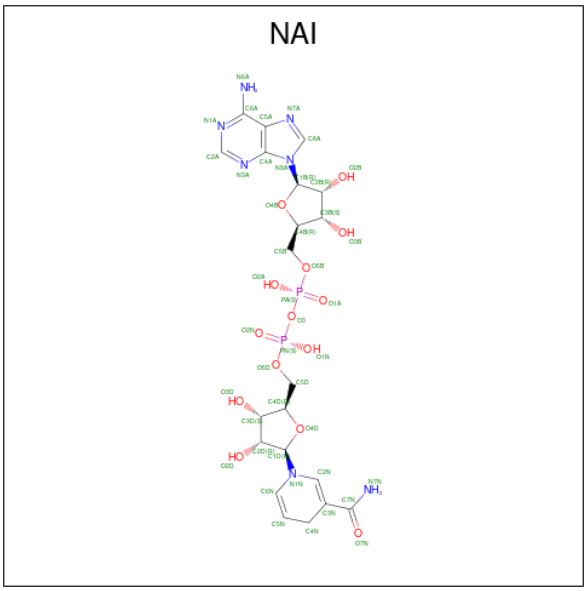
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
47	6	1	8	4	4	0
			Total	Fe	S	
47	9	1	8	4	4	0
			Total	Fe	S	
47	9	1	8	4	4	0

- Molecule 48 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



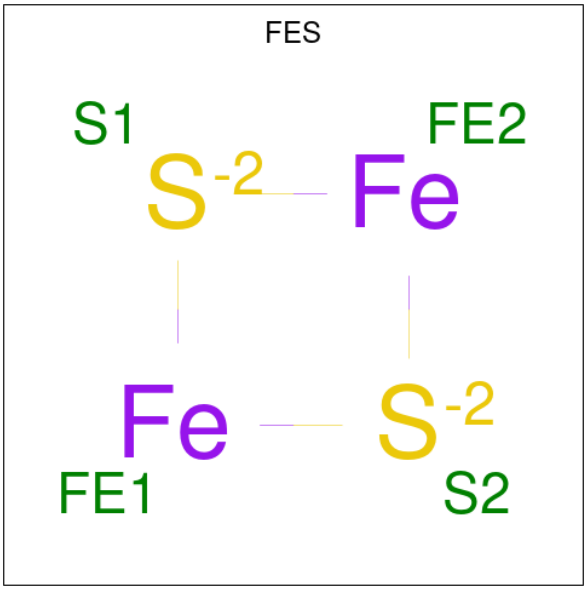
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
48	1	1	31	17	4	9	1	0

- Molecule 49 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (CCD ID: NAI) (formula: $C_{21}H_{29}N_7O_{14}P_2$).



Mol	Chain	Residues	Atoms					AltConf
49	1	1	Total	C	N	O	P	0
			44	21	7	14	2	

- Molecule 50 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms			AltConf
50	2	1	Total	Fe	S	0
			4	2	2	
50	3	1	Total	Fe	S	0
			4	2	2	

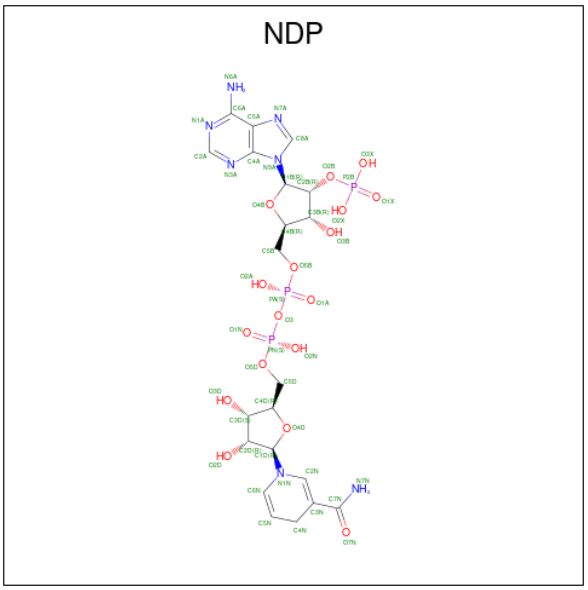
- Molecule 51 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
			Total	K	
51	3	1	1	1	0

- Molecule 52 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
52	b	1	1	1	0

- Molecule 53 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



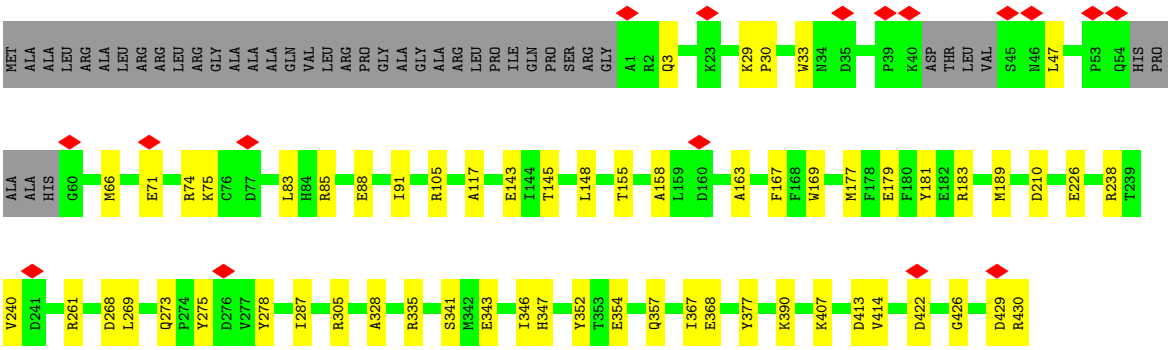
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
53	d	1	48	21	7	17	3	0

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.

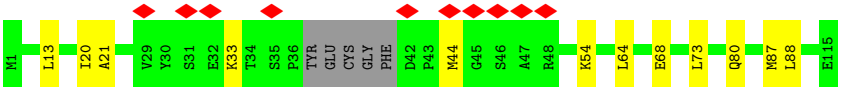
- Molecule 1: Complex I-49kD

Chain 4:



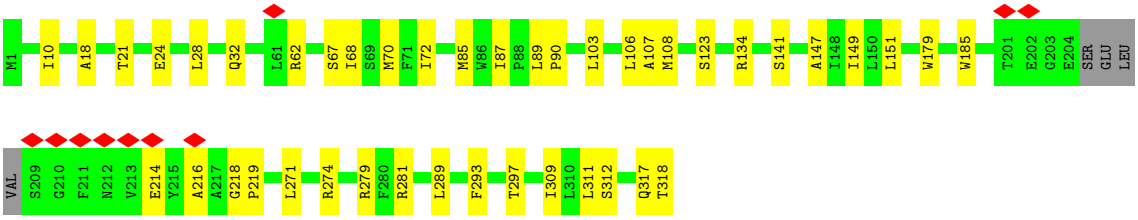
- Molecule 2: NADH-ubiquinone oxidoreductase chain 3

Chain A:



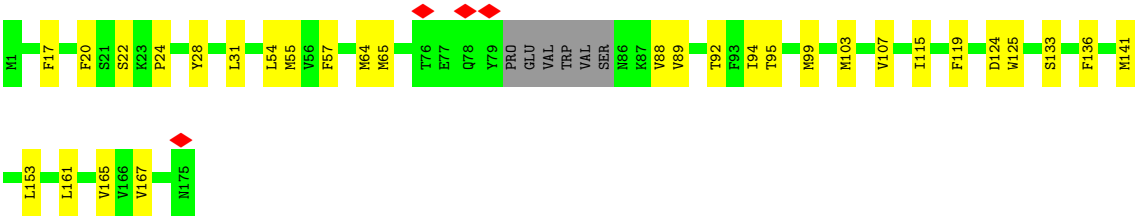
- Molecule 3: NADH-ubiquinone oxidoreductase chain 1

Chain H:



- Molecule 4: NADH-ubiquinone oxidoreductase chain 6

Chain J:

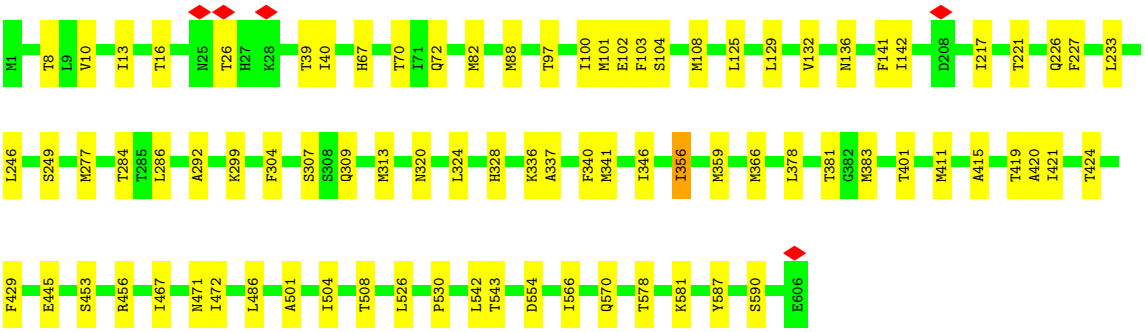


• Molecule 5: NADH-ubiquinone oxidoreductase chain 4L

Chain K:

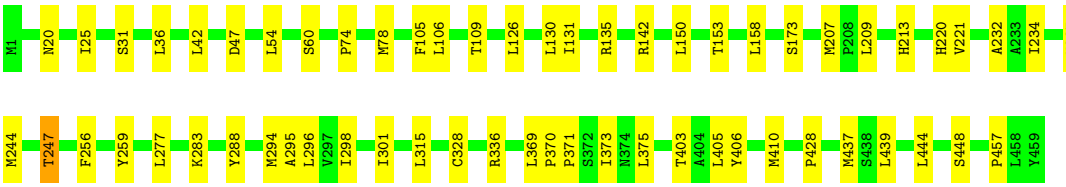
• Molecule 6: NADH-ubiquinone oxidoreductase chain 5

Chain L:



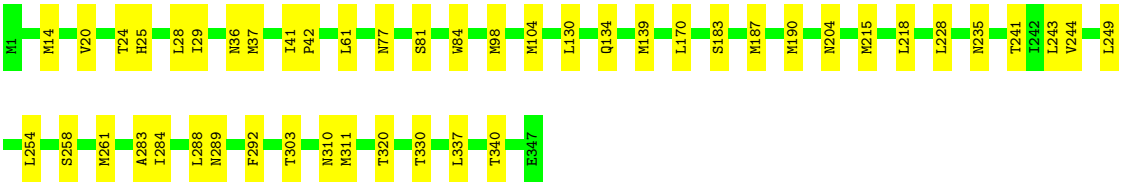
• Molecule 7: NADH-ubiquinone oxidoreductase chain 4

Chain M:



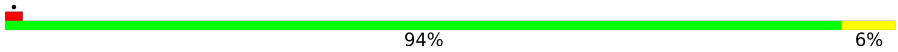
• Molecule 8: NADH-ubiquinone oxidoreductase chain 2

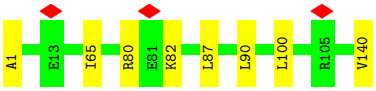
Chain N:



• Molecule 9: Complex I-B14.7

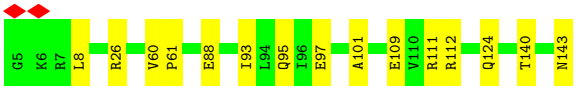
Chain V:





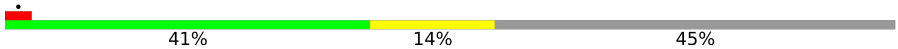
• Molecule 10: Complex I-SGDH

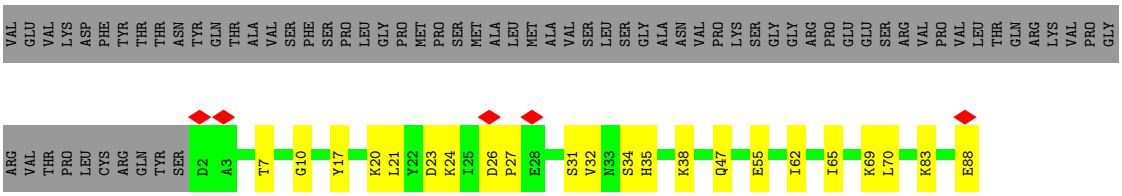
Chain W:



• Molecule 11: Acyl carrier protein

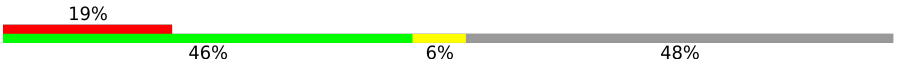
Chain X:

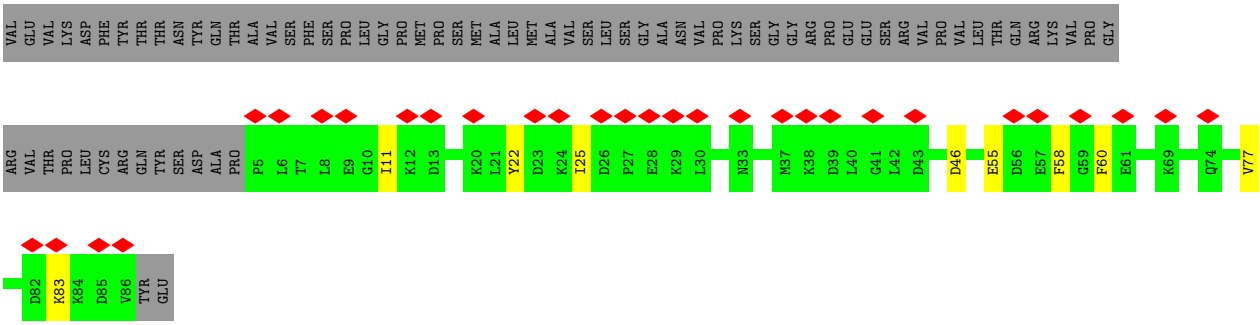




• Molecule 11: Acyl carrier protein

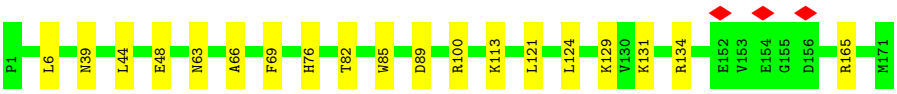
Chain j:





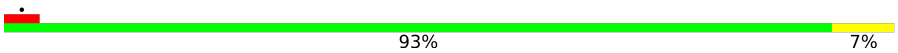
• Molecule 12: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

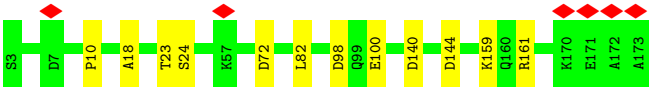
Chain Y:



• Molecule 13: Complex I-PDSW

Chain Z:





• Molecule 14: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

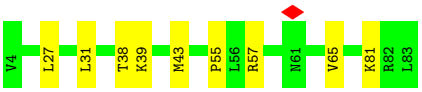
Chain k:

• Molecule 15: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

Chain l:

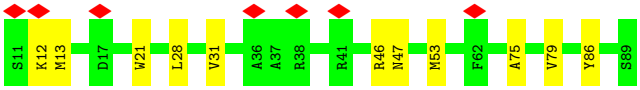
• Molecule 16: Complex I-B9

Chain m:



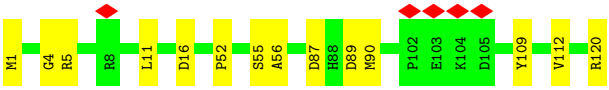
• Molecule 17: Complex I-B12

Chain n:



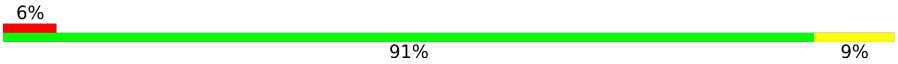
• Molecule 18: NADH dehydrogenase [ubiquinone] 1 subunit C2

Chain o:



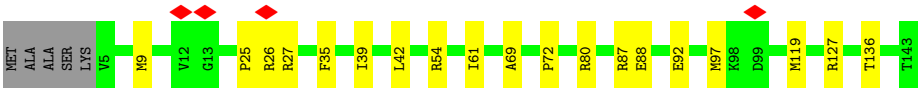
• Molecule 19: NADH:ubiquinone oxidoreductase subunit B4

Chain p:



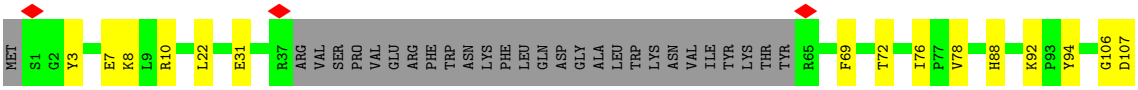
• Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

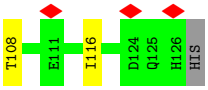
Chain q:



• Molecule 21: Mitochondrial complex I, B17 subunit

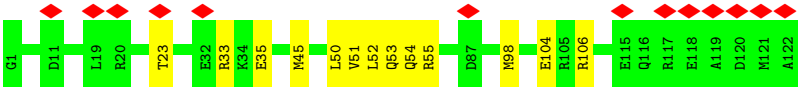
Chain r:





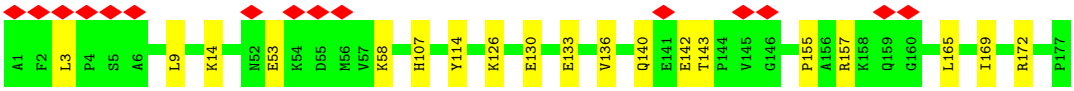
• Molecule 22: Complex I-B18

Chain s:



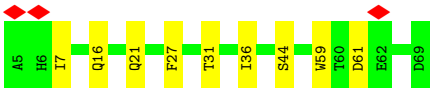
• Molecule 23: Complex I-B22

Chain t:



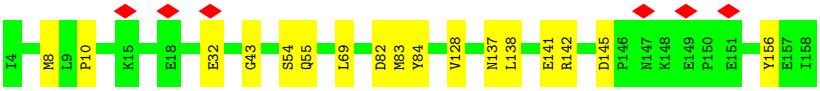
• Molecule 24: Complex I-AGGG

Chain u:



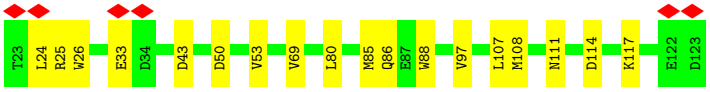
• Molecule 25: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

Chain v:



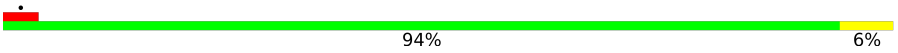
• Molecule 26: Complex I-ESSS

Chain w:



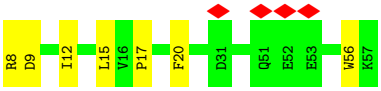
• Molecule 27: Complex I-KFYI

Chain x:



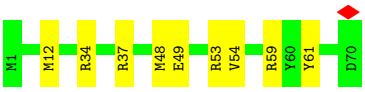
• Molecule 28: Complex I-MNLL

Chain y:



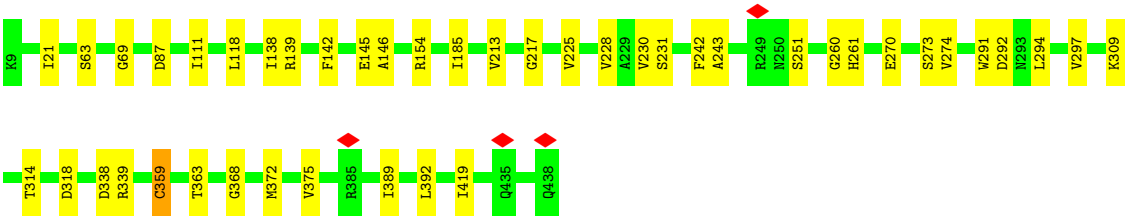
• Molecule 29: Complex I-MWFE

Chain z:



• Molecule 30: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

Chain 1:

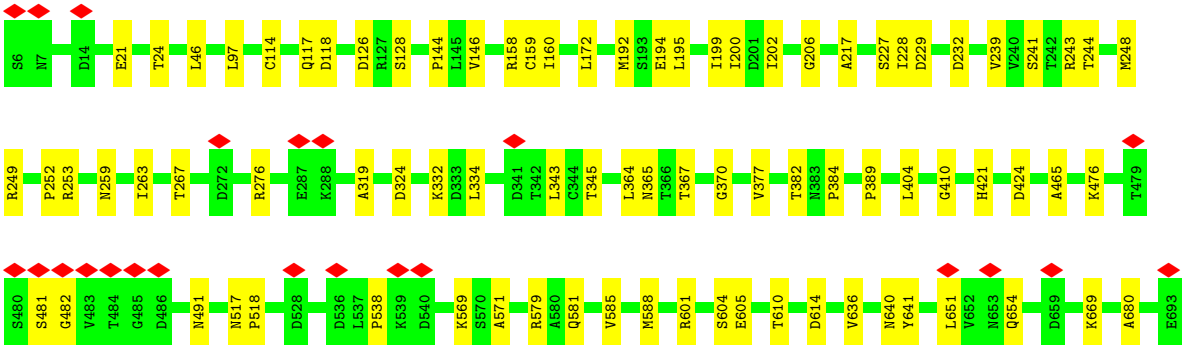


• Molecule 31: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

Chain 2:

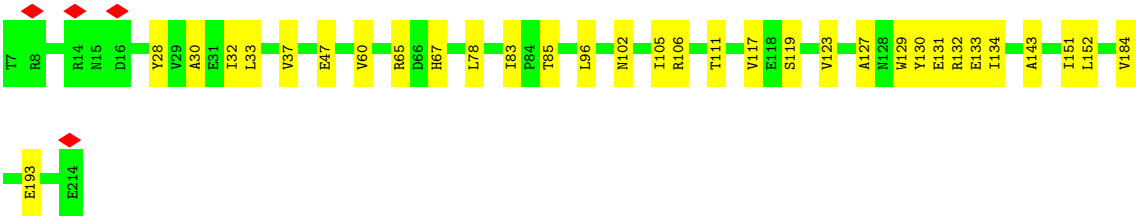
• Molecule 32: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

Chain 3:



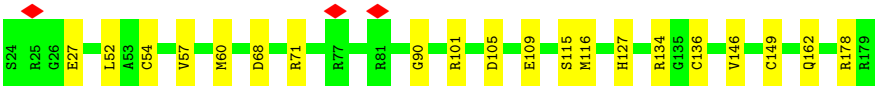
• Molecule 33: Complex I-30kD

Chain 5:



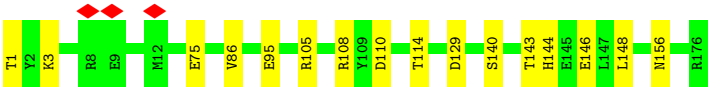
• Molecule 34: Complex I-20kD

Chain 6:



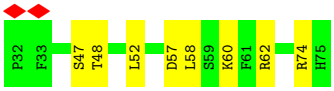
• Molecule 35: Complex I-23kD

Chain 9:



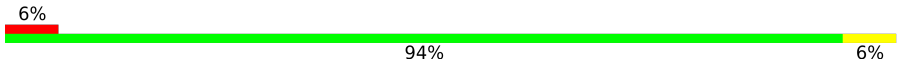
• Molecule 36: Complex I-9kD

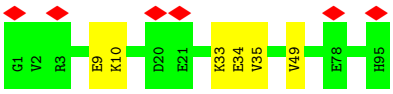
Chain a:



• Molecule 37: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

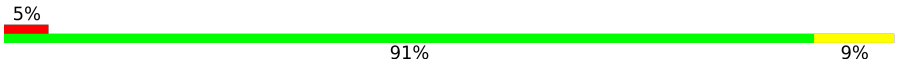
Chain b:

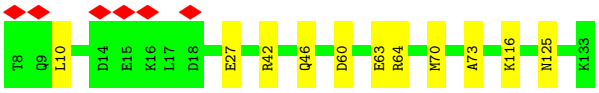




• Molecule 38: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

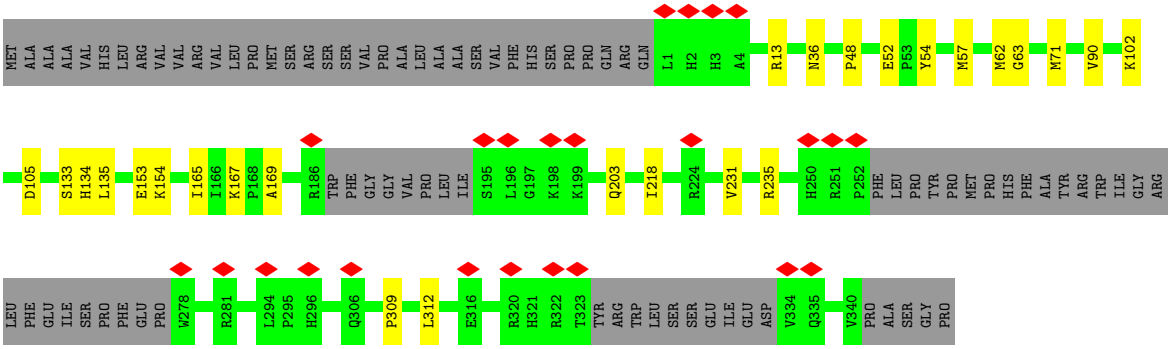
Chain c:





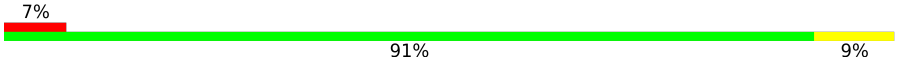
• Molecule 39: NADH:ubiquinone oxidoreductase subunit A9

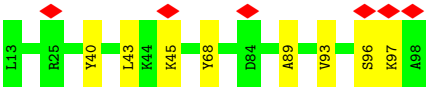
Chain d:



• Molecule 40: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

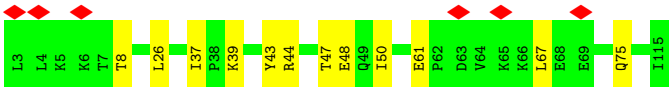
Chain e:





• Molecule 41: Complex I subunit B13

Chain f:

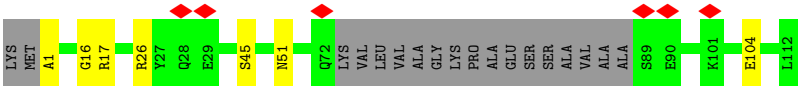


• Molecule 42: Complex I-B14

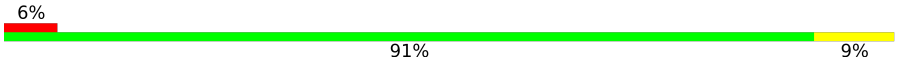
Chain g:

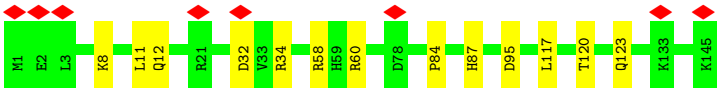
- Molecule 43: Mitochondrial complex I, B14.5a subunit

Chain h:



- Molecule 44: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

Chain i: 



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	97548	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	90	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	120000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.455	Depositor
Minimum map value	-0.078	Depositor
Average map value	0.008	Depositor
Map value standard deviation	0.025	Depositor
Recommended contour level	0.07	Depositor
Map size (Å)	173.24, 201.3, 287.92	wwPDB
Map dimensions	236, 165, 142	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.22, 1.22, 1.22	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: ZN, AYA, FMN, SEP, 2MR, FME, FES, NAI, SF4, ZMP, NDP, MYR, K

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	4	0.14	0/3463	0.31	0/4687
2	A	0.20	0/902	0.47	0/1234
3	H	0.25	1/2572 (0.0%)	0.47	0/3517
4	J	0.20	0/1324	0.46	0/1790
5	K	0.22	0/749	0.44	0/1014
6	L	0.20	0/4924	0.45	0/6698
7	M	0.22	0/3731	0.46	0/5085
8	N	0.22	0/2787	0.44	0/3795
9	V	0.14	0/1041	0.30	0/1412
10	W	0.17	0/1188	0.35	0/1607
11	X	0.15	0/713	0.44	0/963
11	j	0.17	0/670	0.45	0/902
12	Y	0.16	0/1440	0.34	0/1942
13	Z	0.16	0/1475	0.34	0/1989
14	k	0.14	0/2646	0.32	0/3579
15	l	0.16	0/896	0.45	2/1200 (0.2%)
16	m	0.16	0/647	0.40	0/890
17	n	0.16	0/653	0.34	0/882
18	o	0.17	0/1035	0.33	0/1398
19	p	0.16	0/1085	0.32	0/1467
20	q	0.19	0/1171	0.41	0/1579
21	r	0.19	0/874	0.45	0/1188
22	s	0.17	0/1072	0.42	0/1436
23	t	0.15	0/1573	0.37	0/2130
24	u	0.15	0/590	0.35	0/810
25	v	0.14	0/1361	0.34	0/1861
26	w	0.18	0/872	0.39	0/1185
27	x	0.15	0/425	0.36	0/576
28	y	0.23	0/449	0.38	0/605
29	z	0.19	0/591	0.39	0/795
30	1	0.16	0/3386	0.34	0/4575
31	2	0.16	0/1695	0.39	0/2306

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	3	0.15	0/5362	0.35	0/7266
33	5	0.16	0/1776	0.38	0/2417
34	6	0.18	0/1278	0.40	0/1728
35	9	0.17	0/1445	0.37	0/1956
36	a	0.11	0/383	0.27	0/518
37	b	0.12	0/749	0.28	0/1009
38	c	0.16	0/1047	0.36	0/1415
39	d	0.14	0/2424	0.32	0/3276
40	e	0.15	0/702	0.38	0/945
41	f	0.18	0/937	0.39	0/1271
42	g	0.19	0/993	0.41	0/1336
43	h	0.14	0/779	0.33	0/1053
44	i	0.13	0/1250	0.31	0/1698
All	All	0.17	1/67125 (0.0%)	0.39	2/90985 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	4	0	1
32	3	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	87	ILE	C-N	5.68	1.38	1.33

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	l	103	LEU	CA-C-N	5.43	129.00	120.97
15	l	103	LEU	C-N-CA	5.43	129.00	120.97

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
32	3	259	ASN	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	4	275	TYR	Peptide

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	4	3390	0	3334	41	0
2	A	880	0	920	13	0
3	H	2498	0	2609	33	0
4	J	1294	0	1317	26	0
5	K	749	0	793	10	0
6	L	4806	0	4945	52	0
7	M	3647	0	3849	42	0
8	N	2723	0	2930	34	0
9	V	1028	0	1036	5	0
10	W	1155	0	1177	13	0
11	X	701	0	692	17	0
11	j	660	0	662	6	0
12	Y	1403	0	1392	16	0
13	Z	1441	0	1419	11	0
14	k	2596	0	2559	26	0
15	l	874	0	869	9	0
16	m	626	0	635	7	0
17	n	634	0	616	7	0
18	o	1004	0	995	12	0
19	p	1059	0	1062	11	0
20	q	1142	0	1137	19	0
21	r	846	0	864	13	0
22	s	1047	0	1015	12	0
23	t	1520	0	1477	15	0
24	u	563	0	509	7	0
25	v	1307	0	1207	16	0
26	w	846	0	792	15	0
27	x	412	0	411	2	0
28	y	436	0	437	4	0
29	z	576	0	570	7	0
30	1	3312	0	3266	29	0
31	2	1655	0	1668	18	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	3	5275	0	5300	53	0
33	5	1726	0	1676	21	0
34	6	1247	0	1256	13	0
35	9	1414	0	1370	13	0
36	a	371	0	344	6	0
37	b	737	0	710	3	0
38	c	1024	0	1023	11	0
39	d	2372	0	2407	15	0
40	e	691	0	706	5	0
41	f	917	0	958	7	0
42	g	969	0	980	13	0
43	h	769	0	780	6	0
44	i	1209	0	1182	7	0
45	X	31	0	34	1	0
45	j	34	0	40	3	0
46	s	15	0	27	0	0
47	1	8	0	0	0	0
47	3	16	0	0	1	0
47	6	8	0	0	0	0
47	9	16	0	0	0	0
48	1	31	0	19	0	0
49	1	44	0	27	1	0
50	2	4	0	0	1	0
50	3	4	0	0	0	0
51	3	1	0	0	0	0
52	b	1	0	0	0	0
53	d	48	0	26	0	0
All	All	65812	0	66029	585	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 4.

The worst 5 of 585 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:W:124:GLN:HB2	18:o:4:GLY:HA3	1.76	0.67
11:X:20:LYS:HB3	11:X:27:PRO:HB3	1.78	0.66
1:4:328:ALA:HB3	32:3:126:ASP:HB2	1.78	0.64
3:H:141:SER:HB2	3:H:289:LEU:HD22	1.79	0.64
34:6:57:VAL:HA	34:6:60:MET:HE2	1.79	0.64

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	Percentiles	
1	4	414/463 (89%)	401 (97%)	13 (3%)	0	100	100
2	A	106/115 (92%)	102 (96%)	4 (4%)	0	100	100
3	H	310/318 (98%)	302 (97%)	8 (3%)	0	100	100
4	J	165/175 (94%)	155 (94%)	10 (6%)	0	100	100
5	K	96/98 (98%)	93 (97%)	3 (3%)	0	100	100
6	L	604/606 (100%)	577 (96%)	26 (4%)	1 (0%)	43	70
7	M	457/459 (100%)	450 (98%)	7 (2%)	0	100	100
8	N	345/347 (99%)	337 (98%)	8 (2%)	0	100	100
9	V	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
10	W	137/139 (99%)	135 (98%)	2 (2%)	0	100	100
11	X	85/157 (54%)	81 (95%)	4 (5%)	0	100	100
11	j	80/157 (51%)	78 (98%)	2 (2%)	0	100	100
12	Y	169/171 (99%)	166 (98%)	3 (2%)	0	100	100
13	Z	169/171 (99%)	168 (99%)	1 (1%)	0	100	100
14	k	317/320 (99%)	312 (98%)	5 (2%)	0	100	100
15	l	103/105 (98%)	98 (95%)	5 (5%)	0	100	100
16	m	78/80 (98%)	73 (94%)	5 (6%)	0	100	100
17	n	77/79 (98%)	75 (97%)	2 (3%)	0	100	100
18	o	118/120 (98%)	115 (98%)	3 (2%)	0	100	100
19	p	126/128 (98%)	124 (98%)	2 (2%)	0	100	100
20	q	137/144 (95%)	136 (99%)	1 (1%)	0	100	100
21	r	95/128 (74%)	91 (96%)	4 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
22	s	120/122 (98%)	116 (97%)	4 (3%)	0	100	100
23	t	175/177 (99%)	170 (97%)	5 (3%)	0	100	100
24	u	63/65 (97%)	61 (97%)	2 (3%)	0	100	100
25	v	153/155 (99%)	151 (99%)	2 (1%)	0	100	100
26	w	99/101 (98%)	96 (97%)	3 (3%)	0	100	100
27	x	47/49 (96%)	47 (100%)	0	0	100	100
28	y	48/50 (96%)	47 (98%)	1 (2%)	0	100	100
29	z	68/70 (97%)	67 (98%)	1 (2%)	0	100	100
30	1	428/430 (100%)	418 (98%)	10 (2%)	0	100	100
31	2	211/213 (99%)	200 (95%)	11 (5%)	0	100	100
32	3	686/688 (100%)	663 (97%)	23 (3%)	0	100	100
33	5	206/208 (99%)	195 (95%)	11 (5%)	0	100	100
34	6	154/156 (99%)	149 (97%)	5 (3%)	0	100	100
35	9	174/176 (99%)	169 (97%)	5 (3%)	0	100	100
36	a	42/44 (96%)	42 (100%)	0	0	100	100
37	b	93/95 (98%)	91 (98%)	2 (2%)	0	100	100
38	c	124/126 (98%)	121 (98%)	3 (2%)	0	100	100
39	d	289/380 (76%)	283 (98%)	6 (2%)	0	100	100
40	e	84/86 (98%)	82 (98%)	2 (2%)	0	100	100
41	f	111/113 (98%)	107 (96%)	4 (4%)	0	100	100
42	g	112/114 (98%)	107 (96%)	5 (4%)	0	100	100
43	h	92/114 (81%)	90 (98%)	2 (2%)	0	100	100
44	i	143/145 (99%)	142 (99%)	1 (1%)	0	100	100
All	All	8048/8497 (95%)	7819 (97%)	228 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	L	72	GLN

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	4	363/391 (93%)	362 (100%)	1 (0%)	86	86
2	A	99/103 (96%)	99 (100%)	0	100	100
3	H	274/278 (99%)	274 (100%)	0	100	100
4	J	138/144 (96%)	138 (100%)	0	100	100
5	K	86/86 (100%)	85 (99%)	1 (1%)	63	74
6	L	538/538 (100%)	534 (99%)	4 (1%)	76	79
7	M	411/411 (100%)	410 (100%)	1 (0%)	87	87
8	N	315/315 (100%)	313 (99%)	2 (1%)	78	81
9	V	101/101 (100%)	101 (100%)	0	100	100
10	W	122/122 (100%)	122 (100%)	0	100	100
11	X	80/141 (57%)	80 (100%)	0	100	100
11	j	76/141 (54%)	76 (100%)	0	100	100
12	Y	154/154 (100%)	154 (100%)	0	100	100
13	Z	155/155 (100%)	155 (100%)	0	100	100
14	k	283/283 (100%)	282 (100%)	1 (0%)	84	84
15	l	94/94 (100%)	94 (100%)	0	100	100
16	m	69/69 (100%)	69 (100%)	0	100	100
17	n	61/61 (100%)	60 (98%)	1 (2%)	55	70
18	o	107/107 (100%)	107 (100%)	0	100	100
19	p	114/114 (100%)	114 (100%)	0	100	100
20	q	119/122 (98%)	119 (100%)	0	100	100
21	r	95/122 (78%)	95 (100%)	0	100	100
22	s	110/110 (100%)	110 (100%)	0	100	100
23	t	159/159 (100%)	159 (100%)	0	100	100
24	u	59/59 (100%)	59 (100%)	0	100	100
25	v	140/140 (100%)	140 (100%)	0	100	100
26	w	92/92 (100%)	91 (99%)	1 (1%)	65	75
27	x	44/44 (100%)	43 (98%)	1 (2%)	44	65
28	y	46/46 (100%)	46 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	z	59/59 (100%)	58 (98%)	1 (2%)	53	69
30	1	344/344 (100%)	343 (100%)	1 (0%)	86	86
31	2	183/183 (100%)	183 (100%)	0	100	100
32	3	578/578 (100%)	577 (100%)	1 (0%)	87	87
33	5	189/189 (100%)	189 (100%)	0	100	100
34	6	132/132 (100%)	132 (100%)	0	100	100
35	9	151/151 (100%)	151 (100%)	0	100	100
36	a	43/43 (100%)	43 (100%)	0	100	100
37	b	79/79 (100%)	78 (99%)	1 (1%)	61	73
38	c	113/113 (100%)	113 (100%)	0	100	100
39	d	255/326 (78%)	255 (100%)	0	100	100
40	e	76/76 (100%)	76 (100%)	0	100	100
41	f	101/101 (100%)	100 (99%)	1 (1%)	68	75
42	g	107/107 (100%)	107 (100%)	0	100	100
43	h	84/96 (88%)	84 (100%)	0	100	100
44	i	131/131 (100%)	130 (99%)	1 (1%)	73	78
All	All	7129/7410 (96%)	7110 (100%)	19 (0%)	84	86

5 of 19 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
30	1	359	CYS
41	f	26	LEU
44	i	11	LEU
37	b	49	VAL
8	N	235	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 59 such sidechains are listed below:

Mol	Chain	Res	Type
20	q	75	GLN
43	h	24	GLN
25	v	104	HIS
42	g	69	ASN
39	d	148	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)

7 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	2MR	4	85	1	10,12,13	2.42	2 (20%)	5,13,15	1.03	0
43	AYA	h	1	43	6,7,8	1.26	1 (16%)	5,8,10	1.26	1 (20%)
14	SEP	k	36	14	8,9,10	1.56	1 (12%)	8,12,14	1.61	2 (25%)
6	FME	L	1	6	8,9,10	0.93	0	7,9,11	0.87	0
9	AYA	V	1	9	6,7,8	1.25	1 (16%)	5,8,10	1.70	1 (20%)
5	FME	K	1	5	8,9,10	0.93	0	7,9,11	0.86	0
7	FME	M	1	7	8,9,10	0.96	0	7,9,11	0.78	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	2MR	4	85	1	-	2/10/13/15	-
43	AYA	h	1	43	-	0/4/6/8	-
14	SEP	k	36	14	-	3/5/8/10	-
6	FME	L	1	6	-	3/7/9/11	-
9	AYA	V	1	9	-	2/4/6/8	-
5	FME	K	1	5	-	3/7/9/11	-
7	FME	M	1	7	-	3/7/9/11	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	4	85	2MR	CZ-NE	5.13	1.45	1.34
1	4	85	2MR	CZ-NH2	5.03	1.44	1.33
14	k	36	SEP	P-O1P	3.39	1.61	1.50
43	h	1	AYA	CA-N	-2.41	1.44	1.46
9	V	1	AYA	CA-N	-2.33	1.44	1.46

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	V	1	AYA	CB-CA-N	3.01	112.96	109.61
14	k	36	SEP	OG-CB-CA	2.99	111.05	108.14
14	k	36	SEP	P-OG-CB	-2.80	110.57	118.30
43	h	1	AYA	CB-CA-N	2.65	112.55	109.61

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	K	1	FME	O1-CN-N-CA
5	K	1	FME	C-CA-CB-CG
6	L	1	FME	N-CA-CB-CG
7	M	1	FME	C-CA-CB-CG
14	k	36	SEP	CB-OG-P-O1P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 16 ligands modelled in this entry, 2 are monoatomic - leaving 14 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
45	ZMP	j	101	11	27,33,36	0.66	1 (3%)	32,40,45	1.00	1 (3%)
47	SF4	9	202	35	0,12,12	-	-	-		
47	SF4	3	802	32	0,12,12	-	-	-		
48	FMN	1	502	-	33,33,33	1.07	2 (6%)	48,50,50	1.22	6 (12%)
50	FES	3	803	32	0,4,4	-	-	-		
47	SF4	6	300	34	0,12,12	-	-	-		
53	NDP	d	401	-	49,52,52	0.33	0	66,80,80	0.35	0
49	NAI	1	503	-	45,48,48	0.41	1 (2%)	60,73,73	1.66	3 (5%)
47	SF4	9	201	35	0,12,12	-	-	-		
45	ZMP	X	101	11	24,30,36	0.79	1 (4%)	29,37,45	0.93	1 (3%)
47	SF4	3	801	32	0,12,12	-	-	-		
47	SF4	1	501	30	0,12,12	-	-	-		
46	MYR	s	201	22	14,14,15	0.22	0	13,13,15	0.17	0
50	FES	2	300	31	0,4,4	-	-	-		

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
45	ZMP	j	101	11	-	2/38/40/43	-
47	SF4	9	202	35	-	-	0/6/5/5
47	SF4	3	802	32	-	-	0/6/5/5
48	FMN	1	502	-	-	7/18/18/18	0/3/3/3
50	FES	3	803	32	-	-	0/1/1/1
53	NDP	d	401	-	-	9/34/77/77	0/5/5/5
47	SF4	6	300	34	-	-	0/6/5/5
49	NAI	1	503	-	-	8/29/72/72	0/5/5/5
47	SF4	9	201	35	-	-	0/6/5/5
45	ZMP	X	101	11	-	5/35/37/43	-
47	SF4	1	501	30	-	-	0/6/5/5
47	SF4	3	801	32	-	-	0/6/5/5
46	MYR	s	201	22	-	1/11/12/13	-
50	FES	2	300	31	-	-	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	1	502	FMN	C4A-N5	3.68	1.37	1.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	X	101	ZMP	C9-C10	2.62	1.53	1.50
48	1	502	FMN	C10-N1	2.31	1.37	1.33
45	j	101	ZMP	C9-C10	2.26	1.53	1.50
49	1	503	NAI	PA-O5B	2.04	1.67	1.59

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	1	503	NAI	O5B-PA-O1A	-9.76	70.95	109.07
49	1	503	NAI	O2A-PA-O1A	-7.81	73.65	112.24
48	1	502	FMN	C4-N3-C2	-3.24	119.66	125.64
45	j	101	ZMP	O1-C10-C9	-2.85	120.62	123.99
48	1	502	FMN	C4A-C10-N10	2.73	120.47	116.48

There are no chirality outliers.

5 of 32 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
45	X	101	ZMP	C17-C16-N2-C15
45	j	101	ZMP	S1-C11-C12-N1
46	s	201	MYR	C1-C2-C3-C4
48	1	502	FMN	N10-C1'-C2'-O2'
48	1	502	FMN	N10-C1'-C2'-C3'

There are no ring outliers.

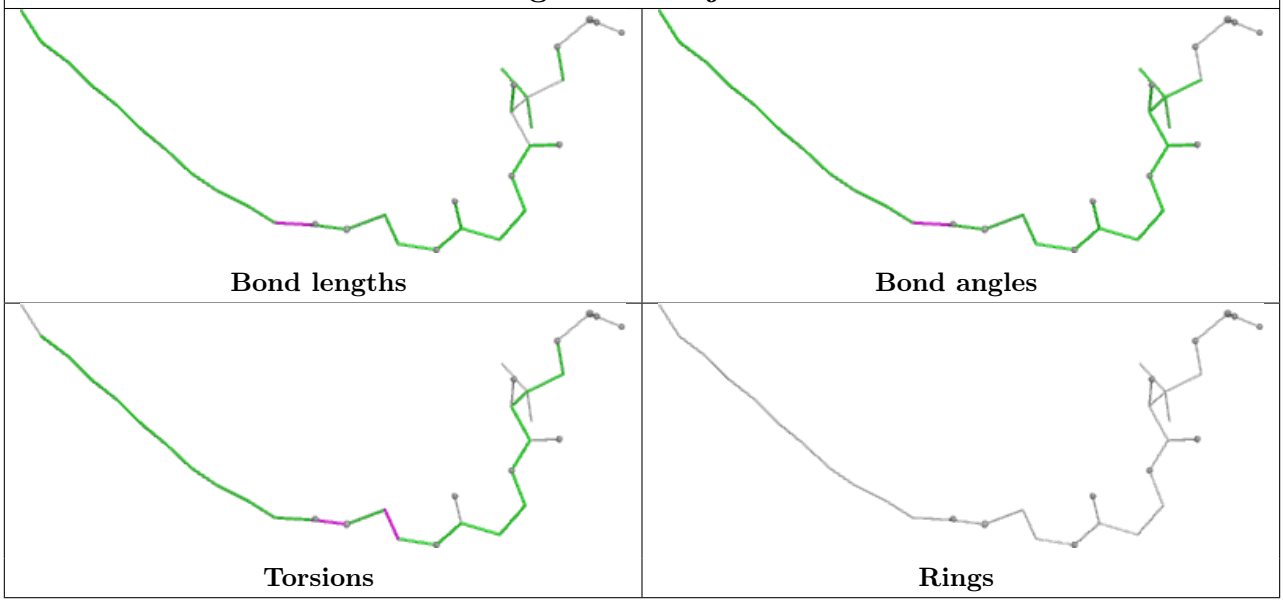
5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
45	j	101	ZMP	3	0
49	1	503	NAI	1	0
45	X	101	ZMP	1	0
47	3	801	SF4	1	0
50	2	300	FES	1	0

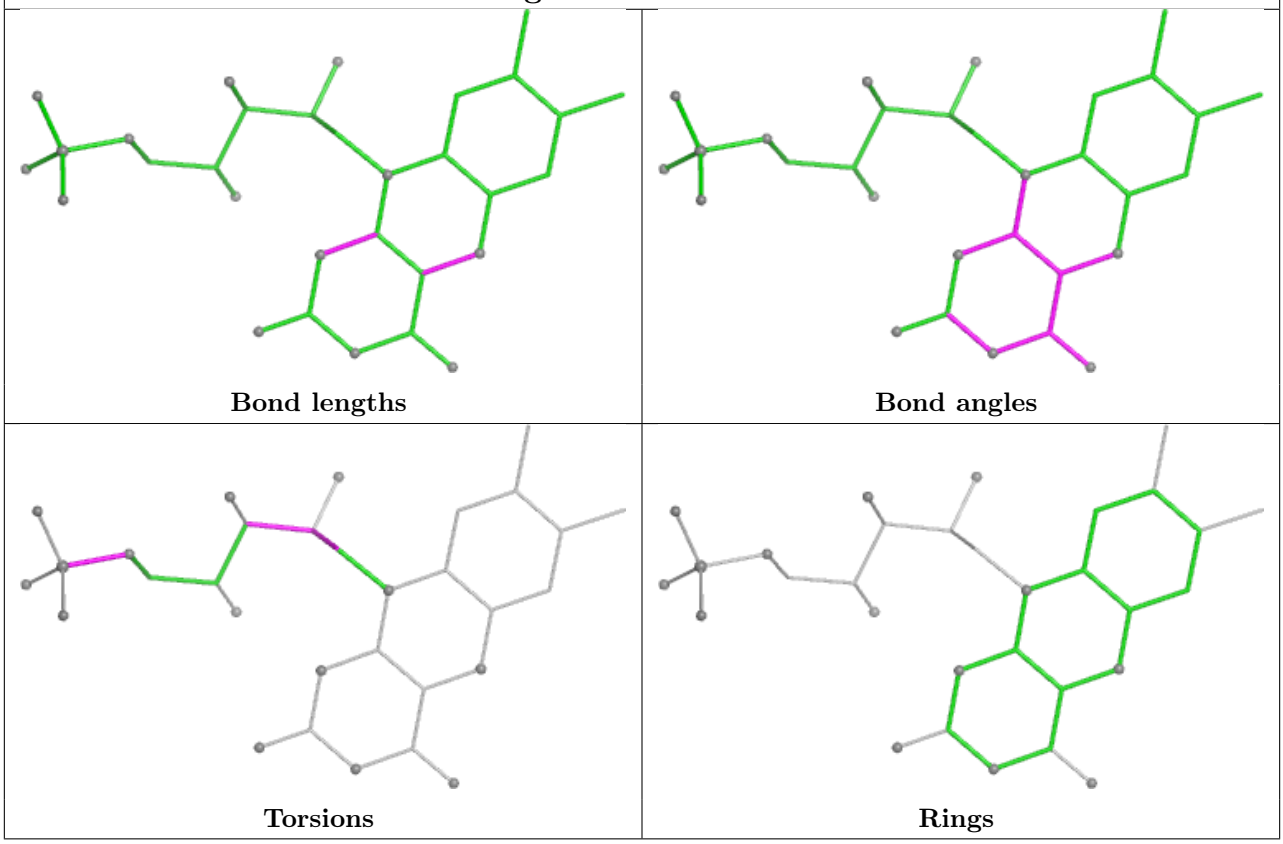
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

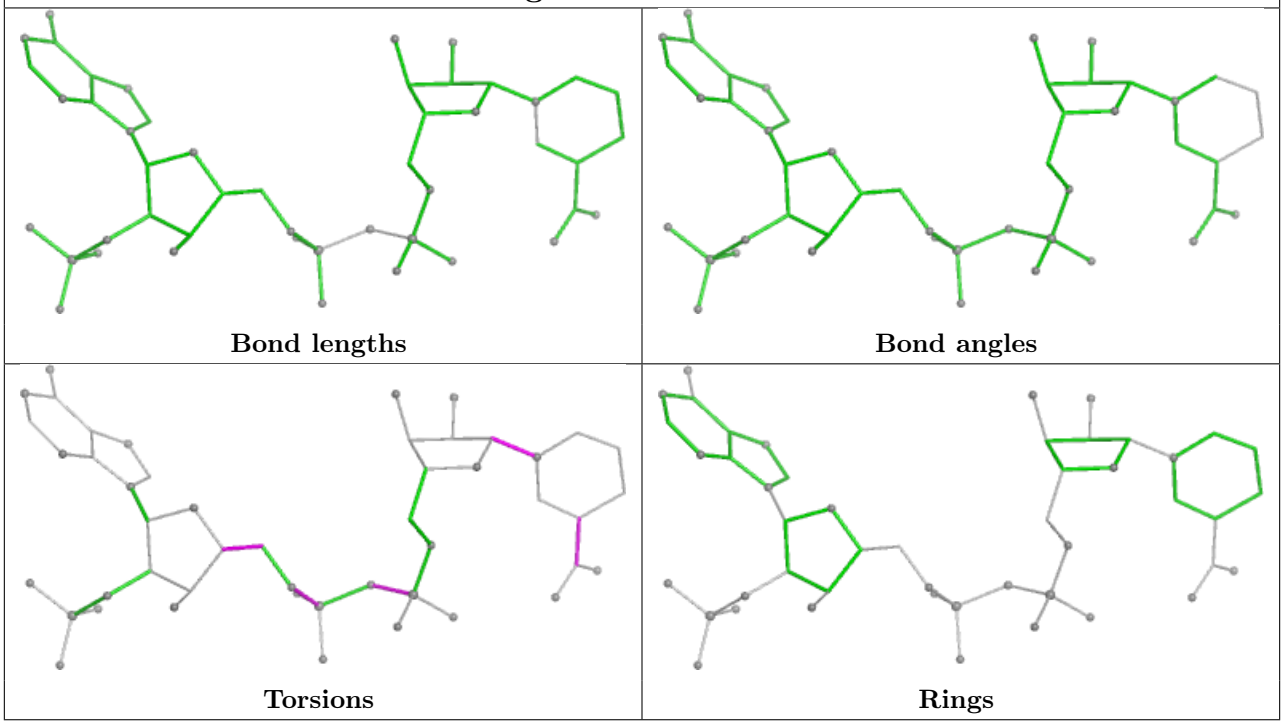
Ligand ZMP j 101



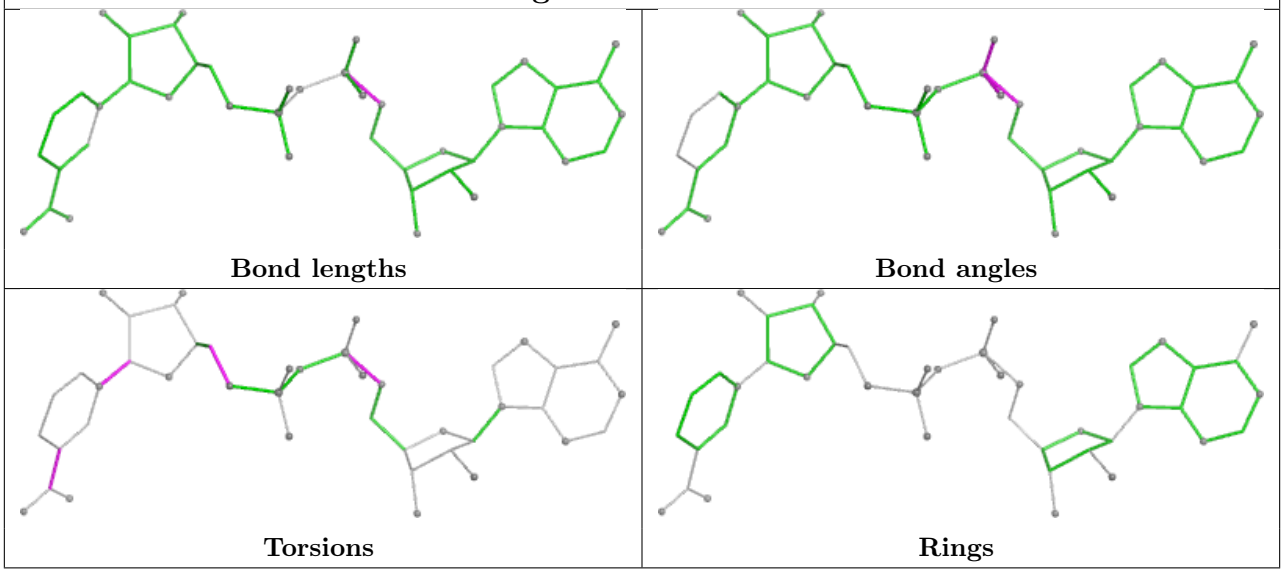
Ligand FMN 1 502

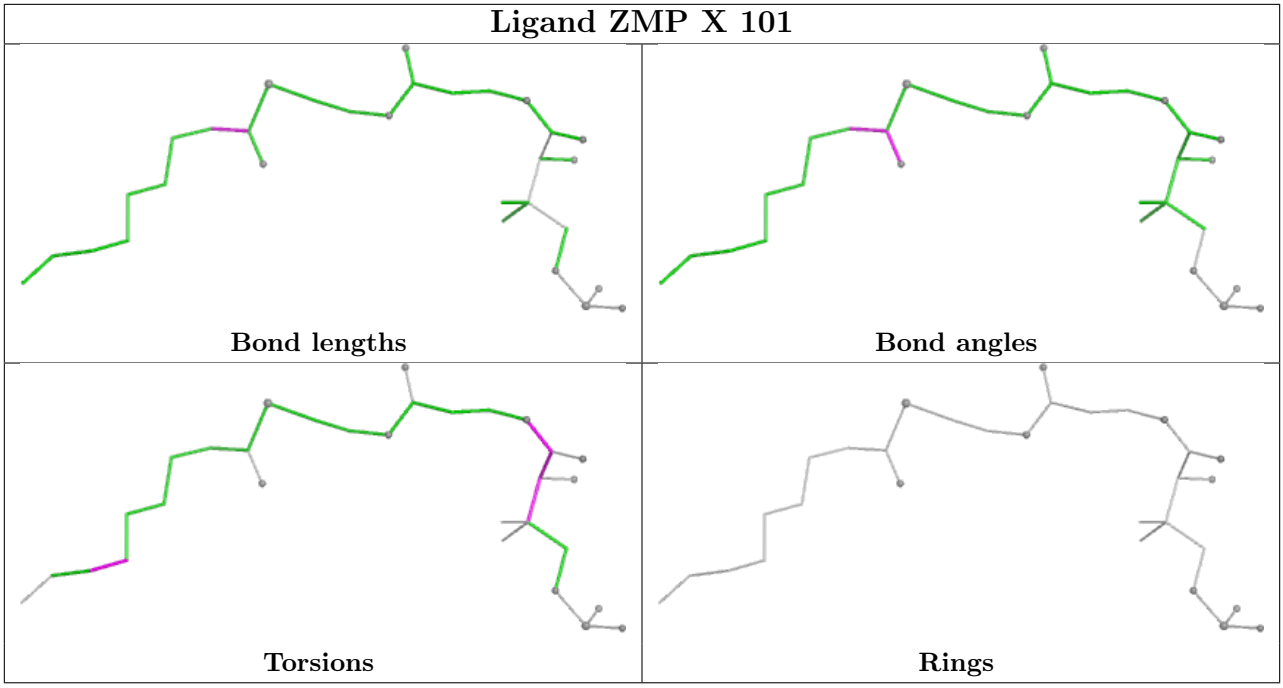


Ligand NDP d 401



Ligand NAI 1 503





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.

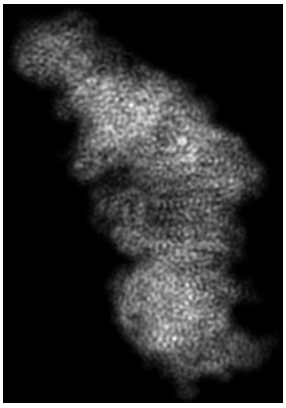
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-14651. These allow visual inspection of the internal detail of the map and identification of artifacts.

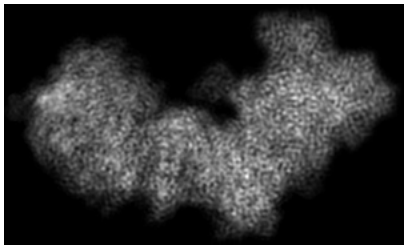
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

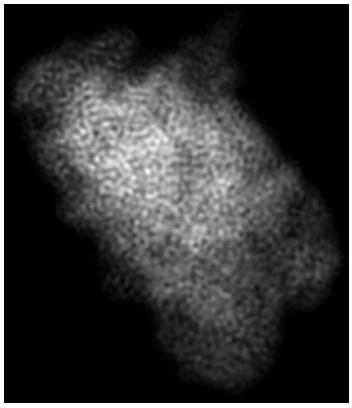
6.1.1 Primary map



X



Y

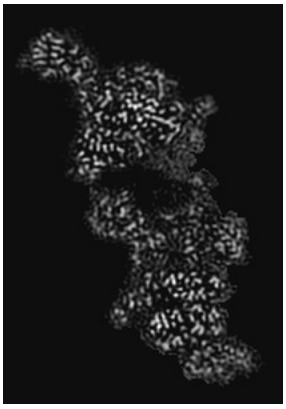


Z

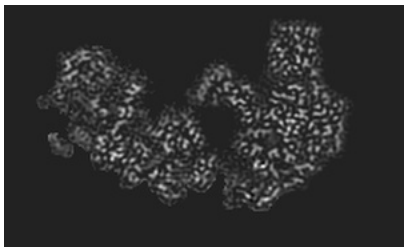
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map



X Index: 71



Y Index: 82

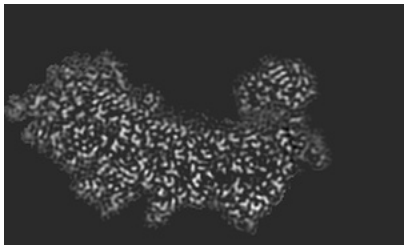
Z Index: 118

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: 50



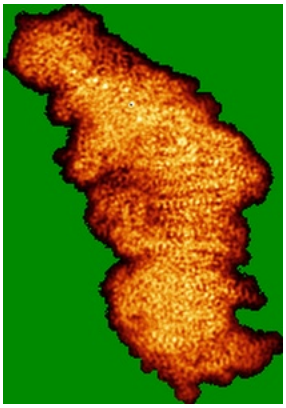
Y Index: 108

Z Index: 143

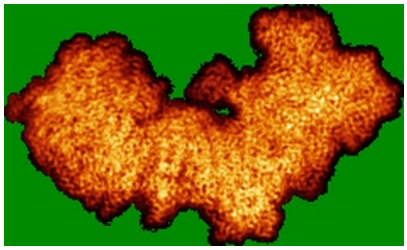
The images above show the largest variance slices of the map in three orthogonal directions.

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

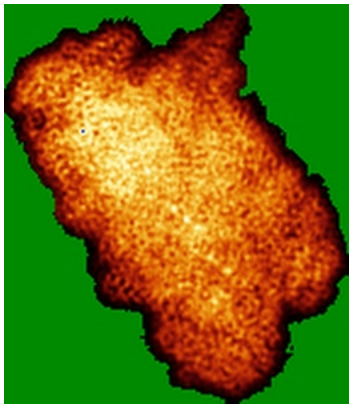
6.4.1 Primary map



X



Y

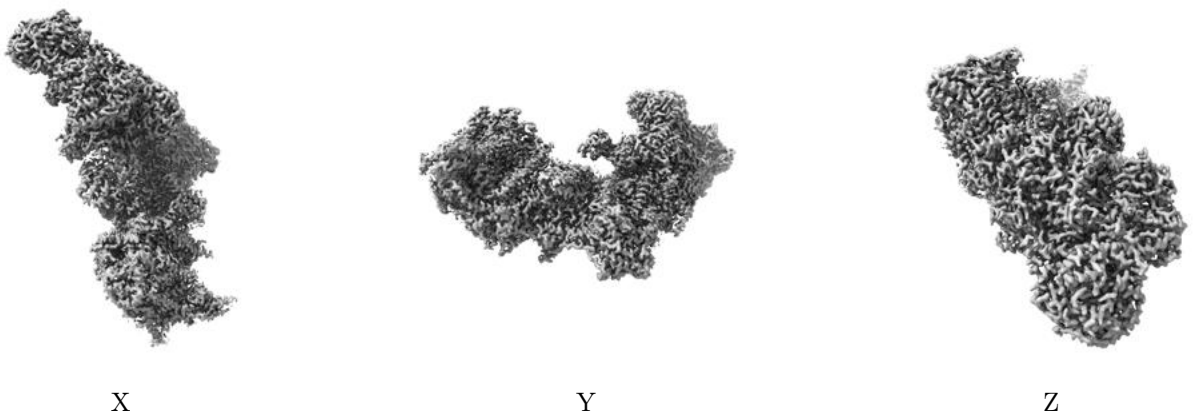


Z

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 0.07. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

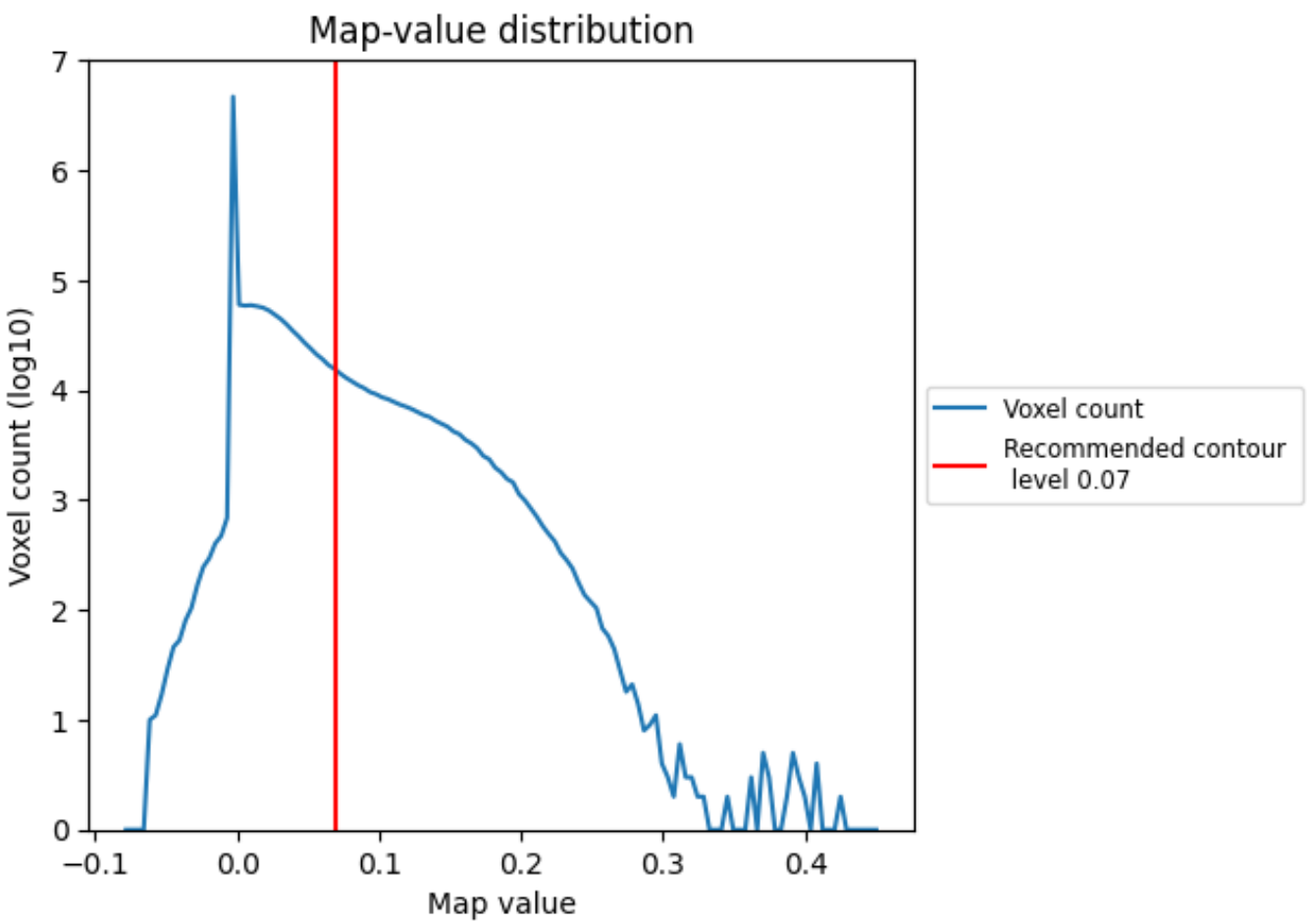
6.6 Mask visualisation (i)

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

7 Map analysis (i)

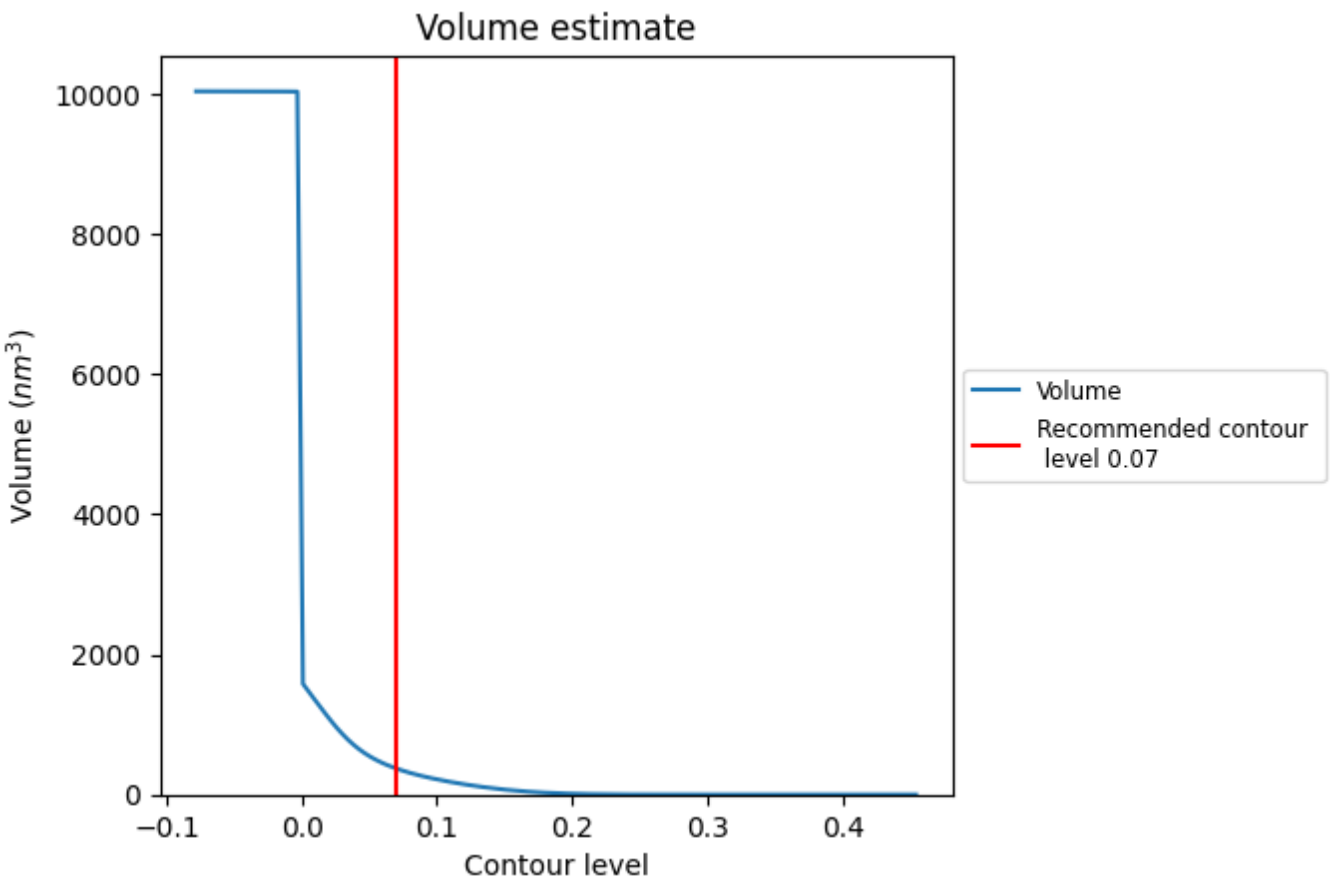
This section contains the results of statistical analysis of the map.

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 371 nm^3; this corresponds to an approximate mass of 336 kDa.

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

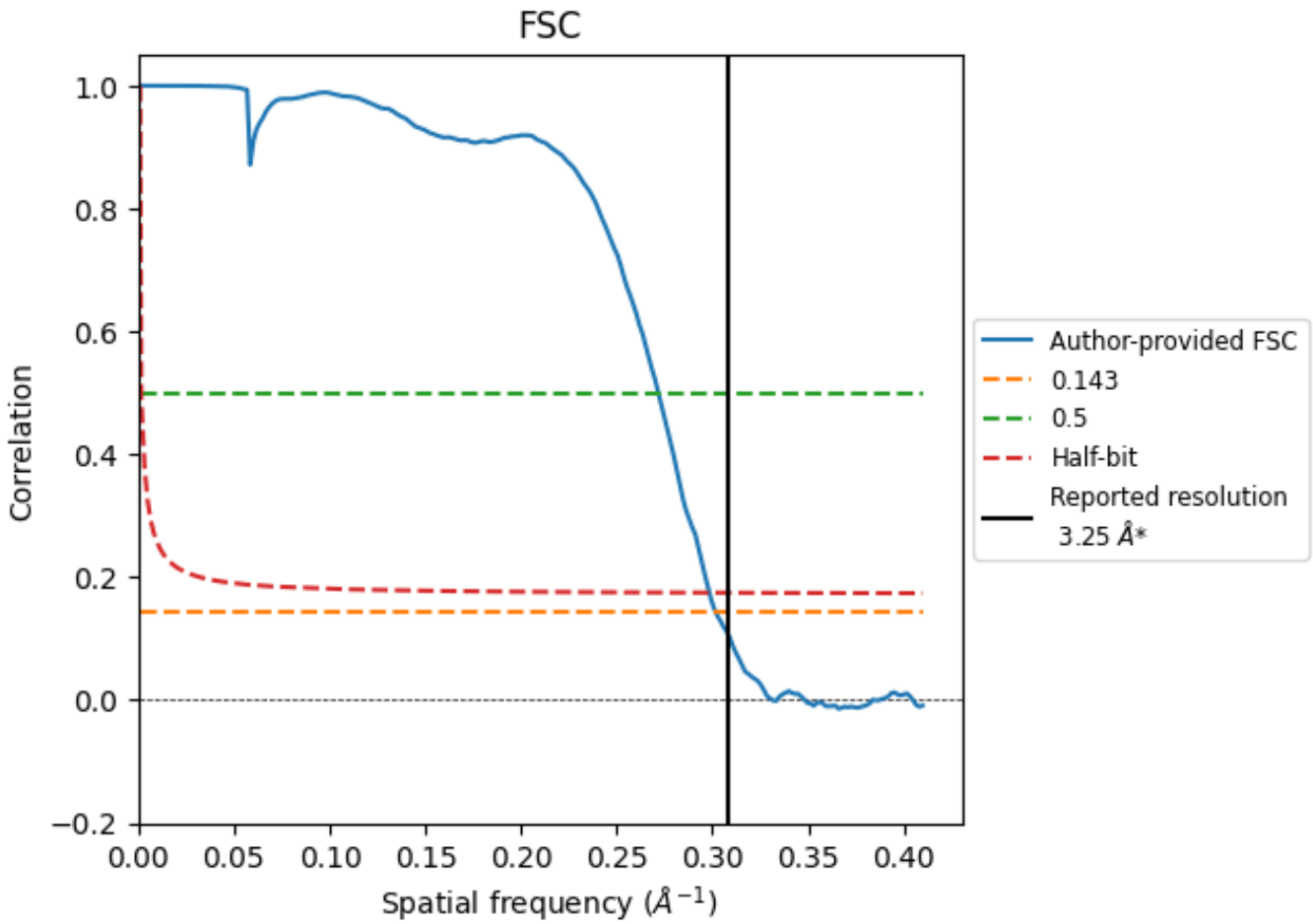
7.3 Rotationally averaged power spectrum (i)

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

8 Fourier-Shell correlation (i)

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 0.308 Å^{-1}

8.2 Resolution estimates (i)

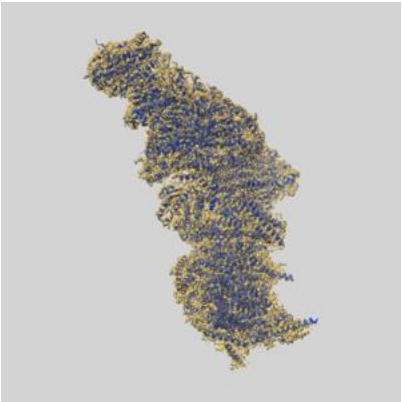
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.25	-	-
Author-provided FSC curve	3.31	3.68	3.35
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

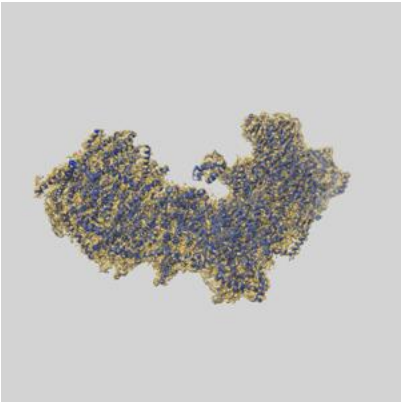
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-14651 and PDB model 7ZDJ. Per-residue inclusion information can be found in section 3 on page 16.

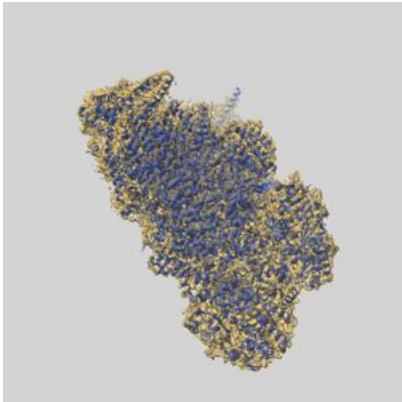
9.1 Map-model overlay (i)



X



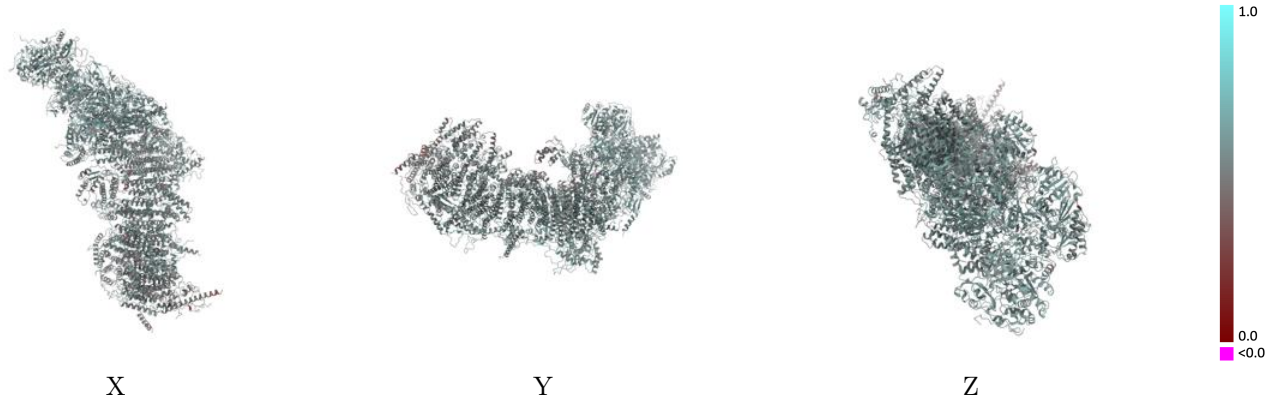
Y



Z

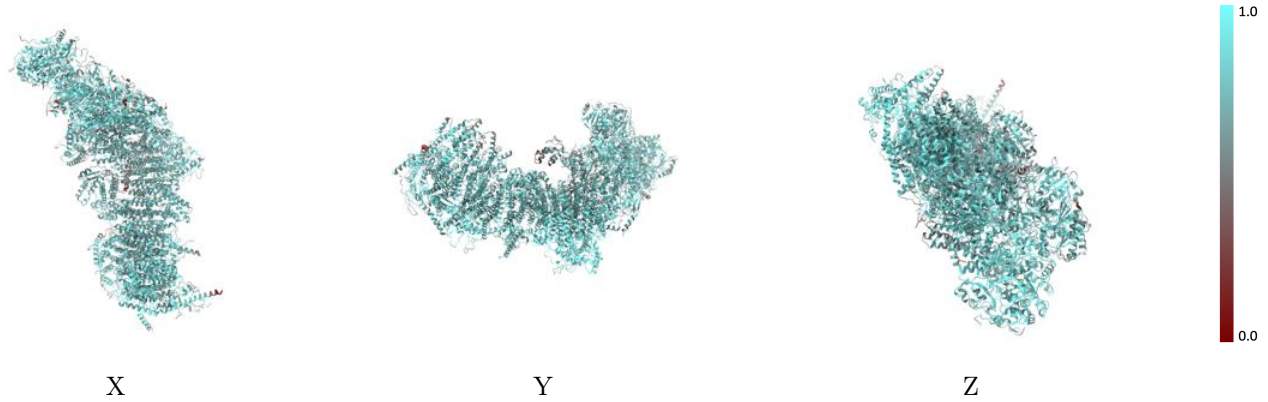
The images above show the 3D surface view of the map at the recommended contour level 0.07 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



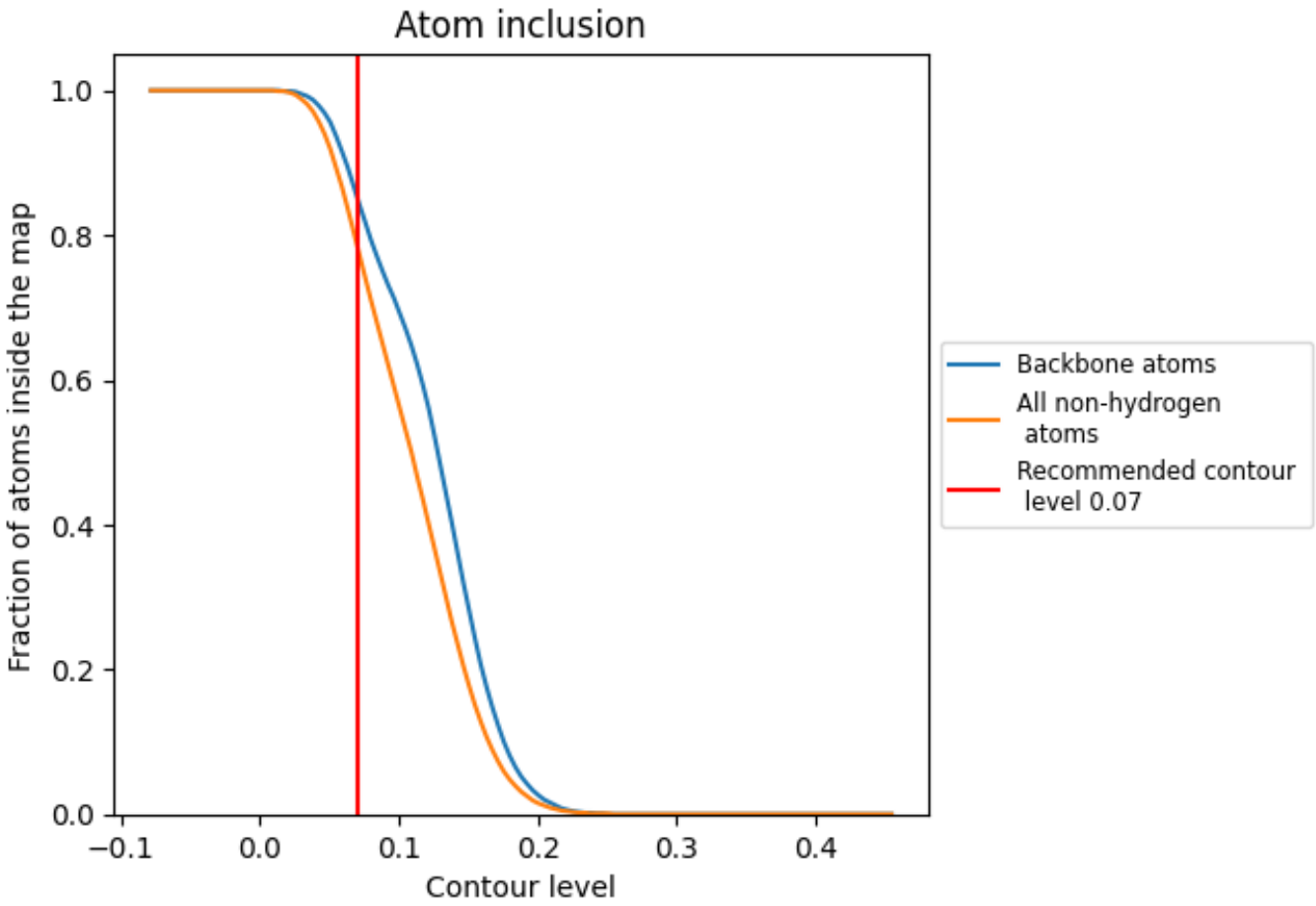
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.07).

9.4 Atom inclusion (i)



At the recommended contour level, 85% of all backbone atoms, 79% 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 (0.07) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7860	0.5470
1	0.8010	0.5540
2	0.7740	0.5510
3	0.7830	0.5640
4	0.7670	0.5710
5	0.8050	0.5800
6	0.8020	0.5710
9	0.8470	0.5730
A	0.7060	0.5090
H	0.8370	0.5510
J	0.7810	0.5320
K	0.8020	0.5460
L	0.8090	0.5300
M	0.8370	0.5570
N	0.8380	0.5610
V	0.7410	0.5280
W	0.8380	0.5540
X	0.7380	0.4930
Y	0.8540	0.5550
Z	0.8120	0.5400
a	0.7620	0.5610
b	0.7310	0.5690
c	0.7560	0.5730
d	0.7230	0.5490
e	0.7540	0.5590
f	0.7020	0.5390
g	0.7150	0.5570
h	0.7300	0.5710
i	0.7620	0.5710
j	0.5220	0.4850
k	0.7440	0.5340
l	0.8250	0.5520
m	0.8360	0.5440
n	0.7300	0.4890
o	0.8240	0.5470

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
p	0.7410	0.5310
q	0.8390	0.5560
r	0.7610	0.5150
s	0.7290	0.4670
t	0.7810	0.5140
u	0.7880	0.4950
v	0.7960	0.5330
w	0.7680	0.5420
x	0.7640	0.5230
y	0.7660	0.5260
z	0.8860	0.5550