



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 07:15 AM UTC

PDB ID : 6VM1 / pdb_00006vm1
EMDB ID : EMD-21235
Title : Chloroplast ATP synthase (C3, CF1FO)
Authors : Yang, J.-H.; Williams, D.; Kandiah, E.; Fromme, P.; Chiu, P.-L.
Deposited on : 2020-01-27
Resolution : 7.90 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

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A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

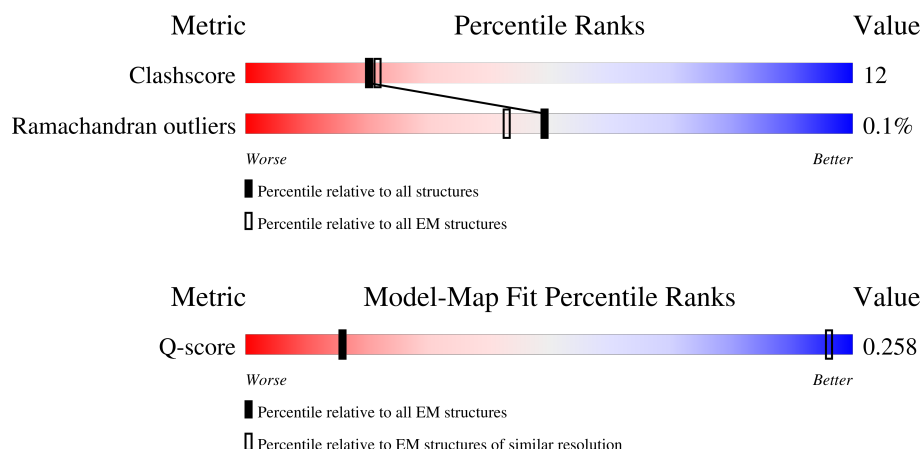
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 7.90 Å.

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



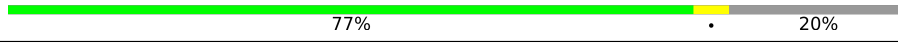
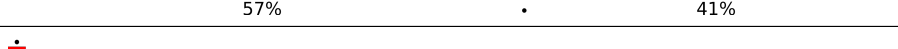
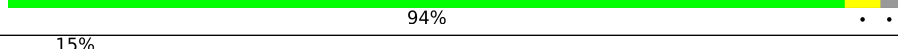
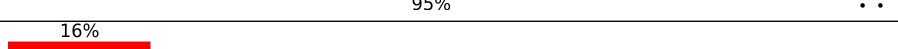
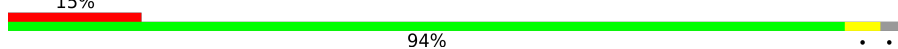
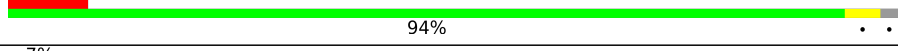
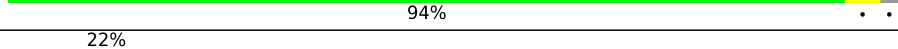
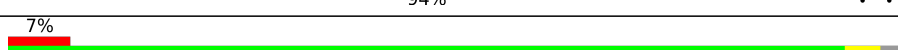
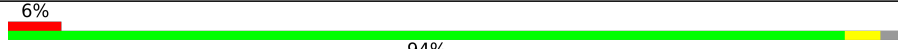
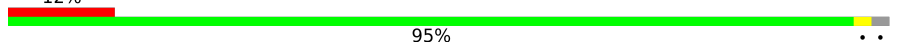
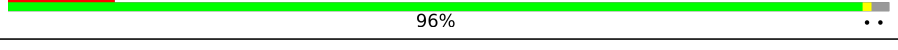
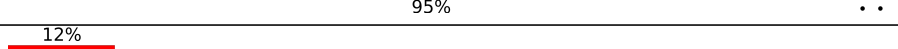
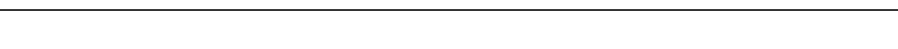
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Q-score	-	25397	366 (7.40 - 8.40)

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 $\leq 5\%$. 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	A	507	
1	B	507	
1	C	507	
2	D	498	
2	E	498	

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Mol	Chain	Length	Quality of chain
2	F	498	
3	I	184	
4	J	222	
5	a	247	
6	d	257	
7	e	134	
8	g	364	
9	M	81	
9	N	81	
9	O	81	
9	P	81	
9	Q	81	
9	R	81	
9	S	81	
9	T	81	
9	U	81	
9	V	81	
9	W	81	
9	X	81	
9	Y	81	
9	Z	81	

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 25331 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 ATP synthase subunit alpha, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	495	Total	C	N	O	0	0
			2436	1446	495	495		
1	B	498	Total	C	N	O	0	0
			2451	1455	498	498		
1	C	501	Total	C	N	O	0	0
			2466	1464	501	501		

- Molecule 2 is a protein called ATP synthase subunit beta, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	D	480	Total	C	N	O	0	0
			2353	1393	480	480		
2	E	478	Total	C	N	O	0	0
			2343	1387	478	478		
2	F	479	Total	C	N	O	0	0
			2348	1390	479	479		

- Molecule 3 is a protein called ATP synthase subunit b, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	I	148	Total	C	N	O	0	0
			731	435	148	148		

- Molecule 4 is a protein called ATP synthase subunit b', chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	J	131	Total	C	N	O	0	0
			651	389	131	131		

- Molecule 5 is a protein called ATP synthase subunit a, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	a	223	Total	C	N	O	0	0
			1096	650	223	223		

- Molecule 6 is a protein called ATP synthase delta chain, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	d	177	Total	C	N	O	0	0
			877	523	177	177		

- Molecule 7 is a protein called ATP synthase epsilon chain, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	e	129	Total	C	N	O	0	0
			637	379	129	129		

- Molecule 8 is a protein called ATP synthase gamma chain, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	g	316	Total	C	N	O	0	0
			1566	934	316	316		

- Molecule 9 is a protein called ATP synthase subunit c, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	R	79	Total	C	N	O	0	0
			384	226	79	79		
9	Q	79	Total	C	N	O	0	0
			384	226	79	79		
9	P	79	Total	C	N	O	0	0
			384	226	79	79		
9	O	79	Total	C	N	O	0	0
			384	226	79	79		
9	N	79	Total	C	N	O	0	0
			384	226	79	79		
9	M	79	Total	C	N	O	0	0
			384	226	79	79		
9	Z	79	Total	C	N	O	0	0
			384	226	79	79		
9	Y	79	Total	C	N	O	0	0
			384	226	79	79		
9	X	79	Total	C	N	O	0	0
			384	226	79	79		

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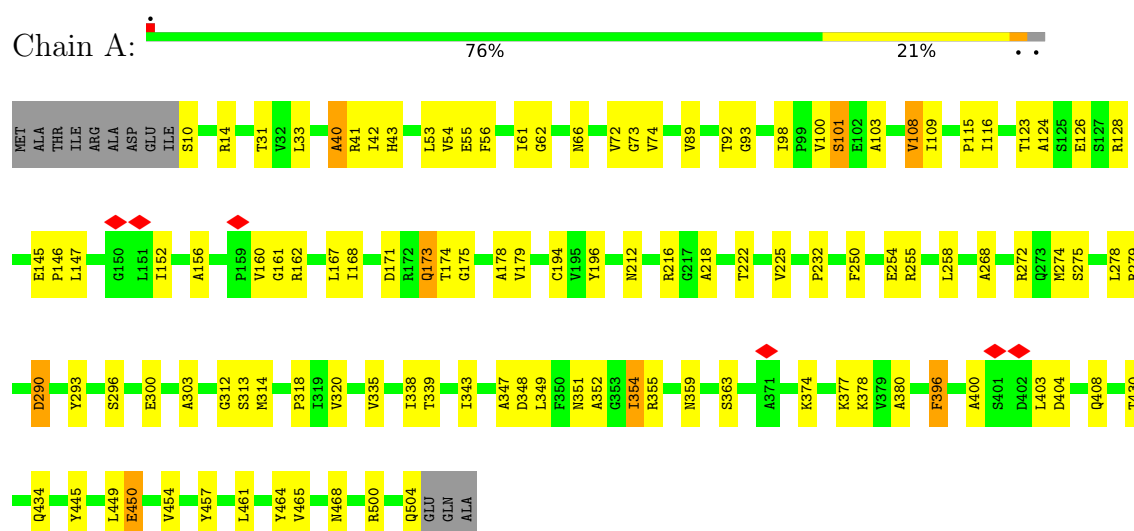
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Mol	Chain	Residues	Atoms				AltConf	Trace
9	W	79	Total 384	C 226	N 79	O 79	0	0
9	V	79	Total 384	C 226	N 79	O 79	0	0
9	U	79	Total 384	C 226	N 79	O 79	0	0
9	T	79	Total 384	C 226	N 79	O 79	0	0
9	S	79	Total 384	C 226	N 79	O 79	0	0

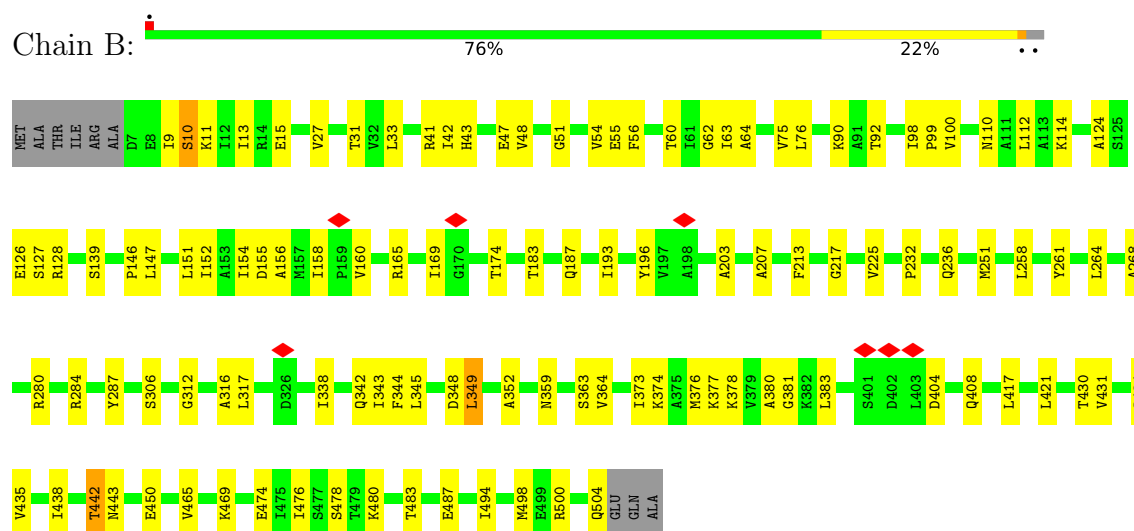
3 Residue-property plots

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.

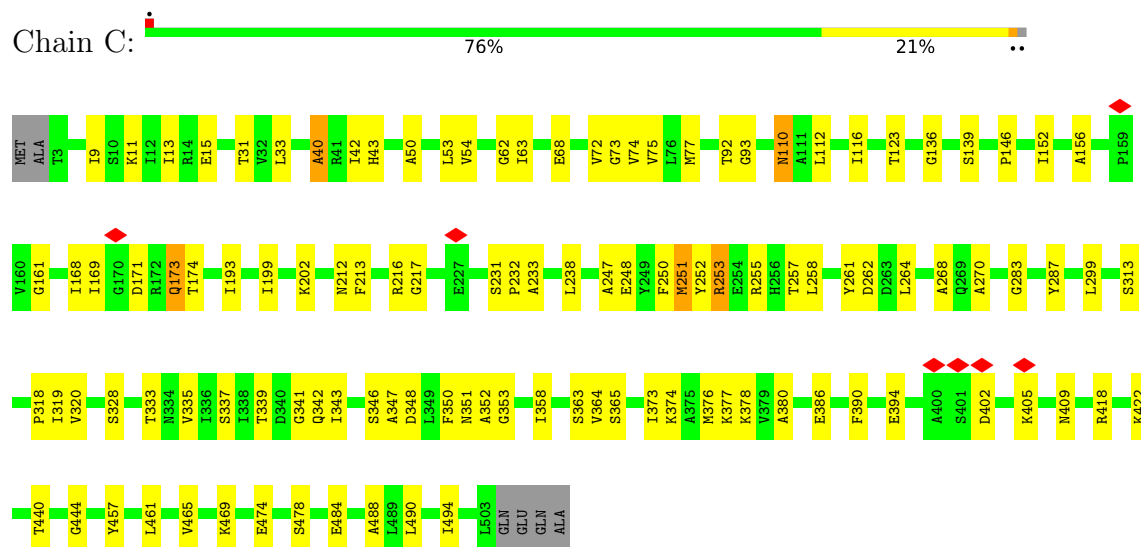
- Molecule 1: ATP synthase subunit alpha, chloroplastic



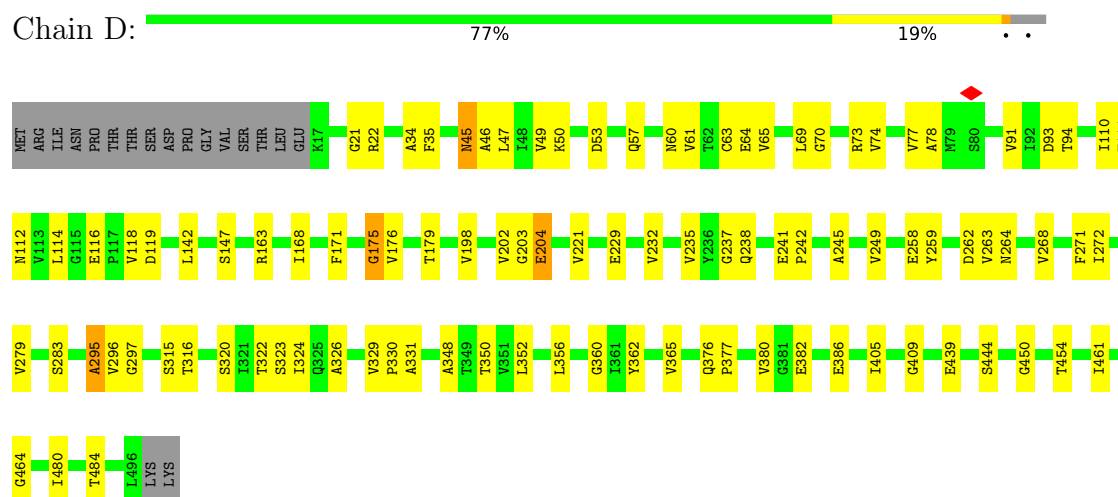
- Molecule 1: ATP synthase subunit alpha, chloroplastic



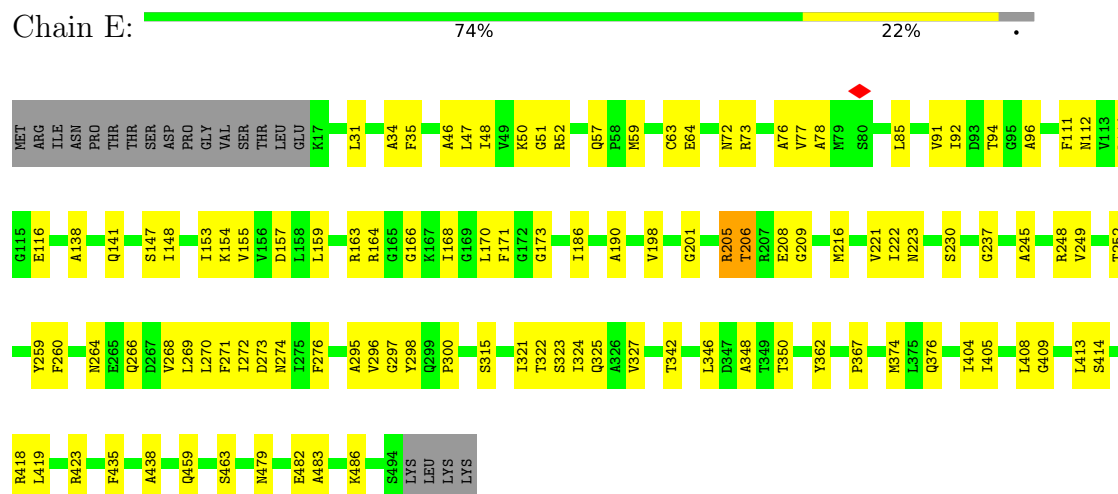
- Molecule 1: ATP synthase subunit alpha, chloroplastic

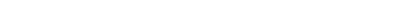


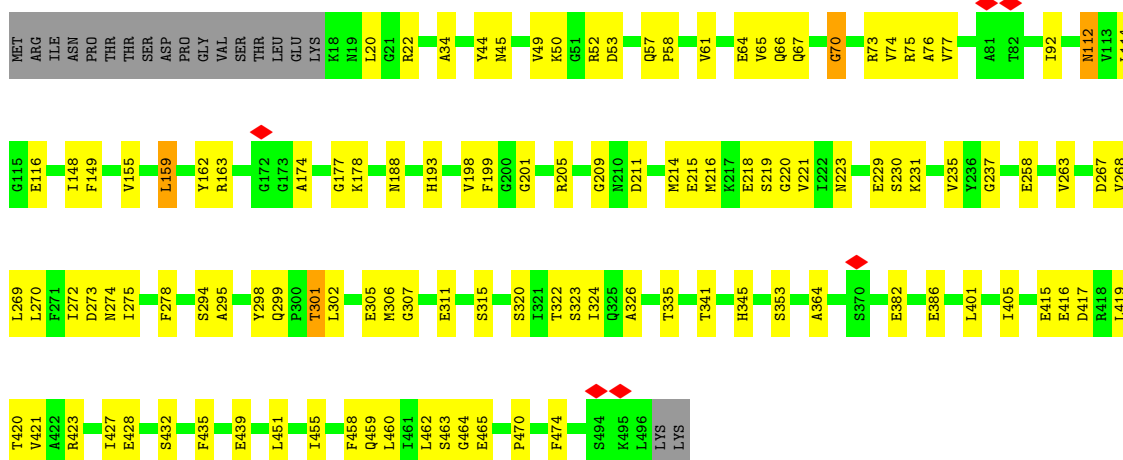
• Molecule 2: ATP synthase subunit beta, chloroplastic

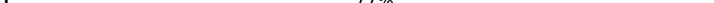


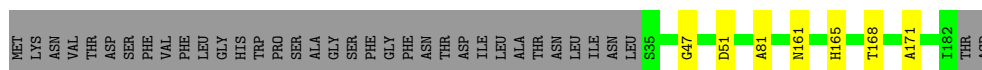
• Molecule 2: ATP synthase subunit beta, chloroplastic



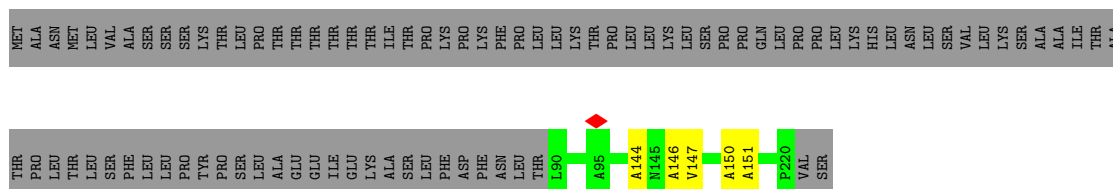
- Chain F:  73% 22% ..



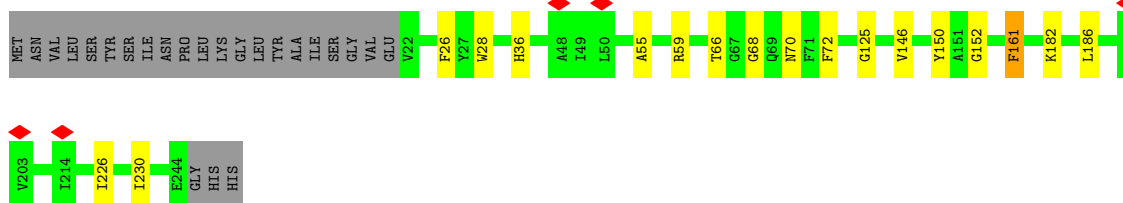
- Chain I:  77% 20%



- Chain J: 57% . 41%



- Chain a: 83% 7% 10%

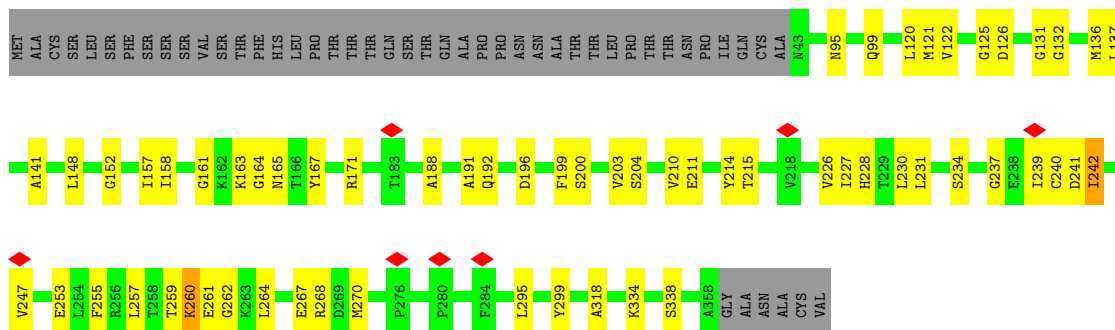


- Chain d: 55% 14% 31%

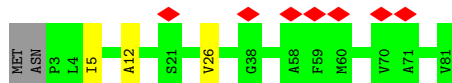
- Molecule 7: ATP synthase epsilon chain, chloroplastic



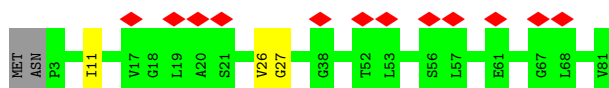
- Molecule 8: ATP synthase gamma chain, chloroplastic



- Molecule 9: ATP synthase subunit c, chloroplastic

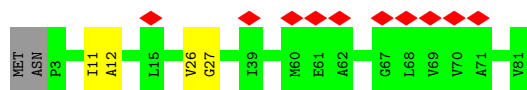


- Molecule 9: ATP synthase subunit c, chloroplastic

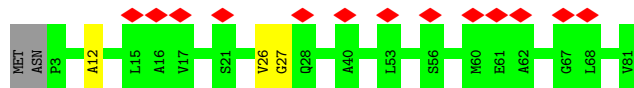


- Molecule 9: ATP synthase subunit c, chloroplasic

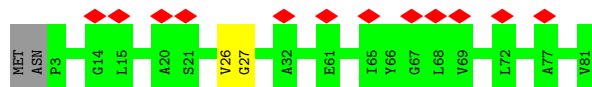




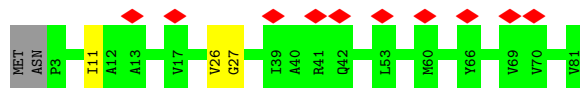
- Molecule 9: ATP synthase subunit c, chloroplastic



- Molecule 9: ATP synthase subunit c, chloroplastic



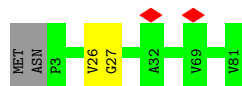
- Molecule 9: ATP synthase subunit c, chloroplastic



- Molecule 9: ATP synthase subunit c, chloroplastic



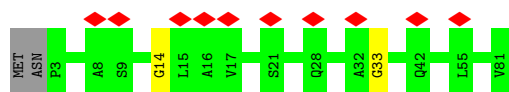
- Molecule 9: ATP synthase subunit c, chloroplastic



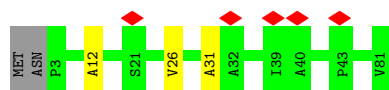
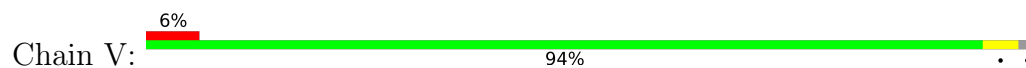
- Molecule 9: ATP synthase subunit c, chloroplastic



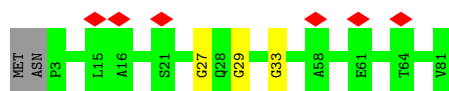
- Molecule 9: ATP synthase subunit c, chloroplastic



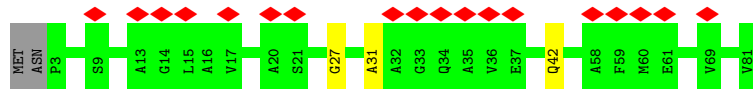
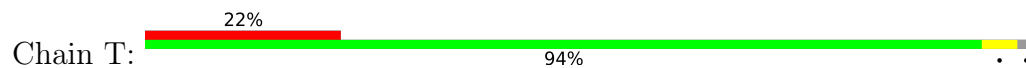
- Molecule 9: ATP synthase subunit c, chloroplastic



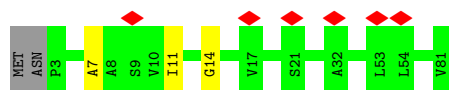
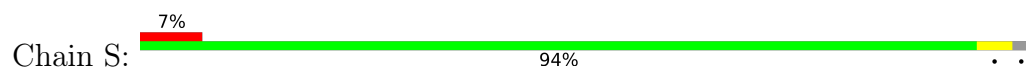
- Molecule 9: ATP synthase subunit c, chloroplastic



- Molecule 9: ATP synthase subunit c, chloroplastic



- Molecule 9: ATP synthase subunit c, chloroplastic



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	13947	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 ($e^-/\text{\AA}^2$)	43.5	Depositor
Minimum defocus (nm)	-1500	Depositor
Maximum defocus (nm)	-4000	Depositor
Magnification	48077	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.038	Depositor
Minimum map value	-0.015	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.00948	Depositor
Map size (Å)	339.84, 339.84, 339.84	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.18, 1.18, 1.18	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	A	0.54	0/2435	0.75	2/3384 (0.1%)
1	B	0.56	0/2450	0.78	0/3405
1	C	0.55	0/2465	0.84	4/3426 (0.1%)
2	D	0.54	0/2352	0.83	2/3263 (0.1%)
2	E	0.55	0/2342	0.78	2/3249 (0.1%)
2	F	0.56	0/2347	0.76	0/3256
3	I	0.42	0/730	0.52	0/1015
4	J	0.37	0/650	0.64	0/906
5	a	0.38	0/1095	0.67	0/1520
6	d	0.55	0/876	0.68	0/1220
7	e	0.52	0/636	0.83	0/884
8	g	0.52	0/1565	0.69	0/2181
9	M	0.31	0/383	0.51	0/528
9	N	0.31	0/383	0.51	0/528
9	O	0.31	0/383	0.51	0/528
9	P	0.32	0/383	0.51	0/528
9	Q	0.31	0/383	0.51	0/528
9	R	0.31	0/383	0.51	0/528
9	S	0.31	0/383	0.52	0/528
9	T	0.31	0/383	0.51	0/528
9	U	0.32	0/383	0.51	0/528
9	V	0.31	0/383	0.51	0/528
9	W	0.31	0/383	0.52	0/528
9	X	0.31	0/383	0.51	0/528
9	Y	0.31	0/383	0.51	0/528
9	Z	0.31	0/383	0.51	0/528
All	All	0.49	0/25305	0.72	10/35101 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	13
1	B	0	12
1	C	0	14
2	D	0	10
2	E	0	9
2	F	0	9
6	d	0	2
8	g	0	2
All	All	0	71

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	362	TYR	CA-C-N	7.61	145.27	127.00
2	D	362	TYR	C-N-CA	7.61	145.27	127.00
2	E	362	TYR	CA-C-N	6.29	142.09	127.00
2	E	362	TYR	C-N-CA	6.29	142.09	127.00
1	C	112	LEU	CA-C-N	6.02	133.04	121.54
1	C	112	LEU	C-N-CA	6.02	133.04	121.54
1	A	355	ARG	CA-C-N	5.58	140.38	127.00
1	A	355	ARG	C-N-CA	5.58	140.38	127.00
1	C	238	LEU	CA-C-N	5.23	126.63	120.09
1	C	238	LEU	C-N-CA	5.23	126.63	120.09

There are no chirality outliers.

All (71) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	101	SER	Peptide
1	A	108	VAL	Peptide
1	A	173	GLN	Peptide
1	A	174	THR	Peptide
1	A	232	PRO	Peptide
1	A	290	ASP	Peptide
1	A	303	ALA	Peptide
1	A	338	ILE	Peptide
1	A	354	ILE	Peptide
1	A	396	PHE	Peptide
1	A	40	ALA	Peptide
1	A	403	LEU	Peptide
1	A	450	GLU	Peptide

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Mol	Chain	Res	Type	Group
1	B	10	SER	Peptide
1	B	112	LEU	Peptide
1	B	146	PRO	Peptide
1	B	174	THR	Peptide
1	B	280	ARG	Peptide
1	B	338	ILE	Peptide
1	B	349	LEU	Peptide
1	B	383	LEU	Peptide
1	B	442	THR	Peptide
1	B	450	GLU	Peptide
1	B	47	GLU	Peptide
1	B	9	ILE	Peptide
1	C	110	ASN	Peptide
1	C	123	THR	Peptide
1	C	173	GLN	Peptide
1	C	174	THR	Peptide
1	C	202	LYS	Peptide
1	C	231	SER	Peptide
1	C	232	PRO	Peptide
1	C	251	MET	Peptide
1	C	253	ARG	Peptide
1	C	299	LEU	Peptide
1	C	318	PRO	Peptide
1	C	328	SER	Peptide
1	C	40	ALA	Peptide
1	C	402	ASP	Peptide
2	D	114	LEU	Peptide
2	D	119	ASP	Peptide
2	D	175	GLY	Peptide
2	D	176	VAL	Peptide
2	D	204	GLU	Peptide
2	D	229	GLU	Peptide
2	D	241	GLU	Peptide
2	D	242	PRO	Peptide
2	D	330	PRO	Peptide
2	D	45	ASN	Peptide
2	E	111	PHE	Peptide
2	E	114	LEU	Peptide
2	E	173	GLY	Peptide
2	E	205	ARG	Peptide
2	E	206	THR	Peptide
2	E	221	VAL	Peptide

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Mol	Chain	Res	Type	Group
2	E	296	VAL	Peptide
2	E	297	GLY	Peptide
2	E	413	LEU	Peptide
2	F	112	ASN	Peptide
2	F	114	LEU	Peptide
2	F	159	LEU	Peptide
2	F	177	GLY	Peptide
2	F	229	GLU	Peptide
2	F	301	THR	Peptide
2	F	335	THR	Peptide
2	F	45	ASN	Peptide
2	F	70	GLY	Peptide
6	d	185	LYS	Peptide
6	d	228	GLU	Peptide
8	g	242	ILE	Peptide
8	g	260	LYS	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	A	2436	0	1164	59	0
1	B	2451	0	1170	65	0
1	C	2466	0	1179	61	0
2	D	2353	0	1107	51	0
2	E	2343	0	1103	56	0
2	F	2348	0	1105	66	0
3	I	731	0	331	4	0
4	J	651	0	304	4	0
5	a	1096	0	501	9	0
6	d	877	0	402	20	0
7	e	637	0	303	17	0
8	g	1566	0	717	33	0
9	M	384	0	216	3	0
9	N	384	0	216	2	0
9	O	384	0	216	3	0
9	P	384	0	216	4	0
9	Q	384	0	216	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	R	384	0	216	4	0
9	S	384	0	216	3	0
9	T	384	0	216	3	0
9	U	384	0	216	3	0
9	V	384	0	216	3	0
9	W	384	0	216	2	0
9	X	384	0	216	1	0
9	Y	384	0	216	2	0
9	Z	384	0	216	3	0
All	All	25331	0	12410	462	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 12.

All (462) 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)
8:g:257:LEU:HA	8:g:267:GLU:H	1.51	0.76
1:A:396:PHE:O	1:A:400:ALA:HB2	1.88	0.73
6:d:224:ARG:HA	6:d:232:LEU:HA	1.70	0.73
6:d:180:VAL:HA	6:d:223:ILE:HA	1.69	0.72
6:d:222:THR:HA	6:d:234:ASP:HA	1.73	0.71
1:A:56:PHE:HA	1:A:89:VAL:HA	1.73	0.69
1:B:165:ARG:HA	1:B:316:ALA:HB3	1.75	0.69
1:C:110:ASN:H	1:C:116:ILE:H	1.39	0.68
2:E:166:GLY:H	2:E:322:THR:HA	1.58	0.68
2:F:66:GLN:H	2:F:76:ALA:HA	1.57	0.68
1:C:484:GLU:O	1:C:488:ALA:HB2	1.95	0.67
1:B:62:GLY:HA2	1:B:76:LEU:HA	1.75	0.67
1:A:54:VAL:HA	1:A:92:THR:H	1.58	0.67
2:E:51:GLY:HA3	2:E:59:MET:HA	1.76	0.66
2:F:315:SER:HA	2:F:320:SER:HA	1.77	0.66
7:e:62:LEU:HA	7:e:81:ALA:HA	1.77	0.66
1:C:62:GLY:HA2	1:C:77:MET:H	1.61	0.65
2:E:47:LEU:HA	2:E:94:THR:H	1.61	0.65
2:D:175:GLY:HA2	2:D:179:THR:H	1.62	0.65
1:C:42:ILE:H	1:C:72:VAL:H	1.44	0.65
6:d:182:SER:HA	6:d:221:PHE:HA	1.79	0.64
2:D:147:SER:H	2:D:163:ARG:HA	1.63	0.64
2:F:52:ARG:HA	2:F:58:PRO:HA	1.79	0.64
2:F:267:ASP:HA	2:F:320:SER:H	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:373:ILE:O	1:C:377:LYS:N	2.30	0.64
1:C:146:PRO:HA	1:C:161:GLY:HA2	1.80	0.63
2:D:49:VAL:HA	2:D:91:VAL:HA	1.80	0.63
2:E:168:ILE:HA	2:E:348:ALA:HB3	1.81	0.63
1:B:54:VAL:HA	1:B:92:THR:H	1.64	0.62
2:F:274:ASN:O	2:F:278:PHE:N	2.33	0.62
1:B:183:THR:O	1:B:187:GLN:N	2.32	0.62
1:C:68:GLU:H	1:C:73:GLY:H	1.46	0.62
1:C:193:ILE:H	1:C:257:THR:HA	1.64	0.62
7:e:53:LEU:N	7:e:56:GLN:O	2.32	0.62
7:e:125:ARG:O	7:e:129:SER:CB	2.48	0.61
1:B:376:MET:O	1:B:380:ALA:C	2.43	0.61
2:E:46:ALA:N	2:E:96:ALA:O	2.32	0.61
6:d:220:GLY:H	6:d:236:SER:HA	1.65	0.61
2:F:415:GLU:O	2:F:419:LEU:N	2.33	0.61
2:F:215:GLU:O	2:F:219:SER:N	2.33	0.61
1:B:154:ILE:O	1:B:158:ILE:N	2.29	0.60
9:R:26:VAL:HA	9:Q:27:GLY:HA3	1.82	0.60
1:C:341:GLY:HA2	1:C:365:SER:HA	1.84	0.60
2:F:205:ARG:O	2:F:209:GLY:N	2.32	0.60
2:E:295:ALA:HB3	2:E:298:TYR:H	1.67	0.60
1:A:147:LEU:N	1:A:160:VAL:O	2.35	0.60
2:F:148:ILE:HA	2:F:163:ARG:HA	1.83	0.59
1:A:347:ALA:O	1:A:351:ASN:N	2.30	0.59
2:F:295:ALA:N	2:F:298:TYR:O	2.35	0.59
1:B:431:VAL:O	1:B:435:VAL:CB	2.50	0.59
2:D:111:PHE:HA	2:D:118:VAL:H	1.66	0.59
5:a:152:GLY:HA3	5:a:161:PHE:HA	1.84	0.59
2:E:63:CYS:HA	2:E:78:ALA:HA	1.83	0.59
2:E:147:SER:O	2:E:164:ARG:N	2.34	0.59
7:e:40:THR:N	7:e:69:ILE:O	2.30	0.59
9:Q:26:VAL:HA	9:P:27:GLY:HA3	1.83	0.59
2:D:382:GLU:O	2:D:386:GLU:CB	2.50	0.59
7:e:126:VAL:O	7:e:130:ASN:N	2.36	0.59
2:E:153:ILE:O	2:E:157:ASP:N	2.33	0.59
2:F:188:ASN:O	2:F:193:HIS:N	2.34	0.58
5:a:66:THR:O	5:a:70:ASN:N	2.36	0.58
1:B:33:LEU:N	1:B:41:ARG:O	2.35	0.58
2:D:69:LEU:H	2:D:74:VAL:HA	1.67	0.58
2:D:50:LYS:HA	2:D:60:ASN:HA	1.86	0.58
2:E:186:ILE:O	2:E:190:ALA:HB3	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:V:26:VAL:HA	9:U:27:GLY:HA3	1.83	0.58
1:C:31:THR:O	1:C:43:HIS:N	2.35	0.58
2:E:112:ASN:O	2:E:116:GLU:N	2.34	0.58
6:d:237:VAL:O	6:d:241:LEU:N	2.34	0.58
1:A:175:GLY:O	1:A:179:VAL:N	2.37	0.57
1:B:417:LEU:O	1:B:421:LEU:N	2.37	0.57
2:E:342:THR:O	2:E:346:LEU:N	2.37	0.57
8:g:167:TYR:O	8:g:171:ARG:N	2.34	0.57
2:F:416:GLU:O	2:F:420:THR:N	2.34	0.57
1:B:376:MET:O	1:B:381:GLY:N	2.37	0.57
8:g:259:THR:HA	8:g:264:LEU:HA	1.85	0.57
8:g:125:GLY:O	8:g:164:GLY:N	2.33	0.57
1:A:212:ASN:O	1:A:216:ARG:N	2.38	0.57
1:B:349:LEU:HA	1:B:352:ALA:HB3	1.85	0.57
1:B:465:VAL:O	1:B:469:LYS:N	2.38	0.57
2:F:53:ASP:N	2:F:57:GLN:O	2.37	0.57
2:D:258:GLU:O	2:D:263:VAL:N	2.34	0.57
2:D:376:GLN:O	2:D:380:VAL:N	2.38	0.57
1:A:152:ILE:O	1:A:156:ALA:HB2	2.05	0.57
2:E:52:ARG:HA	2:E:57:GLN:HA	1.87	0.57
1:B:31:THR:O	1:B:43:HIS:N	2.35	0.57
1:B:345:LEU:HA	1:B:359:ASN:H	1.69	0.56
2:F:149:PHE:N	2:F:162:TYR:O	2.33	0.56
1:B:152:ILE:O	1:B:156:ALA:HB2	2.05	0.56
6:d:121:SER:O	6:d:125:LYS:N	2.32	0.56
2:E:260:PHE:O	2:E:266:GLN:N	2.35	0.56
2:F:201:GLY:O	2:F:237:GLY:N	2.38	0.56
2:F:270:LEU:O	2:F:324:ILE:N	2.33	0.56
2:F:460:LEU:O	2:F:464:GLY:N	2.39	0.56
9:M:26:VAL:HA	9:Z:27:GLY:HA3	1.88	0.56
1:C:169:ILE:N	1:C:343:ILE:O	2.39	0.56
8:g:255:PHE:HA	8:g:268:ARG:HA	1.88	0.56
2:D:22:ARG:O	2:D:34:ALA:N	2.36	0.56
9:R:12:ALA:HB2	9:S:11:ILE:HA	1.88	0.56
1:B:374:LYS:O	1:B:378:LYS:CB	2.54	0.56
1:C:348:ASP:O	1:C:352:ALA:N	2.39	0.56
1:A:457:TYR:O	1:A:461:LEU:CB	2.54	0.55
2:D:168:ILE:N	2:D:323:SER:O	2.36	0.55
1:C:212:ASN:O	1:C:216:ARG:CB	2.55	0.55
2:D:405:ILE:O	2:D:409:GLY:N	2.40	0.55
7:e:61:ALA:O	7:e:82:GLU:N	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:148:ILE:HA	2:E:163:ARG:HA	1.88	0.55
1:A:348:ASP:O	1:A:352:ALA:N	2.38	0.55
1:B:483:THR:O	1:B:487:GLU:N	2.39	0.55
1:C:152:ILE:O	1:C:156:ALA:HB2	2.06	0.55
2:E:270:LEU:O	2:E:324:ILE:N	2.39	0.55
1:C:53:LEU:O	1:C:93:GLY:N	2.40	0.55
1:C:54:VAL:HA	1:C:92:THR:H	1.71	0.55
2:D:110:ILE:O	2:D:118:VAL:N	2.39	0.55
2:F:275:ILE:N	2:F:326:ALA:O	2.40	0.55
2:D:279:VAL:O	2:D:283:SER:CB	2.55	0.55
2:E:459:GLN:O	2:E:463:SER:CB	2.54	0.55
1:B:264:LEU:O	1:B:268:ALA:N	2.39	0.54
7:e:48:ILE:HA	7:e:62:LEU:H	1.72	0.54
1:C:484:GLU:O	1:C:488:ALA:CB	2.55	0.54
7:e:32:GLY:H	9:T:42:GLN:HA	1.73	0.54
1:B:251:MET:HA	1:B:312:GLY:HA3	1.89	0.54
1:C:465:VAL:O	1:C:469:LYS:N	2.41	0.54
2:D:168:ILE:HA	2:D:348:ALA:HB3	1.88	0.54
1:B:438:ILE:O	1:B:442:THR:C	2.51	0.54
2:D:272:ILE:O	2:D:326:ALA:N	2.41	0.54
2:E:198:VAL:O	2:E:271:PHE:N	2.40	0.54
9:P:26:VAL:HA	9:O:27:GLY:HA3	1.89	0.54
1:A:349:LEU:O	1:A:354:ILE:N	2.41	0.54
1:B:213:PHE:O	1:B:217:GLY:N	2.38	0.54
1:C:250:PHE:O	1:C:255:ARG:N	2.40	0.54
2:D:46:ALA:O	2:D:94:THR:N	2.33	0.54
8:g:211:GLU:HA	8:g:230:LEU:H	1.72	0.54
8:g:214:TYR:N	8:g:226:VAL:O	2.35	0.54
1:B:63:ILE:N	1:B:75:VAL:O	2.41	0.54
8:g:199:PHE:O	8:g:203:VAL:CB	2.56	0.54
1:B:169:ILE:N	1:B:343:ILE:O	2.41	0.54
2:F:417:ASP:O	2:F:421:VAL:N	2.41	0.54
1:B:474:GLU:O	1:B:478:SER:CB	2.55	0.54
2:E:435:PHE:H	2:E:438:ALA:HB3	1.73	0.54
1:B:139:SER:O	1:B:306:SER:N	2.42	0.53
1:B:373:ILE:O	1:B:377:LYS:N	2.33	0.53
2:F:382:GLU:O	2:F:386:GLU:CB	2.56	0.53
8:g:126:ASP:HA	8:g:163:LYS:H	1.72	0.53
1:C:264:LEU:O	1:C:268:ALA:N	2.37	0.53
2:E:482:GLU:O	2:E:486:LYS:CB	2.56	0.53
1:B:151:LEU:O	1:B:155:ASP:N	2.32	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:111:PHE:H	2:D:235:VAL:HA	1.74	0.53
1:A:103:ALA:O	1:A:123:THR:N	2.41	0.53
1:B:51:GLY:H	1:B:64:ALA:HB3	1.73	0.53
1:B:348:ASP:O	1:B:352:ALA:N	2.37	0.53
2:D:356:LEU:O	2:D:360:GLY:N	2.42	0.53
7:e:3:LEU:N	7:e:19:VAL:O	2.41	0.53
1:C:390:PHE:O	1:C:394:GLU:CB	2.57	0.53
2:D:45:ASN:H	2:D:65:VAL:H	1.57	0.53
6:d:139:GLN:O	6:d:143:ALA:N	2.36	0.53
1:A:290:ASP:HA	1:A:293:TYR:H	1.74	0.53
9:M:11:ILE:HA	9:Z:12:ALA:HB2	1.91	0.53
1:B:344:PHE:H	1:B:363:SER:HA	1.74	0.53
2:D:64:GLU:N	2:D:77:VAL:O	2.41	0.53
5:a:55:ALA:O	5:a:59:ARG:N	2.38	0.53
1:C:152:ILE:O	1:C:156:ALA:CB	2.56	0.52
2:D:49:VAL:O	2:D:61:VAL:N	2.39	0.52
2:D:272:ILE:N	2:D:324:ILE:O	2.42	0.52
1:B:33:LEU:H	1:B:42:ILE:HA	1.73	0.52
2:D:204:GLU:H	2:D:238:GLN:HA	1.74	0.52
2:F:302:LEU:O	2:F:306:MET:CB	2.58	0.52
2:F:451:LEU:O	2:F:455:ILE:CB	2.57	0.52
6:d:108:GLU:O	6:d:112:TYR:N	2.33	0.52
6:d:113:TYR:HA	6:d:116:ALA:HB3	1.92	0.52
1:B:54:VAL:O	1:B:62:GLY:N	2.42	0.52
6:d:180:VAL:O	6:d:212:VAL:N	2.43	0.52
2:E:259:TYR:O	2:E:264:ASN:N	2.33	0.52
1:B:27:VAL:O	1:B:48:VAL:N	2.39	0.52
1:C:347:ALA:O	1:C:351:ASN:CB	2.57	0.52
2:F:223:ASN:H	2:F:230:SER:HA	1.74	0.52
6:d:225:TYR:O	6:d:231:LYS:N	2.38	0.52
1:A:31:THR:O	1:A:43:HIS:N	2.43	0.52
1:C:418:ARG:O	1:C:422:LYS:N	2.37	0.52
2:F:428:GLU:O	2:F:432:SER:N	2.42	0.52
8:g:228:HIS:HA	8:g:241:ASP:HA	1.92	0.52
2:D:142:LEU:HA	2:D:316:THR:HA	1.92	0.51
8:g:131:GLY:HA3	8:g:318:ALA:HB1	1.92	0.51
2:F:34:ALA:HA	2:F:73:ARG:HA	1.91	0.51
1:C:248:GLU:O	1:C:253:ARG:N	2.42	0.51
1:A:54:VAL:O	1:A:62:GLY:N	2.41	0.51
1:B:10:SER:H	1:B:13:ILE:H	1.58	0.51
2:F:294:SER:H	2:F:299:GLN:HA	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:g:132:GLY:O	8:g:136:MET:N	2.37	0.51
2:D:63:CYS:HA	2:D:78:ALA:HA	1.93	0.51
2:D:329:VAL:O	2:D:331:ALA:N	2.43	0.51
2:E:46:ALA:H	2:E:96:ALA:H	1.59	0.51
9:W:33:GLY:CA	9:V:31:ALA:HA	2.41	0.51
1:A:250:PHE:O	1:A:254:GLU:N	2.41	0.51
1:A:196:TYR:O	1:A:225:VAL:N	2.43	0.51
1:C:171:ASP:O	1:C:173:GLN:N	2.43	0.51
1:C:199:ILE:N	1:C:262:ASP:O	2.42	0.51
2:F:174:ALA:HA	2:F:178:LYS:H	1.76	0.51
2:F:307:GLY:O	2:F:311:GLU:N	2.44	0.51
1:A:54:VAL:N	1:A:62:GLY:O	2.40	0.51
1:B:11:LYS:O	1:B:15:GLU:N	2.40	0.51
1:C:11:LYS:O	1:C:15:GLU:CB	2.59	0.51
2:F:211:ASP:O	2:F:215:GLU:CB	2.59	0.51
1:A:255:ARG:O	1:A:313:SER:N	2.40	0.50
1:B:147:LEU:N	1:B:160:VAL:O	2.42	0.50
2:E:276:PHE:H	2:E:327:VAL:HA	1.77	0.50
2:F:44:TYR:N	2:F:65:VAL:O	2.43	0.50
2:F:201:GLY:N	2:F:235:VAL:O	2.44	0.50
2:D:480:ILE:O	2:D:484:THR:CB	2.60	0.50
2:D:53:ASP:N	2:D:57:GLN:O	2.45	0.50
1:C:376:MET:O	1:C:380:ALA:HB3	2.10	0.50
2:E:205:ARG:O	2:E:208:GLU:N	2.40	0.50
2:F:258:GLU:O	2:F:263:VAL:N	2.30	0.50
8:g:210:VAL:O	8:g:231:LEU:N	2.38	0.50
8:g:240:CYS:HA	8:g:246:CYS:HA	1.94	0.50
1:C:31:THR:N	1:C:43:HIS:O	2.45	0.50
1:A:10:SER:O	1:A:14:ARG:N	2.34	0.50
1:A:33:LEU:H	1:A:42:ILE:HA	1.76	0.50
1:A:171:ASP:O	1:A:173:GLN:N	2.44	0.50
5:a:182:LYS:O	5:a:186:LEU:CB	2.59	0.50
1:A:404:ASP:O	1:A:408:GLN:N	2.39	0.49
1:B:55:GLU:O	1:B:90:LYS:N	2.45	0.49
2:D:268:VAL:O	2:D:322:THR:N	2.42	0.49
2:E:64:GLU:N	2:E:77:VAL:O	2.44	0.49
8:g:122:VAL:N	8:g:158:ILE:O	2.44	0.49
1:A:377:LYS:HA	1:A:380:ALA:HB3	1.95	0.49
9:U:29:GLY:HA3	9:T:27:GLY:C	2.37	0.49
1:C:474:GLU:O	1:C:478:SER:CB	2.60	0.49
3:I:168:THR:HA	3:I:171:ALA:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:221:VAL:O	2:D:232:VAL:N	2.45	0.49
2:E:155:VAL:O	2:E:159:LEU:CB	2.60	0.49
7:e:4:ASN:HA	7:e:18:GLU:HA	1.95	0.49
1:A:296:SER:O	1:A:300:GLU:CB	2.60	0.49
1:C:283:GLY:O	1:C:287:TYR:N	2.46	0.49
7:e:4:ASN:N	7:e:72:ASN:O	2.38	0.49
1:A:108:VAL:O	1:A:116:ILE:N	2.26	0.49
1:B:404:ASP:O	1:B:408:GLN:N	2.35	0.49
1:C:40:ALA:O	1:C:74:VAL:N	2.43	0.49
6:d:181:THR:O	6:d:222:THR:N	2.46	0.49
8:g:234:SER:C	8:g:237:GLY:H	2.21	0.49
1:A:33:LEU:N	1:A:41:ARG:O	2.46	0.49
1:A:359:ASN:O	1:A:363:SER:N	2.31	0.49
1:C:33:LEU:H	1:C:42:ILE:HA	1.77	0.49
2:D:22:ARG:N	2:D:34:ALA:O	2.45	0.49
2:E:31:LEU:N	2:E:76:ALA:O	2.39	0.49
6:d:103:ILE:O	6:d:107:SER:N	2.46	0.49
1:B:98:ILE:O	1:B:128:ARG:N	2.46	0.48
1:B:284:ARG:N	1:B:287:TYR:O	2.44	0.48
2:D:47:LEU:HA	2:D:93:ASP:HA	1.95	0.48
2:F:268:VAL:O	2:F:322:THR:N	2.46	0.48
1:C:346:SER:H	1:C:358:ILE:HA	1.78	0.48
2:E:272:ILE:N	2:E:324:ILE:O	2.46	0.48
9:O:26:VAL:HA	9:N:27:GLY:HA3	1.95	0.48
1:A:152:ILE:O	1:A:156:ALA:CB	2.60	0.48
1:A:168:ILE:O	1:A:320:VAL:N	2.46	0.48
1:A:274:MET:O	1:A:278:LEU:N	2.42	0.48
1:A:42:ILE:N	1:A:72:VAL:O	2.46	0.48
1:B:232:PRO:O	1:B:236:GLN:N	2.39	0.48
8:g:227:ILE:O	8:g:242:ILE:N	2.44	0.48
1:B:196:TYR:O	1:B:225:VAL:N	2.46	0.48
2:D:315:SER:HA	2:D:320:SER:HA	1.96	0.48
6:d:179:VAL:O	6:d:224:ARG:N	2.47	0.48
1:C:63:ILE:O	1:C:75:VAL:N	2.46	0.48
2:F:214:MET:O	2:F:218:GLU:CB	2.62	0.48
5:a:146:VAL:O	5:a:150:TYR:CB	2.62	0.48
1:B:500:ARG:O	1:B:504:GLN:N	2.44	0.48
2:E:206:THR:HA	2:E:209:GLY:H	1.78	0.48
2:F:70:GLY:H	2:F:74:VAL:HA	1.78	0.48
2:F:112:ASN:N	2:F:116:GLU:O	2.35	0.48
8:g:188:ALA:HA	8:g:191:ALA:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:ALA:O	1:A:272:ARG:CB	2.61	0.47
9:Y:26:VAL:HA	9:X:27:GLY:HA3	1.96	0.47
1:B:494:ILE:O	1:B:498:MET:CB	2.62	0.47
1:C:193:ILE:O	1:C:258:LEU:N	2.47	0.47
1:C:342:GLN:O	1:C:364:VAL:N	2.47	0.47
4:J:146:ALA:O	4:J:150:ALA:HB3	2.14	0.47
2:D:295:ALA:O	2:D:297:GLY:N	2.37	0.47
2:F:155:VAL:O	2:F:159:LEU:N	2.47	0.47
6:d:181:THR:N	6:d:222:THR:O	2.46	0.47
6:d:182:SER:O	6:d:214:ASP:N	2.47	0.47
2:E:48:ILE:N	2:E:92:ILE:O	2.47	0.47
2:E:168:ILE:O	2:E:325:GLN:N	2.47	0.47
2:E:248:ARG:O	2:E:252:THR:N	2.44	0.47
1:A:194:CYS:HA	1:A:258:LEU:H	1.80	0.47
1:A:218:ALA:O	1:A:222:THR:N	2.47	0.47
2:E:315:SER:HA	2:E:321:ILE:H	1.80	0.47
1:C:261:TYR:O	1:C:319:ILE:N	2.39	0.47
8:g:200:SER:O	8:g:204:SER:N	2.38	0.47
8:g:215:THR:HA	8:g:226:VAL:H	1.78	0.47
1:B:261:TYR:N	1:B:317:LEU:O	2.41	0.47
1:C:110:ASN:H	1:C:116:ILE:N	2.11	0.47
1:C:213:PHE:O	1:C:217:GLY:N	2.48	0.47
1:C:233:ALA:HB1	1:C:270:ALA:HB1	1.97	0.47
1:C:335:VAL:O	1:C:339:THR:N	2.47	0.47
2:E:245:ALA:O	2:E:249:VAL:N	2.29	0.47
9:Q:11:ILE:HA	9:P:12:ALA:HB2	1.97	0.47
1:A:450:GLU:O	1:A:454:VAL:N	2.40	0.47
2:D:450:GLY:O	2:D:454:THR:N	2.39	0.47
1:A:445:TYR:O	1:A:449:LEU:N	2.48	0.47
1:B:56:PHE:N	1:B:60:THR:O	2.39	0.46
1:C:374:LYS:O	1:C:378:LYS:CB	2.63	0.46
1:A:55:GLU:HA	1:A:61:ILE:HA	1.98	0.46
1:C:247:ALA:O	1:C:251:MET:CB	2.63	0.46
2:E:198:VAL:N	2:E:269:LEU:O	2.47	0.46
2:E:223:ASN:H	2:E:230:SER:HA	1.78	0.46
8:g:121:MET:N	8:g:211:GLU:O	2.37	0.46
1:A:430:THR:O	1:A:434:GLN:N	2.40	0.46
2:D:245:ALA:O	2:D:249:VAL:N	2.48	0.46
2:D:259:TYR:O	2:D:264:ASN:N	2.48	0.46
2:E:112:ASN:N	2:E:116:GLU:O	2.48	0.46
2:F:470:PRO:O	2:F:474:PHE:N	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:464:TYR:O	1:A:468:ASN:CB	2.64	0.46
1:B:54:VAL:N	1:B:62:GLY:O	2.45	0.46
6:d:223:ILE:O	6:d:233:VAL:N	2.46	0.46
1:A:374:LYS:O	1:A:378:LYS:CB	2.64	0.46
2:F:353:SER:N	2:F:364:ALA:O	2.48	0.46
8:g:120:LEU:N	8:g:157:ILE:HA	2.31	0.46
1:C:333:THR:O	1:C:337:SER:N	2.48	0.46
1:A:145:GLU:O	1:A:162:ARG:N	2.49	0.46
9:R:5:ILE:HA	9:S:7:ALA:HB2	1.97	0.46
2:E:35:PHE:N	2:E:72:ASN:O	2.42	0.46
1:B:376:MET:HA	1:B:380:ALA:HB3	1.98	0.46
1:C:386:GLU:O	1:C:390:PHE:CB	2.63	0.46
1:A:167:LEU:O	1:A:343:ILE:N	2.35	0.45
2:E:170:LEU:HA	2:E:350:THR:H	1.82	0.45
6:d:198:VAL:O	6:d:203:GLY:N	2.50	0.45
7:e:42:THR:O	7:e:67:ALA:N	2.49	0.45
1:A:98:ILE:O	1:A:128:ARG:N	2.36	0.45
2:E:405:ILE:O	2:E:409:GLY:N	2.43	0.45
1:A:101:SER:H	1:A:124:ALA:HB1	1.81	0.45
5:a:68:GLY:O	5:a:72:PHE:N	2.43	0.45
8:g:334:LYS:O	8:g:338:SER:CB	2.65	0.45
2:D:171:PHE:N	2:D:350:THR:O	2.49	0.45
7:e:6:CYS:O	7:e:76:ILE:N	2.50	0.45
1:C:50:ALA:H	2:E:85:LEU:N	2.14	0.45
2:E:414:SER:O	2:E:418:ARG:N	2.49	0.45
1:C:136:GLY:C	1:C:139:SER:H	2.25	0.45
1:C:248:GLU:HA	1:C:252:TYR:H	1.82	0.45
2:F:458:PHE:O	2:F:462:LEU:CB	2.65	0.45
1:A:168:ILE:N	1:A:318:PRO:O	2.44	0.45
2:F:50:LYS:H	2:F:92:ILE:H	1.63	0.45
2:F:272:ILE:N	2:F:324:ILE:O	2.30	0.45
1:B:152:ILE:O	1:B:156:ALA:CB	2.65	0.45
2:D:258:GLU:O	2:D:262:ASP:CB	2.65	0.45
2:F:419:LEU:O	2:F:423:ARG:CB	2.65	0.45
1:A:312:GLY:O	1:A:314:MET:N	2.50	0.44
1:C:342:GLN:N	1:C:364:VAL:O	2.32	0.44
2:D:70:GLY:N	2:D:73:ARG:O	2.51	0.44
1:B:31:THR:N	1:B:43:HIS:O	2.46	0.44
2:D:21:GLY:HA2	2:D:35:PHE:HA	1.99	0.44
2:E:50:LYS:N	2:E:91:VAL:HA	2.33	0.44
2:E:268:VAL:O	2:E:322:THR:N	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:374:MET:O	2:E:376:GLN:N	2.51	0.44
1:B:110:ASN:N	1:B:114:LYS:O	2.50	0.44
2:F:401:LEU:O	2:F:405:ILE:CB	2.65	0.44
7:e:39:PRO:HA	7:e:70:GLY:HA2	1.99	0.44
8:g:192:GLN:O	8:g:196:ASP:CB	2.65	0.44
1:A:500:ARG:O	1:A:504:GLN:N	2.51	0.44
2:E:34:ALA:HA	2:E:73:ARG:HA	1.99	0.44
2:F:423:ARG:O	2:F:427:ILE:CB	2.65	0.44
7:e:50:ARG:HA	7:e:59:THR:HA	2.00	0.44
1:A:53:LEU:O	1:A:93:GLY:N	2.36	0.44
2:E:168:ILE:N	2:E:323:SER:O	2.42	0.44
5:a:226:ILE:O	5:a:230:ILE:CB	2.66	0.44
2:E:479:ASN:O	2:E:483:ALA:N	2.51	0.43
2:F:64:GLU:N	2:F:77:VAL:O	2.35	0.43
1:B:126:GLU:O	1:B:128:ARG:N	2.51	0.43
3:I:47:GLY:O	3:I:51:ASP:CB	2.66	0.43
1:A:175:GLY:HA2	1:A:178:ALA:HB3	2.00	0.43
1:A:275:SER:O	1:A:279:ARG:N	2.50	0.43
1:C:440:THR:O	1:C:444:GLY:N	2.42	0.43
2:F:64:GLU:O	2:F:77:VAL:N	2.50	0.43
2:F:270:LEU:H	2:F:323:SER:HA	1.82	0.43
6:d:145:PHE:O	6:d:149:LEU:CB	2.67	0.43
1:B:342:GLN:O	1:B:364:VAL:N	2.50	0.43
1:C:257:THR:N	1:C:313:SER:O	2.51	0.43
2:F:67:GLN:N	2:F:75:ARG:O	2.41	0.43
2:F:216:MET:O	2:F:220:GLY:N	2.51	0.43
8:g:161:GLY:O	8:g:165:ASN:N	2.50	0.43
1:A:66:ASN:O	1:A:73:GLY:N	2.51	0.43
1:B:99:PRO:HA	1:B:127:SER:HA	2.00	0.43
2:D:198:VAL:O	2:D:271:PHE:N	2.52	0.43
1:B:203:ALA:O	1:B:207:ALA:HB2	2.18	0.43
2:F:460:LEU:O	2:F:465:GLU:N	2.39	0.43
9:U:33:GLY:CA	9:T:31:ALA:HA	2.49	0.43
1:C:405:LYS:HA	1:C:409:ASN:H	1.84	0.43
2:D:112:ASN:O	2:D:116:GLU:N	2.52	0.43
8:g:253:GLU:HA	8:g:270:MET:HA	2.01	0.43
3:I:161:ASN:O	3:I:165:HIS:CB	2.67	0.42
1:A:109:ILE:HA	1:A:115:PRO:HA	2.01	0.42
1:B:55:GLU:N	1:B:90:LYS:O	2.52	0.42
1:B:100:VAL:N	1:B:126:GLU:O	2.51	0.42
1:C:168:ILE:O	1:C:320:VAL:N	2.43	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:457:TYR:O	1:C:461:LEU:CB	2.67	0.42
2:E:419:LEU:O	2:E:423:ARG:CB	2.66	0.42
2:F:459:GLN:O	2:F:463:SER:N	2.49	0.42
7:e:49:LEU:N	7:e:60:LEU:O	2.32	0.42
9:N:26:VAL:HA	9:M:27:GLY:HA3	2.01	0.42
1:A:146:PRO:HA	1:A:161:GLY:HA2	2.00	0.42
2:E:138:ALA:HB3	2:E:141:GLN:H	1.83	0.42
2:F:273:ASP:HA	2:F:274:ASN:HA	1.62	0.42
1:C:490:LEU:O	1:C:494:ILE:CB	2.68	0.42
3:I:81:ALA:HB1	4:J:144:ALA:HB2	2.01	0.42
1:A:335:VAL:O	1:A:339:THR:N	2.49	0.42
2:D:49:VAL:N	2:D:61:VAL:O	2.39	0.42
8:g:260:LYS:O	8:g:262:GLY:N	2.53	0.42
8:g:148:LEU:O	8:g:152:GLY:N	2.36	0.42
2:D:439:GLU:HA	2:D:444:SER:H	1.83	0.42
2:E:171:PHE:H	2:E:350:THR:N	2.18	0.42
1:B:430:THR:O	1:B:434:GLN:N	2.41	0.42
1:C:9:ILE:O	1:C:13:ILE:N	2.48	0.42
1:C:350:PHE:C	1:C:353:GLY:H	2.27	0.42
2:D:461:ILE:C	2:D:464:GLY:H	2.27	0.42
2:F:274:ASN:HA	2:F:326:ALA:HB3	2.01	0.42
2:F:455:ILE:O	2:F:459:GLN:CB	2.67	0.42
1:B:438:ILE:O	1:B:442:THR:CB	2.68	0.42
2:F:198:VAL:N	2:F:269:LEU:O	2.53	0.42
2:F:294:SER:N	2:F:298:TYR:O	2.53	0.42
2:E:201:GLY:O	2:E:237:GLY:N	2.52	0.41
4:J:147:VAL:O	4:J:151:ALA:HB2	2.20	0.41
2:D:203:GLY:N	2:D:237:GLY:O	2.41	0.41
5:a:26:PHE:HA	5:a:125:GLY:HA3	2.02	0.41
7:e:108:GLY:O	7:e:112:LYS:N	2.32	0.41
8:g:295:LEU:O	8:g:299:TYR:N	2.51	0.41
2:F:199:PHE:O	2:F:235:VAL:N	2.39	0.41
2:F:435:PHE:O	2:F:439:GLU:N	2.51	0.41
2:E:404:ILE:O	2:E:408:LEU:N	2.40	0.41
2:F:301:THR:O	2:F:305:GLU:N	2.31	0.41
1:B:438:ILE:O	1:B:443:ASN:N	2.53	0.41
2:D:352:LEU:HA	2:D:365:VAL:HA	2.02	0.41
2:E:216:MET:C	2:E:222:ILE:H	2.29	0.41
5:a:28:TRP:HA	5:a:36:HIS:HA	2.01	0.41
1:A:40:ALA:O	1:A:74:VAL:N	2.52	0.41
1:A:461:LEU:O	1:A:465:VAL:CB	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:49:VAL:N	2:F:61:VAL:O	2.34	0.41
2:F:70:GLY:C	2:F:73:ARG:H	2.28	0.41
9:P:11:ILE:HA	9:O:12:ALA:HB2	2.02	0.41
1:A:100:VAL:N	1:A:126:GLU:O	2.54	0.41
4:J:147:VAL:O	4:J:151:ALA:CB	2.69	0.41
8:g:95:ASN:O	8:g:99:GLN:CB	2.68	0.41
8:g:188:ALA:O	8:g:192:GLN:CB	2.68	0.41
1:B:193:ILE:O	1:B:258:LEU:N	2.54	0.41
1:B:438:ILE:O	1:B:442:THR:CA	2.69	0.41
2:D:377:PRO:O	2:D:382:GLU:N	2.54	0.41
2:F:22:ARG:O	2:F:34:ALA:N	2.49	0.41
8:g:239:ILE:O	8:g:247:VAL:N	2.37	0.41
9:W:14:GLY:HA3	9:V:12:ALA:HB1	2.02	0.41
1:A:41:ARG:HA	1:A:73:GLY:HA2	2.03	0.41
2:E:273:ASP:HA	2:E:274:ASN:HA	1.84	0.41
1:C:168:ILE:C	1:C:320:VAL:H	2.26	0.40
9:R:12:ALA:HB1	9:S:14:GLY:HA3	2.02	0.40
2:F:20:LEU:HA	2:F:92:ILE:HA	2.03	0.40
2:F:221:VAL:O	2:F:231:LYS:N	2.54	0.40
8:g:137:LEU:O	8:g:141:ALA:HB2	2.22	0.40
1:B:376:MET:O	1:B:380:ALA:HB3	2.21	0.40
1:C:343:ILE:HA	1:C:363:SER:HA	2.03	0.40
2:E:154:LYS:O	2:E:159:LEU:N	2.48	0.40
9:Z:26:VAL:HA	9:Y:27:GLY:HA3	2.03	0.40
1:B:100:VAL:HA	1:B:124:ALA:HB1	2.02	0.40
1:B:476:ILE:O	1:B:480:LYS:N	2.54	0.40
2:D:202:VAL:HA	2:D:237:GLY:HA3	2.04	0.40
2:F:341:THR:O	2:F:345:HIS:CB	2.70	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	A	493/507 (97%)	411 (83%)	82 (17%)	0	100	100
1	B	496/507 (98%)	404 (82%)	92 (18%)	0	100	100
1	C	499/507 (98%)	400 (80%)	99 (20%)	0	100	100
2	D	478/498 (96%)	400 (84%)	76 (16%)	2 (0%)	30	67
2	E	476/498 (96%)	379 (80%)	95 (20%)	2 (0%)	30	67
2	F	477/498 (96%)	390 (82%)	87 (18%)	0	100	100
3	I	146/184 (79%)	144 (99%)	2 (1%)	0	100	100
4	J	129/222 (58%)	122 (95%)	7 (5%)	0	100	100
5	a	221/247 (90%)	185 (84%)	35 (16%)	1 (0%)	24	63
6	d	175/257 (68%)	149 (85%)	26 (15%)	0	100	100
7	e	127/134 (95%)	91 (72%)	36 (28%)	0	100	100
8	g	314/364 (86%)	260 (83%)	53 (17%)	1 (0%)	36	72
9	M	77/81 (95%)	70 (91%)	7 (9%)	0	100	100
9	N	77/81 (95%)	70 (91%)	7 (9%)	0	100	100
9	O	77/81 (95%)	70 (91%)	7 (9%)	0	100	100
9	P	77/81 (95%)	70 (91%)	7 (9%)	0	100	100
9	Q	77/81 (95%)	70 (91%)	7 (9%)	0	100	100
9	R	77/81 (95%)	70 (91%)	7 (9%)	0	100	100
9	S	77/81 (95%)	70 (91%)	7 (9%)	0	100	100
9	T	77/81 (95%)	70 (91%)	7 (9%)	0	100	100
9	U	77/81 (95%)	70 (91%)	7 (9%)	0	100	100
9	V	77/81 (95%)	70 (91%)	7 (9%)	0	100	100
9	W	77/81 (95%)	70 (91%)	7 (9%)	0	100	100
9	X	77/81 (95%)	70 (91%)	7 (9%)	0	100	100
9	Y	77/81 (95%)	70 (91%)	7 (9%)	0	100	100
9	Z	77/81 (95%)	70 (91%)	7 (9%)	0	100	100
All	All	5109/5557 (92%)	4315 (84%)	788 (15%)	6 (0%)	49	83

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	296	VAL
8	g	261	GLU
2	D	295	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	a	161	PHE
2	E	367	PRO
2	E	300	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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
8	g	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	g	230:LEU	C	231:LEU	N	1.18

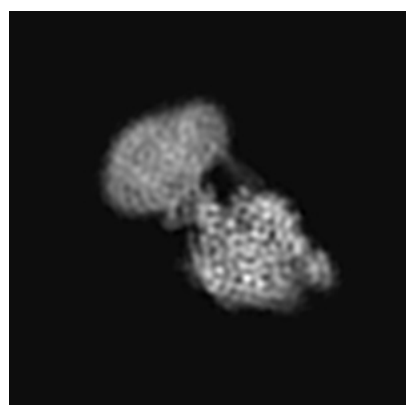
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21235. These allow visual inspection of the internal detail of the map and identification of artifacts.

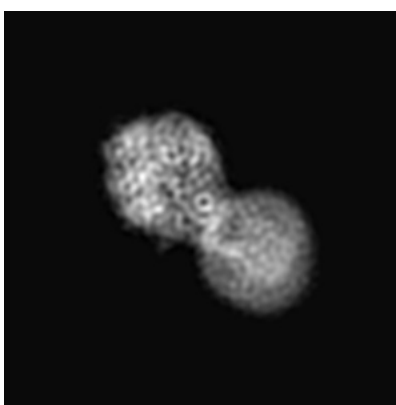
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

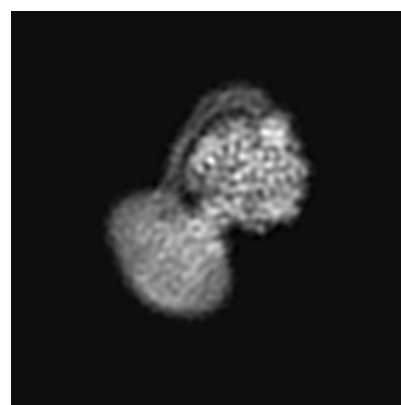
6.1.1 Primary map



X



Y



Z

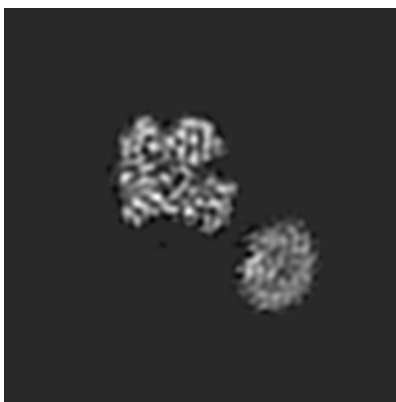
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

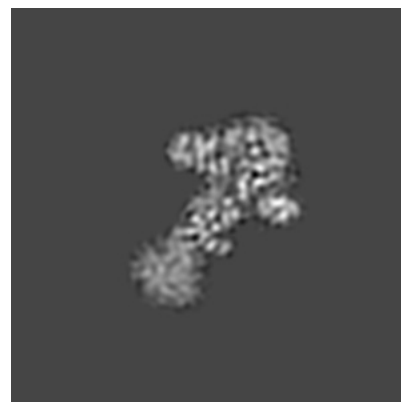
6.2.1 Primary map



X Index: 144



Y Index: 144

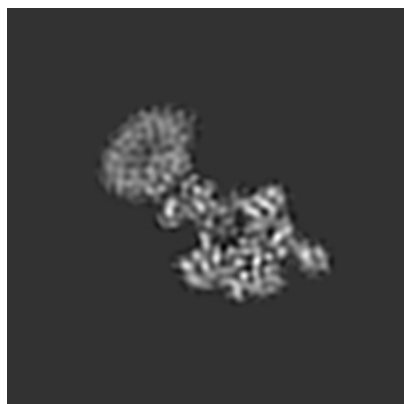


Z Index: 144

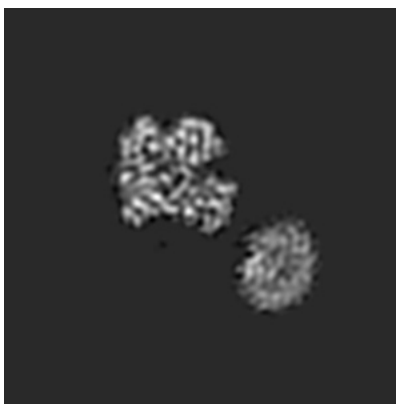
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

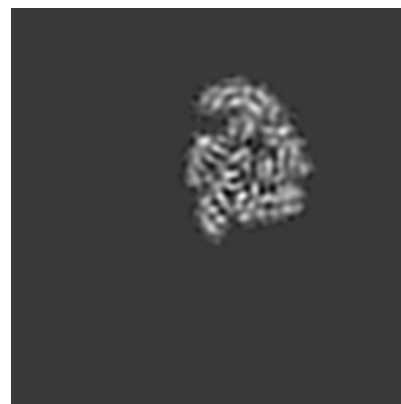
6.3.1 Primary map



X Index: 144



Y Index: 144

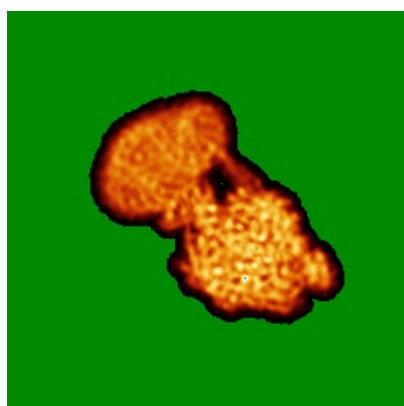


Z Index: 101

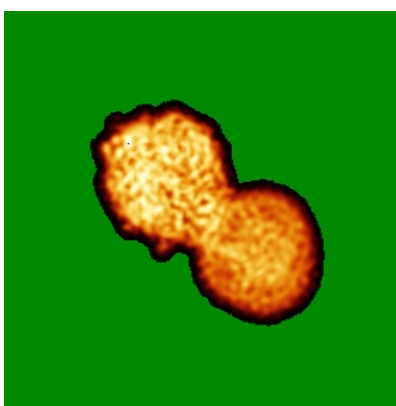
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

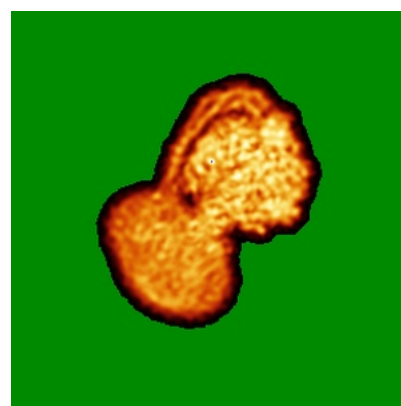
6.4.1 Primary map



X



Y

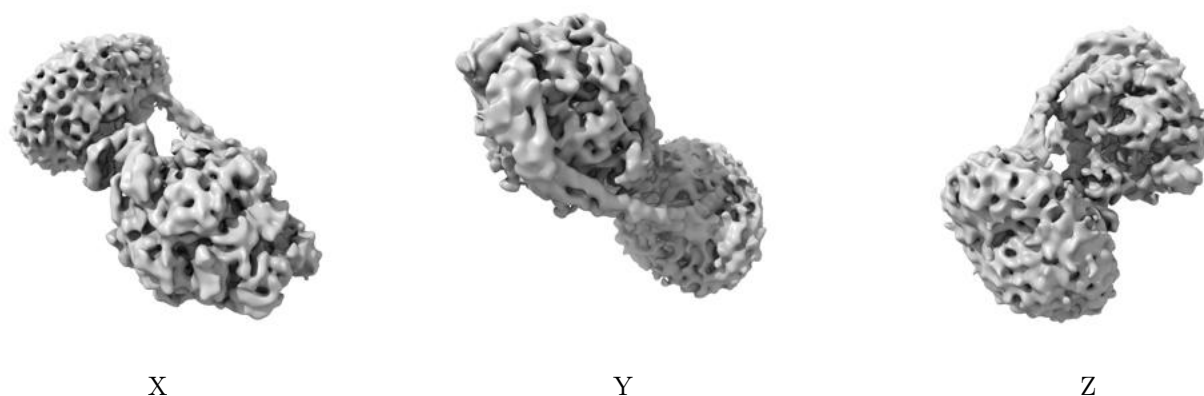


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.00948. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

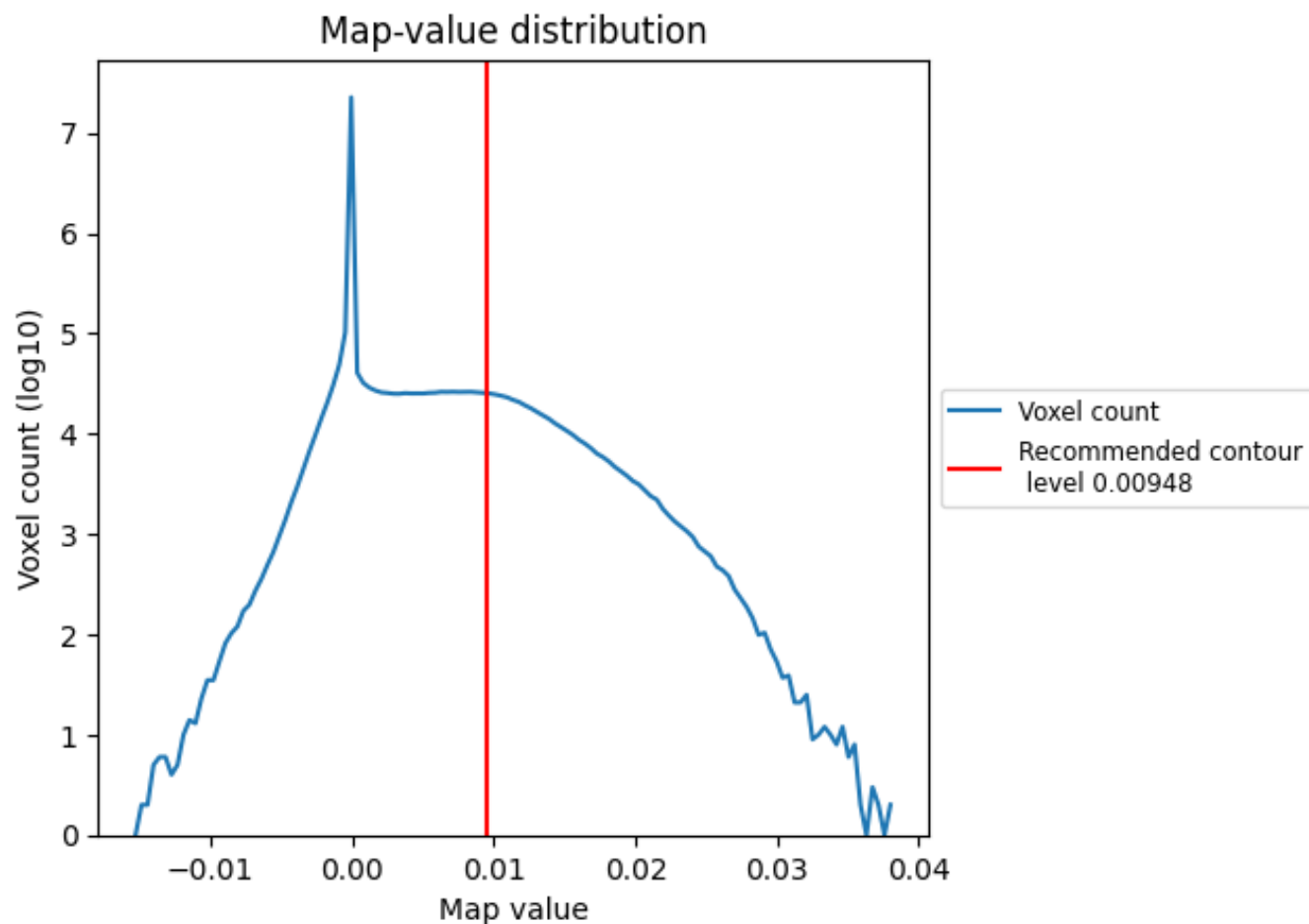
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

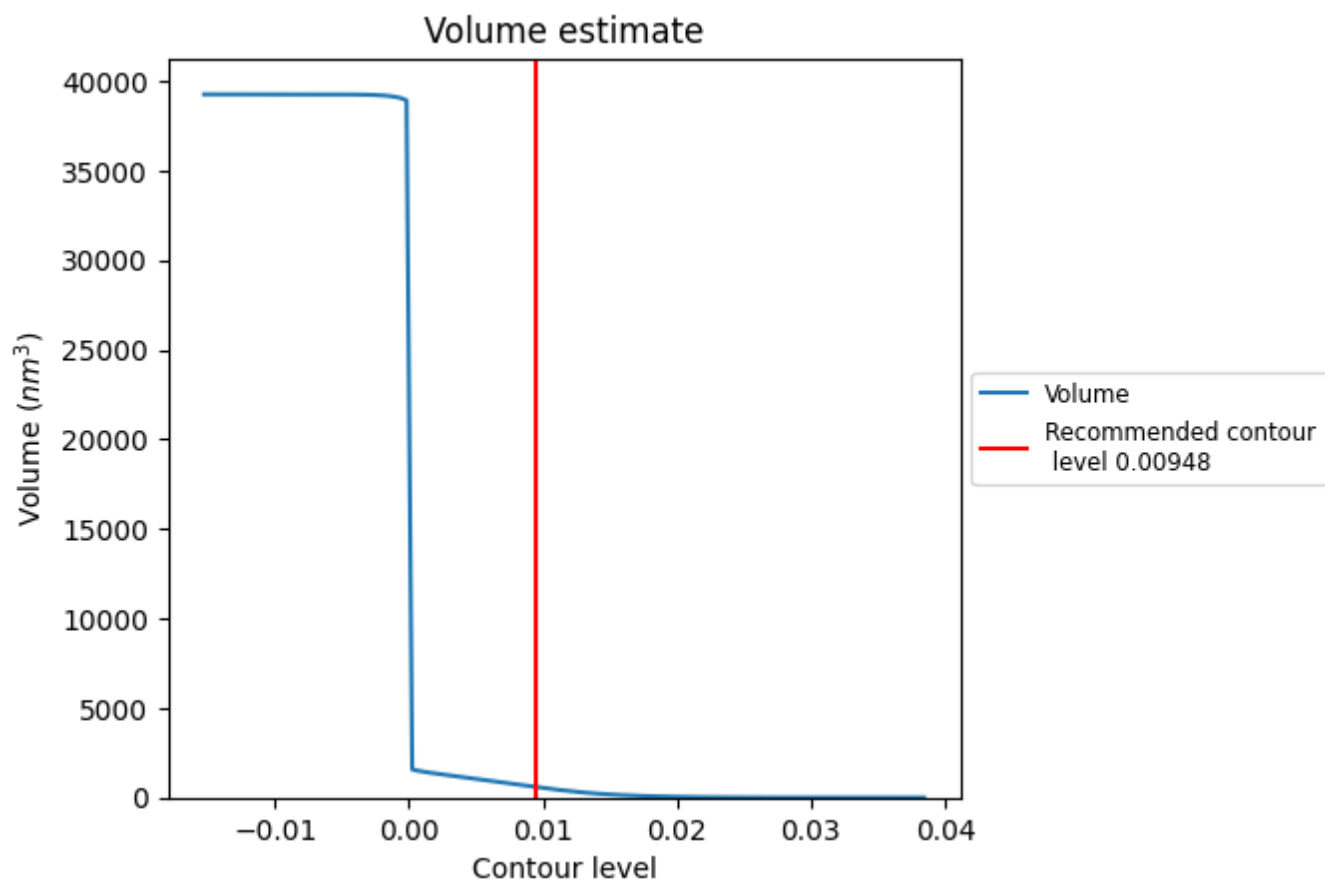
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

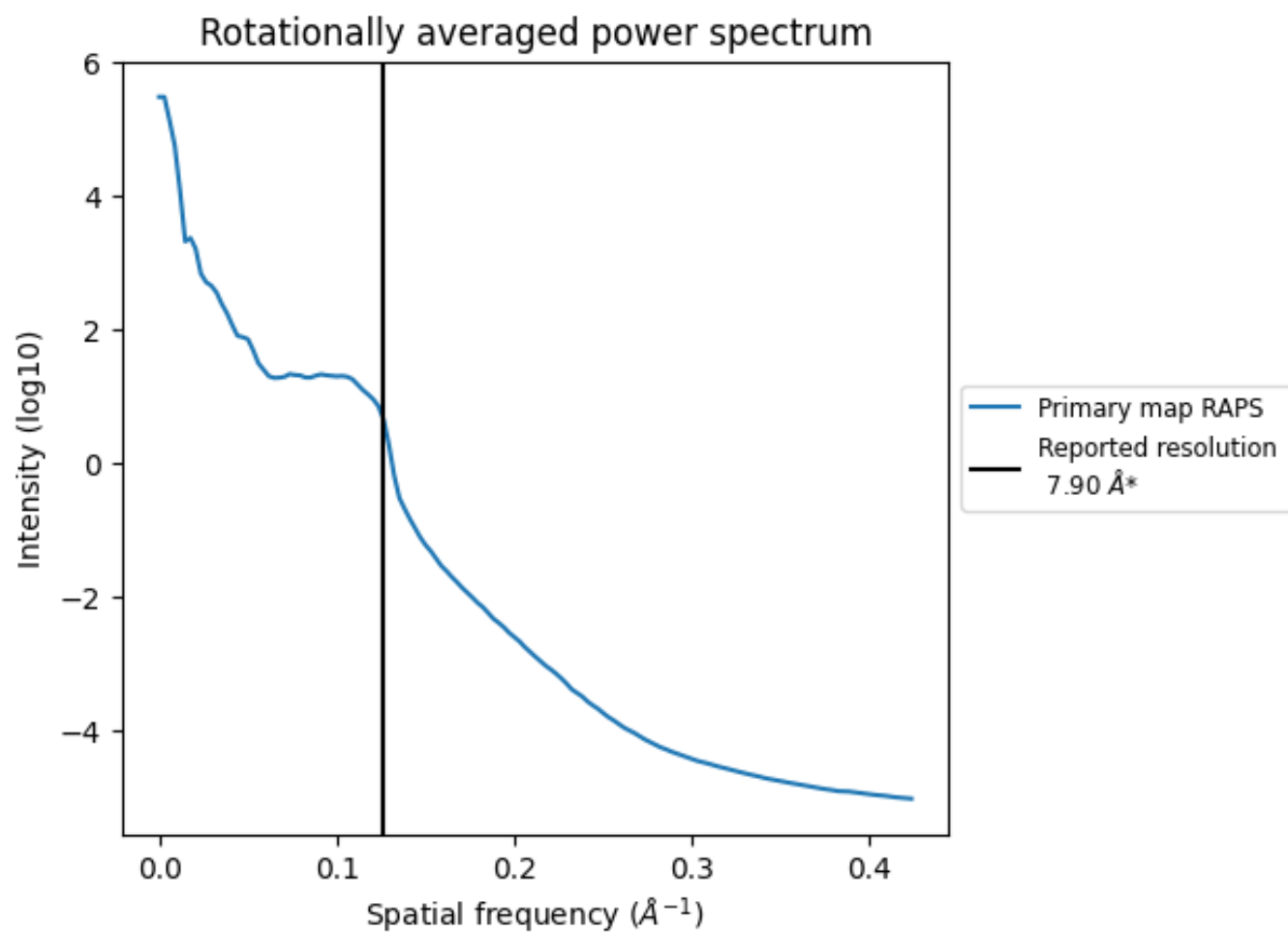
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 591 nm³; this corresponds to an approximate mass of 534 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 ⓘ

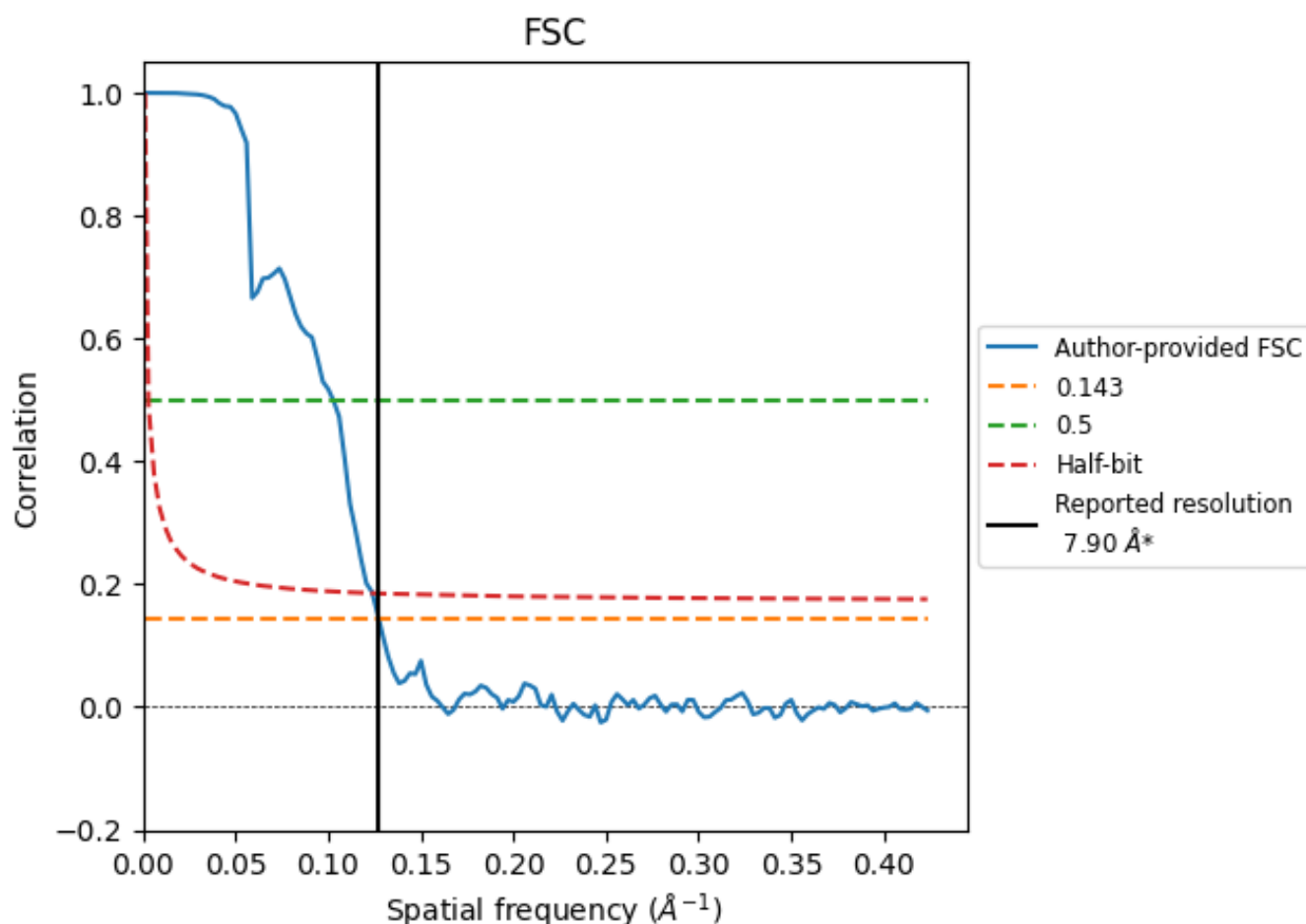


*Reported resolution corresponds to spatial frequency of 0.127 Å⁻¹

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 0.127 Å⁻¹

8.2 Resolution estimates [i](#)

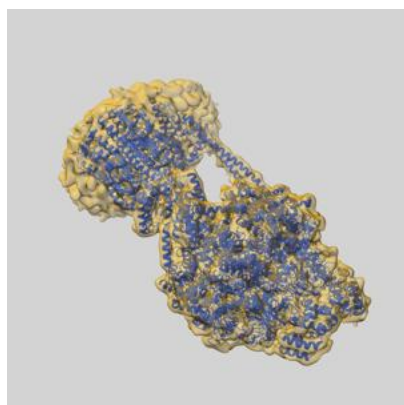
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	7.90	-	-
Author-provided FSC curve	7.85	9.74	8.08
Unmasked-calculated*	-	-	-

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

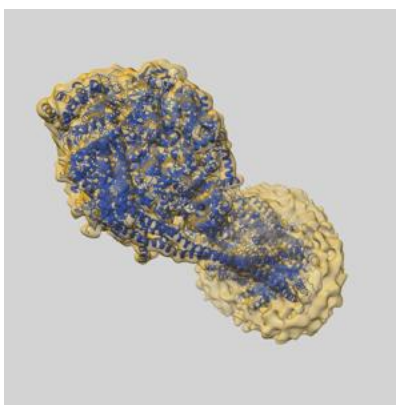
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-21235 and PDB model 6VM1. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

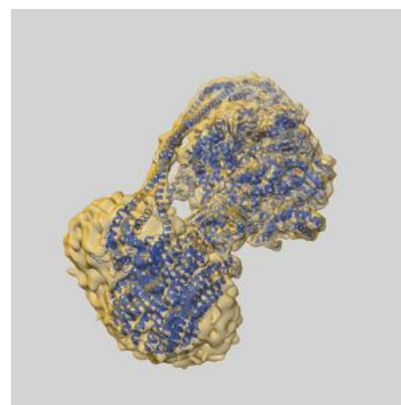
9.1 Map-model overlay [i](#)



X



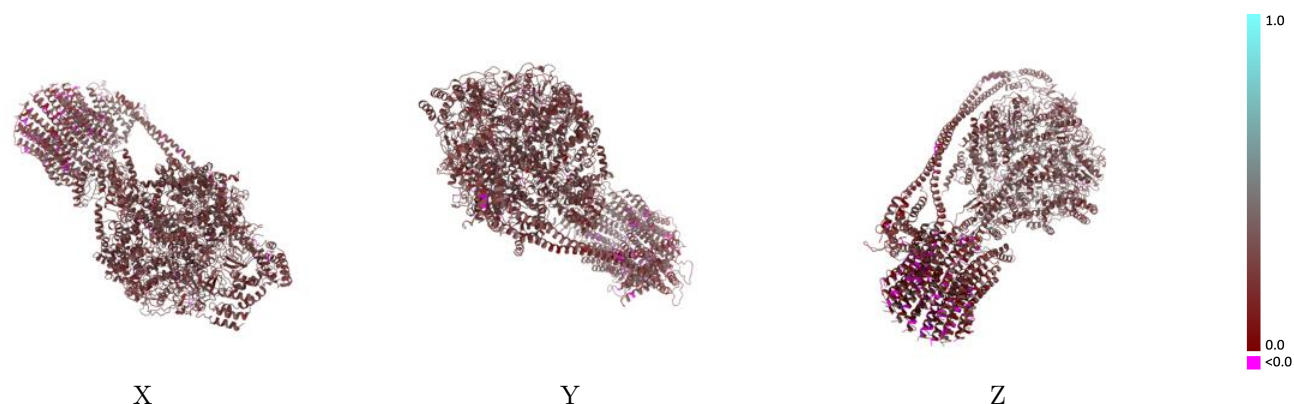
Y



Z

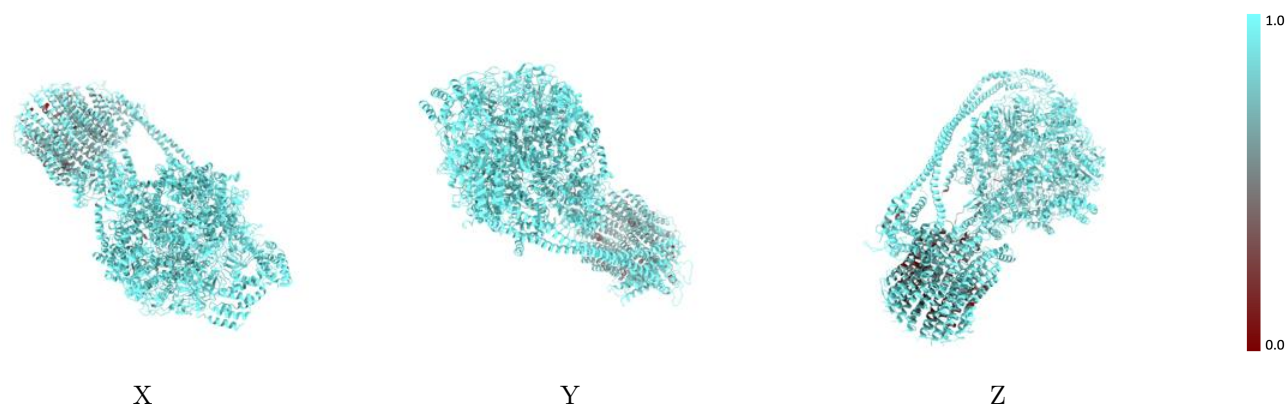
The images above show the 3D surface view of the map at the recommended contour level 0.00948 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



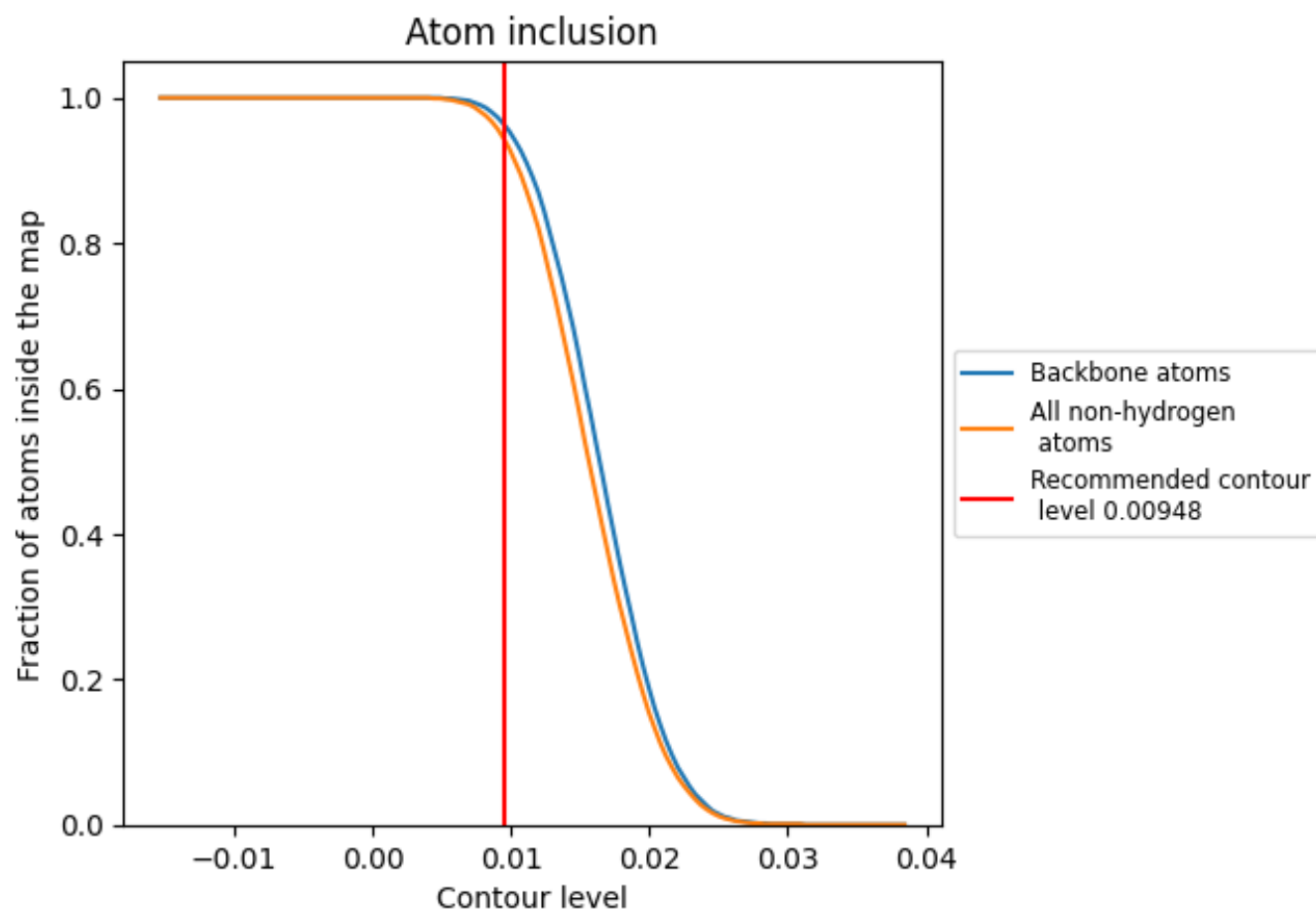
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.00948).

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 94% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.00948) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9440	 0.2580
A	 0.9760	 0.2940
B	 0.9710	 0.2790
C	 0.9700	 0.2870
D	 0.9820	 0.2800
E	 0.9820	 0.2910
F	 0.9700	 0.2860
I	 0.9880	 0.2480
J	 0.9750	 0.2430
M	 0.8310	 0.1760
N	 0.8020	 0.1800
O	 0.7810	 0.1550
P	 0.8440	 0.1610
Q	 0.8200	 0.1740
R	 0.8750	 0.1920
S	 0.8750	 0.1900
T	 0.7920	 0.1490
U	 0.8780	 0.1850
V	 0.8750	 0.1680
W	 0.8540	 0.1780
X	 0.8590	 0.1690
Y	 0.9190	 0.2010
Z	 0.8410	 0.1650
a	 0.9540	 0.2370
d	 0.9980	 0.2850
e	 0.9390	 0.2810
g	 0.9310	 0.2830

