Full wwPDB EM Validation Report (i)

Sep 8, 2026 – 10:08 am BST

PDB ID	:	6QCF / pdb_00006qcf
EMDB ID	:	EMD-4505
Title	:	Ovine respiratory complex I FRC open class 6
Authors	:	Letts, J.A.; Sazanov, L.A.
Deposited on	:	2018-12-27
Resolution	:	6.50 Å(reported)
Based on initial model	:	5LNK

This is a Full wwPDB EM Validation 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:

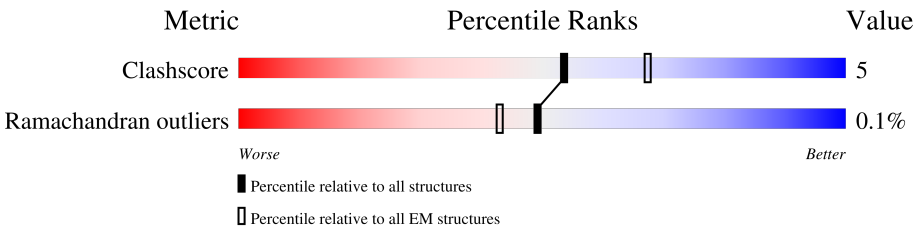
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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

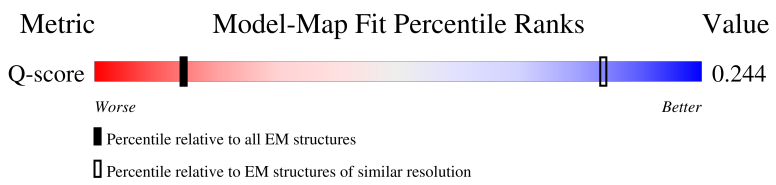
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 6.50 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	-
Q-score	-	25397	556 (6.00 - 7.00)

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	V1	445	12% 91% 6% •
2	V2	217	15% 90% 7% •
3	S1	704	16% 93% 5% •
4	S2	430	29% 96% • •
5	S3	228	23% 83% 7% • 9%

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Mol	Chain	Length	Quality of chain
6	S7	179	23% 86% 13%
7	S8	176	22% 95% 5%
8	V3	75	8% 40% 13% 45%
9	S6	96	21% 95%
10	S4	133	19% 89% 5% 5%
11	A9	338	21% 81% 15%
12	A2	98	6% 79% 5% 16%
13	A5	115	26% 93%
14	A6	127	17% 87% 10%
15	A7	112	41% 74% 10% 14%
16	AL	145	73% 95%
17	AA	88	20% 90% 9%
17	AB	88	25% 95%
18	D3	115	31% 78% 22%
19	D1	318	41% 92% 5%
20	D6	175	54% 94%
21	4L	98	55% 99%
22	D5	606	34% 97%
23	D4	459	29% 98%
24	D2	347	29% 99%
25	AK	140	51% 96%
26	B5	143	24% 97%
27	A8	171	14% 96%
28	BJ	175	17% 92% 6%
29	AJ	320	25% 95% 5%

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Mol	Chain	Length	Quality of chain
30	S5	105	25% 92% • 6%
31	A3	83	46% 87% • 11%
32	B3	97	35% 69% 6% 25%
33	C2	120	22% 92% 6% ••
34	B4	128	22% 95% 5%
35	AM	143	24% 94% • •
36	B6	127	24% 69% 6% • 24%
37	B7	136	24% 82% 5% 12%
38	B9	178	19% 93% 6% •
39	B2	72	31% 83% 7% 10%
40	B8	158	34% 94% 6% •
41	BK	125	18% 80% • 18%
42	C1	49	22% 86% 8% 6%
43	B1	57	40% 89% • 9%
44	A1	70	36% 96% •

2 Entry composition (i)

There are 50 unique types of molecules in this entry. The entry contains 40144 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	V1	430	2099	1239	430	430	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	V2	212	1045	621	212	212	0	0

- Molecule 3 is a protein called NADH:ubiquinone oxidoreductase core subunit S1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	S1	688	3390	2014	688	688	0	0

- Molecule 4 is a protein called NDUFS2.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	S2	424	2090	1242	424	424	0	0

- Molecule 5 is a protein called NADH:ubiquinone oxidoreductase core subunit S3.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	S3	208	1034	618	208	208	0	0

- Molecule 6 is a protein called NDUFS7.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	S7	156	769	457	156	156	0	0

- Molecule 7 is a protein called NDUFS8.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
7	S8	176	871	519	176	176	0	0

- Molecule 8 is a protein called NDUFV3.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
8	V3	41	204	122	41	41	0	0

- Molecule 9 is a protein called NDUFS6.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
9	S6	95	462	272	95	95	0	0

- Molecule 10 is a protein called NADH:ubiquinone oxidoreductase subunit S4.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
10	S4	126	625	373	126	126	0	0

- Molecule 11 is a protein called NADH:ubiquinone oxidoreductase subunit A9.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
11	A9	287	1413	839	287	287	0	0

- Molecule 12 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
12	A2	82	406	242	82	82	0	0

- Molecule 13 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
13	A5	111	550	328	111	111	0	0

- Molecule 14 is a protein called NADH:ubiquinone oxidoreductase subunit A6.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
14	A6	114	567	339	114	114	0	0

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
15	A7	96	476	284	96	96	0	0

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
16	AL	144	708	420	144	144	0	0

- Molecule 17 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
17	AA	80	397	237	80	80	0	0
17	AB	87	432	258	87	87	0	0

- Molecule 18 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
18	D3	90	449	269	90	90	0	0

- Molecule 19 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
19	D1	303	1505	899	303	303	0	0

- Molecule 20 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
20	D6	171	829	487	171	171	0	0

- Molecule 21 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
21	4L	98	486	290	98	98	0	0

- Molecule 22 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
22	D5	606	3001	1789	606	606	0	0

- Molecule 23 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
23	D4	459	2277	1359	459	459	0	0

- Molecule 24 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
24	D2	347	1721	1027	347	347	0	0

- Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
25	AK	140	682	402	140	140	0	0

- Molecule 26 is a protein called NADH:ubiquinone oxidoreductase subunit B5.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
26	B5	139	687	409	139	139	0	0

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-

unit 8.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
27	A8	171	847	505	171	171	0	0

- Molecule 28 is a protein called NDUFB10.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
28	BJ	171	853	511	171	171	0	0

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
29	AJ	319	1575	937	319	319	0	0

- Molecule 30 is a protein called NADH:ubiquinone oxidoreductase subunit S5.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
30	S5	99	490	292	99	99	0	0

- Molecule 31 is a protein called NADH:ubiquinone oxidoreductase subunit A3.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
31	A3	74	367	219	74	74	0	0

- Molecule 32 is a protein called NADH:ubiquinone oxidoreductase subunit B3.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
32	B3	73	356	210	73	73	0	0

- Molecule 33 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
33	C2	119	589	351	119	119	0	0

- Molecule 34 is a protein called NADH:ubiquinone oxidoreductase subunit B4.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
34	B4	128	635	379	128	128	0	0

- Molecule 35 is a protein called NDUFA13.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
35	AM	139	681	403	139	139	0	0

- Molecule 36 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
36	B6	96	477	285	96	96	0	0

- Molecule 37 is a protein called NADH:ubiquinone oxidoreductase subunit B7.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
37	B7	119	592	354	119	119	0	0

- Molecule 38 is a protein called NADH:ubiquinone oxidoreductase subunit B9.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
38	B9	176	874	522	176	176	0	0

- Molecule 39 is a protein called NADH:ubiquinone oxidoreductase subunit B2.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
39	B2	65	323	193	65	65	0	0

- Molecule 40 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
40	B8	157	775	461	157	157	0	0

- Molecule 41 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit

11, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
41	BK	102	506	302	102	102	0	0

- Molecule 42 is a protein called NDUFC1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
42	C1	46	227	135	46	46	0	0

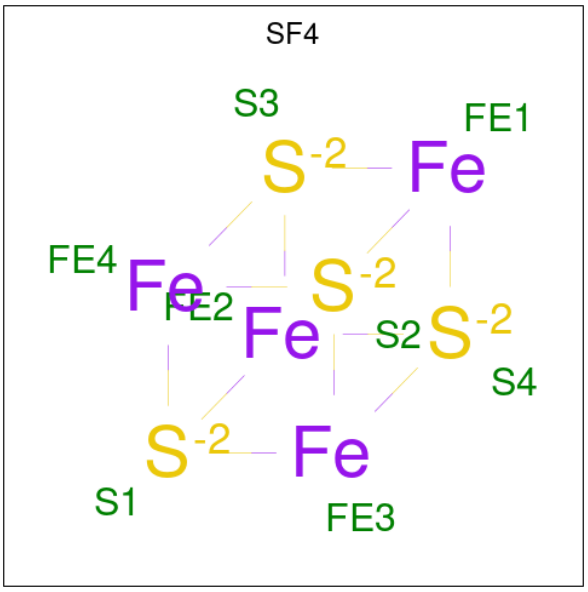
- Molecule 43 is a protein called NDUFB1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
43	B1	52	258	154	52	52	0	0

- Molecule 44 is a protein called NDUFA1.

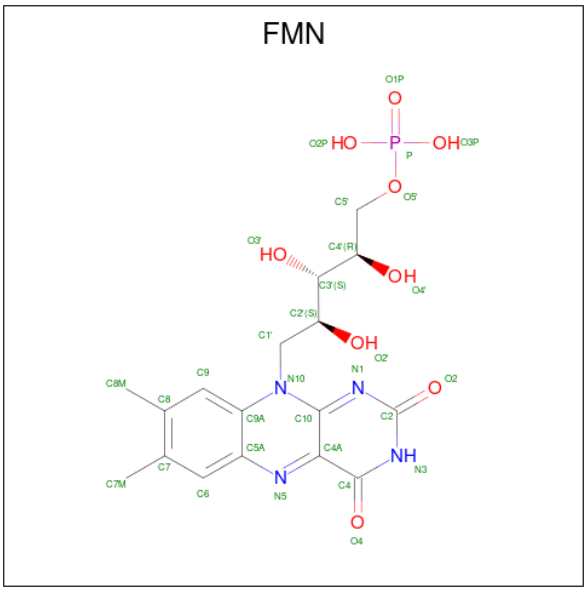
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
44	A1	70	343	203	70	70	0	0

- Molecule 45 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



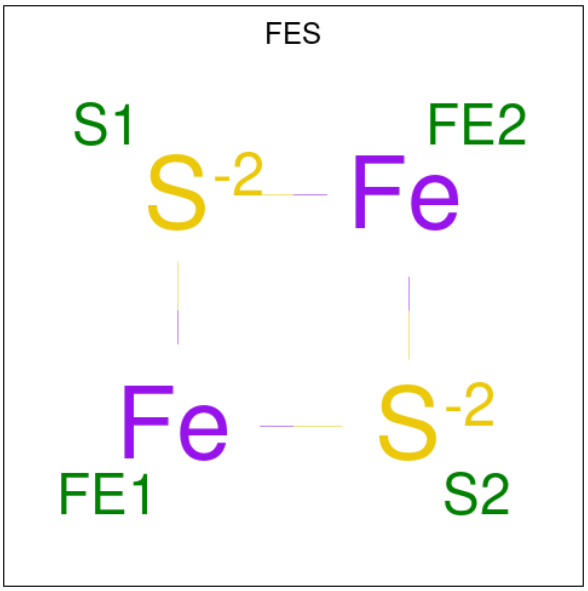
Mol	Chain	Residues	Atoms				AltConf
45	V1	1	Total	Fe	S		0
			8	4	4		
45	S1	1	Total	Fe	S		0
			8	4	4		
45	S1	1	Total	Fe	S		0
			8	4	4		
45	S7	1	Total	Fe	S		0
			8	4	4		
45	S8	1	Total	Fe	S		0
			8	4	4		
45	S8	1	Total	Fe	S		0
			8	4	4		

- Molecule 46 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



Mol	Chain	Residues	Atoms					AltConf
46	V1	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 47 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).

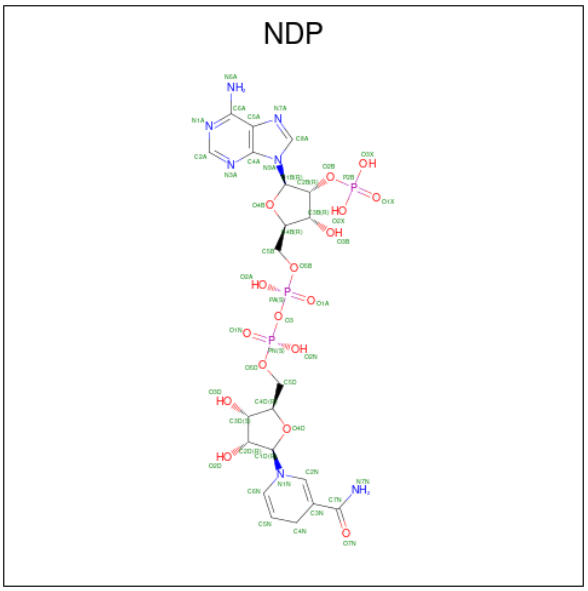


Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
47	V2	1	4	2	2	0
			Total	Fe	S	
47	S1	1	4	2	2	0

- Molecule 48 is ZINC ION (CCD ID: ZN) (formula: Zn).

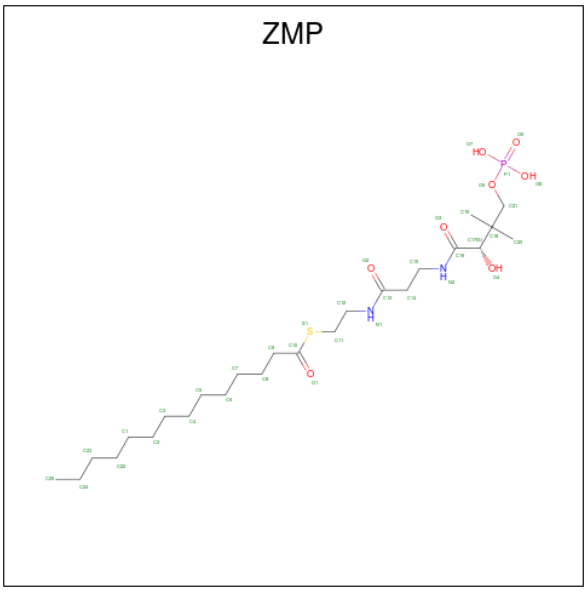
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
48	S6	1	1	1	0

- Molecule 49 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	
49	A9	1	48	21	7	17	3	0

- Molecule 50 is S-[2-({N-[(2S)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] tetradecanethioate (CCD ID: ZMP) (formula: $C_{25}H_{49}N_2O_8PS$).



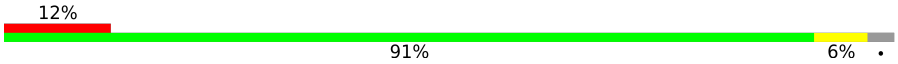
Mol	Chain	Residues	Atoms						AltConf
			Total	C	N	O	P	S	
50	A6	1	34	23	2	7	1	1	0
50	B9	1	31	20	2	7	1	1	0

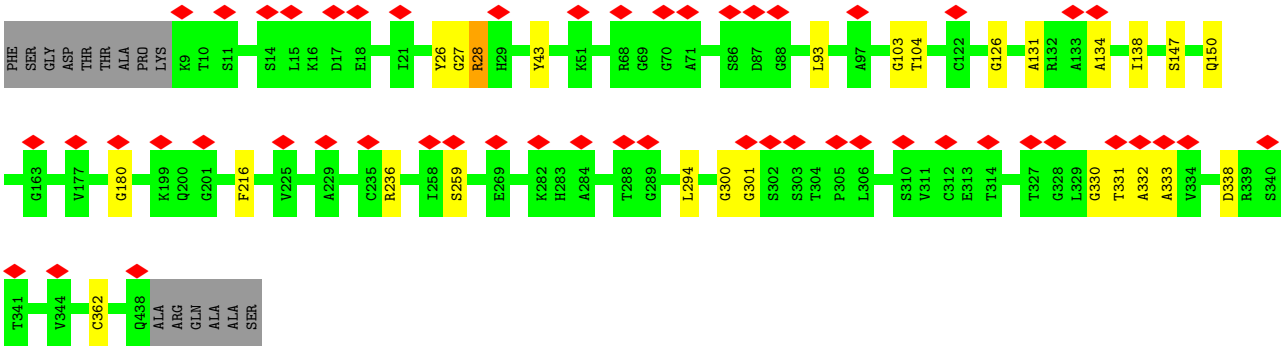
3 Residue-property plots (i)

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: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

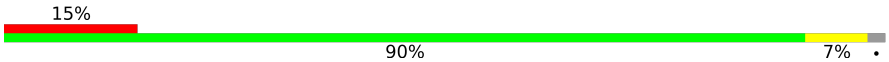
Chain V1:

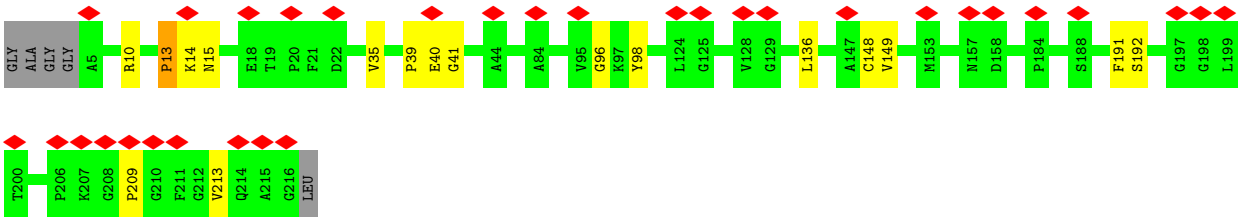




• Molecule 2: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

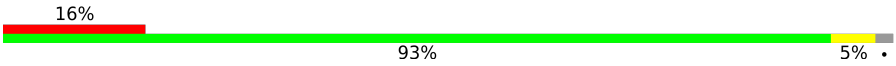
Chain V2:

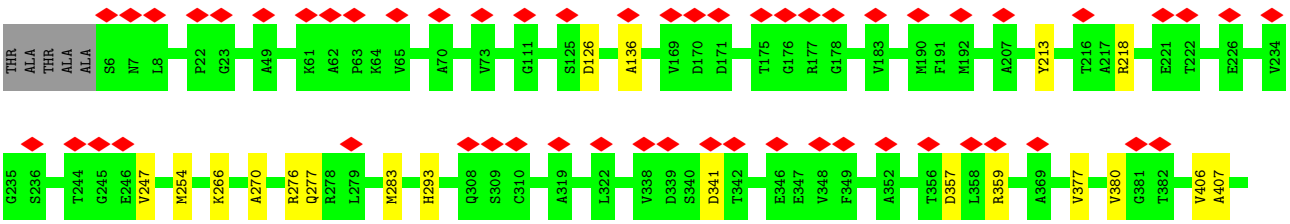


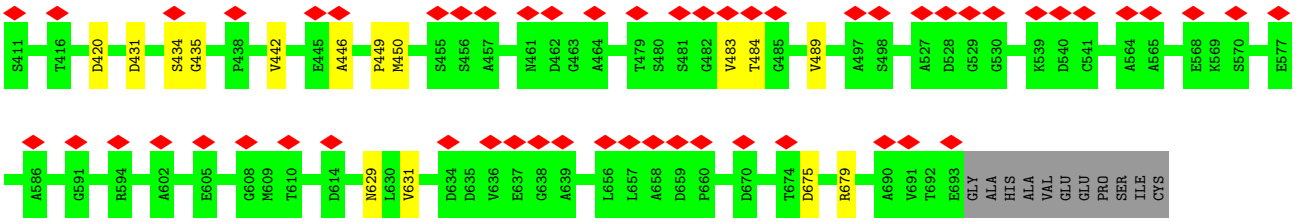


• Molecule 3: NADH:ubiquinone oxidoreductase core subunit S1

Chain S1:

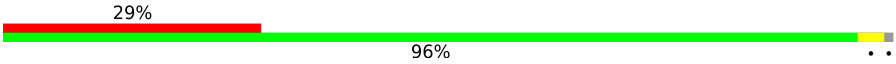


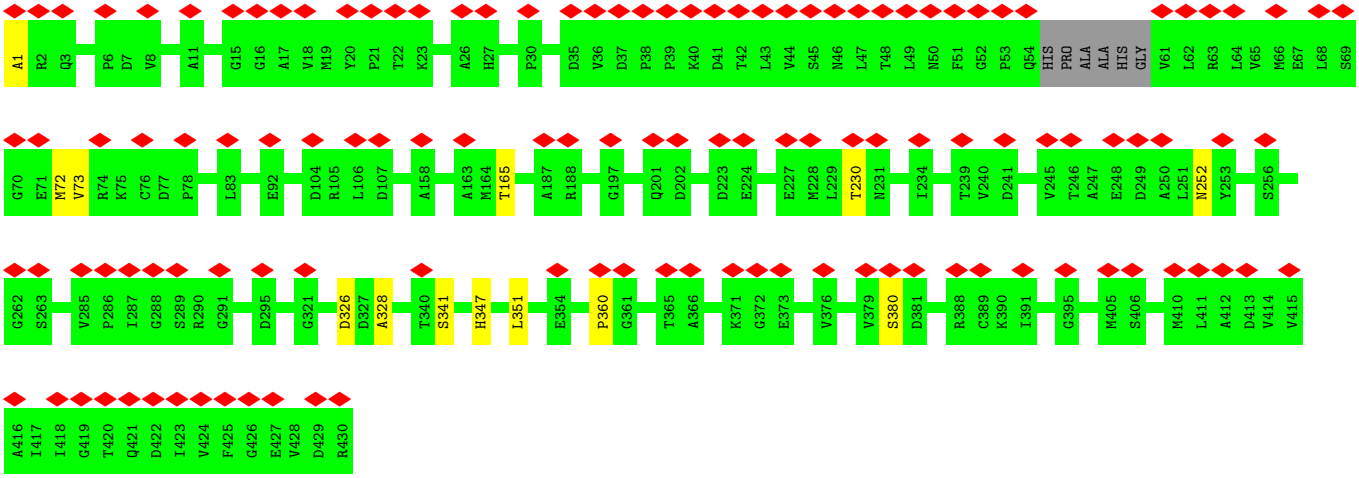




- Molecule 4: NDUFS2

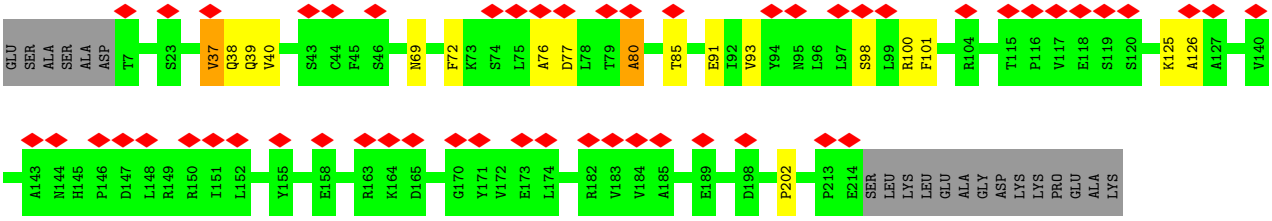
Chain S2:





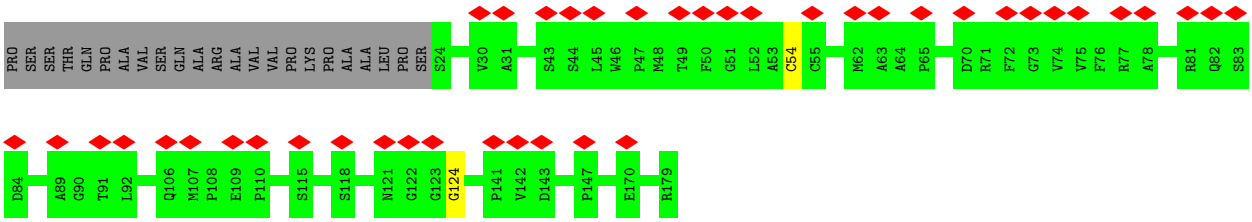
- Molecule 5: NADH:ubiquinone oxidoreductase core subunit S3

Chain S3:



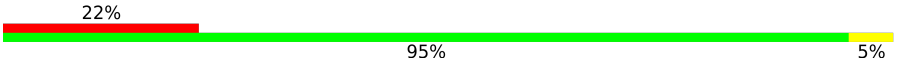
- Molecule 6: NDUFS7

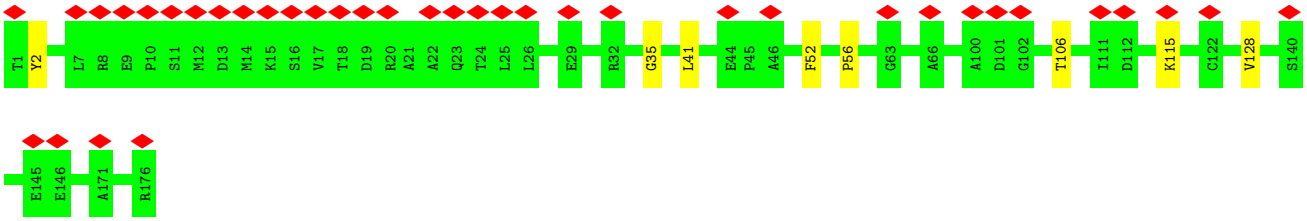
Chain S7:



- Molecule 7: NDUFS8

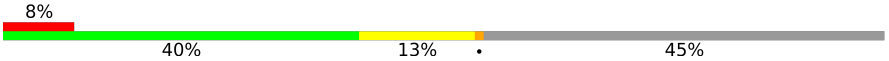
Chain S8:

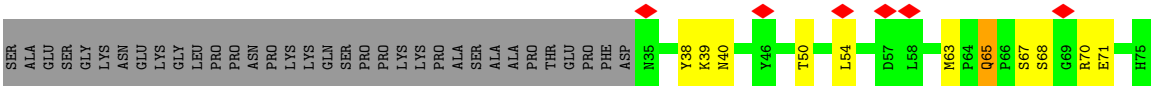




- Molecule 8: NDUFV3

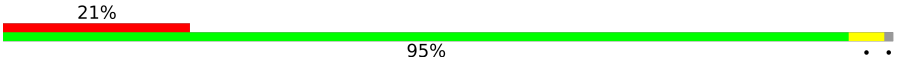
Chain V3:

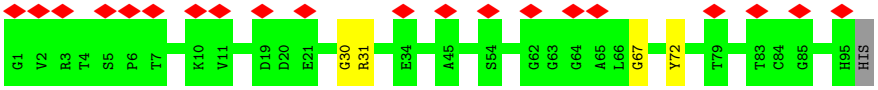




- Molecule 9: NDUFS6

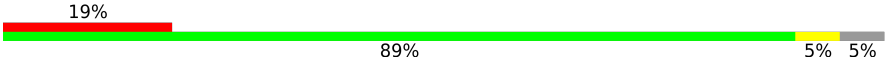
Chain S6:

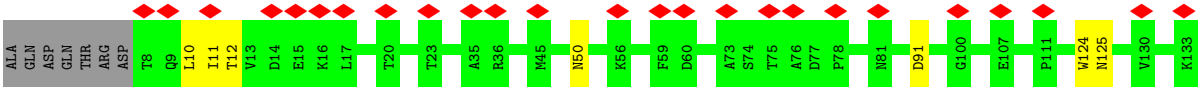




- Molecule 10: NADH:ubiquinone oxidoreductase subunit S4

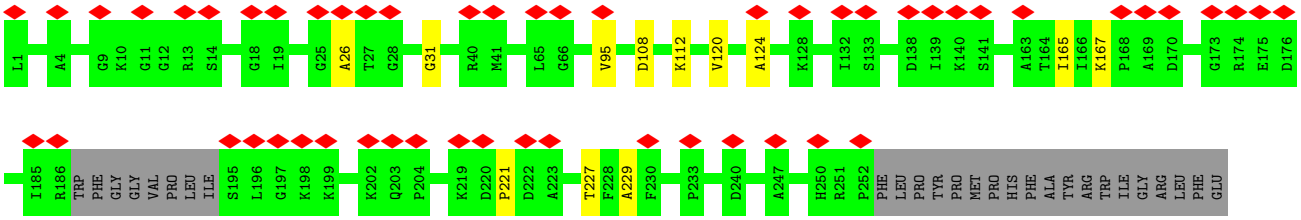
Chain S4:

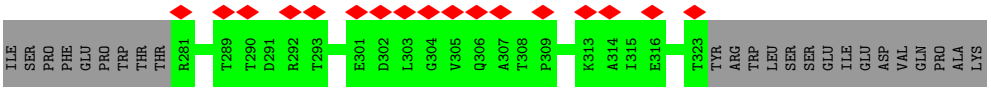




- Molecule 11: NADH:ubiquinone oxidoreductase subunit A9

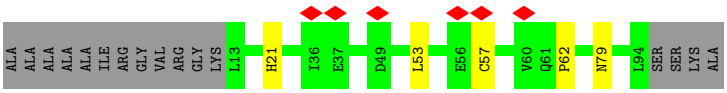
Chain A9:





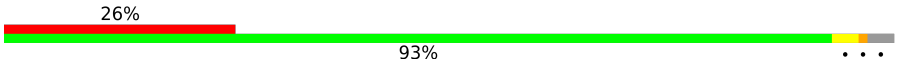
- Molecule 12: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

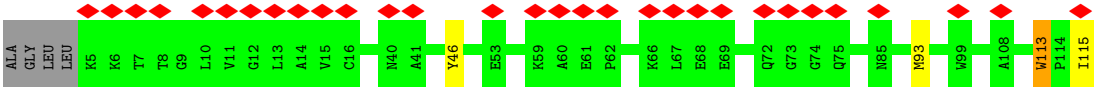
Chain A2:



• Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5

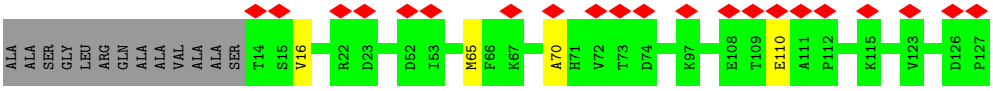
Chain A5:





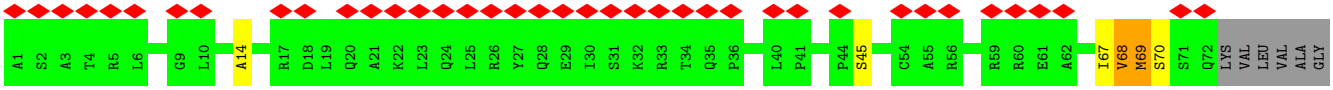
• Molecule 14: NADH:ubiquinone oxidoreductase subunit A6

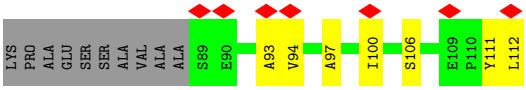
Chain A6:



• Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

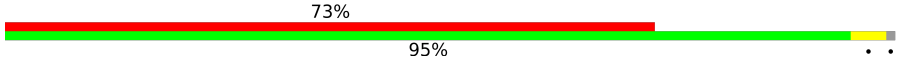
Chain A7:





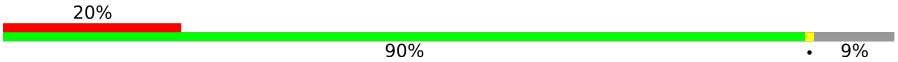
• Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

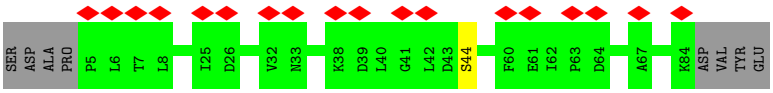
Chain AL:



• Molecule 17: Acyl carrier protein

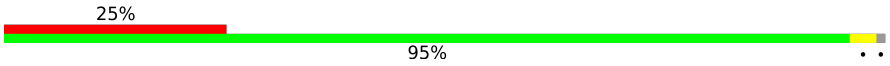
Chain AA:

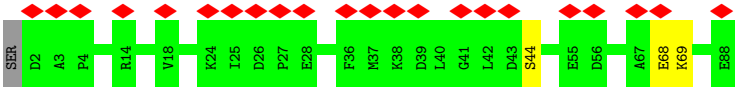




• Molecule 17: Acyl carrier protein

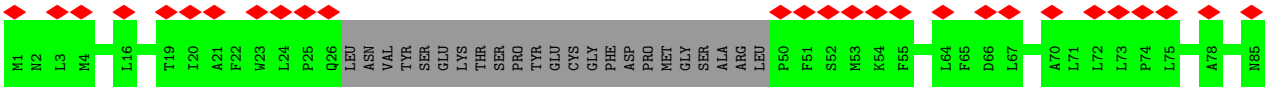
Chain AB:

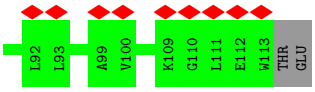




• Molecule 18: NADH-ubiquinone oxidoreductase chain 3

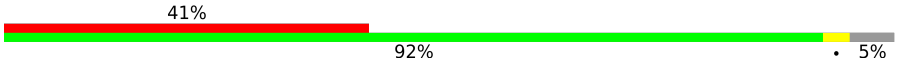
Chain D3:

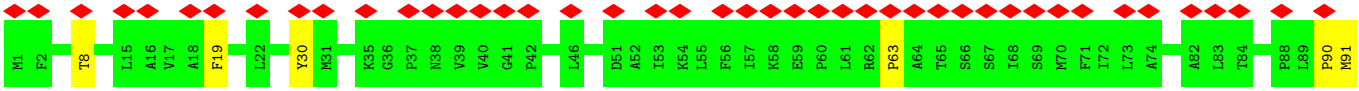


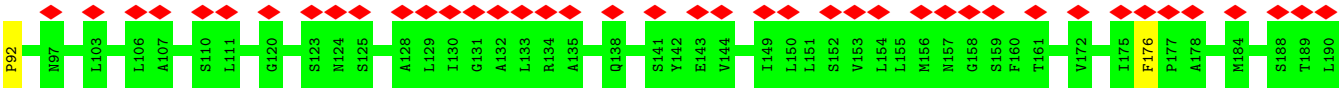


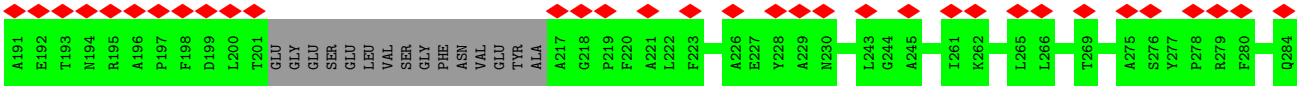
• Molecule 19: NADH-ubiquinone oxidoreductase chain 1

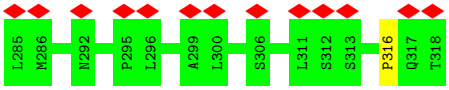
Chain D1:





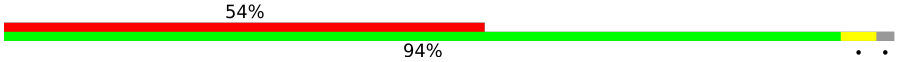


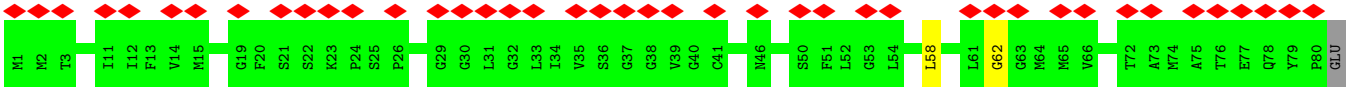


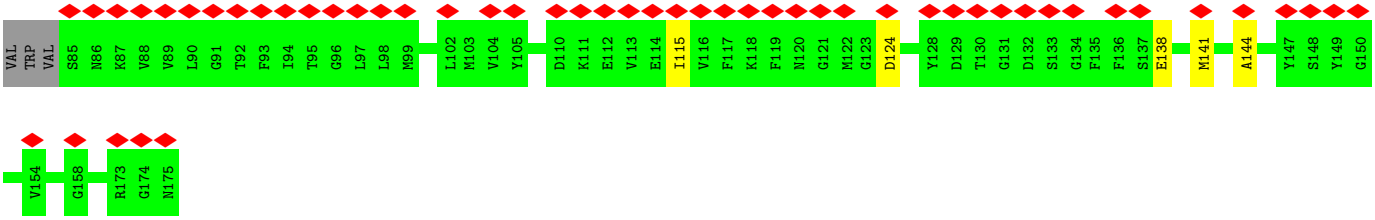


• Molecule 20: NADH-ubiquinone oxidoreductase chain 6

Chain D6:

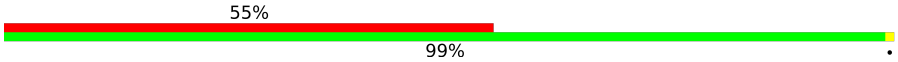


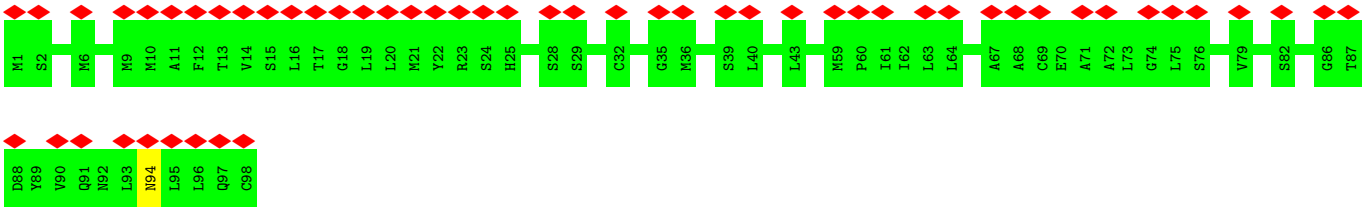




• Molecule 21: NADH-ubiquinone oxidoreductase chain 4L

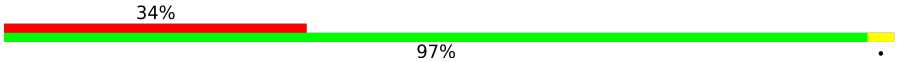
Chain 4L:

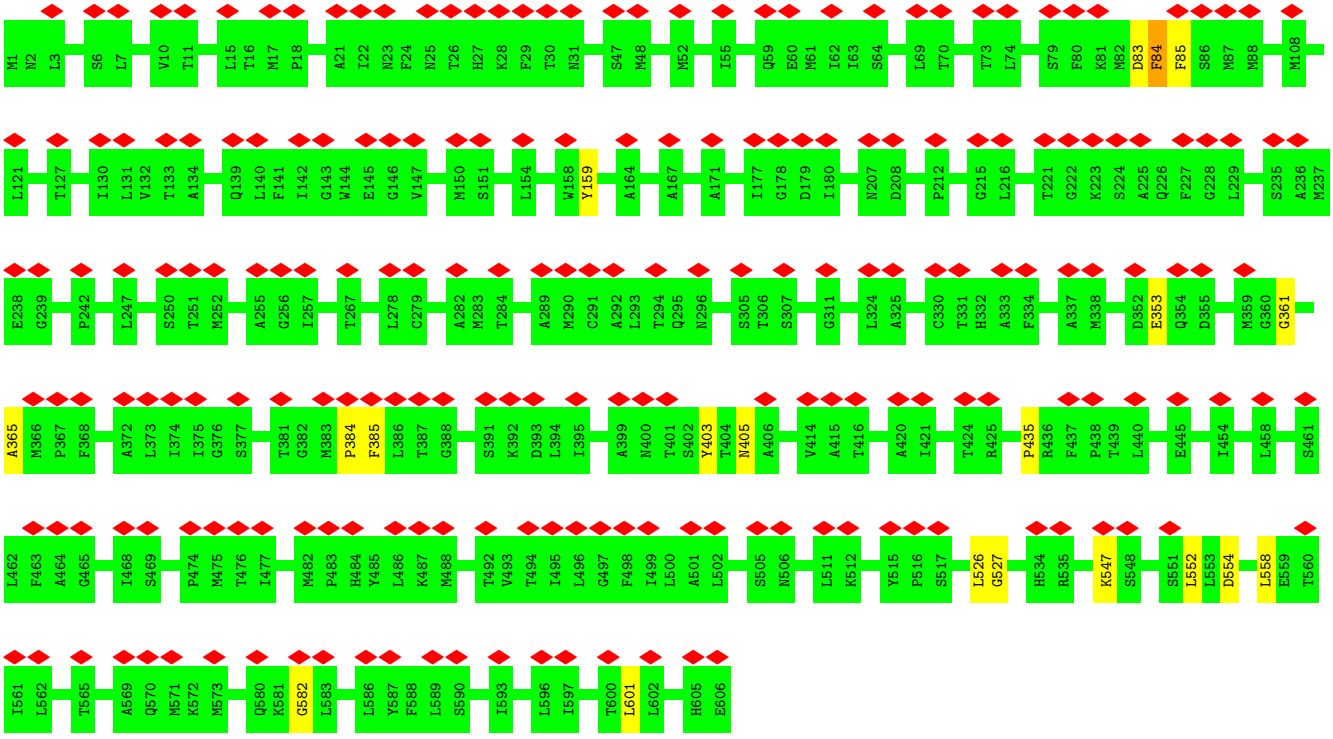




• Molecule 22: NADH-ubiquinone oxidoreductase chain 5

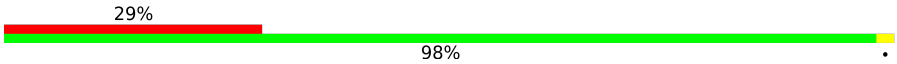
Chain D5:

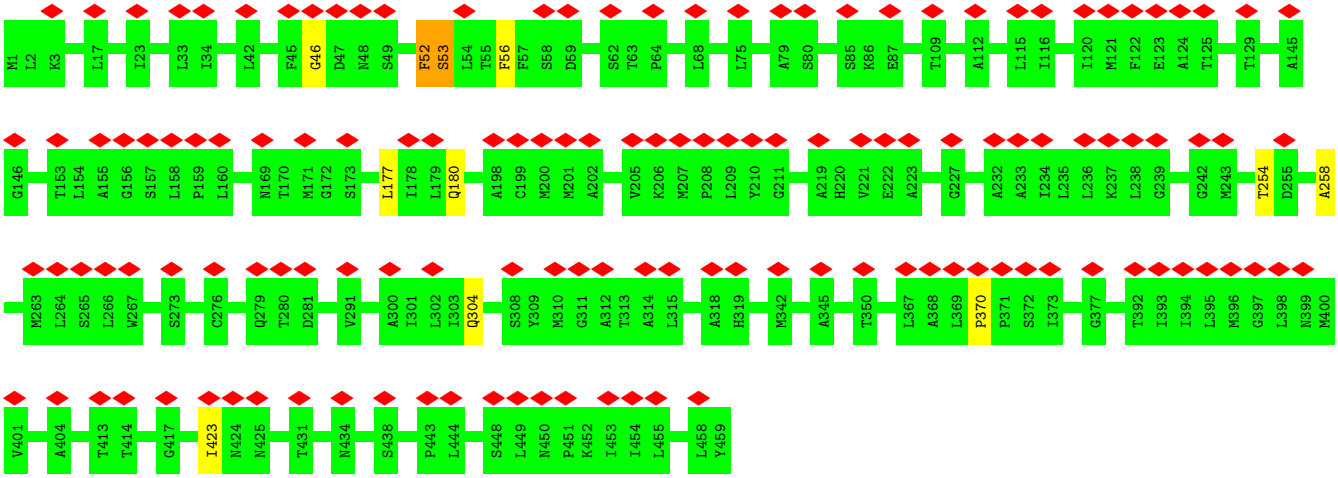




• Molecule 23: NADH-ubiquinone oxidoreductase chain 4

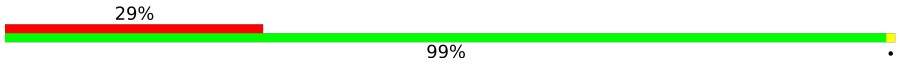
Chain D4:

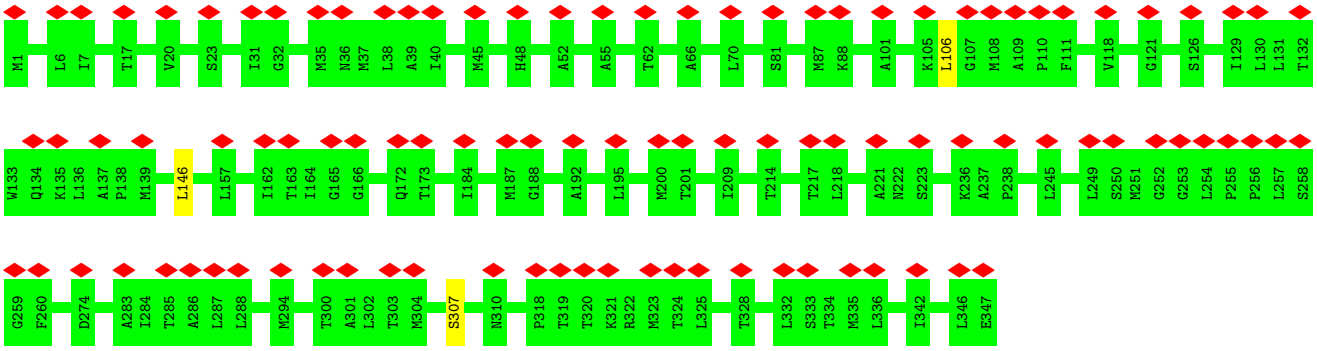




- Molecule 24: NADH-ubiquinone oxidoreductase chain 2

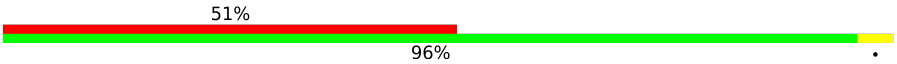
Chain D2:

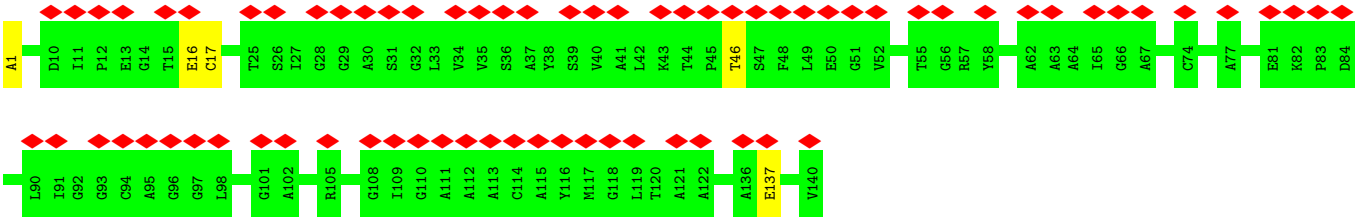




- Molecule 25: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

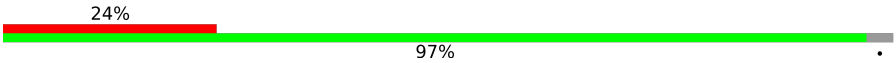
Chain AK:

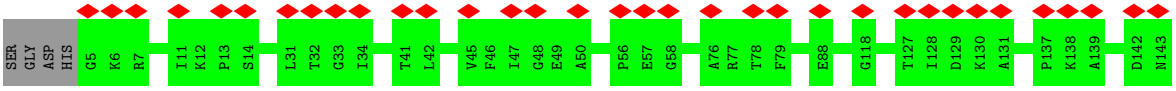




- Molecule 26: NADH:ubiquinone oxidoreductase subunit B5

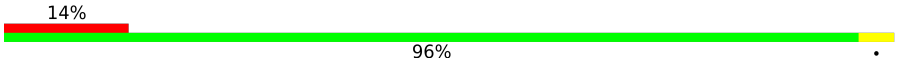
Chain B5:

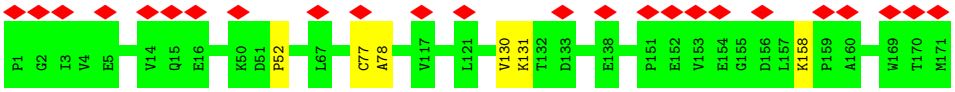




- Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

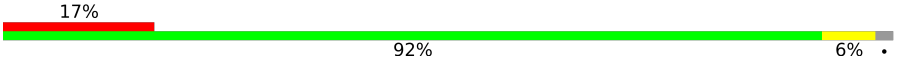
Chain A8:

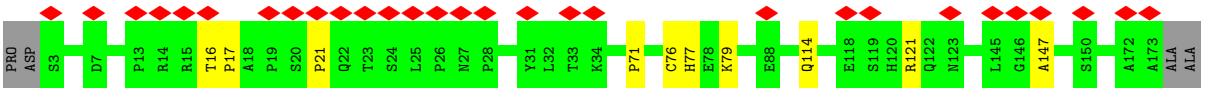




• Molecule 28: NDUFB10

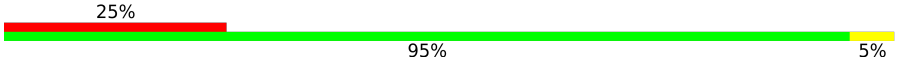
Chain BJ:

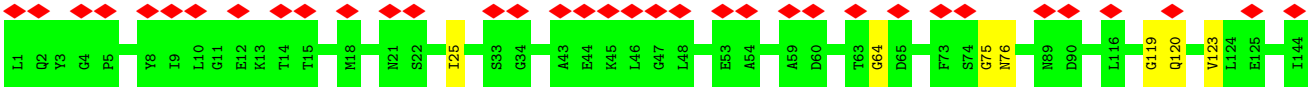


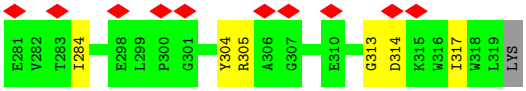


• Molecule 29: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain AJ:

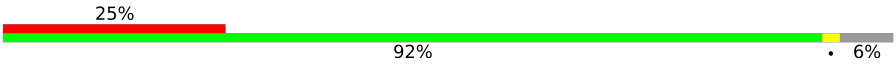


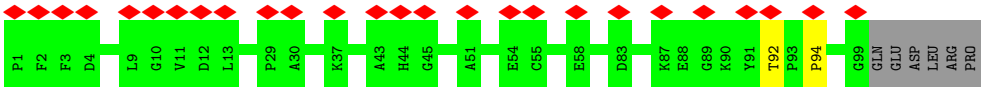




• Molecule 30: NADH:ubiquinone oxidoreductase subunit S5

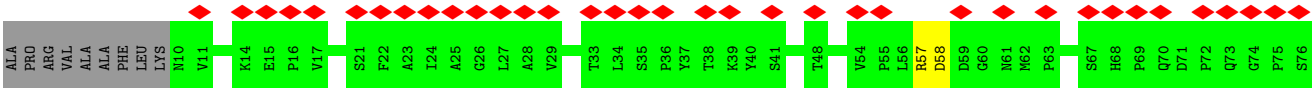
Chain S5:





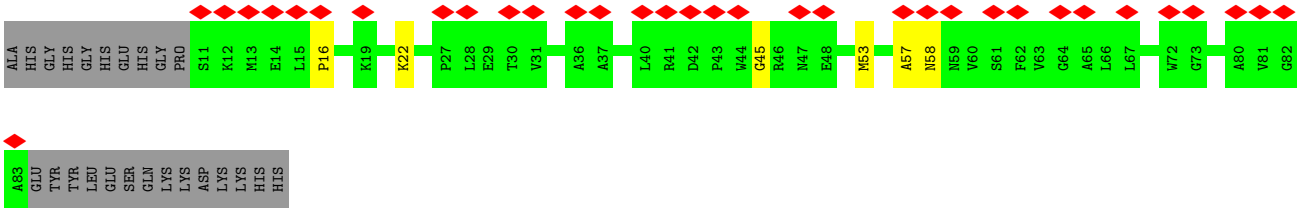
• Molecule 31: NADH:ubiquinone oxidoreductase subunit A3

Chain A3:



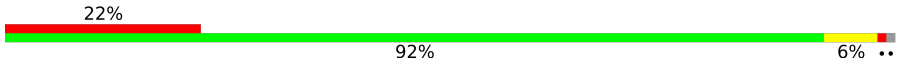
• Molecule 32: NADH:ubiquinone oxidoreductase subunit B3

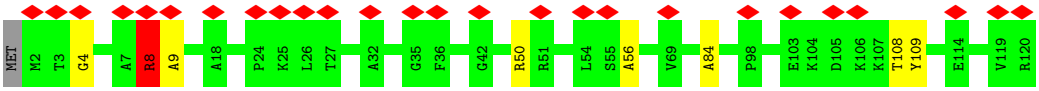
Chain B3:



- Molecule 33: NADH dehydrogenase [ubiquinone] 1 subunit C2

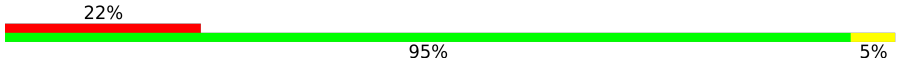
Chain C2:

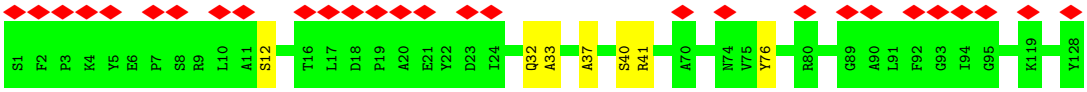




- Molecule 34: NADH:ubiquinone oxidoreductase subunit B4

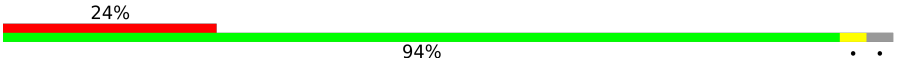
Chain B4:

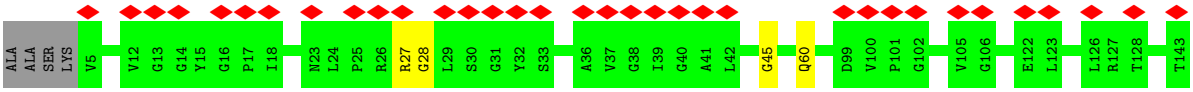




- Molecule 35: NDUFA13

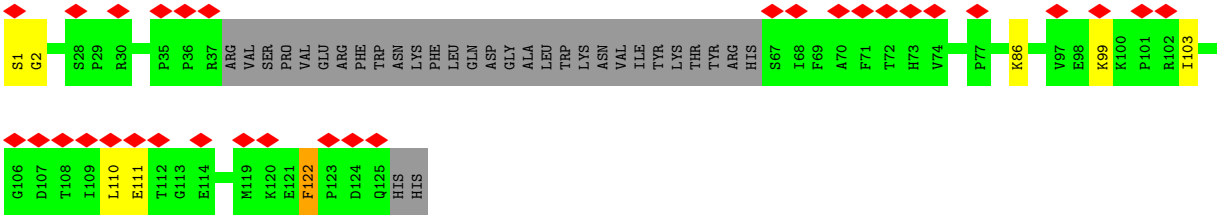
Chain AM:





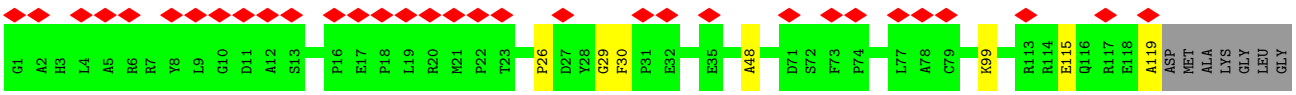
- Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

Chain B6:



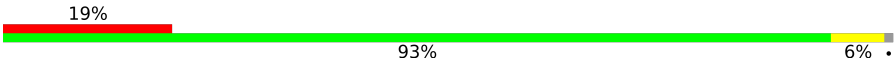
- Molecule 37: NADH:ubiquinone oxidoreductase subunit B7

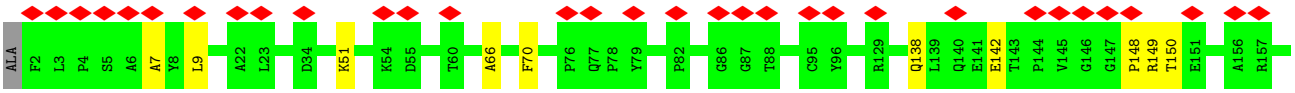
Chain B7:



• Molecule 38: NADH:ubiquinone oxidoreductase subunit B9

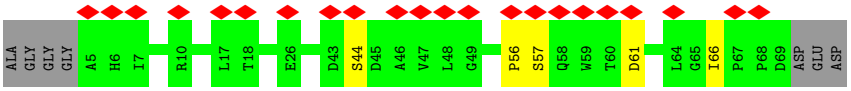
Chain B9:





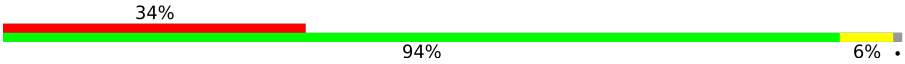
• Molecule 39: NADH:ubiquinone oxidoreductase subunit B2

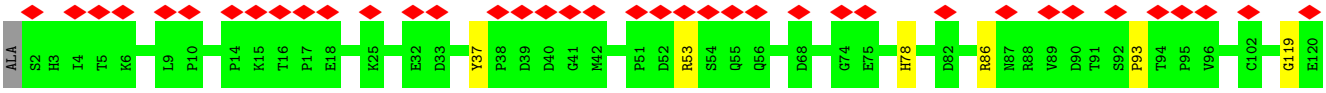
Chain B2:

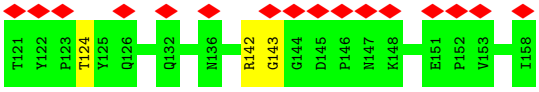


• Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

Chain B8:

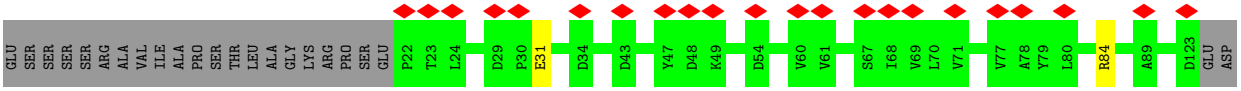






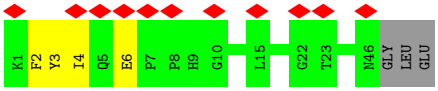
• Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

Chain BK:



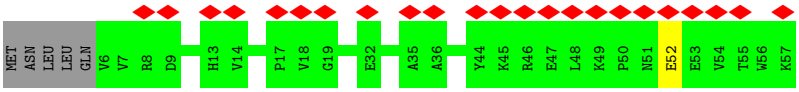
• Molecule 42: NDUFC1

Chain C1:



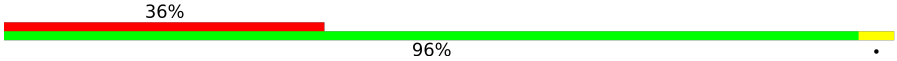
• Molecule 43: NDUFB1

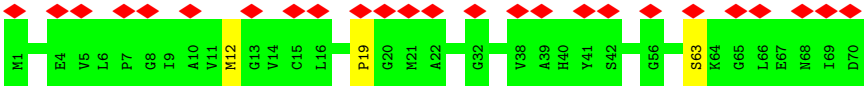
Chain B1:



• Molecule 44: NDUFA1

Chain A1:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	14487	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	51	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	100000	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.494	Depositor
Minimum map value	-0.124	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	716.8, 716.8, 716.8	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.4, 1.4, 1.4	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: FES, ZMP, SF4, FMN, NDP, ZN

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	V1	0.28	0/2098	0.69	1/2905 (0.0%)
2	V2	0.32	0/1044	0.86	2/1451 (0.1%)
3	S1	0.27	0/3389	0.69	3/4713 (0.1%)
4	S2	0.32	0/2088	0.69	4/2902 (0.1%)
5	S3	0.31	0/1033	0.79	2/1441 (0.1%)
6	S7	0.32	0/768	0.71	0/1067
7	S8	0.33	0/870	0.67	0/1211
8	V3	0.31	0/203	0.76	0/282
9	S6	0.22	0/461	0.53	0/636
10	S4	0.24	0/624	0.69	2/869 (0.2%)
11	A9	0.27	0/1410	0.68	2/1956 (0.1%)
12	A2	0.25	0/405	0.67	2/563 (0.4%)
13	A5	0.26	0/549	0.72	0/764
14	A6	0.27	0/566	0.73	2/789 (0.3%)
15	A7	0.28	0/474	0.74	0/658
16	AL	0.26	0/707	0.71	0/981
17	AA	0.26	0/396	0.74	0/551
17	AB	0.25	0/431	0.59	0/600
18	D3	0.28	0/447	0.63	0/622
19	D1	0.34	0/1503	0.79	2/2095 (0.1%)
20	D6	0.27	0/827	0.74	0/1139
21	4L	0.33	0/485	0.70	0/675
22	D5	0.32	0/3000	0.79	0/4181
23	D4	0.34	0/2276	0.80	3/3174 (0.1%)
24	D2	0.34	1/1720 (0.1%)	0.97	2/2398 (0.1%)
25	AK	0.28	0/681	0.76	4/941 (0.4%)
26	B5	0.26	0/686	0.57	0/954
27	A8	0.27	0/846	0.71	0/1178
28	BJ	0.29	0/852	0.72	2/1190 (0.2%)
29	AJ	0.28	0/1574	0.76	2/2190 (0.1%)
30	S5	0.40	1/489 (0.2%)	0.75	0/680
31	A3	0.27	0/366	0.75	0/509

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	B3	0.32	0/355	0.93	1/490 (0.2%)
33	C2	0.32	0/588	0.81	4/818 (0.5%)
34	B4	0.25	0/634	0.62	0/883
35	AM	0.28	0/680	0.68	0/942
36	B6	0.30	0/475	0.83	1/660 (0.2%)
37	B7	0.27	0/591	0.74	2/824 (0.2%)
38	B9	0.27	0/873	0.70	2/1217 (0.2%)
39	B2	0.33	0/322	0.94	4/448 (0.9%)
40	B8	0.30	0/774	0.95	4/1076 (0.4%)
41	BK	0.26	0/505	0.72	0/703
42	C1	0.27	0/226	0.75	2/313 (0.6%)
43	B1	0.24	0/257	0.68	0/357
44	A1	0.27	0/342	0.62	0/473
All	All	0.30	2/39890 (0.0%)	0.75	55/55469 (0.1%)

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	V1	0	2
2	V2	0	3
3	S1	0	6
4	S2	0	2
5	S3	0	2
7	S8	0	1
8	V3	0	2
10	S4	0	1
13	A5	0	2
15	A7	0	2
19	D1	0	2
20	D6	0	2
22	D5	0	5
23	D4	0	2
25	AK	0	2
27	A8	0	1
28	BJ	0	1
29	AJ	0	2
30	S5	0	1
31	A3	0	1
32	B3	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
33	C2	0	1
34	B4	0	1
36	B6	0	2
37	B7	0	1
39	B2	0	1
40	B8	0	2
42	C1	0	1
43	B1	0	1
44	A1	0	1
All	All	0	56

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	S5	94	PRO	C-N	6.68	1.39	1.33
24	D2	146	LEU	C-N	5.88	1.38	1.33

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	D2	106	LEU	N-CA-C	29.24	146.06	112.72
24	D2	106	LEU	CB-CA-C	-15.73	84.98	110.94
28	BJ	21	PRO	CA-C-N	7.69	135.54	121.70
28	BJ	21	PRO	C-N-CA	7.69	135.54	121.70
29	AJ	229	GLU	CA-C-N	7.58	135.33	121.70
29	AJ	229	GLU	C-N-CA	7.58	135.33	121.70
19	D1	63	PRO	CA-C-N	7.23	134.71	121.70
19	D1	63	PRO	C-N-CA	7.23	134.71	121.70
39	B2	44	SER	CA-C-N	7.03	134.36	121.70
39	B2	44	SER	C-N-CA	7.03	134.36	121.70
14	A6	110	GLU	CA-C-N	7.02	134.33	121.70
14	A6	110	GLU	C-N-CA	7.02	134.33	121.70
33	C2	8	ARG	CA-C-N	6.78	133.91	121.70
33	C2	8	ARG	C-N-CA	6.78	133.91	121.70
3	S1	434	SER	CA-C-N	6.69	133.75	121.70
3	S1	434	SER	C-N-CA	6.69	133.75	121.70
25	AK	17	CYS	CA-C-N	6.67	134.29	121.54
25	AK	17	CYS	C-N-CA	6.67	134.29	121.54
40	B8	78	HIS	CA-C-N	6.37	129.11	120.38
40	B8	78	HIS	C-N-CA	6.37	129.11	120.38
4	S2	230	THR	CA-C-N	6.32	133.61	121.54
4	S2	230	THR	C-N-CA	6.32	133.61	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	S4	10	LEU	CA-C-N	6.00	130.45	120.62
10	S4	10	LEU	C-N-CA	6.00	130.45	120.62
32	B3	45	GLY	N-CA-C	5.97	117.42	111.21
33	C2	4	GLY	CA-C-N	5.96	132.43	121.70
33	C2	4	GLY	C-N-CA	5.96	132.43	121.70
39	B2	61	ASP	CA-C-N	5.90	132.81	121.54
39	B2	61	ASP	C-N-CA	5.90	132.81	121.54
1	V1	332	ALA	N-CA-CB	-5.73	107.63	114.17
5	S3	37	VAL	CA-C-N	5.66	132.65	122.46
5	S3	37	VAL	C-N-CA	5.66	132.65	122.46
38	B9	9	LEU	CA-C-N	5.52	132.08	121.54
38	B9	9	LEU	C-N-CA	5.52	132.08	121.54
2	V2	14	LYS	CA-C-N	5.50	132.05	121.54
2	V2	14	LYS	C-N-CA	5.50	132.05	121.54
3	S1	631	VAL	N-CA-C	-5.46	108.17	113.53
40	B8	37	TYR	CA-C-N	5.35	139.84	127.00
40	B8	37	TYR	C-N-CA	5.35	139.84	127.00
11	A9	221	PRO	CA-C-N	5.27	135.41	125.66
11	A9	221	PRO	C-N-CA	5.27	135.41	125.66
37	B7	26	PRO	CA-C-N	5.24	131.55	121.54
37	B7	26	PRO	C-N-CA	5.24	131.55	121.54
25	AK	137	GLU	CA-C-N	5.20	139.48	127.00
25	AK	137	GLU	C-N-CA	5.20	139.48	127.00
4	S2	72	MET	N-CA-C	-5.19	99.75	110.80
4	S2	165	THR	N-CA-C	5.16	121.22	109.81
23	D4	370	PRO	N-CA-C	5.10	116.92	110.70
42	C1	4	ILE	CA-C-N	5.09	131.26	121.54
42	C1	4	ILE	C-N-CA	5.09	131.26	121.54
23	D4	423	ILE	CA-C-N	5.09	131.26	121.54
23	D4	423	ILE	C-N-CA	5.09	131.26	121.54
12	A2	79	ASN	CA-C-N	5.03	129.55	122.46
12	A2	79	ASN	C-N-CA	5.03	129.55	122.46
36	B6	122	PHE	N-CA-C	5.02	120.89	109.81

There are no chirality outliers.

All (56) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
44	A1	63	SER	Peptide
31	A3	57	ARG	Peptide
13	A5	113	TRP	Peptide
13	A5	93	MET	Peptide

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Mol	Chain	Res	Type	Group
15	A7	68	VAL	Peptide
15	A7	69	MET	Peptide
27	A8	52	PRO	Peptide
29	AJ	216	GLU	Peptide
29	AJ	278	PHE	Peptide
25	AK	16	GLU	Peptide
25	AK	46	THR	Peptide
43	B1	52	GLU	Peptide
39	B2	56	PRO	Peptide
32	B3	16	PRO	Peptide
32	B3	22	LYS	Peptide
32	B3	58	ASN	Peptide
34	B4	76	TYR	Peptide
36	B6	122	PHE	Peptide
36	B6	86	LYS	Peptide
37	B7	30	PHE	Peptide
40	B8	53	ARG	Peptide
40	B8	86	ARG	Peptide
28	BJ	79	LYS	Peptide
42	C1	6	GLU	Peptide
33	C2	8	ARG	Peptide
19	D1	90	PRO	Peptide
19	D1	91	MET	Peptide
23	D4	52	PHE	Peptide
23	D4	53	SER	Peptide
22	D5	159	TYR	Peptide
22	D5	353	GLU	Peptide
22	D5	365	ALA	Peptide
22	D5	526	LEU	Peptide
22	D5	84	PHE	Mainchain
20	D6	115	ILE	Peptide
20	D6	124	ASP	Peptide
3	S1	213	TYR	Peptide
3	S1	218	ARG	Peptide
3	S1	247	VAL	Peptide
3	S1	254	MET	Peptide
3	S1	341	ASP	Peptide
3	S1	380	VAL	Peptide
4	S2	341	SER	Peptide
4	S2	73	VAL	Peptide
5	S3	76	ALA	Peptide
5	S3	80	ALA	Mainchain

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Mol	Chain	Res	Type	Group
10	S4	11	ILE	Peptide
30	S5	92	THR	Peptide
7	S8	106	THR	Peptide
1	V1	28	ARG	Peptide
1	V1	331	THR	Peptide
2	V2	10	ARG	Peptide
2	V2	13	PRO	Peptide
2	V2	35	VAL	Peptide
8	V3	63	MET	Peptide
8	V3	65	GLN	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	V1	2099	0	993	24	0
2	V2	1045	0	462	20	0
3	S1	3390	0	1573	20	0
4	S2	2090	0	930	9	0
5	S3	1034	0	445	63	0
6	S7	769	0	351	1	0
7	S8	871	0	401	8	0
8	V3	204	0	78	19	0
9	S6	462	0	211	8	0
10	S4	625	0	274	8	0
11	A9	1413	0	639	6	0
12	A2	406	0	178	3	0
13	A5	550	0	239	2	0
14	A6	567	0	236	6	0
15	A7	476	0	210	58	0
16	AL	708	0	294	11	0
17	AA	397	0	168	2	0
17	AB	432	0	183	8	0
18	D3	449	0	203	0	0
19	D1	1505	0	676	5	0
20	D6	829	0	381	3	0
21	4L	486	0	222	1	0
22	D5	3001	0	1331	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	D4	2277	0	1004	7	0
24	D2	1721	0	744	2	0
25	AK	682	0	358	1	0
26	B5	687	0	302	0	0
27	A8	847	0	364	14	0
28	BJ	853	0	375	21	0
29	AJ	1575	0	694	20	0
30	S5	490	0	215	0	0
31	A3	367	0	157	12	0
32	B3	356	0	178	1	0
33	C2	589	0	254	18	0
34	B4	635	0	281	31	0
35	AM	681	0	302	3	0
36	B6	477	0	187	24	0
37	B7	592	0	260	13	0
38	B9	874	0	374	35	0
39	B2	323	0	136	8	0
40	B8	775	0	318	6	0
41	BK	506	0	214	3	0
42	C1	227	0	97	3	0
43	B1	258	0	109	0	0
44	A1	343	0	159	2	0
45	S1	16	0	0	0	0
45	S7	8	0	0	0	0
45	S8	16	0	0	0	0
45	V1	8	0	0	1	0
46	V1	31	0	19	1	0
47	S1	4	0	0	0	0
47	V2	4	0	0	0	0
48	S6	1	0	0	0	0
49	A9	48	0	26	1	0
50	A6	34	0	40	5	0
50	B9	31	0	34	9	0
All	All	40144	0	17879	299	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 5.

All (299) 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)
1:V1:150:GLN:CB	8:V3:54:LEU:CB	1.77	1.61
5:S3:38:GLN:CA	15:A7:70:SER:HA	1.24	1.57
34:B4:32:GLN:CB	38:B9:7:ALA:HB1	1.39	1.51
5:S3:101:PHE:CB	15:A7:97:ALA:HB3	1.37	1.49
5:S3:38:GLN:HA	15:A7:70:SER:CA	1.00	1.46
34:B4:37:ALA:CA	38:B9:149:ARG:HA	1.44	1.44
5:S3:38:GLN:HA	15:A7:70:SER:C	1.40	1.43
5:S3:38:GLN:C	15:A7:70:SER:HA	1.43	1.43
5:S3:38:GLN:CA	15:A7:70:SER:CA	1.85	1.42
37:B7:99:LYS:HA	39:B2:57:SER:CB	1.53	1.36
5:S3:80:ALA:HA	5:S3:91:GLU:O	1.17	1.35
36:B6:103:ILE:O	37:B7:48:ALA:HB2	1.28	1.32
3:S1:431:ASP:O	3:S1:435:GLY:HA2	1.31	1.31
3:S1:431:ASP:O	3:S1:435:GLY:CA	1.81	1.28
28:BJ:16:THR:O	36:B6:110:LEU:N	1.65	1.27
34:B4:32:GLN:C	38:B9:7:ALA:CB	2.06	1.27
34:B4:32:GLN:CA	38:B9:7:ALA:HB1	1.67	1.23
34:B4:37:ALA:HA	38:B9:149:ARG:CA	1.67	1.22
1:V1:26:TYR:CB	2:V2:192:SER:CB	2.18	1.20
34:B4:32:GLN:CB	38:B9:7:ALA:CB	2.21	1.17
14:A6:70:ALA:HA	50:A6:201:ZMP:O2	1.43	1.16
34:B4:32:GLN:C	38:B9:7:ALA:HB1	1.67	1.13
34:B4:40:SER:CB	38:B9:150:THR:N	2.12	1.12
1:V1:27:GLY:CA	8:V3:40:ASN:H	1.47	1.12
5:S3:101:PHE:CB	15:A7:97:ALA:CB	2.28	1.12
17:AB:69:LYS:CB	36:B6:2:GLY:HA2	1.79	1.12
1:V1:28:ARG:O	8:V3:39:LYS:CB	1.80	1.11
5:S3:101:PHE:O	15:A7:97:ALA:CB	1.98	1.11
1:V1:27:GLY:HA2	8:V3:40:ASN:N	1.02	1.10
2:V2:40:GLU:O	8:V3:67:SER:HA	1.49	1.10
36:B6:103:ILE:O	37:B7:48:ALA:CB	1.99	1.10
28:BJ:17:PRO:C	36:B6:110:LEU:CB	2.25	1.09
34:B4:32:GLN:C	38:B9:7:ALA:HB2	1.76	1.09
5:S3:40:VAL:N	15:A7:68:VAL:H	1.54	1.06
5:S3:101:PHE:CA	15:A7:97:ALA:HB3	1.85	1.05
5:S3:38:GLN:O	15:A7:70:SER:HA	1.54	1.05
3:S1:449:PRO:O	3:S1:489:VAL:HA	1.57	1.04
9:S6:30:GLY:O	16:AL:121:PRO:HA	1.58	1.04
34:B4:37:ALA:CB	38:B9:149:ARG:HA	1.85	1.04
5:S3:38:GLN:N	15:A7:69:MET:O	1.92	1.01
1:V1:27:GLY:CA	8:V3:40:ASN:N	1.97	1.01
34:B4:40:SER:CB	38:B9:150:THR:H	1.70	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V2:191:PHE:CB	8:V3:38:TYR:CB	2.39	1.00
5:S3:40:VAL:CB	15:A7:68:VAL:CB	2.40	0.99
5:S3:40:VAL:H	15:A7:68:VAL:N	1.58	0.99
10:S4:12:THR:CB	14:A6:16:VAL:H	1.74	0.98
3:S1:431:ASP:O	3:S1:435:GLY:HA3	1.62	0.98
27:A8:130:VAL:O	31:A3:58:ASP:CA	2.11	0.98
5:S3:38:GLN:CA	15:A7:70:SER:C	2.23	0.98
38:B9:66:ALA:HB1	50:B9:201:ZMP:H6	1.46	0.97
17:AB:69:LYS:CB	36:B6:2:GLY:CA	2.42	0.97
28:BJ:17:PRO:O	36:B6:110:LEU:CB	2.13	0.97
50:A6:201:ZMP:P1	17:AA:44:SER:CB	2.53	0.96
34:B4:37:ALA:HA	38:B9:149:ARG:HA	0.98	0.96
22:D5:403:TYR:HA	40:B8:124:THR:O	1.66	0.95
28:BJ:17:PRO:HA	36:B6:110:LEU:N	1.81	0.95
34:B4:37:ALA:CB	38:B9:149:ARG:CB	2.46	0.94
5:S3:80:ALA:CA	5:S3:91:GLU:O	2.14	0.94
28:BJ:16:THR:O	36:B6:110:LEU:CA	2.15	0.94
27:A8:131:LYS:CA	31:A3:58:ASP:CB	2.46	0.93
5:S3:38:GLN:HA	15:A7:70:SER:N	1.82	0.93
17:AB:44:SER:CB	50:B9:201:ZMP:P1	2.56	0.92
37:B7:99:LYS:CA	39:B2:57:SER:CB	2.46	0.92
5:S3:38:GLN:O	15:A7:70:SER:CA	2.18	0.91
34:B4:37:ALA:CB	38:B9:149:ARG:CA	2.50	0.90
21:4L:94:ASN:HA	22:D5:582:GLY:O	1.70	0.90
37:B7:29:GLY:HA3	39:B2:66:ILE:C	1.97	0.89
37:B7:29:GLY:HA3	39:B2:66:ILE:O	1.72	0.89
5:S3:101:PHE:O	15:A7:97:ALA:HB1	1.70	0.89
34:B4:37:ALA:HA	38:B9:149:ARG:C	1.96	0.89
28:BJ:17:PRO:HA	36:B6:110:LEU:H	1.33	0.88
34:B4:32:GLN:O	38:B9:7:ALA:HB2	1.73	0.87
29:AJ:317:ILE:HA	33:C2:56:ALA:HA	1.54	0.86
27:A8:130:VAL:C	31:A3:58:ASP:CB	2.49	0.86
19:D1:19:PHE:CB	44:A1:12:MET:CB	2.54	0.85
34:B4:37:ALA:HB1	38:B9:149:ARG:CB	2.05	0.85
28:BJ:76:CYS:O	33:C2:108:THR:CA	2.24	0.85
27:A8:131:LYS:HA	31:A3:58:ASP:CB	2.07	0.85
5:S3:37:VAL:C	15:A7:69:MET:O	2.20	0.84
28:BJ:76:CYS:O	33:C2:108:THR:CB	2.25	0.84
5:S3:40:VAL:H	15:A7:68:VAL:H	0.83	0.82
2:V2:40:GLU:O	8:V3:67:SER:CA	2.28	0.82
5:S3:39:GLN:HA	15:A7:68:VAL:O	1.79	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:BJ:76:CYS:O	33:C2:108:THR:HA	1.78	0.82
27:A8:130:VAL:O	31:A3:58:ASP:N	2.13	0.80
5:S3:80:ALA:HA	5:S3:91:GLU:C	2.07	0.80
27:A8:131:LYS:N	31:A3:58:ASP:CB	2.45	0.80
34:B4:37:ALA:CA	38:B9:149:ARG:CA	2.35	0.80
9:S6:30:GLY:O	16:AL:121:PRO:CA	2.31	0.79
5:S3:37:VAL:O	15:A7:70:SER:N	2.15	0.79
28:BJ:17:PRO:CA	36:B6:110:LEU:H	1.96	0.79
5:S3:101:PHE:C	15:A7:97:ALA:HB3	2.07	0.78
5:S3:38:GLN:CA	15:A7:70:SER:N	2.44	0.78
37:B7:29:GLY:HA3	39:B2:66:ILE:N	1.98	0.78
27:A8:130:VAL:O	31:A3:58:ASP:CB	2.31	0.78
28:BJ:16:THR:C	36:B6:110:LEU:H	1.91	0.77
10:S4:12:THR:CB	14:A6:16:VAL:O	2.32	0.77
4:S2:326:ASP:CB	15:A7:45:SER:CB	2.62	0.77
3:S1:136:ALA:CB	9:S6:72:TYR:O	2.34	0.76
29:AJ:305:ARG:CB	33:C2:50:ARG:C	2.59	0.76
34:B4:32:GLN:O	38:B9:7:ALA:CB	2.28	0.76
28:BJ:16:THR:O	36:B6:110:LEU:CB	2.33	0.76
27:A8:130:VAL:O	31:A3:58:ASP:HA	1.87	0.74
34:B4:12:SER:O	40:B8:93:PRO:CB	2.35	0.74
36:B6:103:ILE:O	37:B7:48:ALA:CA	2.34	0.74
5:S3:202:PRO:HA	10:S4:50:ASN:CB	2.18	0.74
1:V1:43:TYR:CB	2:V2:209:PRO:CB	2.66	0.73
6:S7:124:GLY:HA2	7:S8:115:LYS:HA	1.70	0.73
5:S3:40:VAL:N	15:A7:68:VAL:O	2.22	0.73
34:B4:37:ALA:HB2	38:B9:149:ARG:CB	2.18	0.73
5:S3:37:VAL:C	15:A7:69:MET:C	2.56	0.73
5:S3:39:GLN:CA	15:A7:68:VAL:O	2.36	0.73
3:S1:126:ASP:CB	4:S2:328:ALA:HB3	2.19	0.72
5:S3:38:GLN:CB	15:A7:70:SER:C	2.63	0.72
29:AJ:317:ILE:CA	33:C2:56:ALA:HA	2.19	0.72
3:S1:442:VAL:O	3:S1:446:ALA:HB2	1.89	0.71
34:B4:37:ALA:HB1	38:B9:149:ARG:CA	2.20	0.71
37:B7:29:GLY:CA	39:B2:66:ILE:O	2.38	0.71
3:S1:276:ARG:O	16:AL:135:GLN:CB	2.38	0.70
1:V1:216:PHE:O	10:S4:124:TRP:HA	1.91	0.70
5:S3:101:PHE:C	15:A7:97:ALA:CB	2.62	0.70
34:B4:37:ALA:HB1	38:B9:149:ARG:HA	1.73	0.70
2:V2:39:PRO:CB	8:V3:65:GLN:CB	2.70	0.70
23:D4:177:LEU:O	23:D4:180:GLN:C	2.35	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:BJ:121:ARG:CB	40:B8:142:ARG:O	2.41	0.69
5:S3:38:GLN:O	15:A7:70:SER:CB	2.41	0.69
5:S3:38:GLN:C	15:A7:69:MET:O	2.35	0.68
10:S4:12:THR:CB	14:A6:16:VAL:N	2.52	0.68
34:B4:32:GLN:CB	38:B9:7:ALA:O	2.42	0.67
29:AJ:64:GLY:HA2	42:C1:3:TYR:HA	1.76	0.67
34:B4:37:ALA:C	38:B9:149:ARG:HA	2.17	0.67
13:A5:46:TYR:CB	15:A7:93:ALA:HB2	2.25	0.66
29:AJ:64:GLY:C	42:C1:2:PHE:O	2.39	0.66
4:S2:252:ASN:O	5:S3:126:ALA:N	2.29	0.66
2:V2:39:PRO:CA	8:V3:65:GLN:CB	2.74	0.66
27:A8:131:LYS:CB	31:A3:58:ASP:CB	2.73	0.66
38:B9:66:ALA:CB	50:B9:201:ZMP:H6	2.22	0.66
17:AB:69:LYS:CB	36:B6:2:GLY:N	2.59	0.65
7:S8:35:GLY:O	15:A7:14:ALA:HB1	1.96	0.65
29:AJ:317:ILE:HA	33:C2:56:ALA:CA	2.26	0.65
28:BJ:17:PRO:CA	36:B6:110:LEU:CB	2.75	0.65
5:S3:38:GLN:CA	15:A7:69:MET:O	2.45	0.65
29:AJ:304:TYR:C	33:C2:50:ARG:O	2.40	0.65
23:D4:46:GLY:H	41:BK:84:ARG:HA	1.60	0.64
1:V1:126:GLY:HA2	1:V1:131:ALA:HB3	1.79	0.64
5:S3:39:GLN:C	15:A7:68:VAL:O	2.40	0.64
9:S6:31:ARG:HA	16:AL:121:PRO:O	1.98	0.64
1:V1:259:SER:CB	2:V2:149:VAL:HA	2.28	0.64
2:V2:41:GLY:HA2	8:V3:70:ARG:O	1.98	0.63
5:S3:38:GLN:HA	15:A7:70:SER:O	1.93	0.63
1:V1:27:GLY:HA2	8:V3:40:ASN:H	0.81	0.63
20:D6:58:LEU:O	20:D6:62:GLY:HA3	1.98	0.62
24:D2:307:SER:N	29:AJ:284:ILE:O	2.33	0.62
5:S3:38:GLN:CA	15:A7:70:SER:O	2.47	0.61
5:S3:40:VAL:CA	15:A7:68:VAL:H	2.13	0.61
29:AJ:305:ARG:CB	33:C2:50:ARG:O	2.49	0.61
5:S3:38:GLN:N	15:A7:69:MET:C	2.59	0.61
38:B9:51:LYS:O	50:B9:201:ZMP:O3	2.18	0.60
23:D4:304:GLN:O	28:BJ:147:ALA:HB2	2.00	0.60
1:V1:93:LEU:O	1:V1:134:ALA:HA	2.00	0.60
34:B4:33:ALA:N	38:B9:7:ALA:HB2	2.15	0.60
4:S2:1:ALA:H2	41:BK:31:GLU:CB	2.15	0.60
37:B7:29:GLY:CA	39:B2:66:ILE:C	2.74	0.59
7:S8:2:TYR:O	15:A7:106:SER:N	2.21	0.59
28:BJ:16:THR:C	36:B6:110:LEU:CB	2.76	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S3:38:GLN:CA	15:A7:69:MET:C	2.76	0.59
34:B4:33:ALA:N	38:B9:7:ALA:CB	2.62	0.59
27:A8:130:VAL:H	31:A3:58:ASP:HA	1.68	0.58
12:A2:21:HIS:O	12:A2:62:PRO:HA	2.02	0.58
37:B7:115:GLU:O	37:B7:119:ALA:HB3	2.04	0.58
22:D5:547:LYS:O	22:D5:552:LEU:CB	2.51	0.58
27:A8:130:VAL:C	31:A3:58:ASP:CA	2.74	0.57
1:V1:300:GLY:HA2	1:V1:330:GLY:H	1.70	0.57
5:S3:37:VAL:C	15:A7:70:SER:N	2.62	0.57
5:S3:69:ASN:CB	15:A7:94:VAL:O	2.53	0.57
37:B7:29:GLY:HA3	39:B2:66:ILE:CA	2.33	0.57
5:S3:69:ASN:CB	15:A7:94:VAL:C	2.78	0.57
5:S3:100:ARG:O	15:A7:100:ILE:N	2.38	0.57
22:D5:601:LEU:O	25:AK:1:ALA:HB2	2.05	0.56
1:V1:294:LEU:HA	1:V1:338:ASP:HA	1.86	0.56
28:BJ:77:HIS:HA	33:C2:108:THR:HA	1.88	0.56
23:D4:177:LEU:O	23:D4:180:GLN:O	2.23	0.56
3:S1:357:ASP:CB	12:A2:53:LEU:HA	2.36	0.56
5:S3:77:ASP:O	5:S3:93:VAL:O	2.23	0.56
5:S3:38:GLN:C	15:A7:69:MET:C	2.73	0.55
3:S1:136:ALA:HB2	9:S6:72:TYR:O	2.05	0.55
2:V2:40:GLU:O	8:V3:67:SER:CB	2.54	0.55
1:V1:216:PHE:O	10:S4:124:TRP:CA	2.55	0.55
1:V1:301:GLY:HA2	1:V1:333:ALA:HB3	1.89	0.55
29:AJ:305:ARG:N	33:C2:50:ARG:CB	2.69	0.55
22:D5:361:GLY:H	22:D5:435:PRO:HA	1.72	0.54
3:S1:377:VAL:HA	3:S1:450:MET:O	2.07	0.54
5:S3:37:VAL:O	15:A7:70:SER:O	2.25	0.54
24:D2:307:SER:O	29:AJ:284:ILE:N	2.33	0.53
23:D4:52:PHE:O	23:D4:56:PHE:CB	2.57	0.53
1:V1:27:GLY:N	8:V3:40:ASN:H	2.03	0.53
3:S1:629:ASN:CB	12:A2:57:CYS:CB	2.86	0.53
28:BJ:114:GLN:O	36:B6:99:LYS:HA	2.09	0.53
19:D1:316:PRO:CB	35:AM:60:GLN:CB	2.87	0.52
1:V1:103:GLY:C	2:V2:148:CYS:CB	2.83	0.51
22:D5:83:ASP:O	22:D5:85:PHE:N	2.43	0.51
27:A8:130:VAL:C	31:A3:58:ASP:HA	2.34	0.51
17:AB:68:GLU:CB	36:B6:1:SER:N	2.74	0.51
16:AL:6:VAL:O	16:AL:10:GLY:N	2.40	0.51
29:AJ:25:ILE:O	29:AJ:123:VAL:HA	2.11	0.51
20:D6:141:MET:HA	20:D6:144:ALA:HB3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:B4:41:ARG:HA	38:B9:148:PRO:CB	2.40	0.50
5:S3:101:PHE:CB	15:A7:97:ALA:CA	2.89	0.50
28:BJ:16:THR:O	36:B6:111:GLU:N	2.45	0.50
23:D4:254:THR:O	23:D4:258:ALA:HB2	2.11	0.50
3:S1:407:ALA:HA	3:S1:420:ASP:O	2.12	0.50
14:A6:70:ALA:CA	50:A6:201:ZMP:O2	2.37	0.50
19:D1:8:THR:O	44:A1:19:PRO:CB	2.60	0.50
3:S1:277:GLN:HA	16:AL:135:GLN:O	2.12	0.50
3:S1:266:LYS:O	3:S1:270:ALA:HB2	2.13	0.49
7:S8:52:PHE:O	16:AL:61:TRP:HA	2.13	0.49
9:S6:30:GLY:O	16:AL:121:PRO:O	2.30	0.49
36:B6:103:ILE:O	37:B7:48:ALA:HA	2.11	0.49
38:B9:138:GLN:O	38:B9:142:GLU:CB	2.60	0.49
4:S2:252:ASN:O	5:S3:125:LYS:C	2.56	0.48
20:D6:58:LEU:O	20:D6:62:GLY:CA	2.60	0.48
38:B9:70:PHE:HA	50:B9:201:ZMP:C2	2.43	0.48
1:V1:236:ARG:O	2:V2:213:VAL:CB	2.61	0.48
28:BJ:76:CYS:O	33:C2:109:TYR:N	2.46	0.48
2:V2:96:GLY:HA3	2:V2:136:LEU:H	1.77	0.48
5:S3:40:VAL:O	15:A7:68:VAL:N	2.46	0.48
3:S1:450:MET:HA	3:S1:489:VAL:O	2.13	0.48
4:S2:360:PRO:HA	4:S2:380:SER:O	2.14	0.48
28:BJ:17:PRO:CA	36:B6:110:LEU:N	2.61	0.48
17:AB:68:GLU:CB	36:B6:1:SER:H3	2.26	0.48
46:V1:501:FMN:O5'	46:V1:501:FMN:O3'	2.30	0.47
34:B4:12:SER:O	40:B8:93:PRO:HA	2.14	0.47
9:S6:30:GLY:O	16:AL:121:PRO:C	2.57	0.47
27:A8:158:LYS:O	33:C2:84:ALA:HB1	2.14	0.47
5:S3:72:PHE:HA	5:S3:98:SER:HA	1.97	0.47
11:A9:120:VAL:O	11:A9:124:ALA:HB2	2.14	0.47
11:A9:167:LYS:O	11:A9:229:ALA:HA	2.14	0.47
50:B9:201:ZMP:O2	50:B9:201:ZMP:N2	2.45	0.47
8:V3:68:SER:CB	10:S4:125:ASN:CB	2.93	0.47
23:D4:254:THR:O	23:D4:258:ALA:CB	2.62	0.47
34:B4:12:SER:O	40:B8:93:PRO:CA	2.62	0.47
2:V2:39:PRO:N	8:V3:65:GLN:CB	2.78	0.47
5:S3:40:VAL:O	15:A7:67:ILE:C	2.58	0.47
5:S3:101:PHE:O	15:A7:97:ALA:HB2	2.05	0.47
35:AM:27:ARG:HA	35:AM:28:GLY:HA3	1.71	0.47
5:S3:37:VAL:O	15:A7:69:MET:C	2.54	0.47
5:S3:101:PHE:CA	15:A7:97:ALA:CB	2.74	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:D5:384:PRO:HA	22:D5:385:PHE:HA	1.54	0.47
29:AJ:305:ARG:CB	33:C2:50:ARG:CB	2.93	0.47
38:B9:66:ALA:HB1	50:B9:201:ZMP:C6	2.33	0.46
2:V2:41:GLY:HA2	8:V3:71:GLU:HA	1.98	0.46
4:S2:347:HIS:O	4:S2:351:LEU:CB	2.64	0.46
32:B3:53:MET:HA	32:B3:57:ALA:HB2	1.96	0.46
17:AB:44:SER:CB	50:B9:201:ZMP:O7	2.64	0.46
5:S3:38:GLN:C	15:A7:70:SER:CA	2.34	0.45
29:AJ:64:GLY:CA	42:C1:3:TYR:HA	2.45	0.45
1:V1:103:GLY:CA	2:V2:148:CYS:CB	2.94	0.45
3:S1:483:VAL:HA	3:S1:484:THR:HA	1.65	0.45
4:S2:1:ALA:N	41:BK:31:GLU:CB	2.79	0.45
3:S1:675:ASP:O	3:S1:679:ARG:CB	2.64	0.45
15:A7:111:TYR:HA	15:A7:112:LEU:HA	1.63	0.45
7:S8:41:LEU:HA	19:D1:30:TYR:O	2.16	0.45
7:S8:128:VAL:HA	9:S6:67:GLY:O	2.16	0.45
33:C2:8:ARG:H	33:C2:9:ALA:HB3	1.81	0.45
3:S1:377:VAL:O	3:S1:406:VAL:HA	2.16	0.45
11:A9:95:VAL:O	49:A9:401:NDP:O3D	2.33	0.45
2:V2:13:PRO:HA	2:V2:15:ASN:H	1.82	0.44
3:S1:283:MET:HA	3:S1:293:HIS:HA	2.00	0.44
22:D5:405:ASN:O	40:B8:119:GLY:CA	2.65	0.44
38:B9:66:ALA:HB2	50:B9:201:ZMP:H7A	1.99	0.44
5:S3:38:GLN:N	15:A7:70:SER:N	2.66	0.43
11:A9:108:ASP:O	11:A9:112:LYS:CB	2.66	0.43
7:S8:56:PRO:HA	16:AL:92:CYS:CB	2.48	0.43
1:V1:138:ILE:O	1:V1:180:GLY:N	2.52	0.43
7:S8:56:PRO:CB	16:AL:92:CYS:CB	2.97	0.43
11:A9:26:ALA:HA	11:A9:31:GLY:HA3	2.01	0.43
1:V1:147:SER:CB	8:V3:50:THR:CB	2.96	0.43
5:S3:85:THR:HA	10:S4:91:ASP:CB	2.49	0.43
2:V2:39:PRO:HA	8:V3:65:GLN:CB	2.48	0.43
29:AJ:317:ILE:C	33:C2:56:ALA:HA	2.43	0.42
4:S2:252:ASN:CB	5:S3:125:LYS:CB	2.98	0.42
14:A6:65:MET:CB	50:A6:201:ZMP:H4	2.49	0.42
1:V1:104:THR:N	2:V2:148:CYS:CB	2.82	0.42
50:A6:201:ZMP:O6	17:AA:44:SER:CB	2.65	0.42
29:AJ:317:ILE:CA	33:C2:56:ALA:CA	2.93	0.42
1:V1:362:CYS:N	45:V1:500:SF4:S2	2.77	0.42
5:S3:40:VAL:N	15:A7:68:VAL:N	2.36	0.42
22:D5:554:ASP:O	22:D5:558:LEU:CB	2.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:AJ:317:ILE:HA	33:C2:56:ALA:CB	2.50	0.42
2:V2:98:TYR:H	2:V2:136:LEU:HA	1.85	0.42
19:D1:176:PHE:C	35:AM:45:GLY:HA3	2.45	0.42
29:AJ:75:GLY:HA3	29:AJ:76:ASN:HA	1.73	0.41
29:AJ:119:GLY:HA3	29:AJ:120:GLN:HA	1.83	0.41
27:A8:77:CYS:HA	27:A8:78:ALA:HA	1.70	0.41
29:AJ:313:GLY:HA3	29:AJ:314:ASP:HA	1.72	0.41
34:B4:32:GLN:CB	38:B9:7:ALA:C	2.94	0.41
11:A9:165:ILE:O	11:A9:227:THR:HA	2.21	0.41
17:AB:69:LYS:CB	36:B6:2:GLY:H	2.31	0.40
13:A5:113:TRP:O	13:A5:115:ILE:N	2.54	0.40

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	V1	428/445 (96%)	381 (89%)	47 (11%)	0	100	100
2	V2	210/217 (97%)	167 (80%)	43 (20%)	0	100	100
3	S1	686/704 (97%)	614 (90%)	71 (10%)	1 (0%)	48	83
4	S2	420/430 (98%)	380 (90%)	40 (10%)	0	100	100
5	S3	206/228 (90%)	180 (87%)	26 (13%)	0	100	100
6	S7	154/179 (86%)	136 (88%)	17 (11%)	1 (1%)	21	59
7	S8	174/176 (99%)	157 (90%)	17 (10%)	0	100	100
8	V3	39/75 (52%)	32 (82%)	7 (18%)	0	100	100
9	S6	93/96 (97%)	88 (95%)	5 (5%)	0	100	100
10	S4	124/133 (93%)	108 (87%)	16 (13%)	0	100	100
11	A9	281/338 (83%)	244 (87%)	37 (13%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	A2	80/98 (82%)	72 (90%)	8 (10%)	0	100	100
13	A5	109/115 (95%)	96 (88%)	13 (12%)	0	100	100
14	A6	112/127 (88%)	105 (94%)	7 (6%)	0	100	100
15	A7	92/112 (82%)	77 (84%)	15 (16%)	0	100	100
16	AL	142/145 (98%)	119 (84%)	23 (16%)	0	100	100
17	AA	78/88 (89%)	67 (86%)	11 (14%)	0	100	100
17	AB	85/88 (97%)	76 (89%)	9 (11%)	0	100	100
18	D3	86/115 (75%)	81 (94%)	5 (6%)	0	100	100
19	D1	299/318 (94%)	273 (91%)	25 (8%)	1 (0%)	36	72
20	D6	167/175 (95%)	145 (87%)	21 (13%)	1 (1%)	21	59
21	4L	96/98 (98%)	90 (94%)	6 (6%)	0	100	100
22	D5	604/606 (100%)	533 (88%)	69 (11%)	2 (0%)	36	72
23	D4	457/459 (100%)	411 (90%)	45 (10%)	1 (0%)	43	78
24	D2	345/347 (99%)	319 (92%)	26 (8%)	0	100	100
25	AK	138/140 (99%)	129 (94%)	9 (6%)	0	100	100
26	B5	137/143 (96%)	124 (90%)	13 (10%)	0	100	100
27	A8	169/171 (99%)	136 (80%)	33 (20%)	0	100	100
28	BJ	169/175 (97%)	151 (89%)	17 (10%)	1 (1%)	21	59
29	AJ	317/320 (99%)	276 (87%)	41 (13%)	0	100	100
30	S5	97/105 (92%)	80 (82%)	17 (18%)	0	100	100
31	A3	72/83 (87%)	60 (83%)	12 (17%)	0	100	100
32	B3	71/97 (73%)	58 (82%)	13 (18%)	0	100	100
33	C2	117/120 (98%)	105 (90%)	12 (10%)	0	100	100
34	B4	126/128 (98%)	111 (88%)	15 (12%)	0	100	100
35	AM	137/143 (96%)	126 (92%)	11 (8%)	0	100	100
36	B6	92/127 (72%)	79 (86%)	13 (14%)	0	100	100
37	B7	117/136 (86%)	100 (86%)	17 (14%)	0	100	100
38	B9	174/178 (98%)	148 (85%)	26 (15%)	0	100	100
39	B2	63/72 (88%)	54 (86%)	9 (14%)	0	100	100
40	B8	155/158 (98%)	117 (76%)	37 (24%)	1 (1%)	21	59
41	BK	100/125 (80%)	81 (81%)	19 (19%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
42	C1	44/49 (90%)	38 (86%)	6 (14%)	0	100	100
43	B1	50/57 (88%)	46 (92%)	4 (8%)	0	100	100
44	A1	68/70 (97%)	64 (94%)	4 (6%)	0	100	100
All	All	7980/8509 (94%)	7034 (88%)	937 (12%)	9 (0%)	49	83

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
22	D5	84	PHE
23	D4	53	SER
3	S1	359	ARG
6	S7	54	CYS
22	D5	527	GLY
20	D6	138	GLU
40	B8	143	GLY
28	BJ	71	PRO
19	D1	92	PRO

5.3.2 Protein sidechains (i)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 13 ligands modelled in this entry, 1 is monoatomic - leaving 12 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	$\#\|Z\| > 2$
50	ZMP	B9	201	-	24,30,36	0.76	1 (4%)	29,37,45	1.29	3 (10%)
45	SF4	S8	202	-	0,12,12	-	-	-		
47	FES	S1	803	-	0,4,4	-	-	-		
45	SF4	S1	801	-	0,12,12	-	-	-		
50	ZMP	A6	201	-	27,33,36	0.65	1 (3%)	32,40,45	1.00	1 (3%)
45	SF4	S1	802	-	0,12,12	-	-	-		
45	SF4	S8	201	-	0,12,12	-	-	-		
45	SF4	V1	500	-	0,12,12	-	-	-		
46	FMN	V1	501	-	33,33,33	0.27	0	48,50,50	0.41	0
47	FES	V2	300	-	0,4,4	-	-	-		
49	NDP	A9	401	-	49,52,52	0.44	1 (2%)	66,80,80	0.44	0
45	SF4	S7	300	-	0,12,12	-	-	-		

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
50	ZMP	B9	201	-	-	16/35/37/43	-
45	SF4	S7	300	-	-	-	0/6/5/5
45	SF4	S8	202	-	-	-	0/6/5/5
47	FES	S1	803	-	-	-	0/1/1/1
45	SF4	S1	801	-	-	-	0/6/5/5
50	ZMP	A6	201	-	-	15/38/40/43	-
45	SF4	S1	802	-	-	-	0/6/5/5
45	SF4	S8	201	-	-	-	0/6/5/5
45	SF4	V1	500	-	-	-	0/6/5/5
47	FES	V2	300	-	-	-	0/1/1/1
49	NDP	A9	401	-	-	13/34/77/77	0/5/5/5
46	FMN	V1	501	-	-	7/18/18/18	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	B9	201	ZMP	C9-C10	2.32	1.53	1.50
49	A9	401	NDP	P2B-O2B	2.27	1.63	1.59
50	A6	201	ZMP	C9-C10	2.09	1.53	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
50	B9	201	ZMP	O1-C10-C9	-3.36	120.02	123.99
50	A6	201	ZMP	O1-C10-C9	-2.58	120.94	123.99
50	B9	201	ZMP	C11-C12-N1	-2.49	107.18	112.42
50	B9	201	ZMP	C15-C14-C13	-2.46	108.25	112.36

There are no chirality outliers.

All (51) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
46	V1	501	FMN	C2'-C3'-C4'-O4'
46	V1	501	FMN	C2'-C3'-C4'-C5'
46	V1	501	FMN	O3'-C3'-C4'-C5'
46	V1	501	FMN	C5'-O5'-P-O2P
46	V1	501	FMN	C5'-O5'-P-O3P
49	A9	401	NDP	C5B-O5B-PA-O1A
49	A9	401	NDP	C5B-O5B-PA-O2A
49	A9	401	NDP	C1B-C2B-O2B-P2B
50	A6	201	ZMP	C9-C10-S1-C11
50	A6	201	ZMP	C7-C8-C9-C10
50	B9	201	ZMP	C17-C18-C21-O5
50	B9	201	ZMP	C12-C11-S1-C10
50	B9	201	ZMP	O1-C10-S1-C11
50	B9	201	ZMP	C9-C10-S1-C11
50	A6	201	ZMP	C14-C13-N1-C12
50	B9	201	ZMP	C14-C13-N1-C12
46	V1	501	FMN	O3'-C3'-C4'-O4'
50	A6	201	ZMP	O2-C13-N1-C12
50	B9	201	ZMP	O2-C13-N1-C12
50	B9	201	ZMP	C5-C6-C7-C8
50	B9	201	ZMP	C3-C4-C5-C6
50	B9	201	ZMP	C6-C7-C8-C9
50	A6	201	ZMP	C2-C1-C22-C23
46	V1	501	FMN	C5'-O5'-P-O1P
50	A6	201	ZMP	O4-C17-C18-C19
50	B9	201	ZMP	S1-C11-C12-N1

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Mol	Chain	Res	Type	Atoms
50	B9	201	ZMP	N2-C16-C17-C18
50	A6	201	ZMP	O1-C10-S1-C11
49	A9	401	NDP	PN-O3-PA-O5B
49	A9	401	NDP	C2B-O2B-P2B-O3X
50	A6	201	ZMP	O4-C17-C18-C21
50	B9	201	ZMP	O3-C16-C17-O4
50	B9	201	ZMP	C19-C18-C21-O5
50	B9	201	ZMP	C20-C18-C21-O5
49	A9	401	NDP	O4D-C1D-N1N-C6N
50	A6	201	ZMP	O4-C17-C18-C20
49	A9	401	NDP	C2D-C1D-N1N-C6N
50	B9	201	ZMP	O3-C16-C17-C18
50	A6	201	ZMP	C11-C12-N1-C13
50	A6	201	ZMP	C12-C11-S1-C10
50	A6	201	ZMP	C4-C5-C6-C7
50	A6	201	ZMP	C16-C17-C18-C19
50	A6	201	ZMP	C16-C17-C18-C20
49	A9	401	NDP	C5B-O5B-PA-O3
49	A9	401	NDP	C4B-C5B-O5B-PA
49	A9	401	NDP	C2D-C1D-N1N-C2N
49	A9	401	NDP	O4B-C4B-C5B-O5B
49	A9	401	NDP	PA-O3-PN-O2N
50	B9	201	ZMP	C4-C5-C6-C7
49	A9	401	NDP	O4D-C1D-N1N-C2N
50	A6	201	ZMP	C16-C17-C18-C21

There are no ring outliers.

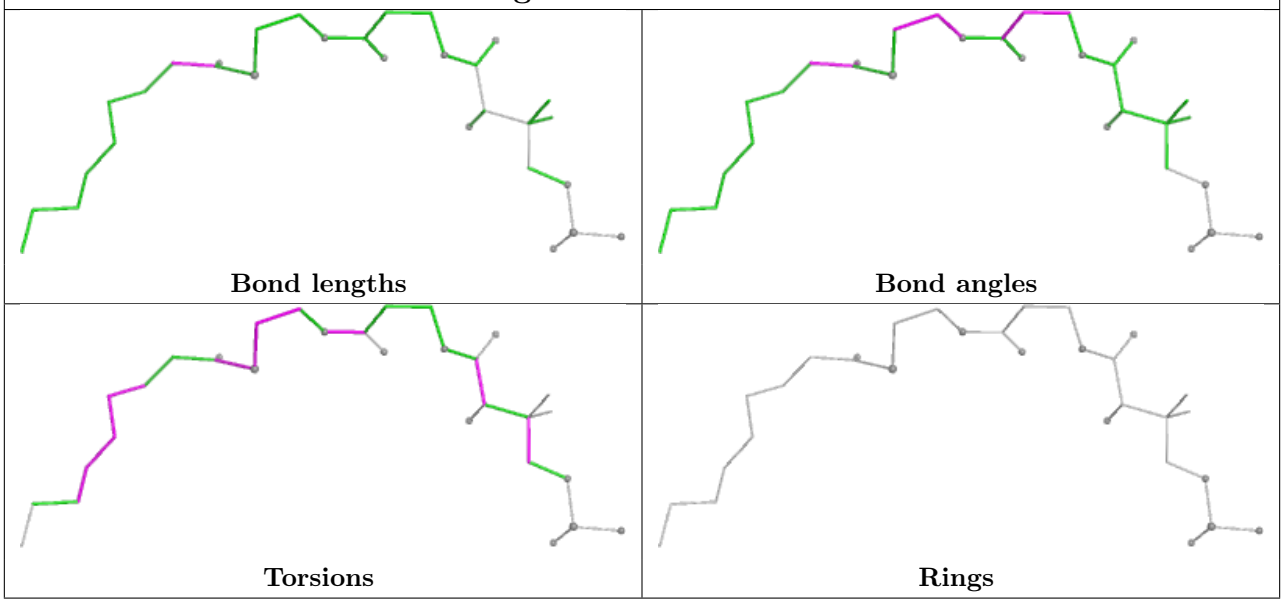
5 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
50	B9	201	ZMP	9	0
50	A6	201	ZMP	5	0
45	V1	500	SF4	1	0
46	V1	501	FMN	1	0
49	A9	401	NDP	1	0

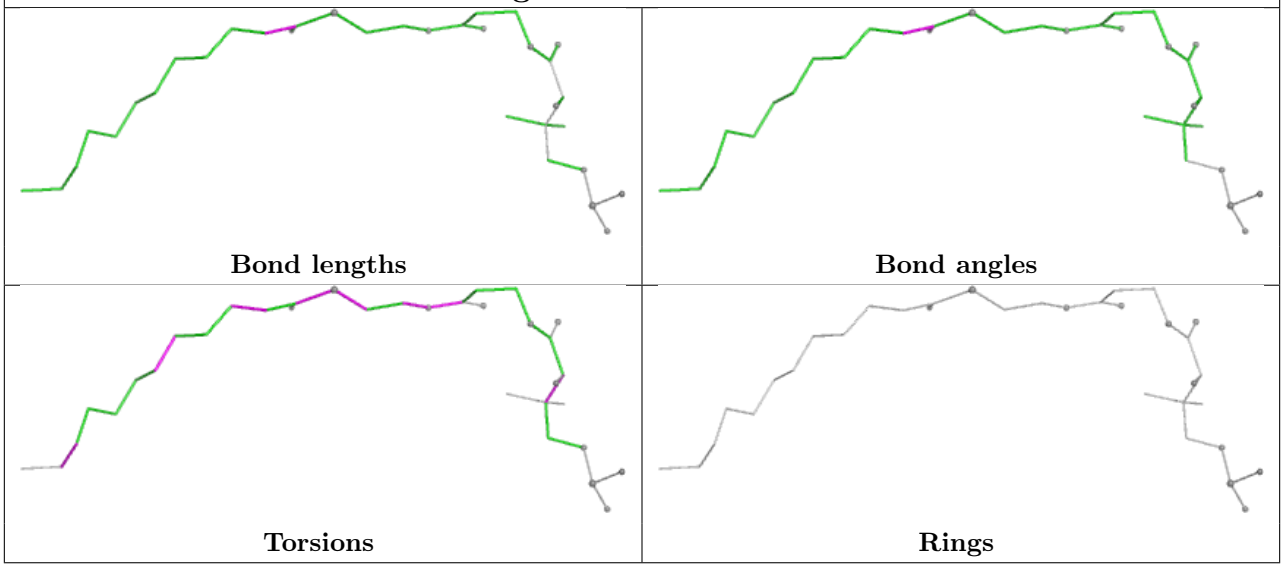
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

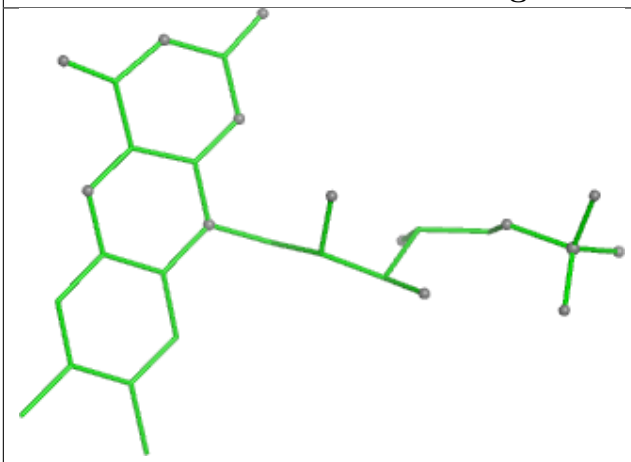
Ligand ZMP B9 201



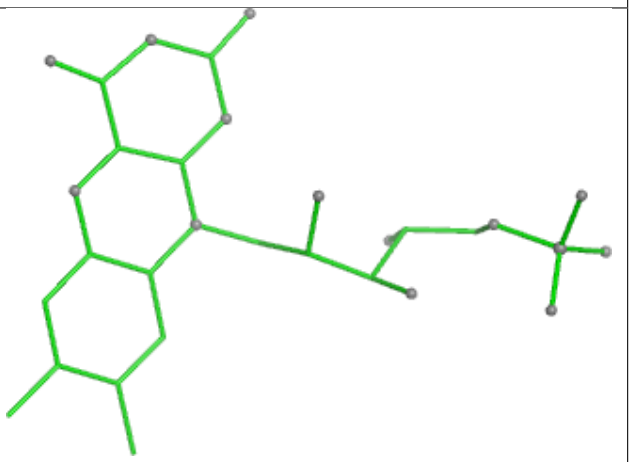
Ligand ZMP A6 201



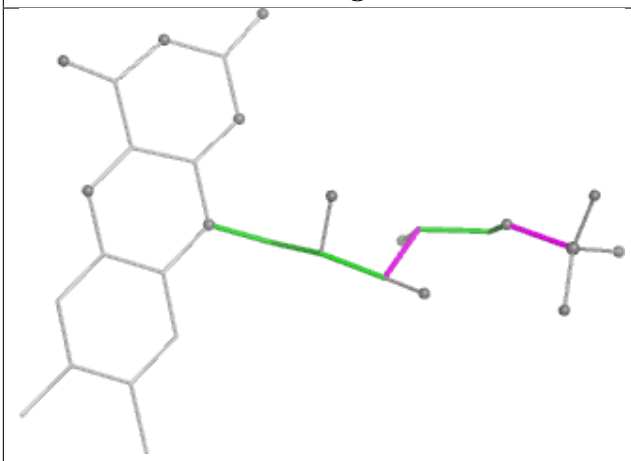
Ligand FMN V1 501



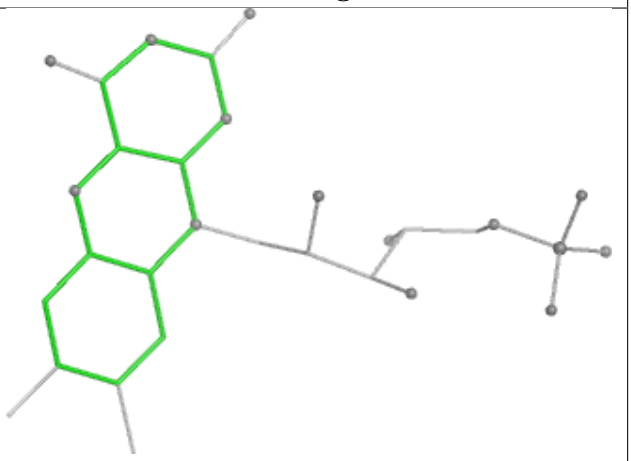
Bond lengths



Bond angles

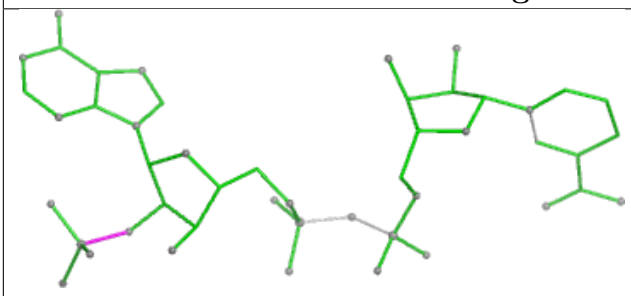


Torsions

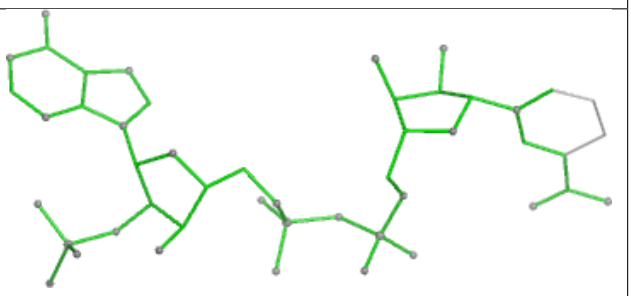


Rings

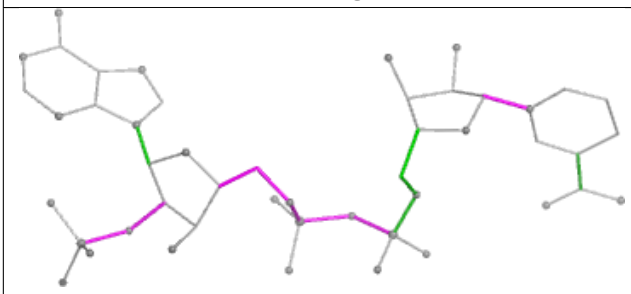
Ligand NDP A9 401



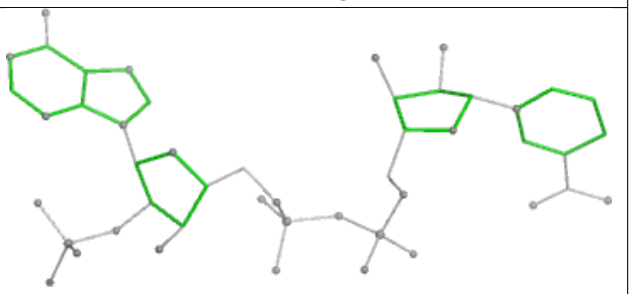
Bond lengths



Bond angles



Torsions



Rings

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.

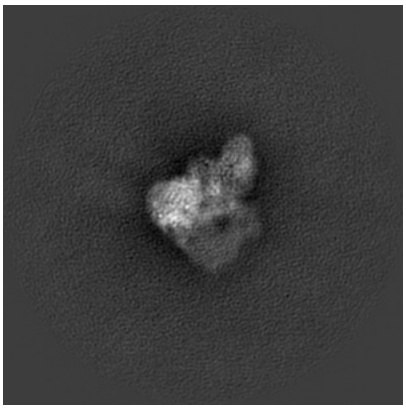
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-4505. These allow visual inspection of the internal detail of the map and identification of artifacts.

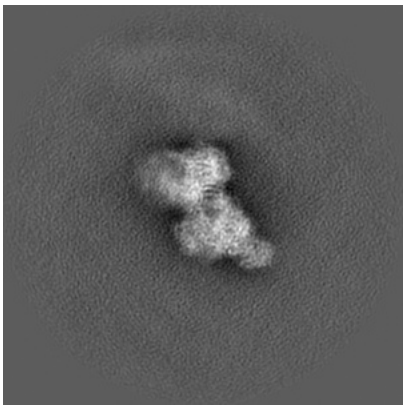
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

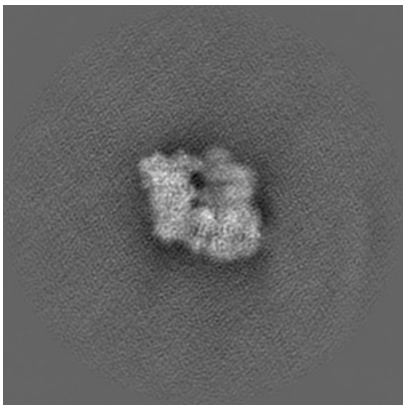
6.1.1 Primary map



X

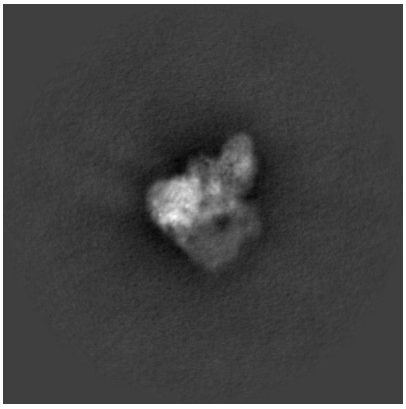


Y

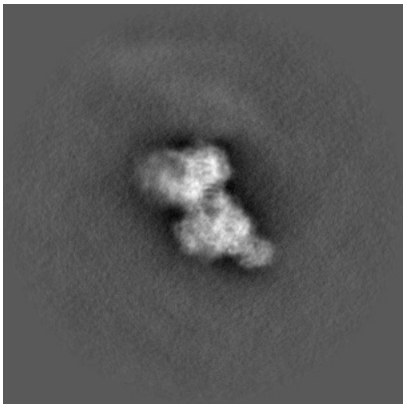


Z

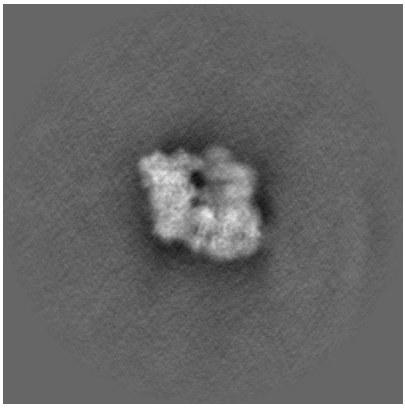
6.1.2 Raw map



X



Y

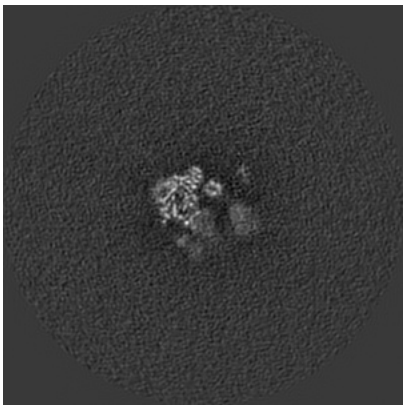


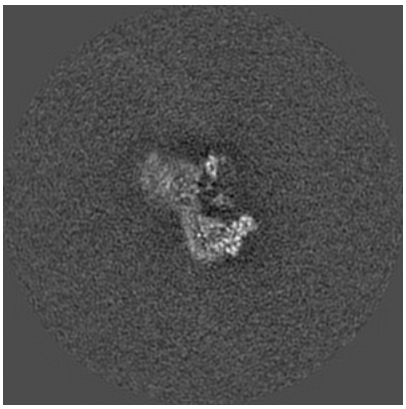
Z

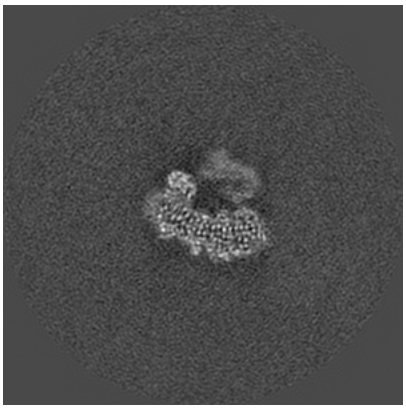
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

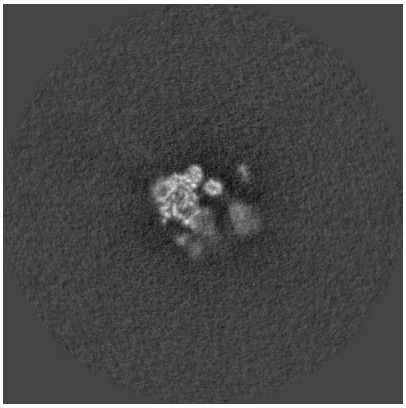
6.2.1 Primary map

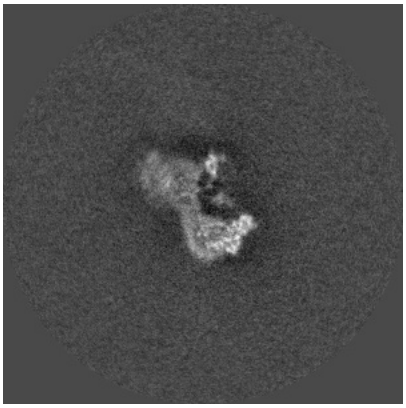

X Index: 256

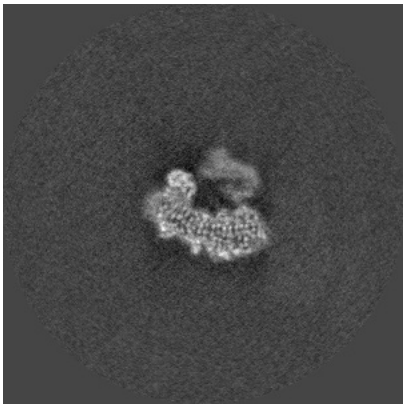

Y Index: 256


Z Index: 256

6.2.2 Raw map


X Index: 256

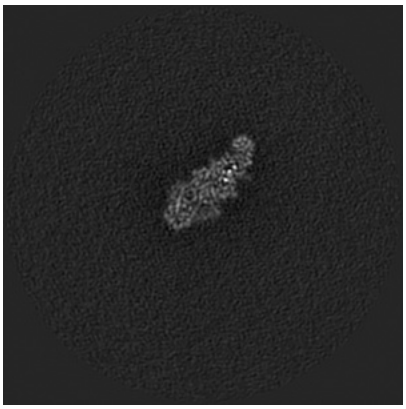

Y Index: 256

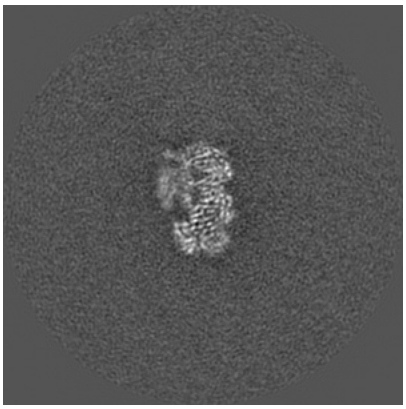

Z Index: 256

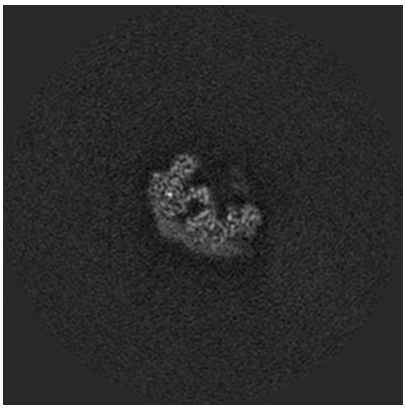
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

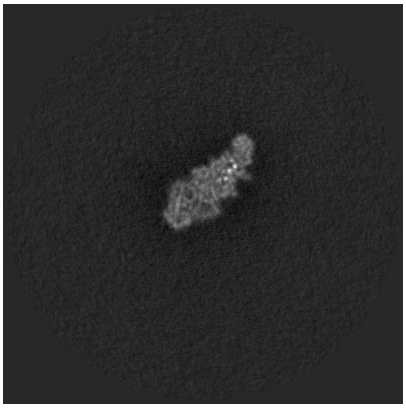
6.3.1 Primary map

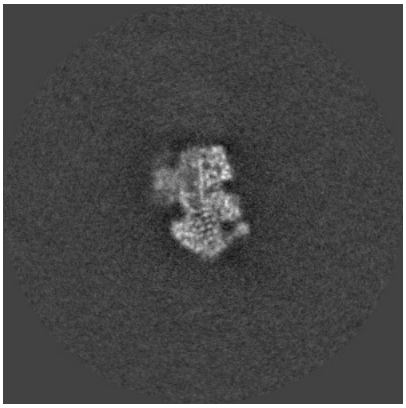

X Index: 205

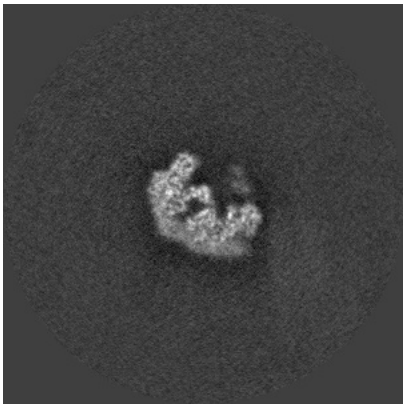

Y Index: 230


Z Index: 280

6.3.2 Raw map


X Index: 206

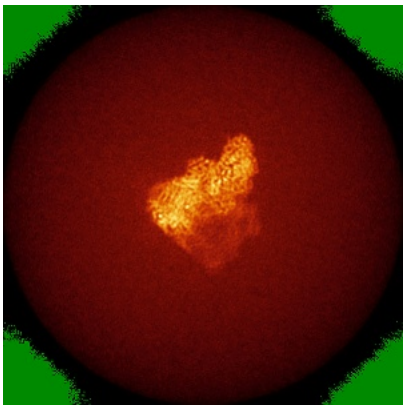

Y Index: 237

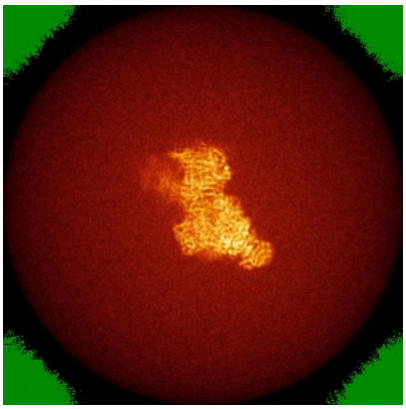

Z Index: 279

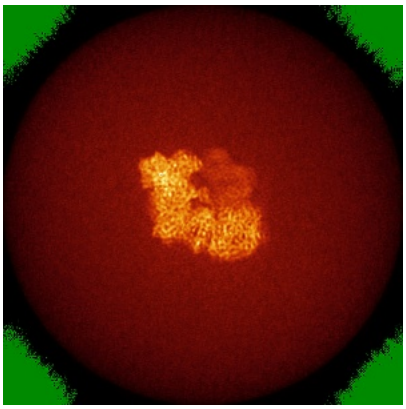
The images above show the largest variance slices of the map in three orthogonal directions.

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

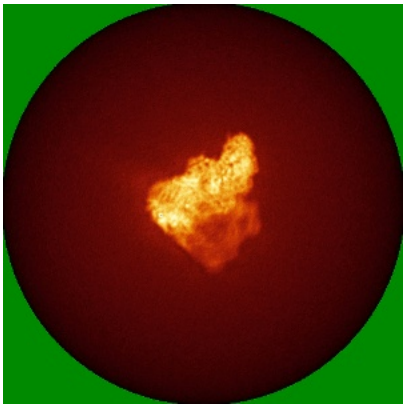
6.4.1 Primary map

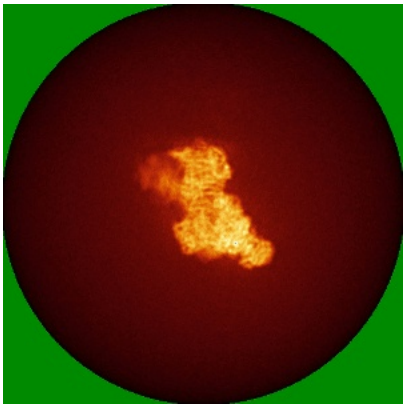

X

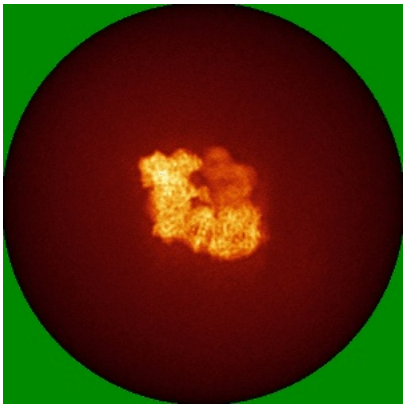

Y


Z

6.4.2 Raw map


X

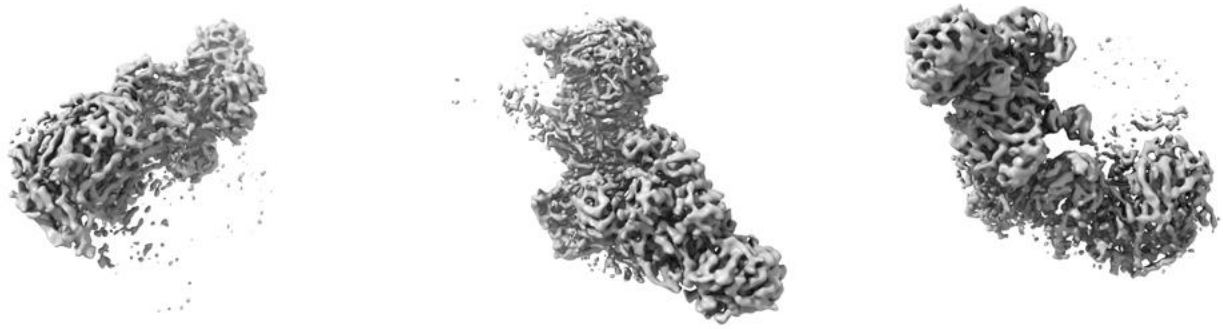

Y


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)

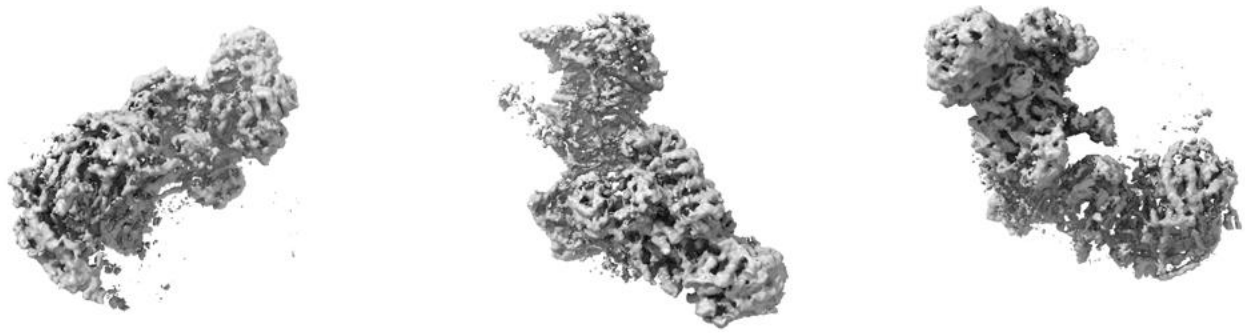
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.1. 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



X Y Z

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.

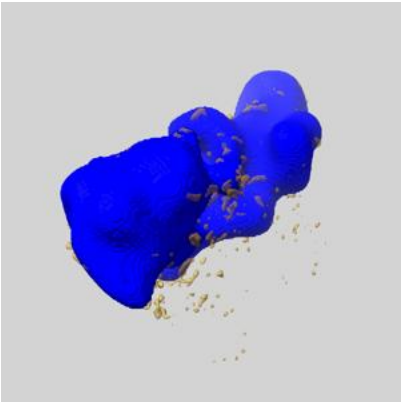
6.6 Mask visualisation (i)

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

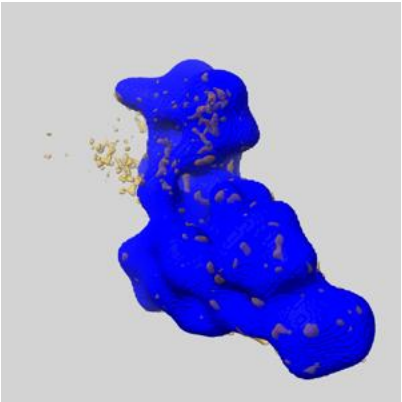
A mask typically either:

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

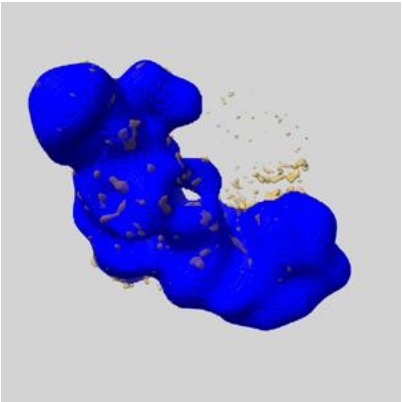
6.6.1 emd_4505_msk_1.map (i)



X



Y

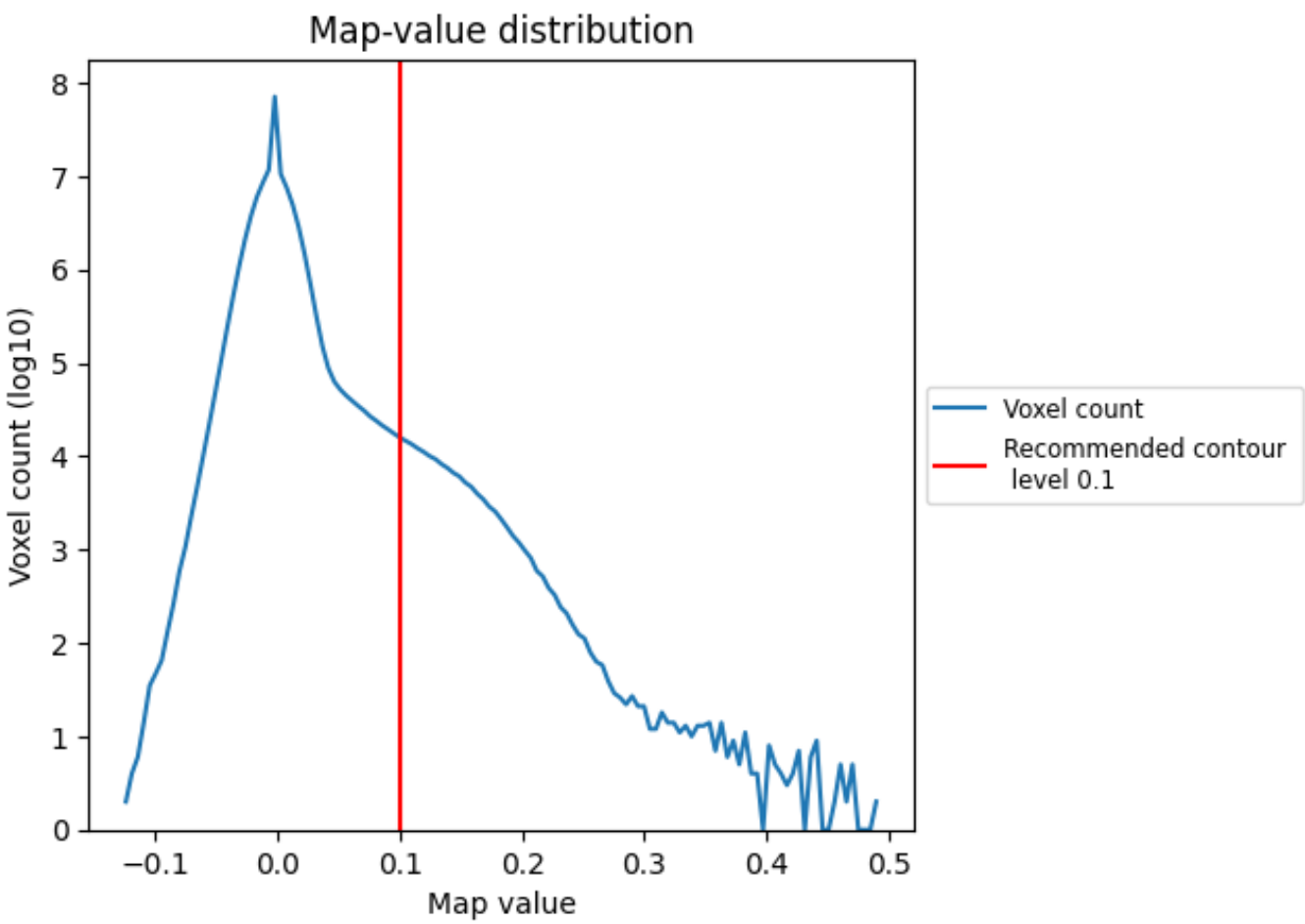


Z

7 Map analysis (i)

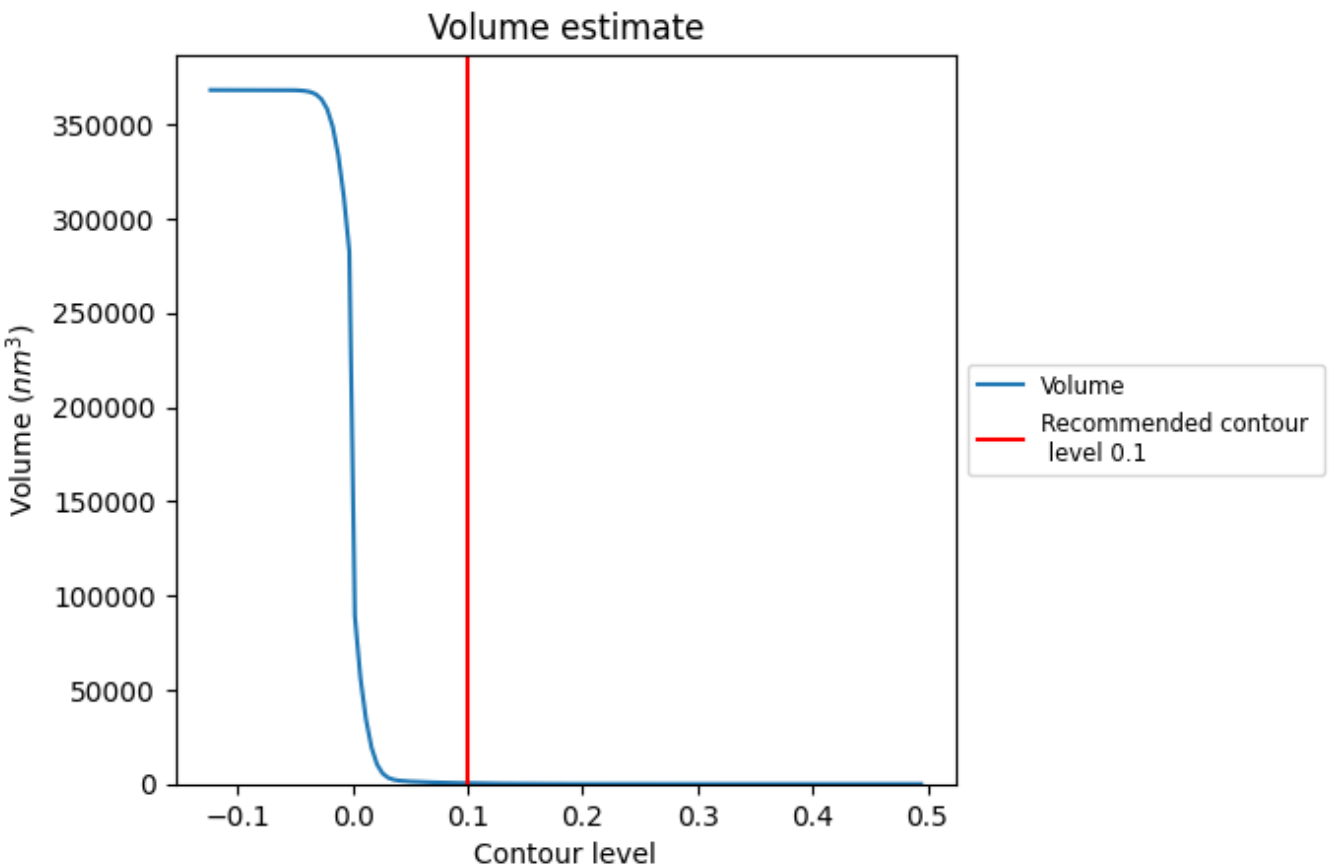
This section contains the results of statistical analysis of the map.

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.

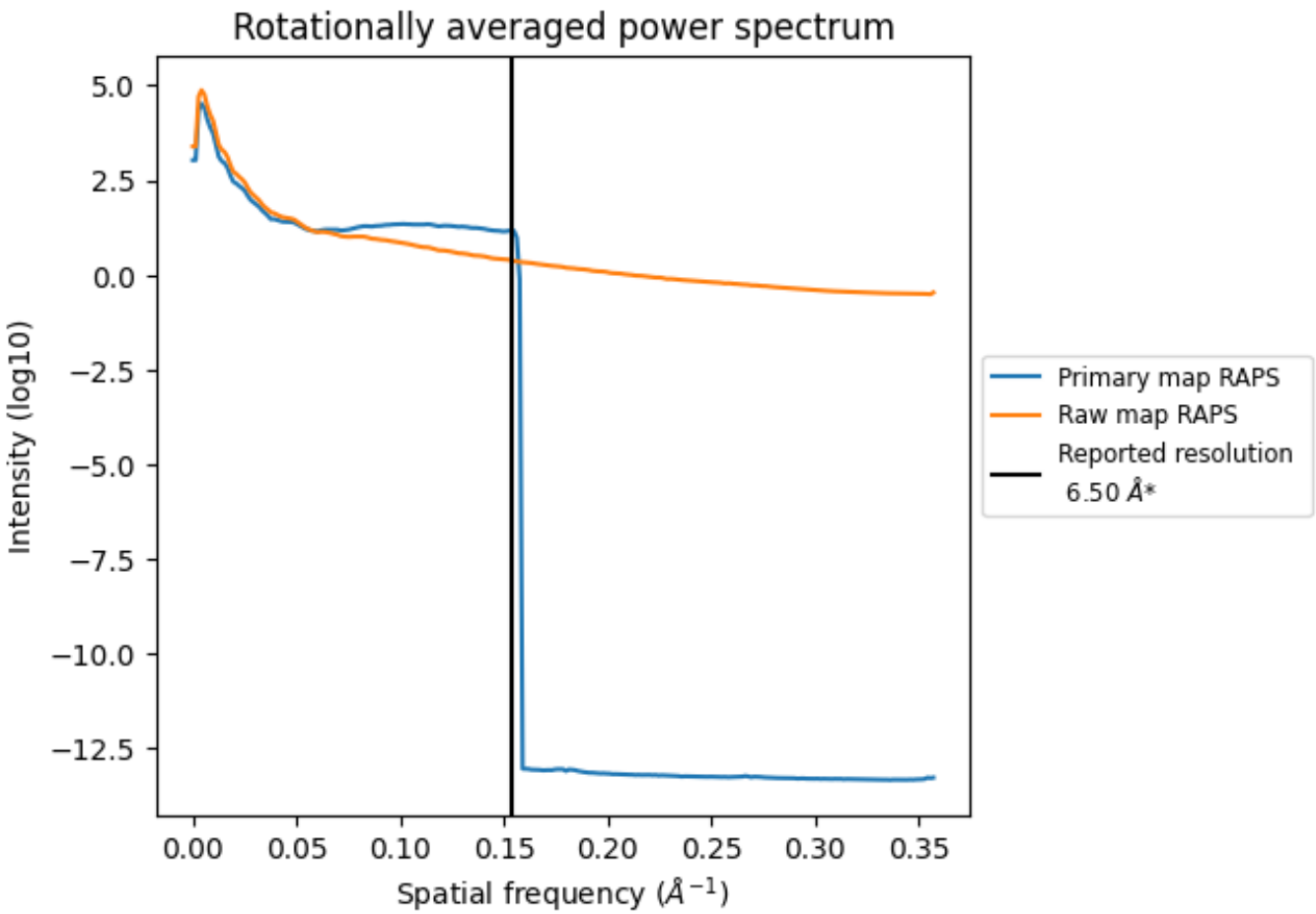
7.2 Volume estimate (i)



The volume at the recommended contour level is 413 nm^3; this corresponds to an approximate mass of 373 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)

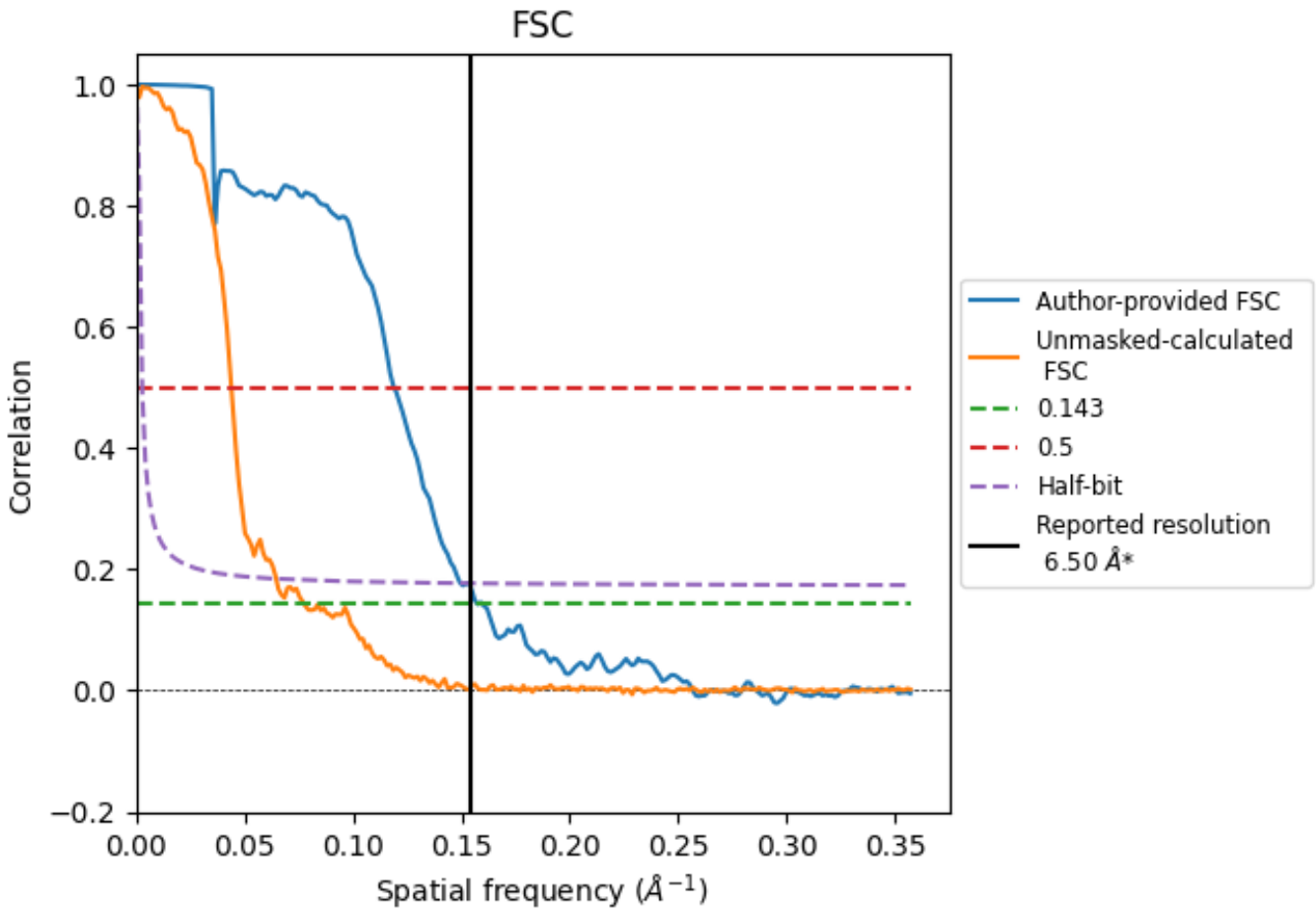


*Reported resolution corresponds to spatial frequency of 0.154 Å^{-1}

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 0.154 Å^{-1}

8.2 Resolution estimates (i)

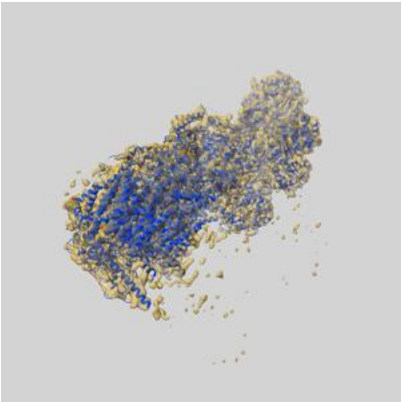
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.50	-	-
Author-provided FSC curve	6.35	8.40	6.68
Unmasked-calculated*	12.92	22.78	15.50

*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 12.92 differs from the reported value 6.5 by more than 10 %

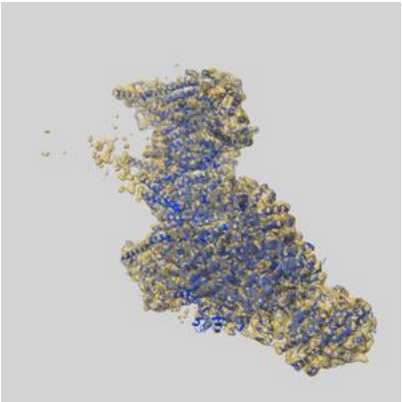
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-4505 and PDB model 6QCF. Per-residue inclusion information can be found in section 3 on page 15.

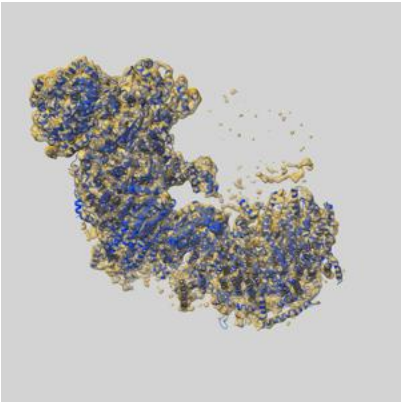
9.1 Map-model overlay (i)



X



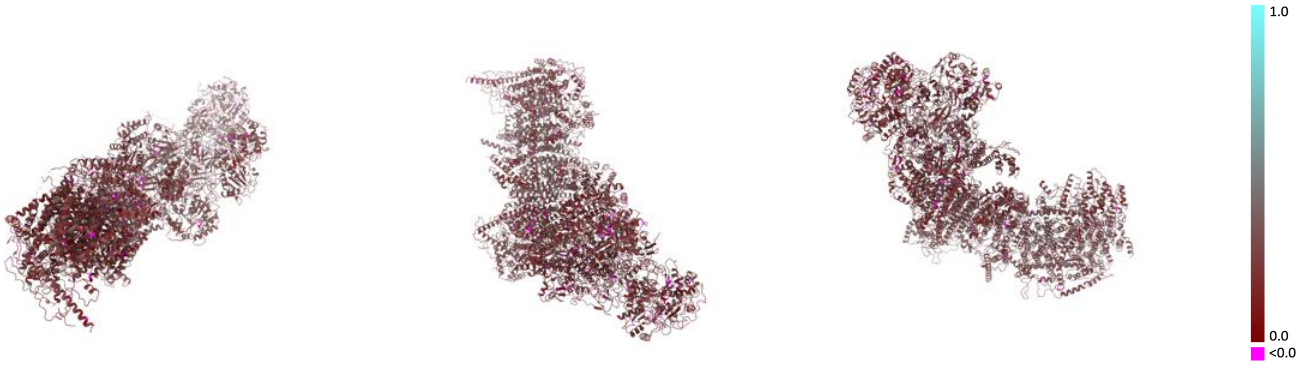
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.1 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.

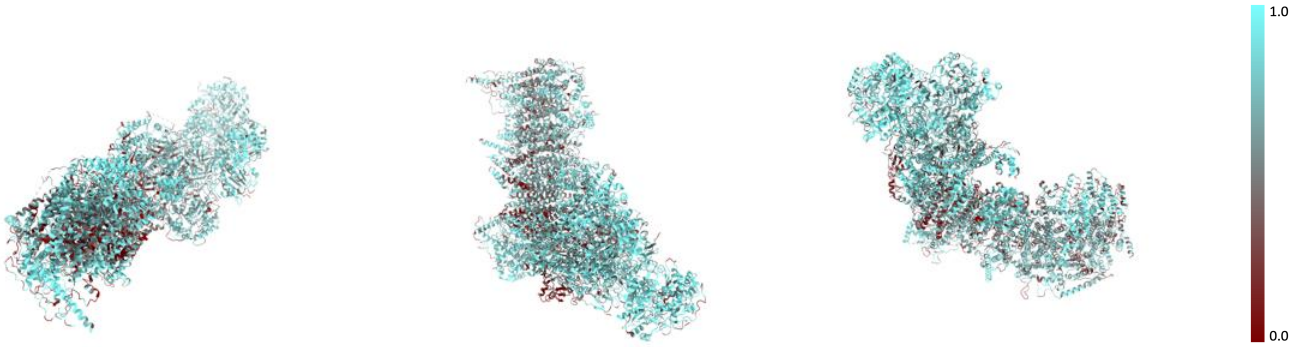
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

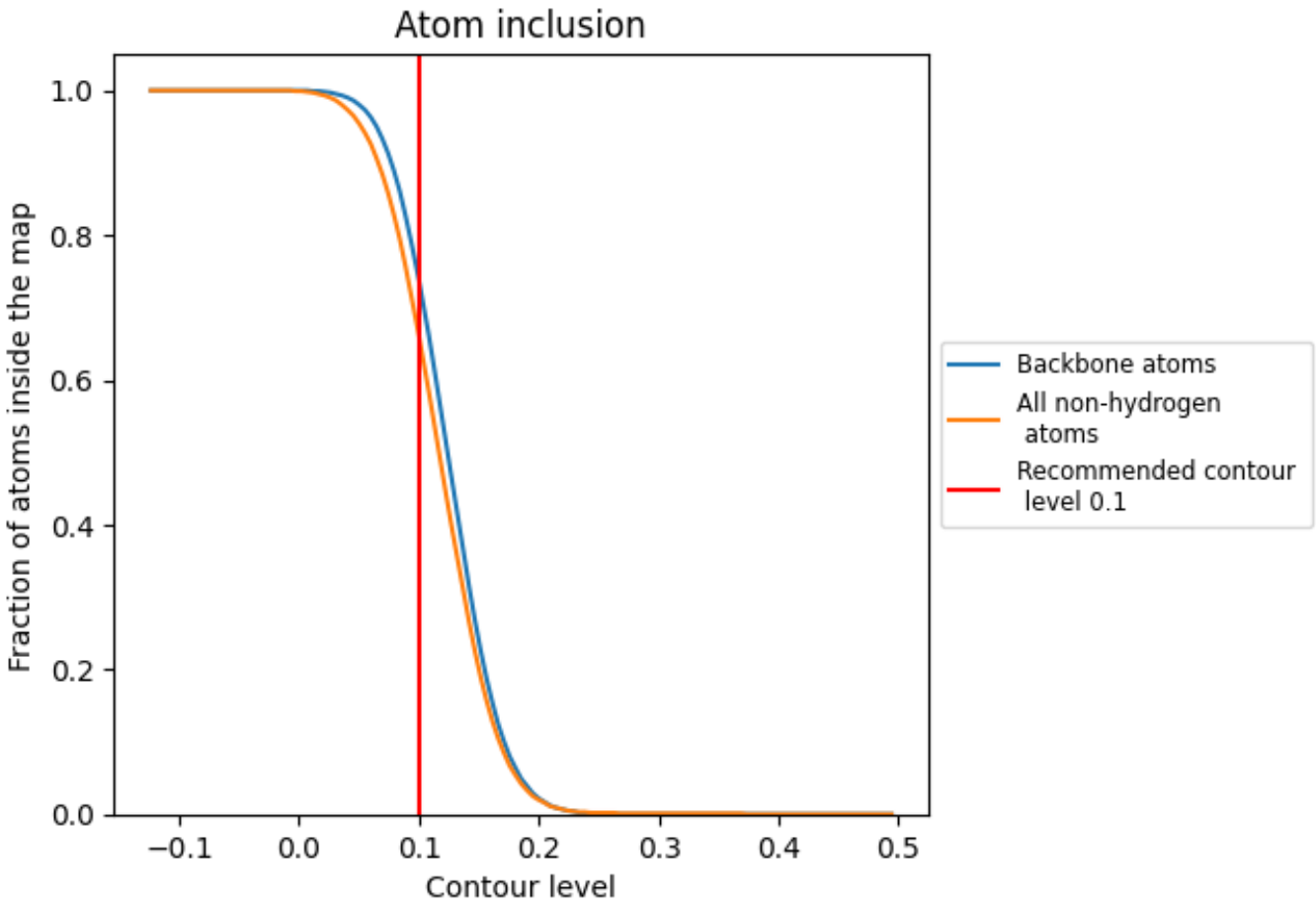
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.1).

9.4 Atom inclusion (i)



At the recommended contour level, 74% of all backbone atoms, 66% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6610	0.2440
4L	0.4110	0.2310
A1	0.6590	0.2210
A2	0.8520	0.2420
A3	0.4820	0.2360
A5	0.6910	0.2400
A6	0.7120	0.2620
A7	0.5150	0.2180
A8	0.7830	0.2630
A9	0.6790	0.2510
AA	0.7410	0.2440
AB	0.6850	0.2190
AJ	0.6930	0.2450
AK	0.4750	0.2400
AL	0.2730	0.1920
AM	0.7060	0.2390
B1	0.5580	0.2540
B2	0.5940	0.2480
B3	0.4800	0.2210
B4	0.6930	0.2400
B5	0.6960	0.2340
B6	0.6520	0.2390
B7	0.7100	0.2250
B8	0.6030	0.2420
B9	0.7240	0.2550
BJ	0.7670	0.2480
BK	0.7130	0.2660
C1	0.7400	0.2500
C2	0.7200	0.2450
D1	0.5260	0.2410
D2	0.6270	0.2530
D3	0.5460	0.2490
D4	0.6250	0.2530
D5	0.5970	0.2460
D6	0.4280	0.2320

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Chain	Atom inclusion	Q-score
S1	0.7570	0.2490
S2	0.6500	0.2500
S3	0.6930	0.2540
S4	0.7200	0.2760
S5	0.6780	0.2370
S6	0.6930	0.2500
S7	0.6690	0.2350
S8	0.7110	0.2410
V1	0.8000	0.2370
V2	0.7850	0.2360
V3	0.8140	0.2390