Full wwPDB EM Validation Report (i)

Nov 6, 2022 – 08:11 PM EST

PDB ID	:	6NBQ
EMDB ID	:	EMD-0415
Title	:	T.elongatus NDH (data-set 1)
Authors	:	Laughlin, T.G.; Bayne, A.; Trempe, J.-F.; Savage, D.F.; Davies, K.M.
Deposited on	:	2018-12-09
Resolution	:	3.10 Å(reported)
Based on initial models	:	4HEA, 3C4S

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:

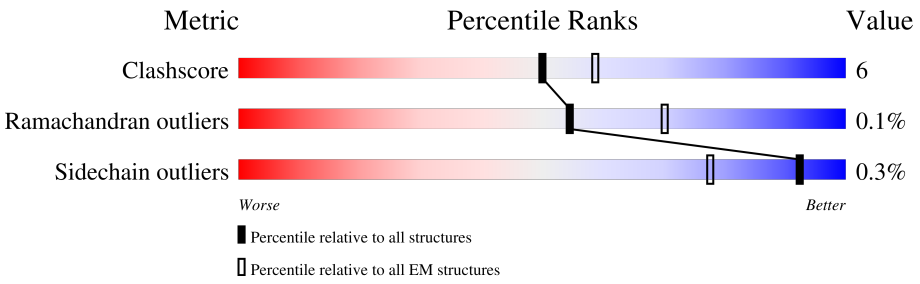
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.10 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	H	394	• 78% 21% ••
2	J	168	5% 81% 14% • •
3	K	237	10% 70% 19% 11%
4	I	196	15% 77% 17% • 6%
5	N	150	5% 87% 12% •
6	L	76	17% 70% 17% 13%
7	M	111	5% 85% 15%
8	O	70	6% 86% 13% •

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Mol	Chain	Length	Quality of chain
9	S	110	21% 38% 13% 48%
10	A	372	19% 83% 13%
11	C	132	17% 62% 8% 30%
12	E	101	5% 85% 15%
13	P	44	23% 89% 7% 5%
14	F	656	57% 79% 10% 11%
15	D	529	5% 81% 14% 5%
16	B	515	76% 18% 6%
17	G	200	22% 84% 12%

2 Entry composition (i)

There are 18 unique types of molecules in this entry. The entry contains 28296 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 NAD(P)H-quinone oxidoreductase subunit H.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	H	392	3105	2010	541	535	19	0	0

- Molecule 2 is a protein called NAD(P)H-quinone oxidoreductase subunit J.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	J	161	1295	832	223	235	5	0	0

- Molecule 3 is a protein called NAD(P)H-quinone oxidoreductase subunit K.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	K	212	1615	1040	282	279	14	0	0

- Molecule 4 is a protein called NAD(P)H-quinone oxidoreductase subunit I.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	I	184	1444	922	249	260	13	0	0

- Molecule 5 is a protein called NAD(P)H-quinone oxidoreductase subunit N.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	N	148	1158	755	201	201	1	0	0

- Molecule 6 is a protein called NAD(P)H-quinone oxidoreductase subunit L.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	L	66	536	369	83	83	1	0	0

- Molecule 7 is a protein called NAD(P)H-quinone oxidoreductase subunit M.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	M	111	866	542	161	161	2	0	0

- Molecule 8 is a protein called NAD(P)H-quinone oxidoreductase subunit O.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
8	O	69	543	352	93	98	0	0

- Molecule 9 is a protein called Tlr0636 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	S	57	440	286	71	81	2	0	0

- Molecule 10 is a protein called NdhA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	A	359	2614	1757	422	425	10	0	0

- Molecule 11 is a protein called NAD(P)H-quinone oxidoreductase subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	C	93	732	519	105	106	2	0	0

- Molecule 12 is a protein called NAD(P)H-quinone oxidoreductase subunit 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	E	101	772	512	128	128	4	0	0

- Molecule 13 is a protein called Proton-translocating NADH-quinone dehydrogenase subunit P NdhP.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	P	42	318	212	51	53	2	0	0

- Molecule 14 is a protein called NADH dehydrogenase subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	F	582	4077	2688	656	705	28	0	0

- Molecule 15 is a protein called NAD(P)H-quinone oxidoreductase chain 4 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	D	504	3805	2565	603	616	21	0	0

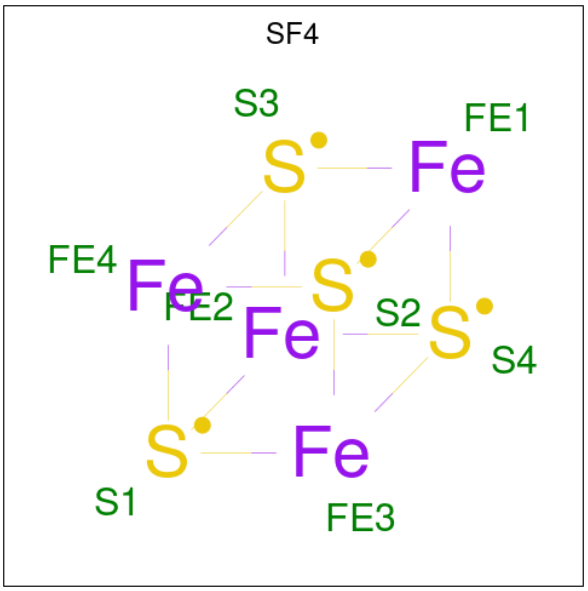
- Molecule 16 is a protein called NAD(P)H-quinone oxidoreductase subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	B	483	3579	2393	563	607	16	0	0

- Molecule 17 is a protein called NADH-quinone oxidoreductase subunit J.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	G	191	1373	914	217	238	4	0	0

- Molecule 18 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).

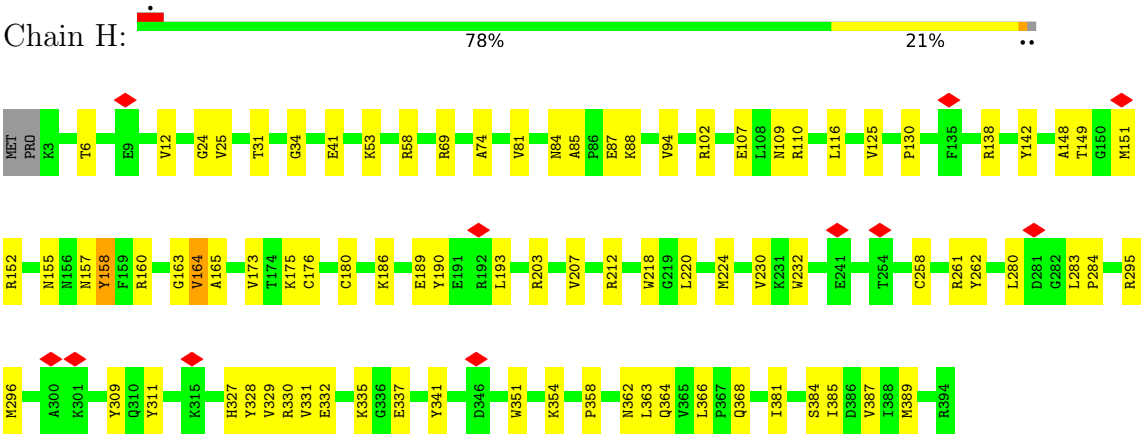


Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
18	K	1	8	4	4	0
			Total	Fe	S	
18	I	1	16	8	8	0
			Total	Fe	S	
18	I	1	16	8	8	0

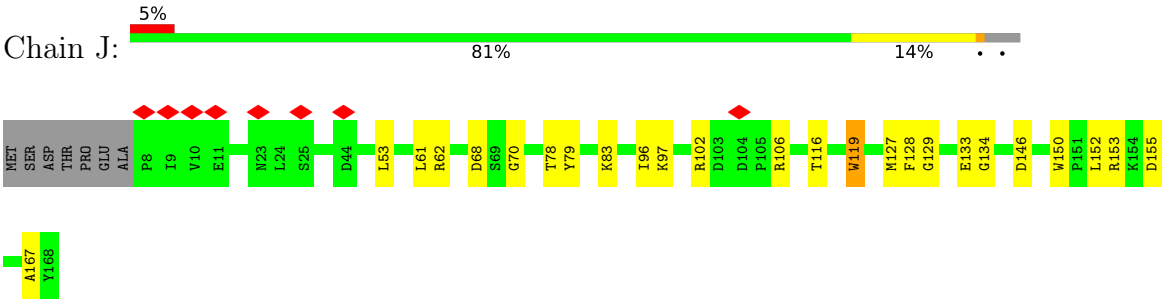
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

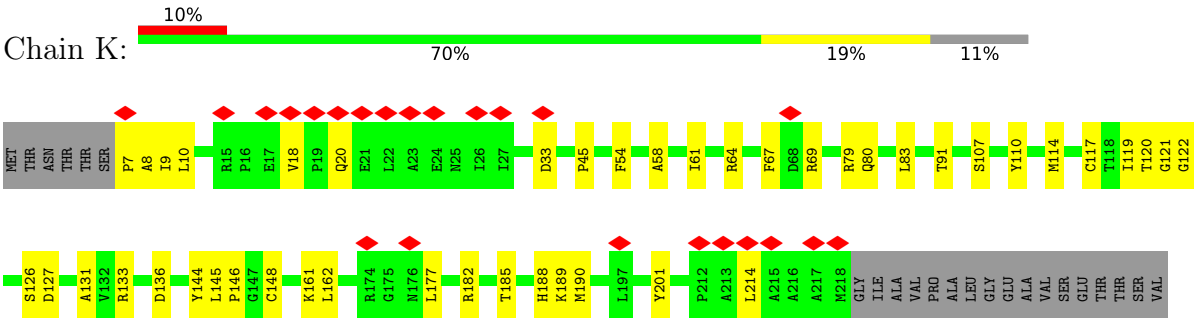
• Molecule 1: NAD(P)H-quinone oxidoreductase subunit H



• Molecule 2: NAD(P)H-quinone oxidoreductase subunit J



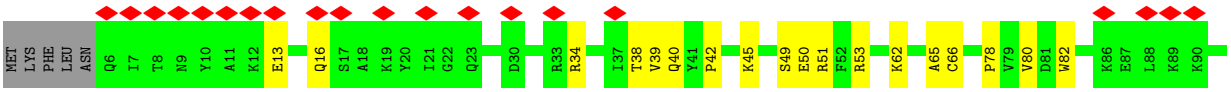
• Molecule 3: NAD(P)H-quinone oxidoreductase subunit K

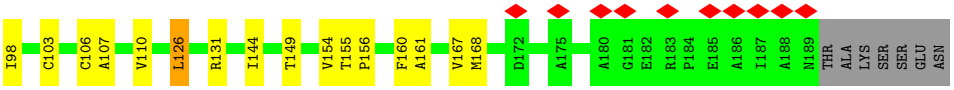


ALA
GLU

- Molecule 4: NAD(P)H-quinone oxidoreductase subunit I

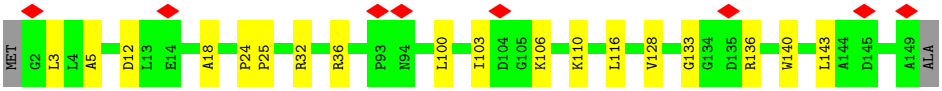
Chain I:





- Molecule 5: NAD(P)H-quinone oxidoreductase subunit N

Chain N:

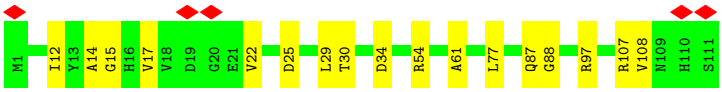


- Molecule 6: NAD(P)H-quinone oxidoreductase subunit L

Chain L:

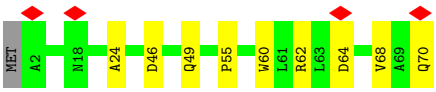
- Molecule 7: NAD(P)H-quinone oxidoreductase subunit M

Chain M:



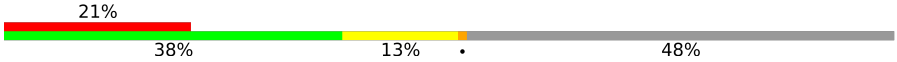
- Molecule 8: NAD(P)H-quinone oxidoreductase subunit O

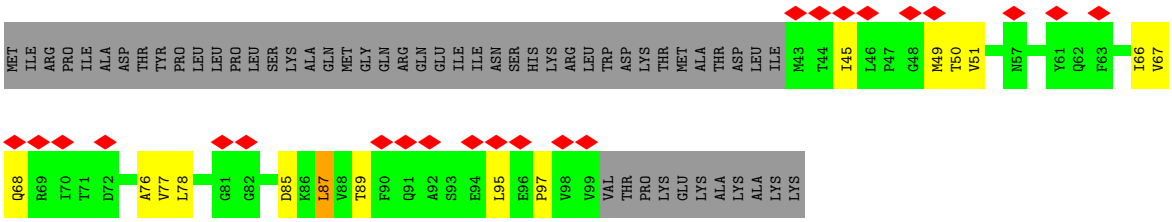
Chain O:



- Molecule 9: Tlr0636 protein

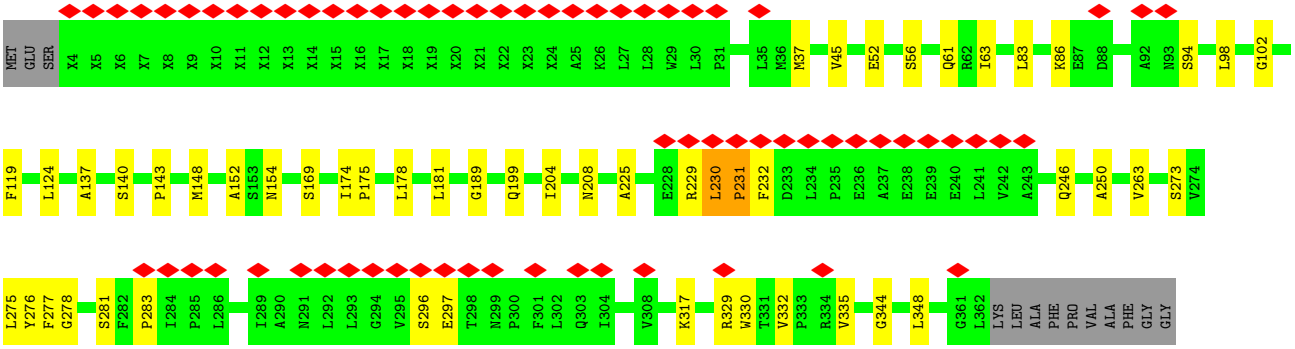
Chain S:





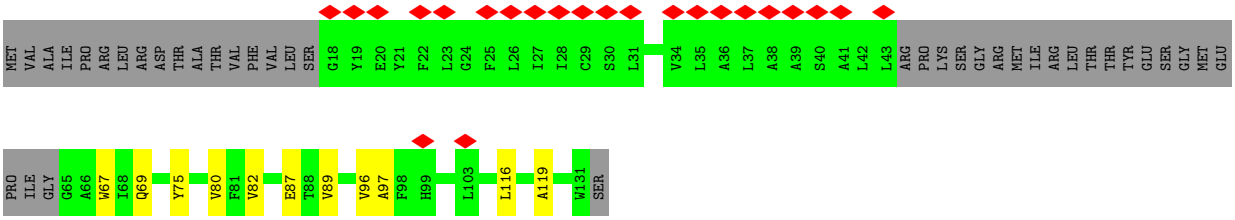
- Molecule 10: NdhA

Chain A:



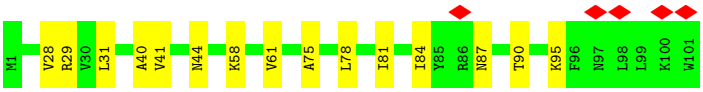
- Molecule 11: NAD(P)H-quinone oxidoreductase subunit 3

Chain C:



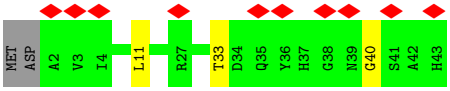
- Molecule 12: NAD(P)H-quinone oxidoreductase subunit 4L

Chain E:



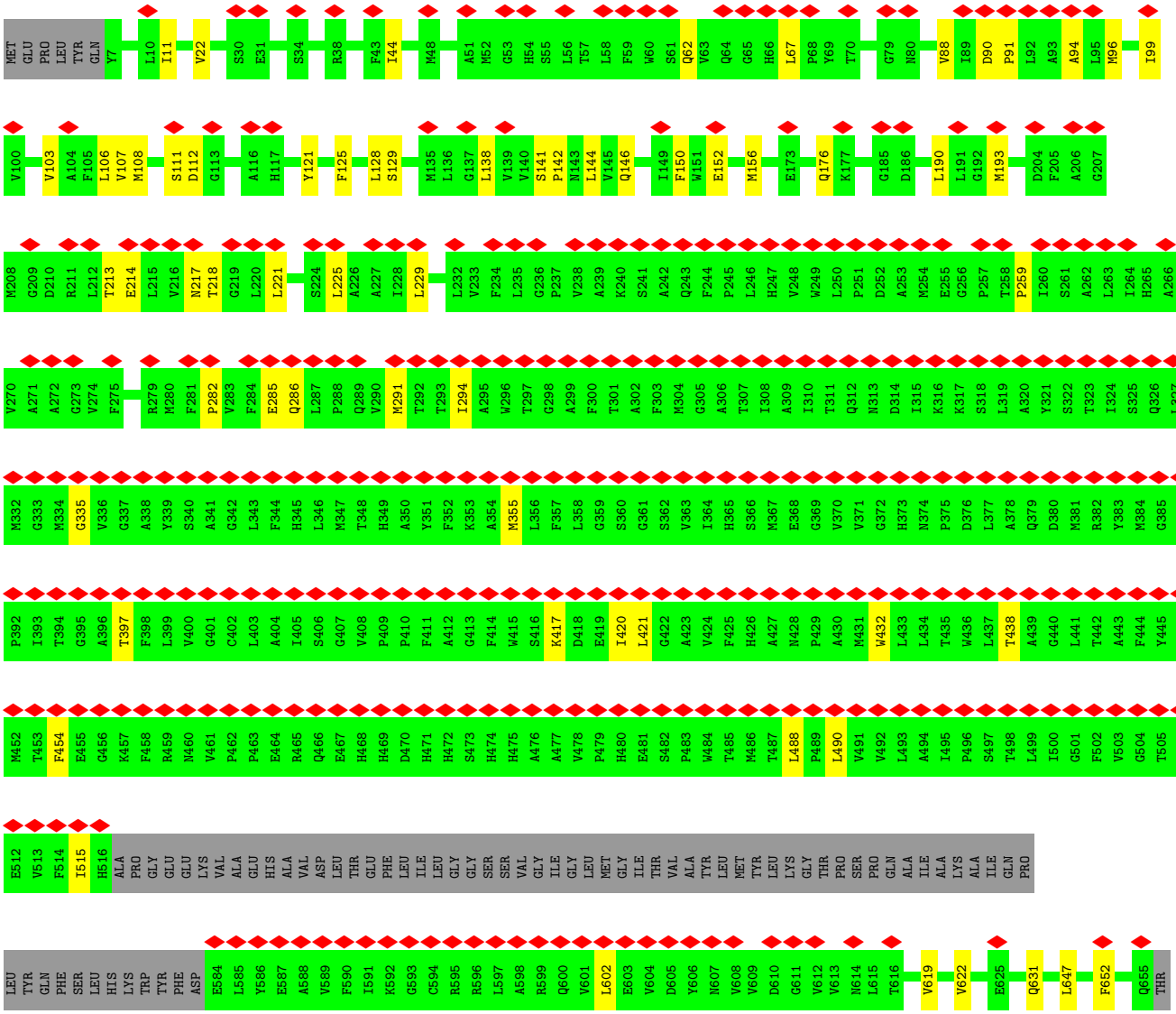
- Molecule 13: Proton-translocating NADH-quinone dehydrogenase subunit P NdhP

Chain P:



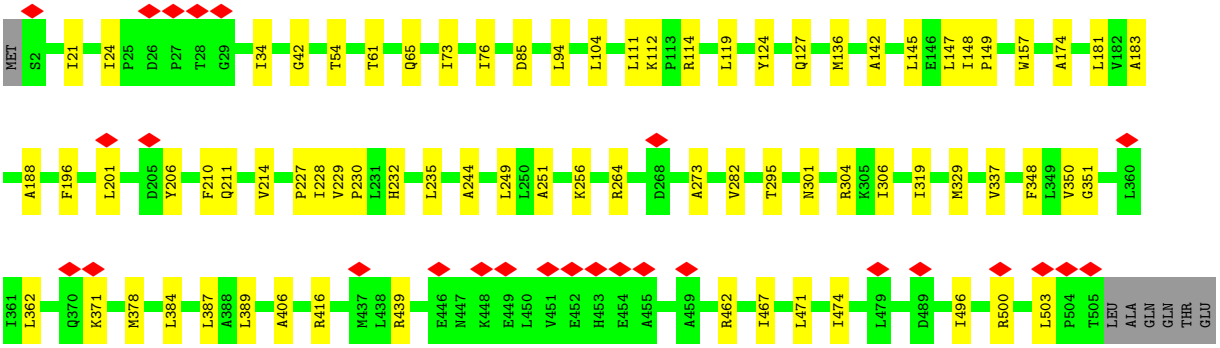
- Molecule 14: NADH dehydrogenase subunit 5

Chain F:



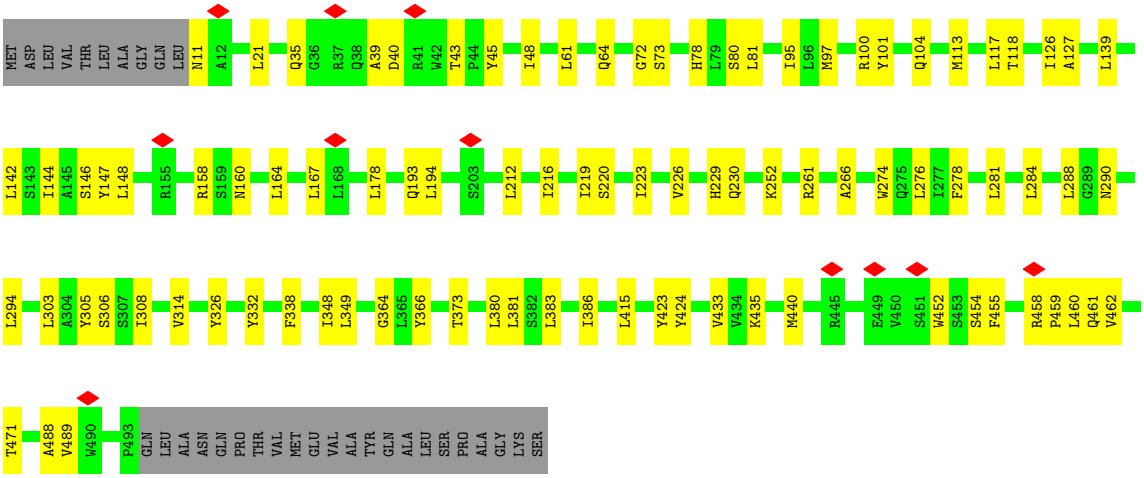
- Molecule 15: NAD(P)H-quinone oxidoreductase chain 4 1

Chain D:



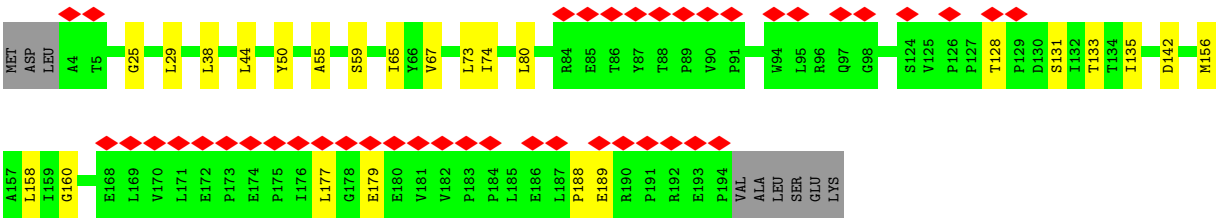
- Molecule 16: NAD(P)H-quinone oxidoreductase subunit 2

Chain B:



- Molecule 17: NADH-quinone oxidoreductase subunit J

Chain G:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	81670	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 ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.324	Depositor
Minimum map value	-0.132	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	384.47998, 384.47998, 384.47998	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.068, 1.068, 1.068	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: SF4

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	H	0.42	0/3187	0.56	0/4325
2	J	0.39	0/1332	0.53	1/1816 (0.1%)
3	K	0.45	0/1657	0.60	0/2258
4	I	0.44	0/1481	0.59	1/2013 (0.0%)
5	N	0.35	0/1190	0.54	0/1619
6	L	0.34	0/556	0.56	0/760
7	M	0.36	0/882	0.50	0/1198
8	O	0.36	0/555	0.52	0/755
9	S	0.31	0/449	0.65	1/612 (0.2%)
10	A	0.37	0/2575	0.59	2/3531 (0.1%)
11	C	0.39	0/757	0.53	0/1039
12	E	0.34	0/782	0.56	0/1063
13	P	0.33	0/327	0.57	0/445
14	F	0.30	0/4178	0.53	1/5725 (0.0%)
15	D	0.37	0/3912	0.57	1/5350 (0.0%)
16	B	0.40	0/3665	0.59	0/5008
17	G	0.35	0/1401	0.55	0/1926
All	All	0.38	0/28886	0.56	7/39443 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	K	0	1
4	I	0	1
11	C	0	1
17	G	0	1
All	All	0	4

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	F	488	LEU	CA-CB-CG	6.99	131.39	115.30
2	J	119	TRP	CA-CB-CG	6.25	125.58	113.70
10	A	230	LEU	CA-CB-CG	6.06	129.24	115.30
9	S	87	LEU	CA-CB-CG	5.94	128.97	115.30
4	I	126	LEU	CA-CB-CG	5.40	127.73	115.30
15	D	362	LEU	CA-CB-CG	5.14	127.13	115.30
10	A	124	LEU	CA-CB-CG	5.09	127.02	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	C	67	TRP	Peptide
17	G	179	GLU	Peptide
4	I	103	CYS	Peptide
3	K	121	GLY	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	H	3105	0	3060	53	0
2	J	1295	0	1254	19	0
3	K	1615	0	1657	37	0
4	I	1444	0	1399	26	0
5	N	1158	0	1170	16	0
6	L	536	0	539	9	0
7	M	866	0	847	16	0
8	O	543	0	553	6	0
9	S	440	0	440	10	0
10	A	2614	0	2603	33	0
11	C	732	0	741	9	0
12	E	772	0	827	14	0
13	P	318	0	309	2	0
14	F	4077	0	3782	37	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	D	3805	0	3918	43	0
16	B	3579	0	3707	67	0
17	G	1373	0	1396	22	0
18	I	16	0	0	1	0
18	K	8	0	0	0	0
All	All	28296	0	28202	340	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 6.

All (340) 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)
3:K:7:PRO:HG3	7:M:88:GLY:HA3	1.42	1.02
3:K:7:PRO:HD3	7:M:87:GLN:C	1.87	0.94
3:K:7:PRO:HD3	7:M:87:GLN:O	1.71	0.90
15:D:21:ILE:HG23	15:D:34:ILE:HD11	1.75	0.69
1:H:69:ARG:NH2	3:K:148:CYS:SG	2.66	0.69
4:I:144:ILE:HG23	9:S:89:THR:HG21	1.73	0.68
12:E:61:VAL:HG22	17:G:135:ILE:HG13	1.76	0.66
1:H:155:ASN:O	4:I:53:ARG:NH1	2.28	0.65
1:H:138:ARG:NH1	1:H:142:TYR:OH	2.32	0.63
11:C:89:VAL:HG11	17:G:65:ILE:HD11	1.82	0.62
5:N:106:LYS:HG2	5:N:133:GLY:H	1.65	0.62
1:H:157:ASN:HD21	4:I:106:CYS:HB2	1.65	0.61
1:H:58:ARG:NH2	3:K:126:SER:OG	2.32	0.61
14:F:96:MET:HA	14:F:99:ILE:HD12	1.83	0.61
3:K:136:ASP:OD2	4:I:131:ARG:NH2	2.34	0.60
10:A:102:GLY:HA2	10:A:148:MET:HG3	1.83	0.60
1:H:173:VAL:HG23	1:H:280:LEU:HD22	1.82	0.60
16:B:220:SER:HA	16:B:223:ILE:HG12	1.82	0.60
16:B:118:THR:HG21	17:G:156:MET:HB2	1.82	0.60
1:H:175:LYS:HG3	4:I:161:ALA:HA	1.83	0.60
14:F:213:THR:O	14:F:217:ASN:ND2	2.34	0.60
10:A:199:GLN:HE21	10:A:208:ASN:H	1.48	0.59
16:B:305:TYR:HA	16:B:308:ILE:HD12	1.84	0.59
1:H:24:GLY:HA3	1:H:389:MET:HB2	1.84	0.59
2:J:167:ALA:O	4:I:131:ARG:NH1	2.36	0.58
2:J:102:ARG:NH1	2:J:155:ASP:OD2	2.36	0.58
10:A:225:ALA:HA	10:A:231:PRO:HG2	1.84	0.58
12:E:84:ILE:HG22	16:B:160:ASN:HB3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:D:500:ARG:HD3	15:D:503:LEU:HD12	1.85	0.58
1:H:41:GLU:HB3	3:K:201:TYR:HB2	1.86	0.58
10:A:278:GLY:O	10:A:317:LYS:NZ	2.34	0.58
16:B:80:SER:HB2	16:B:261:ARG:HH12	1.68	0.58
7:M:15:GLY:HA2	7:M:25:ASP:HB2	1.86	0.57
15:D:227:PRO:HG3	15:D:235:LEU:HD22	1.85	0.57
16:B:226:VAL:HG11	16:B:288:LEU:HB3	1.86	0.57
6:L:24:VAL:HA	6:L:27:ILE:HD12	1.84	0.57
14:F:176:GLN:OE1	15:D:439:ARG:NH1	2.38	0.57
12:E:31:LEU:HD21	16:B:167:LEU:HD21	1.87	0.56
3:K:79:ARG:HB3	10:A:250:ALA:HB2	1.87	0.56
9:S:78:LEU:HD11	9:S:85:ASP:HB3	1.87	0.56
15:D:229:VAL:O	15:D:232:HIS:ND1	2.38	0.56
16:B:226:VAL:HA	16:B:229:HIS:HB3	1.86	0.56
1:H:110:ARG:NH2	1:H:332:GLU:O	2.38	0.56
14:F:421:LEU:HD13	14:F:432:TRP:HE1	1.71	0.56
12:E:87:ASN:OD1	16:B:160:ASN:ND2	2.39	0.56
10:A:231:PRO:HD2	10:A:232:PHE:HD2	1.71	0.56
16:B:364:GLY:HA3	16:B:440:MET:HB3	1.87	0.56
14:F:285:GLU:HG3	14:F:286:GLN:HG3	1.87	0.56
3:K:18:VAL:O	3:K:20:GLN:NE2	2.39	0.55
14:F:144:LEU:HB3	14:F:193:MET:HG2	1.88	0.55
16:B:216:ILE:HA	16:B:219:ILE:HB	1.89	0.55
1:H:295:ARG:NH2	1:H:309:TYR:O	2.39	0.55
10:A:143:PRO:HG3	10:A:169:SER:HB2	1.87	0.55
11:C:82:VAL:HG21	17:G:73:LEU:HD22	1.88	0.55
1:H:358:PRO:O	1:H:362:ASN:ND2	2.38	0.55
1:H:176:CYS:O	1:H:180:CYS:N	2.33	0.55
2:J:78:THR:HG22	2:J:97:LYS:HG2	1.89	0.55
5:N:32:ARG:HH21	5:N:36:ARG:HH22	1.55	0.55
11:C:97:ALA:HB2	17:G:133:THR:HG22	1.87	0.55
3:K:80:GLN:NE2	10:A:246:GLN:O	2.40	0.55
16:B:95:ILE:HG23	16:B:113:MET:HE2	1.89	0.54
4:I:45:LYS:H	4:I:154:VAL:HG13	1.73	0.54
9:S:45:ILE:HA	9:S:49:MET:HE2	1.88	0.54
1:H:218:TRP:NE1	1:H:368:GLN:OE1	2.40	0.54
14:F:62:GLN:NE2	14:F:67:LEU:O	2.40	0.54
16:B:212:LEU:HD11	16:B:274:TRP:HB3	1.88	0.54
3:K:119:ILE:HG22	3:K:120:THR:HG23	1.90	0.54
4:I:38:THR:HG21	10:A:63:ILE:HG12	1.90	0.54
6:L:25:PRO:HB3	6:L:58:LEU:HD23	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:74:ALA:O	1:H:109:ASN:ND2	2.40	0.54
5:N:136:ARG:O	6:L:68:ARG:NH1	2.41	0.54
14:F:22:VAL:HG21	14:F:44:ILE:HD11	1.89	0.54
14:F:108:MET:HG2	14:F:128:LEU:HD13	1.89	0.54
17:G:50:TYR:HB3	17:G:55:ALA:HB3	1.90	0.54
4:I:62:LYS:HE3	9:S:68:GLN:HE21	1.73	0.53
1:H:53:LYS:NZ	2:J:153:ARG:O	2.41	0.53
12:E:40:ALA:O	12:E:44:ASN:ND2	2.41	0.53
1:H:366:LEU:HD12	1:H:385:ILE:HD12	1.89	0.53
8:O:46:ASP:OD2	8:O:62:ARG:NH2	2.42	0.53
15:D:104:LEU:O	15:D:462:ARG:NH1	2.41	0.53
3:K:117:CYS:HA	3:K:122:GLY:H	1.74	0.53
1:H:125:VAL:O	1:H:203:ARG:NH1	2.41	0.53
1:H:102:ARG:NH2	1:H:160:ARG:O	2.42	0.53
5:N:18:ALA:HB1	5:N:143:LEU:HD12	1.91	0.53
8:O:62:ARG:NH1	8:O:64:ASP:OD1	2.42	0.53
1:H:142:TYR:HB3	1:H:152:ARG:HD2	1.90	0.53
4:I:13:GLU:O	4:I:16:GLN:NE2	2.38	0.53
6:L:35:ARG:NH2	6:L:43:GLU:OE1	2.42	0.53
9:S:76:ALA:HA	9:S:89:THR:HA	1.90	0.53
15:D:24:ILE:O	15:D:114:ARG:NH1	2.37	0.53
1:H:107:GLU:OE2	1:H:110:ARG:NH1	2.42	0.52
1:H:203:ARG:HH22	10:A:335:VAL:HA	1.74	0.52
3:K:133:ARG:NH1	8:O:55:PRO:O	2.42	0.52
16:B:458:ARG:NH1	16:B:461:GLN:OE1	2.43	0.52
5:N:116:LEU:HD22	5:N:128:VAL:HG11	1.89	0.52
11:C:87:GLU:HB2	11:C:116:LEU:HD22	1.91	0.52
10:A:208:ASN:HB2	10:A:276:TYR:HA	1.92	0.52
1:H:351:TRP:HZ2	2:J:70:GLY:HA2	1.75	0.51
10:A:56:SER:HG	10:A:330:TRP:HE1	1.58	0.51
15:D:127:GLN:HE22	15:D:249:LEU:HB3	1.74	0.51
5:N:136:ARG:HD2	6:L:70:GLN:HA	1.93	0.51
15:D:148:ILE:HG13	16:B:386:ILE:HD13	1.93	0.51
10:A:296:SER:OG	10:A:297:GLU:N	2.42	0.51
4:I:78:PRO:HB3	4:I:98:ILE:HG12	1.92	0.51
15:D:228:ILE:HG22	15:D:230:PRO:HD2	1.92	0.51
1:H:130:PRO:HG2	1:H:193:LEU:HD21	1.93	0.51
2:J:106:ARG:NH1	2:J:133:GLU:OE2	2.40	0.51
15:D:136:MET:HB2	15:D:196:PHE:HD1	1.76	0.51
4:I:66:CYS:N	18:I:202:SF4:S3	2.82	0.51
10:A:94:SER:HA	10:A:154:ASN:HD22	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:273:SER:HA	10:A:277:PHE:HB2	1.92	0.51
15:D:183:ALA:HB1	15:D:214:VAL:HG13	1.93	0.51
3:K:182:ARG:NH1	7:M:34:ASP:O	2.43	0.50
5:N:5:ALA:O	5:N:36:ARG:NH1	2.43	0.50
2:J:68:ASP:HB2	2:J:128:PHE:HE1	1.77	0.50
15:D:301:ASN:HB3	15:D:304:ARG:HB2	1.93	0.50
16:B:380:LEU:HD23	16:B:383:LEU:HD12	1.94	0.50
9:S:67:VAL:HA	9:S:77:VAL:HA	1.93	0.50
10:A:52:GLU:OE2	10:A:329:ARG:NH2	2.45	0.50
1:H:94:VAL:HG13	1:H:163:GLY:HA2	1.93	0.50
14:F:112:ASP:OD1	14:F:121:TYR:OH	2.30	0.50
14:F:156:MET:HB2	15:D:389:LEU:HD11	1.92	0.49
3:K:114:MET:HG3	3:K:145:LEU:HD23	1.93	0.49
3:K:127:ASP:N	3:K:127:ASP:OD1	2.44	0.49
15:D:251:ALA:O	15:D:256:LYS:NZ	2.44	0.49
6:L:40:SER:OG	6:L:41:SER:N	2.43	0.49
14:F:138:LEU:HB3	14:F:150:PHE:HB2	1.92	0.49
1:H:328:TYR:HE2	2:J:62:ARG:HD3	1.77	0.49
1:H:363:LEU:HD13	1:H:387:VAL:HG11	1.94	0.49
5:N:12:ASP:OD2	5:N:140:TRP:NE1	2.45	0.49
14:F:141:SER:HB2	14:F:146:GLN:HB3	1.94	0.49
1:H:186:LYS:NZ	1:H:189:GLU:OE1	2.42	0.49
2:J:129:GLY:HA3	2:J:153:ARG:HH21	1.77	0.49
14:F:125:PHE:O	14:F:129:SER:OG	2.27	0.49
16:B:61:LEU:HB3	16:B:81:LEU:HD11	1.95	0.49
1:H:190:TYR:O	1:H:262:TYR:OH	2.31	0.49
3:K:45:PRO:HG3	3:K:83:LEU:HD23	1.94	0.49
3:K:146:PRO:HG2	4:I:126:LEU:HG	1.93	0.49
16:B:349:LEU:HD21	16:B:452:TRP:HH2	1.76	0.49
16:B:381:LEU:HB3	16:B:386:ILE:HG12	1.95	0.49
16:B:101:TYR:OH	17:G:189:GLU:OE1	2.30	0.48
17:G:128:THR:HB	17:G:131:SER:HB3	1.95	0.48
13:P:11:LEU:HB2	15:D:54:THR:HG21	1.95	0.48
14:F:152:GLU:O	14:F:156:MET:N	2.44	0.48
12:E:29:ARG:NH2	17:G:29:LEU:O	2.46	0.48
16:B:294:LEU:HD12	16:B:424:TYR:HB3	1.95	0.48
16:B:366:TYR:HB2	16:B:373:THR:HG21	1.95	0.48
1:H:85:ALA:HA	1:H:329:VAL:HG21	1.96	0.48
14:F:221:LEU:HB2	14:F:225:LEU:HD22	1.94	0.48
14:F:619:VAL:HA	14:F:622:VAL:HG22	1.96	0.48
16:B:97:MET:HB3	16:B:348:ILE:HD13	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:B:338:PHE:O	16:B:471:THR:OG1	2.30	0.48
9:S:51:VAL:HA	9:S:97:PRO:HA	1.95	0.48
12:E:78:LEU:HD11	17:G:74:ILE:HD13	1.94	0.48
4:I:49:SER:OG	4:I:50:GLU:N	2.46	0.48
4:I:160:PHE:HE1	4:I:168:MET:HG2	1.78	0.48
3:K:110:TYR:HB3	3:K:162:LEU:HD11	1.94	0.48
16:B:229:HIS:HD2	16:B:308:ILE:HD13	1.79	0.48
11:C:80:VAL:HG12	17:G:158:LEU:HD11	1.96	0.47
1:H:261:ARG:NH1	1:H:384:SER:OG	2.47	0.47
3:K:33:ASP:OD2	5:N:36:ARG:NH2	2.46	0.47
16:B:40:ASP:HA	16:B:43:THR:HG22	1.96	0.47
1:H:283:LEU:HD12	1:H:284:PRO:HD2	1.96	0.47
14:F:631:GLN:NE2	16:B:230:GLN:O	2.48	0.47
14:F:331:VAL:O	14:F:335:GLY:N	2.47	0.47
10:A:189:GLY:HA2	11:C:96:VAL:HG13	1.97	0.47
14:F:91:PRO:HB2	14:F:515:ILE:HA	1.96	0.47
2:J:150:TRP:HD1	8:O:24:ALA:HA	1.79	0.47
3:K:119:ILE:HG12	3:K:144:TYR:HD1	1.80	0.47
10:A:137:ALA:O	10:A:140:SER:OG	2.32	0.47
15:D:384:LEU:HD23	15:D:387:LEU:HD12	1.97	0.47
16:B:127:ALA:O	16:B:261:ARG:NH1	2.48	0.47
14:F:103:VAL:HA	14:F:106:LEU:HB2	1.96	0.47
16:B:126:ILE:HD11	16:B:139:LEU:HA	1.97	0.47
15:D:282:VAL:HG12	15:D:319:ILE:HA	1.96	0.46
12:E:58:LYS:NZ	17:G:142:ASP:OD2	2.48	0.46
1:H:175:LYS:NZ	4:I:167:VAL:O	2.49	0.46
1:H:232:TRP:HZ2	2:J:62:ARG:HH22	1.64	0.46
9:S:50:THR:HG22	9:S:66:ILE:HG12	1.96	0.46
3:K:61:ILE:HA	3:K:67:PHE:HB2	1.96	0.46
3:K:189:LYS:HB2	7:M:61:ALA:HB1	1.97	0.46
5:N:3:LEU:HD11	6:L:63:PRO:HB2	1.98	0.46
6:L:35:ARG:HE	6:L:35:ARG:HB3	1.60	0.46
10:A:174:ILE:HG23	10:A:175:PRO:HD3	1.98	0.46
10:A:281:SER:O	10:A:317:LYS:NZ	2.38	0.46
14:F:107:VAL:HG13	14:F:259:PRO:HB2	1.96	0.46
9:S:51:VAL:HG21	9:S:95:LEU:HD13	1.97	0.46
10:A:98:LEU:HB3	10:A:152:ALA:HB2	1.97	0.46
15:D:111:LEU:HB3	15:D:157:TRP:HE1	1.80	0.46
15:D:112:LYS:NZ	16:B:433:VAL:O	2.49	0.46
15:D:147:LEU:HD21	15:D:174:ALA:HB2	1.97	0.46
17:G:50:TYR:HB2	17:G:59:SER:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:364:GLN:HB3	2:J:119:TRP:CD1	2.51	0.46
2:J:127:MET:HB3	2:J:152:LEU:HB2	1.97	0.46
2:J:79:TYR:HB2	2:J:96:ILE:HB	1.98	0.45
1:H:158:TYR:O	1:H:165:ALA:N	2.48	0.45
7:M:17:VAL:HG23	7:M:30:THR:HG21	1.98	0.45
10:A:178:LEU:HD23	10:A:181:LEU:HD12	1.97	0.45
10:A:230:LEU:HD13	10:A:332:VAL:HG21	1.98	0.45
11:C:119:ALA:HB1	17:G:158:LEU:HD23	1.99	0.45
15:D:119:LEU:HD22	15:D:149:PRO:HA	1.99	0.45
16:B:35:GLN:HB2	16:B:39:ALA:HB2	1.98	0.45
16:B:72:GLY:O	16:B:193:GLN:NE2	2.41	0.45
16:B:104:GLN:HE22	17:G:177:LEU:HB2	1.81	0.45
15:D:306:ILE:HG13	15:D:350:VAL:HG21	1.98	0.45
16:B:61:LEU:HD23	16:B:64:GLN:HG3	1.99	0.45
1:H:81:VAL:HG22	1:H:331:VAL:HB	1.99	0.45
3:K:64:ARG:O	4:I:39:VAL:N	2.50	0.45
16:B:100:ARG:NE	16:B:104:GLN:OE1	2.44	0.45
16:B:252:LYS:HE2	16:B:252:LYS:HB3	1.74	0.45
1:H:34:GLY:N	11:C:69:GLN:OE1	2.50	0.45
2:J:134:GLY:HA3	3:K:214:LEU:HD22	1.99	0.45
4:I:155:THR:O	4:I:155:THR:OG1	2.32	0.45
15:D:378:MET:HB3	15:D:467:ILE:HG21	1.99	0.45
15:D:406:ALA:HA	15:D:416:ARG:HD2	1.99	0.45
16:B:142:LEU:O	16:B:146:SER:OG	2.28	0.45
16:B:226:VAL:O	16:B:229:HIS:ND1	2.47	0.45
1:H:12:VAL:HA	1:H:31:THR:HA	1.98	0.45
1:H:337:GLU:OE1	2:J:62:ARG:NE	2.41	0.45
17:G:25:GLY:HA3	17:G:38:LEU:HD13	1.99	0.45
10:A:344:GLY:HA2	10:A:348:LEU:HB2	1.99	0.44
15:D:188:ALA:HA	15:D:201:LEU:HD21	1.98	0.44
3:K:7:PRO:CG	7:M:88:GLY:HA3	2.31	0.44
16:B:226:VAL:HG22	16:B:284:LEU:HB3	2.00	0.44
16:B:435:LYS:HA	16:B:435:LYS:HD2	1.88	0.44
7:M:14:ALA:HA	7:M:29:LEU:HD23	2.00	0.44
12:E:41:VAL:HG11	16:B:178:LEU:HD13	2.00	0.44
14:F:397:THR:HB	14:F:490:LEU:HD11	1.99	0.44
1:H:258:CYS:SG	1:H:261:ARG:NH1	2.90	0.44
15:D:73:ILE:HG22	15:D:76:ILE:H	1.82	0.44
16:B:101:TYR:CZ	17:G:188:PRO:HD2	2.53	0.44
16:B:278:PHE:HA	16:B:281:LEU:HB2	2.00	0.44
5:N:100:LEU:HD23	5:N:100:LEU:HA	1.86	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:229:ARG:HB2	10:A:329:ARG:HD2	2.00	0.44
14:F:282:PRO:HA	14:F:285:GLU:HG2	1.99	0.44
16:B:11:ASN:OD1	16:B:11:ASN:N	2.51	0.44
1:H:220:LEU:HD13	1:H:224:MET:HG2	2.00	0.44
16:B:294:LEU:HD11	16:B:423:TYR:HD2	1.83	0.44
1:H:335:LYS:HE2	1:H:335:LYS:HB3	1.72	0.43
14:F:111:SER:HB3	14:F:259:PRO:HG3	2.00	0.43
5:N:110:LYS:HD3	5:N:110:LYS:HA	1.90	0.43
16:B:290:ASN:OD1	16:B:424:TYR:OH	2.32	0.43
1:H:212:ARG:HG3	1:H:230:VAL:HG22	1.99	0.43
1:H:164:VAL:HG12	1:H:311:TYR:HB2	2.01	0.43
1:H:341:TYR:HB3	1:H:354:LYS:HB3	2.01	0.43
16:B:21:LEU:HD23	16:B:21:LEU:HA	1.87	0.43
12:E:28:VAL:HG22	12:E:81:ILE:HG21	2.01	0.43
16:B:100:ARG:NH2	16:B:455:PHE:O	2.43	0.43
16:B:97:MET:HA	16:B:460:LEU:HD13	2.01	0.43
9:S:76:ALA:HB1	9:S:87:LEU:HD13	2.00	0.43
10:A:199:GLN:NE2	10:A:275:LEU:O	2.51	0.43
10:A:230:LEU:HG	10:A:231:PRO:HD3	2.01	0.43
16:B:21:LEU:HD22	16:B:117:LEU:HD22	2.01	0.43
3:K:188:HIS:HD2	3:K:190:MET:H	1.66	0.43
4:I:149:THR:HA	4:I:156:PRO:HG3	2.00	0.43
7:M:17:VAL:HG22	7:M:22:VAL:HG22	2.01	0.43
14:F:329:TYR:OH	14:F:438:THR:OG1	2.32	0.43
1:H:207:VAL:HG12	1:H:381:ILE:HD11	2.01	0.43
3:K:69:ARG:NH1	4:I:40:GLN:HG3	2.34	0.43
4:I:107:ALA:HB1	4:I:110:VAL:HG22	2.01	0.43
10:A:204:ILE:HD11	10:A:283:PRO:HD3	2.01	0.43
14:F:229:LEU:HD23	14:F:229:LEU:HA	1.85	0.42
15:D:211:GLN:HB3	15:D:273:ALA:HB2	2.00	0.42
16:B:144:ILE:HD13	16:B:147:TYR:HE2	1.83	0.42
6:L:39:ALA:O	6:L:44:ARG:NH2	2.45	0.42
1:H:148:ALA:O	4:I:51:ARG:NH2	2.52	0.42
12:E:90:THR:HG21	12:E:95:LYS:HE3	1.99	0.42
16:B:45:TYR:HA	16:B:48:ILE:HD12	2.01	0.42
3:K:7:PRO:HB2	3:K:8:ALA:H	1.64	0.42
14:F:291:MET:HA	14:F:294:ILE:HG12	2.01	0.42
1:H:84:ASN:ND2	1:H:87:GLU:OE2	2.52	0.42
15:D:244:ALA:HB1	15:D:348:PHE:HA	2.02	0.42
8:O:68:VAL:HG22	8:O:70:GLN:H	1.84	0.42
14:F:90:ASP:O	14:F:94:ALA:N	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:B:326:TYR:HB2	16:B:489:VAL:HG13	2.01	0.42
16:B:78:HIS:HB2	16:B:488:ALA:HA	2.01	0.42
16:B:194:LEU:HD22	16:B:266:ALA:HB2	2.01	0.42
15:D:371:LYS:HA	15:D:371:LYS:HD3	1.87	0.42
1:H:296:MET:HE3	1:H:296:MET:HB2	1.76	0.42
7:M:12:ILE:HD11	7:M:77:LEU:HD12	2.02	0.42
12:E:84:ILE:HD13	16:B:164:LEU:HD22	2.01	0.42
14:F:88:VAL:HG13	14:F:142:PRO:HB3	2.02	0.42
15:D:329:MET:HB2	15:D:496:ILE:HD11	2.02	0.42
1:H:88:LYS:HB2	1:H:327:HIS:HE1	1.85	0.42
14:F:190:LEU:HA	14:F:193:MET:HE2	2.01	0.42
15:D:42:GLY:HA2	15:D:124:TYR:HE2	1.85	0.42
16:B:294:LEU:HD11	16:B:423:TYR:CD2	2.55	0.42
3:K:91:THR:HA	3:K:131:ALA:HA	2.02	0.41
3:K:161:LYS:HD2	5:N:103:ILE:HD12	2.01	0.41
4:I:42:PRO:HB2	5:N:25:PRO:HB2	2.01	0.41
10:A:45:VAL:HG21	10:A:263:VAL:HG22	2.02	0.41
10:A:83:LEU:HD23	10:A:86:LYS:HE2	2.00	0.41
17:G:131:SER:O	17:G:131:SER:OG	2.32	0.41
2:J:53:LEU:HD12	2:J:96:ILE:HD11	2.01	0.41
11:C:75:TYR:OH	12:E:75:ALA:O	2.38	0.41
16:B:303:LEU:HA	16:B:306:SER:HB3	2.02	0.41
5:N:100:LEU:HB2	5:N:128:VAL:HG12	2.03	0.41
14:F:652:PHE:HE2	16:B:276:LEU:HG	1.85	0.41
1:H:116:LEU:HD12	1:H:116:LEU:HA	1.92	0.41
14:F:214:GLU:O	14:F:218:THR:OG1	2.30	0.41
15:D:61:THR:HG23	15:D:65:GLN:HE21	1.85	0.41
15:D:181:LEU:HD23	16:B:415:LEU:HD21	2.01	0.41
16:B:158:ARG:NH2	17:G:189:GLU:O	2.53	0.41
16:B:314:VAL:HG22	16:B:332:TYR:HD2	1.84	0.41
5:N:24:PRO:HA	5:N:25:PRO:HD3	1.87	0.41
10:A:178:LEU:HA	10:A:181:LEU:HB2	2.02	0.41
16:B:459:PRO:HA	16:B:462:VAL:HG12	2.02	0.41
3:K:54:PHE:O	3:K:58:ALA:N	2.43	0.41
3:K:185:THR:O	7:M:54:ARG:NH2	2.53	0.41
4:I:80:VAL:HG12	4:I:82:TRP:HD1	1.85	0.41
10:A:37:MET:HG2	10:A:119:PHE:HZ	1.85	0.41
14:F:602:LEU:HA	15:D:295:THR:HG23	2.02	0.41
15:D:85:ASP:OD2	15:D:264:ARG:NH2	2.53	0.41
1:H:6:THR:HG21	17:G:80:LEU:HA	2.02	0.41
3:K:9:ILE:HG12	7:M:108:VAL:HG12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:107:SER:OG	3:K:177:LEU:O	2.39	0.41
12:E:41:VAL:HG11	16:B:178:LEU:HB3	2.02	0.41
14:F:387:LEU:N	14:F:454:PHE:O	2.54	0.41
15:D:206:TYR:HB3	15:D:210:PHE:HD2	1.85	0.41
2:J:83:LYS:HE3	2:J:83:LYS:HB2	1.81	0.41
3:K:10:LEU:N	7:M:107:ARG:O	2.52	0.41
14:F:417:LYS:HA	14:F:420:ILE:HG12	2.03	0.41
15:D:94:LEU:HD13	15:D:337:VAL:HG13	2.02	0.41
16:B:73:SER:O	16:B:73:SER:OG	2.36	0.41
4:I:34:ARG:HH11	10:A:61:GLN:HE22	1.67	0.41
8:O:49:GLN:HB2	8:O:60:TRP:CE2	2.56	0.41
15:D:471:LEU:HA	15:D:474:ILE:HB	2.03	0.41
15:D:496:ILE:O	15:D:500:ARG:N	2.53	0.41
16:B:454:SER:OG	16:B:455:PHE:N	2.53	0.41
15:D:244:ALA:HB2	15:D:351:GLY:HA3	2.04	0.40
2:J:61:LEU:HD23	2:J:116:THR:HB	2.03	0.40
7:M:77:LEU:HD23	7:M:77:LEU:HA	1.92	0.40
14:F:647:LEU:HD23	14:F:647:LEU:HA	1.95	0.40
15:D:142:ALA:HA	15:D:145:LEU:HB2	2.02	0.40
3:K:45:PRO:HG2	3:K:67:PHE:CZ	2.57	0.40
4:I:45:LYS:HD2	4:I:154:VAL:HG21	2.03	0.40
7:M:97:ARG:H	7:M:97:ARG:HG2	1.70	0.40
13:P:40:GLY:HA2	15:D:111:LEU:HD12	2.04	0.40
16:B:148:LEU:HD13	17:G:160:GLY:HA3	2.04	0.40
17:G:44:LEU:HG	17:G:67:VAL:HG21	2.02	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	H	390/394 (99%)	355 (91%)	34 (9%)	1 (0%)	41 73

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	J	159/168 (95%)	145 (91%)	14 (9%)	0	100	100
3	K	210/237 (89%)	184 (88%)	26 (12%)	0	100	100
4	I	182/196 (93%)	161 (88%)	20 (11%)	1 (0%)	29	64
5	N	146/150 (97%)	140 (96%)	6 (4%)	0	100	100
6	L	64/76 (84%)	56 (88%)	8 (12%)	0	100	100
7	M	109/111 (98%)	94 (86%)	15 (14%)	0	100	100
8	O	67/70 (96%)	60 (90%)	7 (10%)	0	100	100
9	S	55/110 (50%)	47 (86%)	8 (14%)	0	100	100
10	A	337/372 (91%)	312 (93%)	24 (7%)	1 (0%)	41	73
11	C	89/132 (67%)	84 (94%)	5 (6%)	0	100	100
12	E	99/101 (98%)	93 (94%)	6 (6%)	0	100	100
13	P	40/44 (91%)	36 (90%)	4 (10%)	0	100	100
14	F	578/656 (88%)	525 (91%)	53 (9%)	0	100	100
15	D	502/529 (95%)	468 (93%)	34 (7%)	0	100	100
16	B	481/515 (93%)	443 (92%)	38 (8%)	0	100	100
17	G	189/200 (94%)	172 (91%)	17 (9%)	0	100	100
All	All	3697/4061 (91%)	3375 (91%)	319 (9%)	3 (0%)	54	83

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	151	MET
4	I	65	ALA
10	A	231	PRO

5.3.2 Protein sidechains (i)

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

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	317/338 (94%)	312 (98%)	5 (2%)	62	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	J	137/148 (93%)	136 (99%)	1 (1%)	84	93
3	K	172/196 (88%)	172 (100%)	0	100	100
4	I	153/172 (89%)	153 (100%)	0	100	100
5	N	117/120 (98%)	117 (100%)	0	100	100
6	L	54/63 (86%)	54 (100%)	0	100	100
7	M	91/96 (95%)	91 (100%)	0	100	100
8	O	57/59 (97%)	57 (100%)	0	100	100
9	S	48/97 (50%)	48 (100%)	0	100	100
10	A	245/285 (86%)	245 (100%)	0	100	100
11	C	68/109 (62%)	68 (100%)	0	100	100
12	E	79/82 (96%)	79 (100%)	0	100	100
13	P	32/37 (86%)	31 (97%)	1 (3%)	40	70
14	F	352/527 (67%)	350 (99%)	2 (1%)	86	94
15	D	378/424 (89%)	378 (100%)	0	100	100
16	B	367/413 (89%)	367 (100%)	0	100	100
17	G	137/166 (82%)	137 (100%)	0	100	100
All	All	2804/3332 (84%)	2795 (100%)	9 (0%)	92	96

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	25	VAL
1	H	149	THR
1	H	158	TYR
1	H	164	VAL
1	H	330	ARG
2	J	146	ASP
13	P	33	THR
14	F	11	ILE
14	F	355	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	60	ASN

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Mol	Chain	Res	Type
1	H	78	ASN
1	H	84	ASN
1	H	157	ASN
1	H	327	HIS
3	K	20	GLN
3	K	32	ASN
4	I	150	GLN
5	N	63	HIS
7	M	9	HIS
7	M	79	HIS
8	O	49	GLN
8	O	65	GLN
10	A	61	GLN
10	A	154	ASN
10	A	199	GLN
10	A	201	GLN
10	A	212	GLN
12	E	44	ASN
14	F	217	ASN
14	F	313	ASN
14	F	349	HIS
15	D	127	GLN
16	B	11	ASN
17	G	54	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

3 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
18	SF4	K	301	-	0,12,12	-	-	-		
18	SF4	I	202	-	0,12,12	-	-	-		
18	SF4	I	201	-	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
18	SF4	K	301	-	-	-	0/6/5/5
18	SF4	I	202	-	-	-	0/6/5/5
18	SF4	I	201	-	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	I	202	SF4	1	0

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)

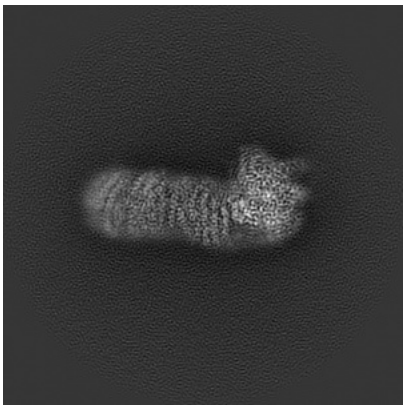
This section contains visualisations of the EMDB entry EMD-0415. These allow visual inspection of the internal detail of the map and identification of artifacts.

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.

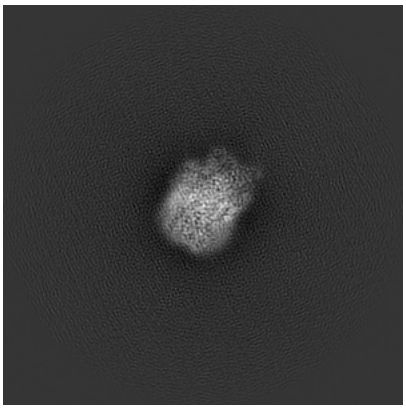
6.1 Orthogonal projections (i)

6.1.1 Primary map

X



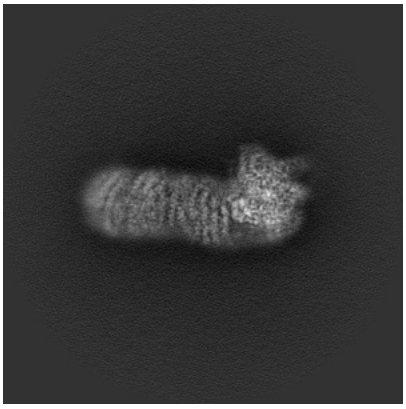
Y



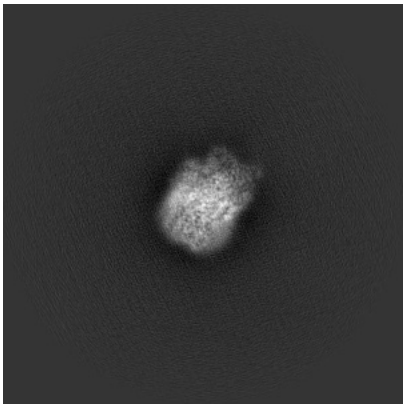
Z

6.1.2 Raw map

X



Y

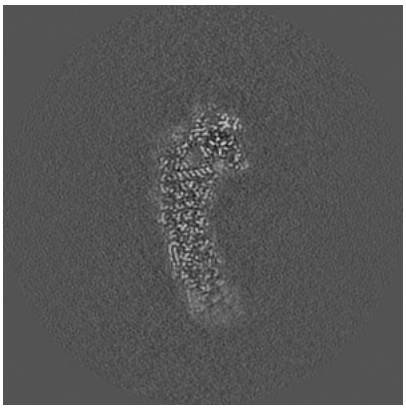


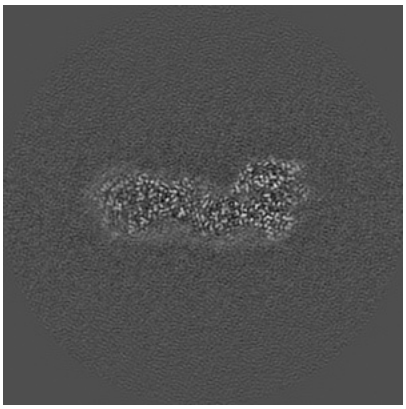
Z

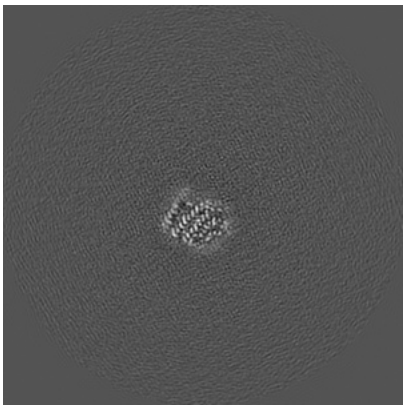
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

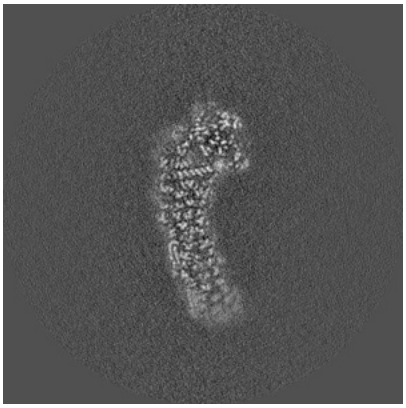
6.2.1 Primary map

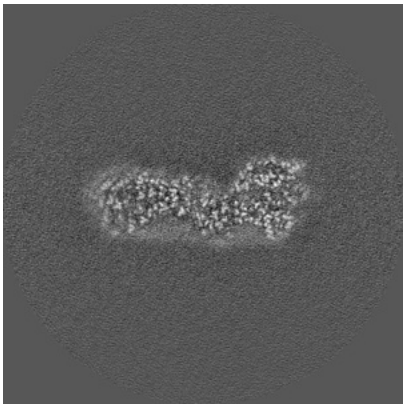

X Index: 180

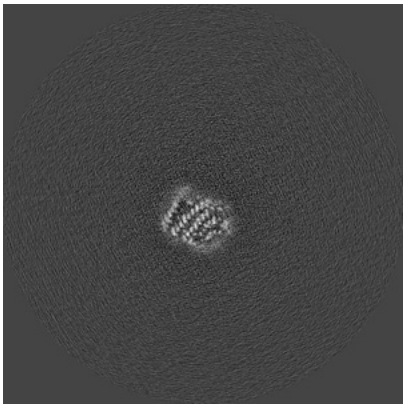

Y Index: 180


Z Index: 180

6.2.2 Raw map


X Index: 180

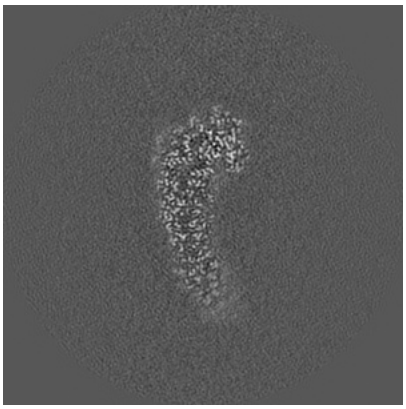

Y Index: 180

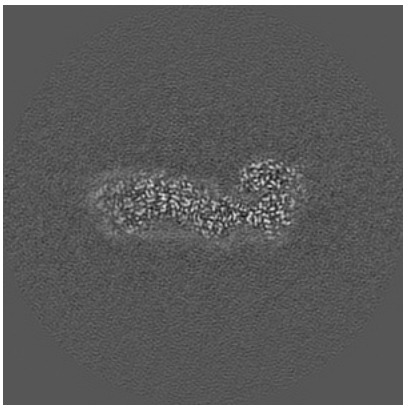

Z Index: 180

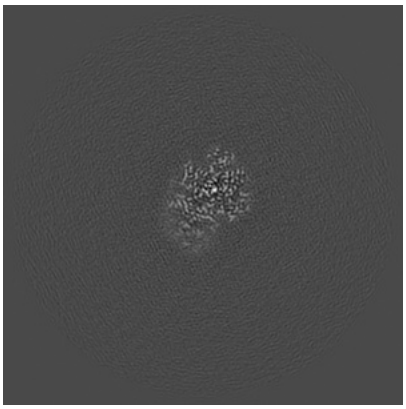
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map

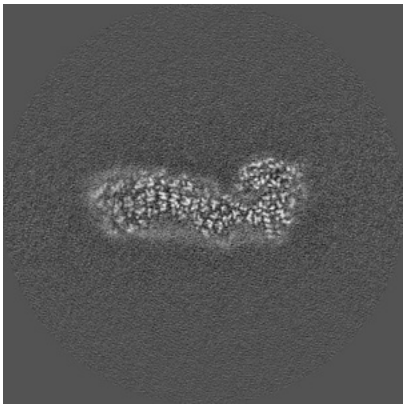

X Index: 173

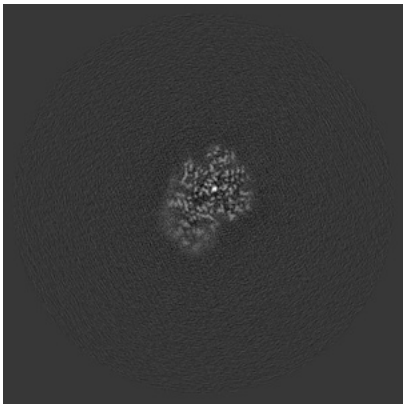

Y Index: 178


Z Index: 239

6.3.2 Raw map

X Index: 181

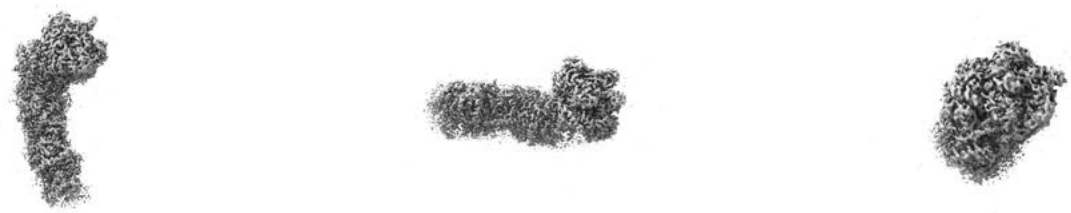

Y Index: 178


Z Index: 239

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

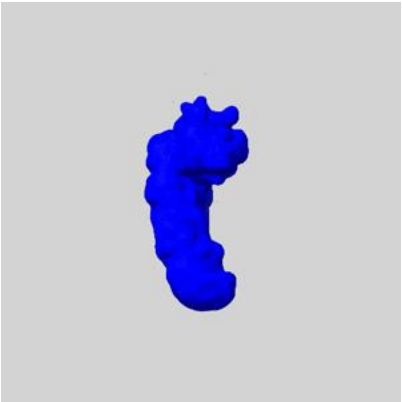
6.5 Mask visualisation (i)

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

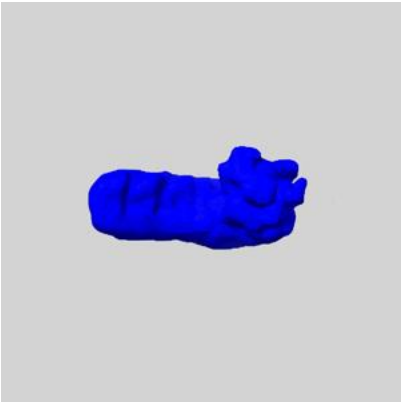
A mask typically either:

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

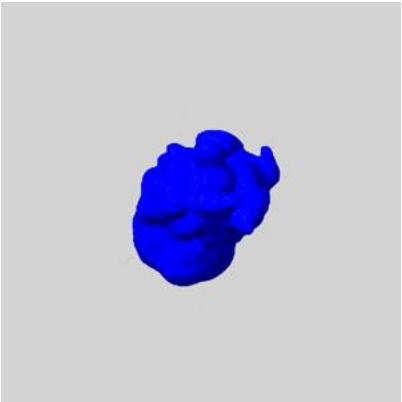
6.5.1 emd_0415_msk_1.map (i)



X



Y

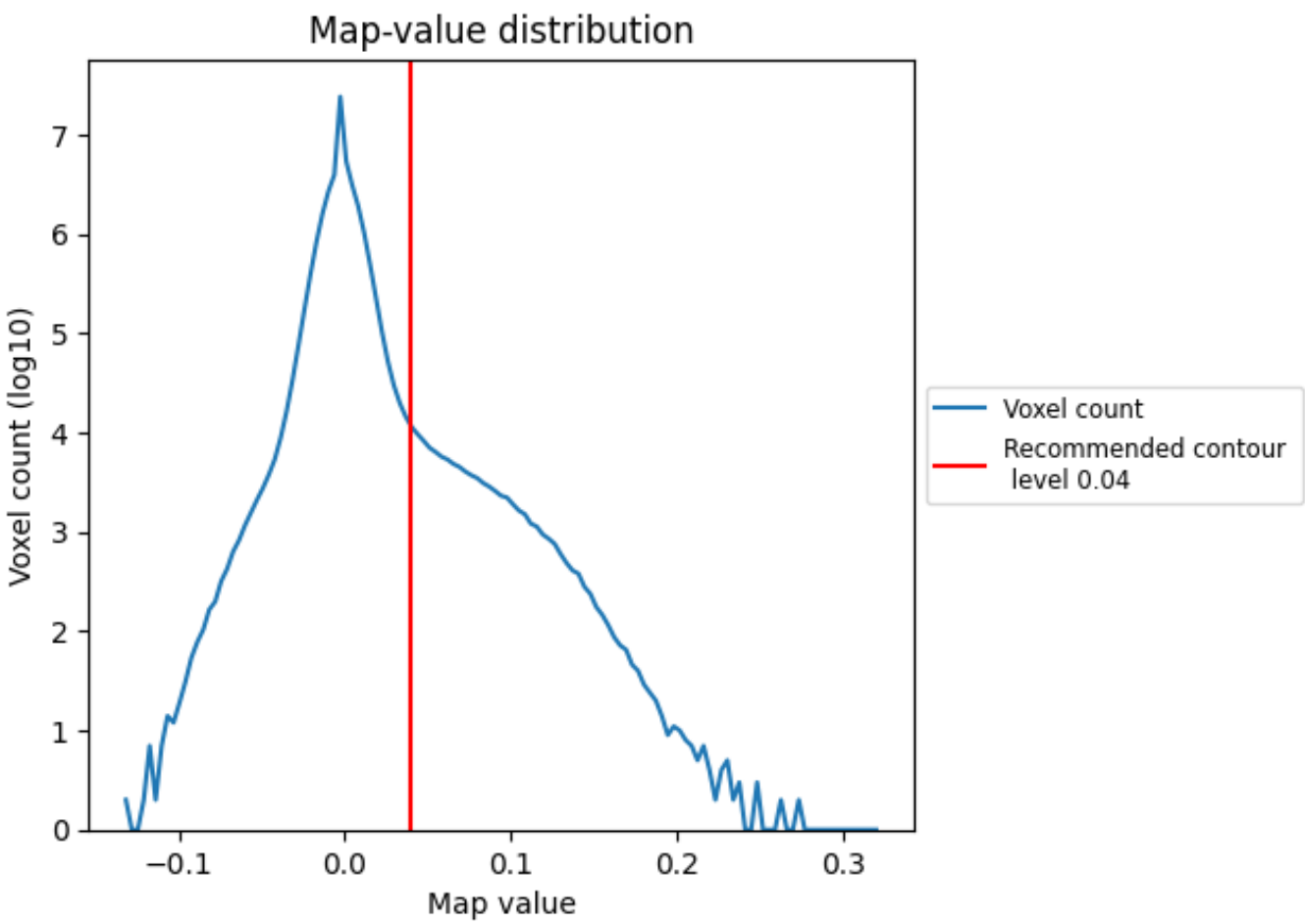


Z

7 Map analysis (i)

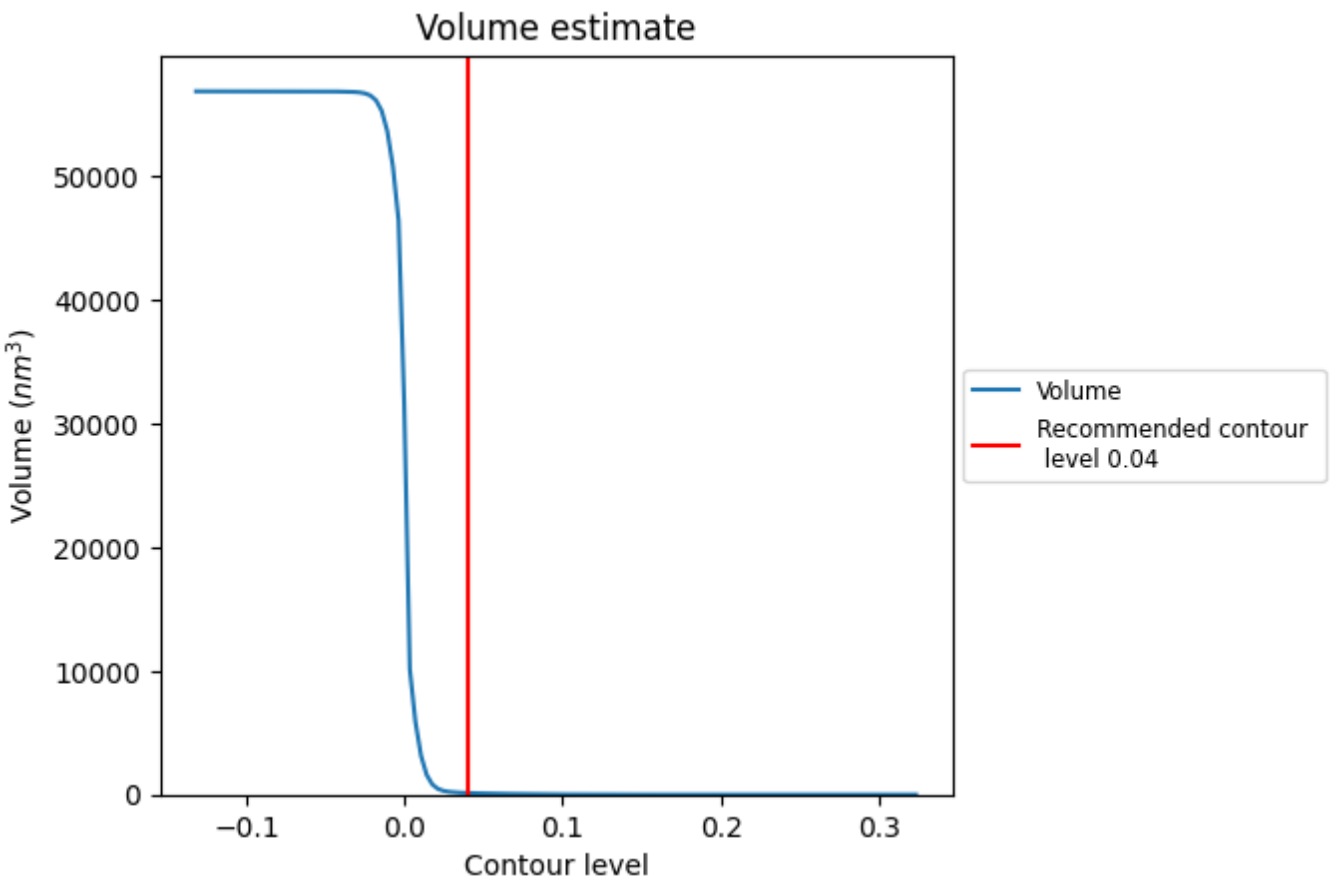
This section contains the results of statistical analysis of the map.

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.

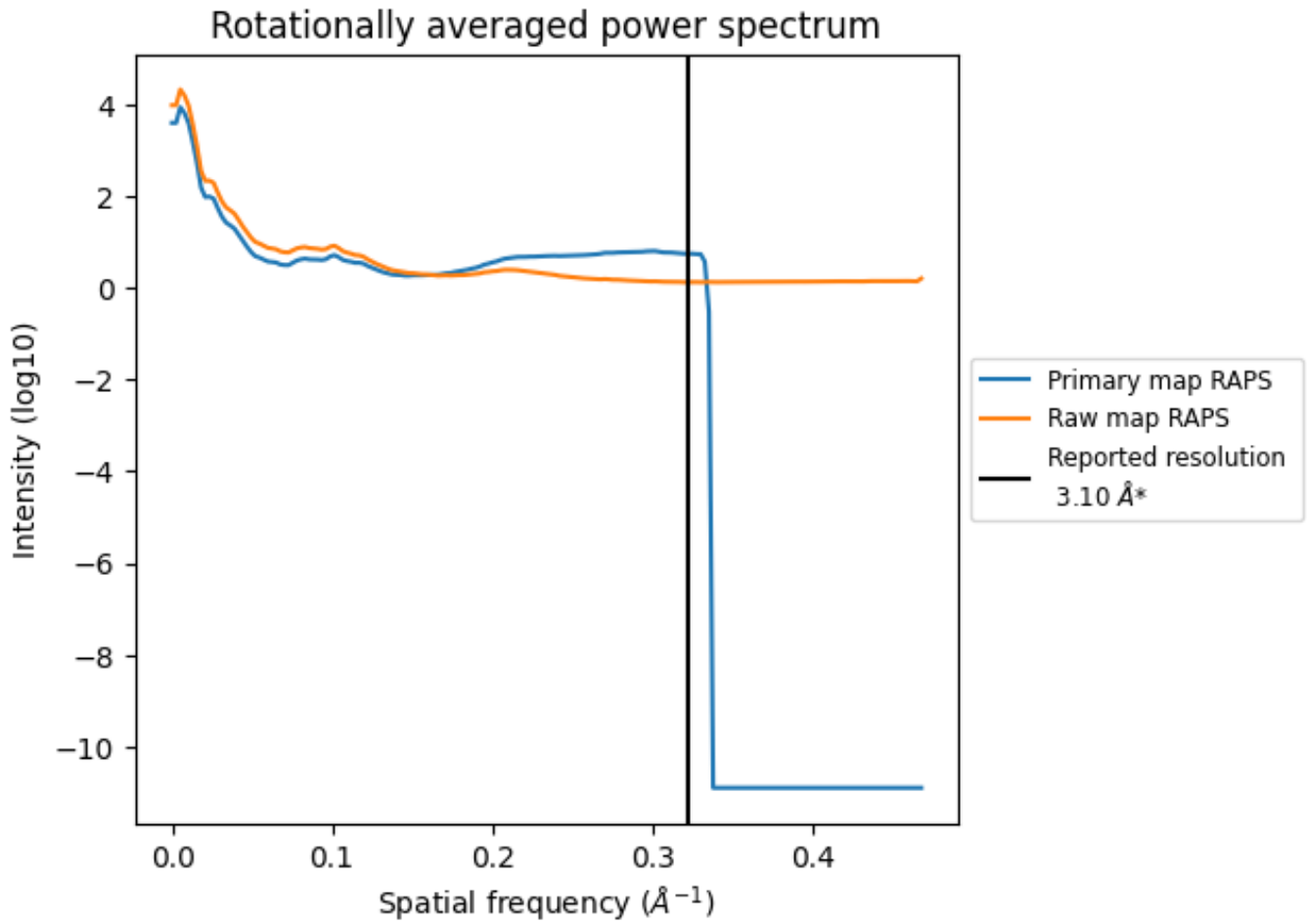
7.2 Volume estimate (i)



The volume at the recommended contour level is 125 nm^3; this corresponds to an approximate mass of 113 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)

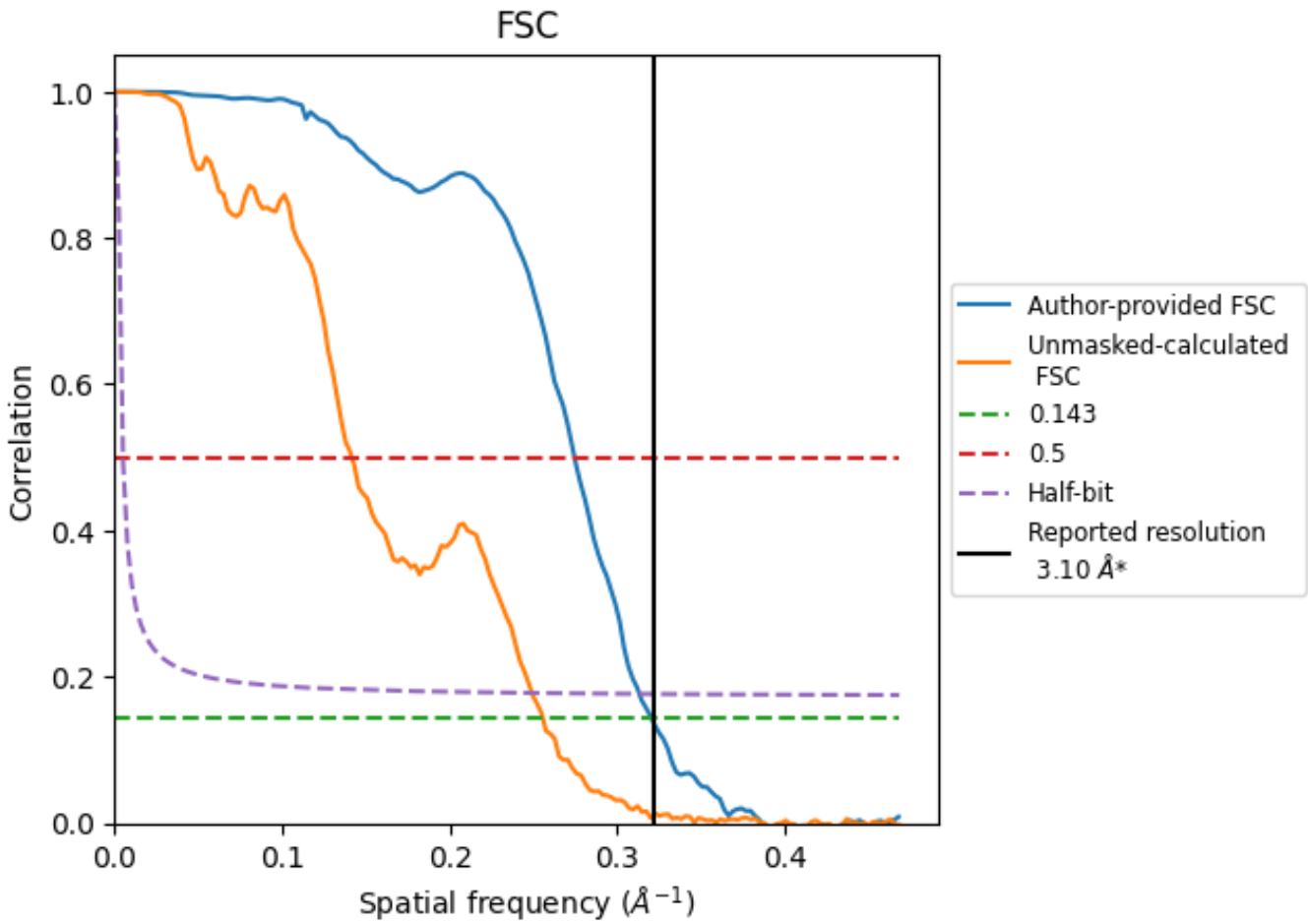


*Reported resolution corresponds to spatial frequency of 0.323 Å^{-1}

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 0.323 Å^{-1}

8.2 Resolution estimates (i)

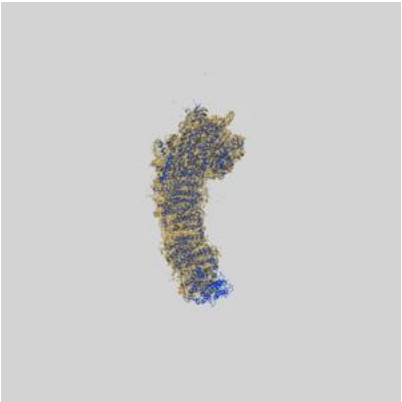
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.12	3.64	3.19
Unmasked-calculated*	3.91	7.06	4.01

*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 3.91 differs from the reported value 3.1 by more than 10 %

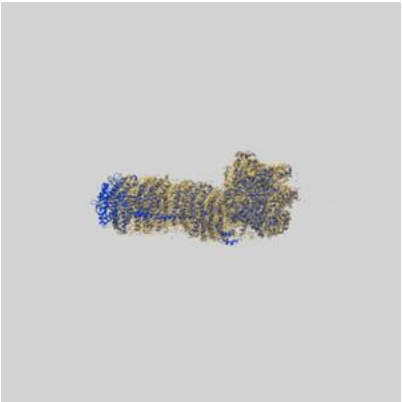
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-0415 and PDB model 6NBQ. Per-residue inclusion information can be found in section 3 on page 8.

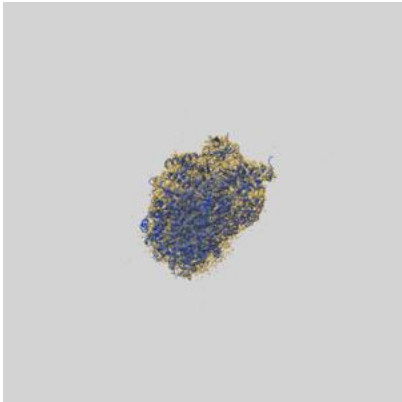
9.1 Map-model overlay (i)



X



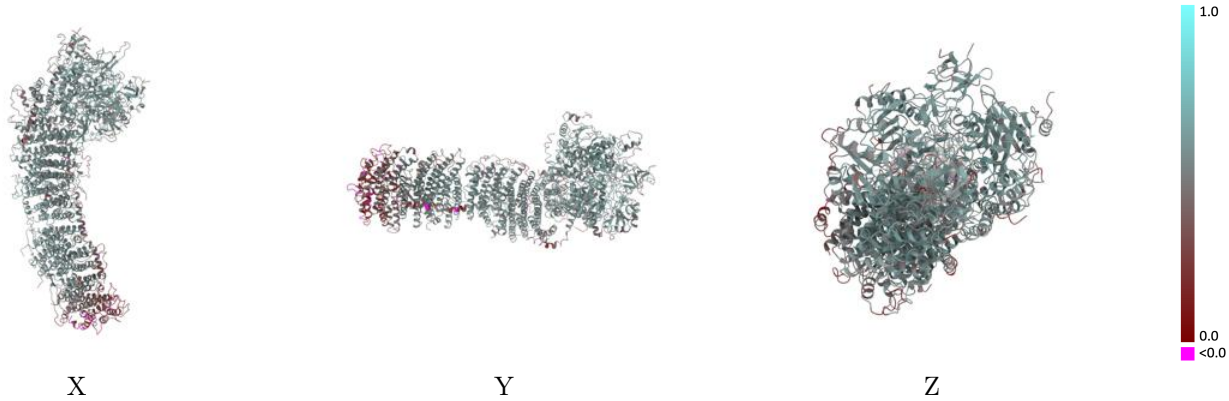
Y



Z

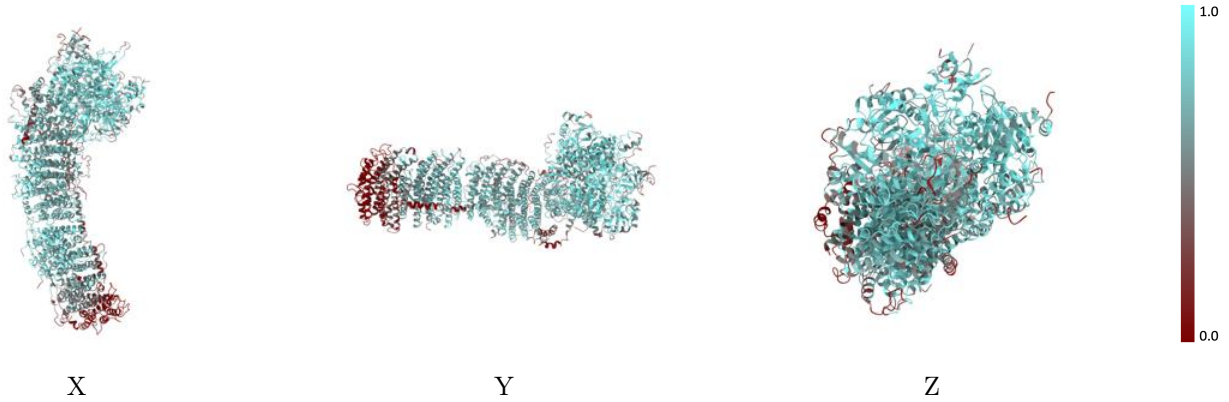
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



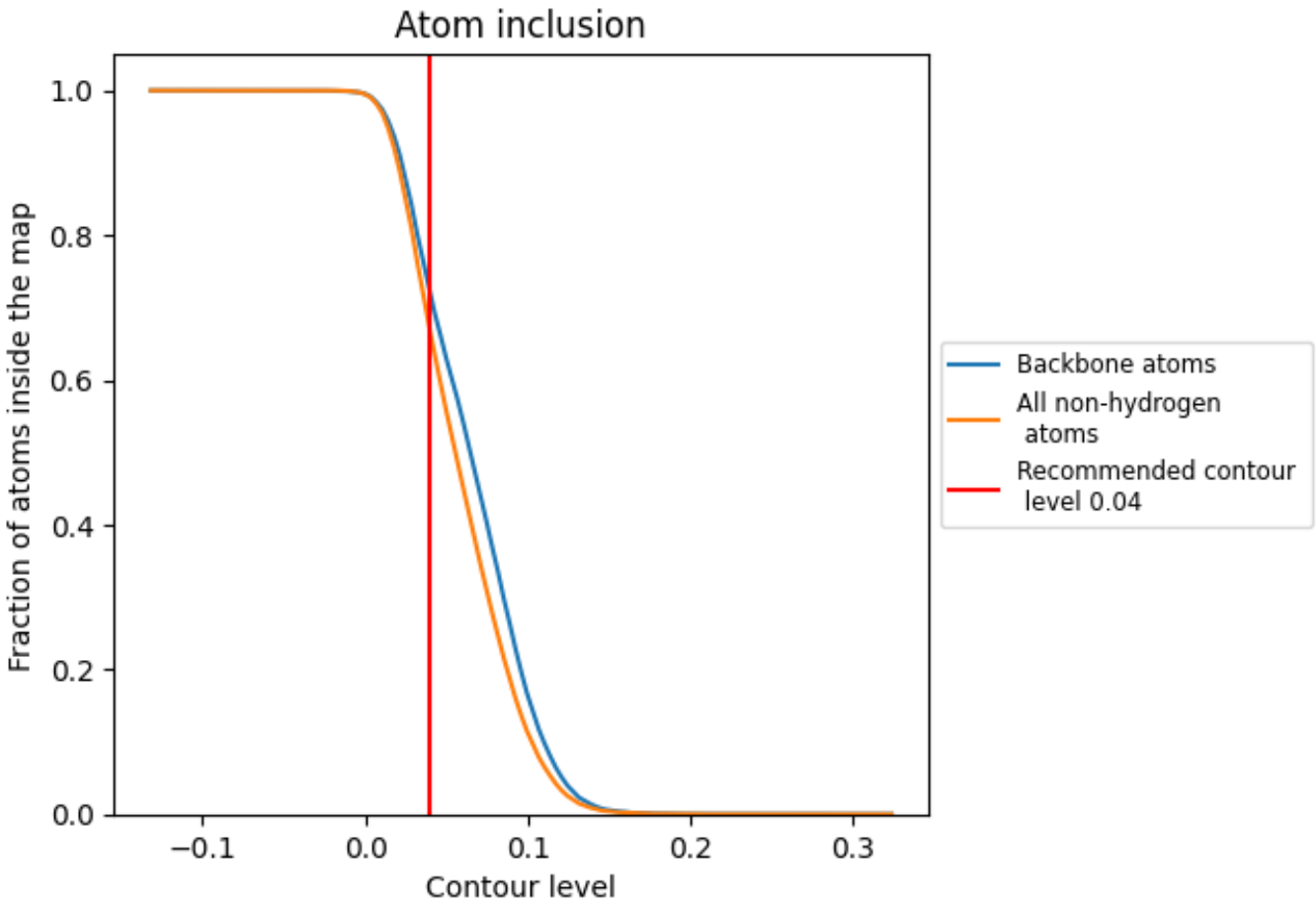
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model (i)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.04).

9.4 Atom inclusion (i)



At the recommended contour level, 72% of all backbone atoms, 67% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6654	0.5100
A	0.6683	0.5110
B	0.7657	0.5550
C	0.6347	0.5240
D	0.7405	0.5410
E	0.7510	0.5470
F	0.3135	0.3550
G	0.6444	0.5140
H	0.7855	0.5560
I	0.7097	0.5210
J	0.7771	0.5410
K	0.7443	0.5370
L	0.6084	0.5010
M	0.7621	0.5460
N	0.7381	0.5420
O	0.7608	0.5430
P	0.6433	0.4720
S	0.4184	0.4690