



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 09:03 AM UTC

PDB ID : 7O01 / pdb_00007o01
EMDB ID : EMD-12672
Title : Dimeric Photosystem I of a temperature sensitive mutant *Chlamydomonas reinhardtii*
Authors : Caspy, I.; Nelson, N.
Deposited on : 2021-03-25
Resolution : 17.10 Å(reported)
Based on initial model : 6JO5

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 ⓘ 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:

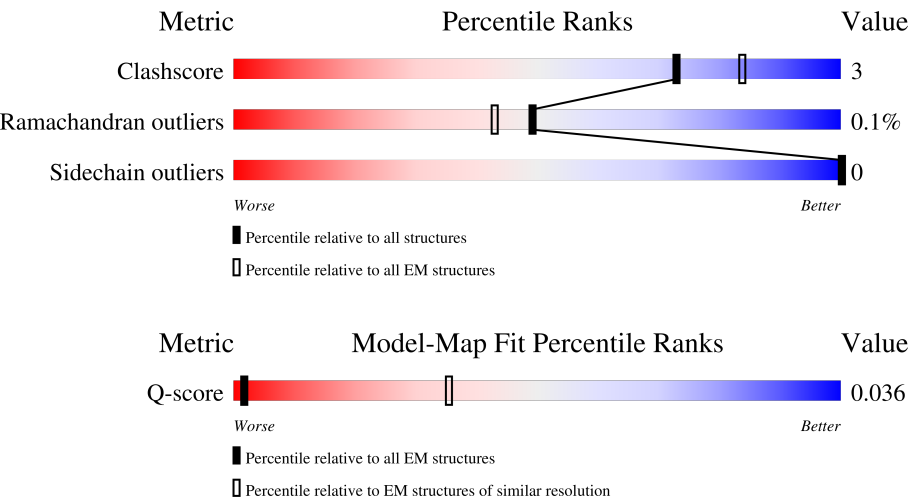
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
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 i

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

The reported resolution of this entry is 17.10 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	34 (16.80 - 17.60)

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	741	
1	a	741	
2	B	733	
2	b	733	

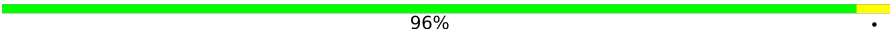
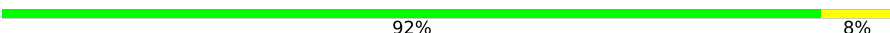
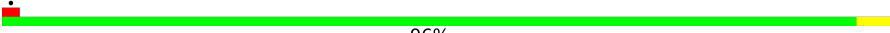
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Mol	Chain	Length	Quality of chain
3	C	80	
3	c	80	
4	D	144	
4	d	144	
5	E	63	
5	e	63	
6	F	165	
6	f	165	
7	G	91	
7	g	91	
8	I	37	
8	i	37	
9	J	39	
9	j	39	
10	K	84	
10	k	84	
11	L	138	
11	l	138	
12	1	194	
12	Z	194	
12	p	194	
12	z	194	
13	3	219	
13	q	219	
14	7	213	

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Mol	Chain	Length	Quality of chain
14	r	213	 96% .
15	8	217	 89% 11%
15	s	217	 92% 8%
16	4	210	 9% 90% 10%
16	t	210	 87% 13%
17	5	227	 96% .
17	u	227	 93% 7%
18	6	229	 94% 6%
18	v	229	 91% 9%
19	2	198	 85% 15%
20	9	183	 89% 11%

2 Entry composition [i](#)

There are 20 unique types of molecules in this entry. The entry contains 64554 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 Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	741	Total	C	N	O	S	0	0
			5820	3805	993	1000	22		
1	a	741	Total	C	N	O	S	0	0
			5820	3805	993	1000	22		

- Molecule 2 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	733	Total	C	N	O	S	0	0
			5825	3825	977	1005	18		
2	b	733	Total	C	N	O	S	0	0
			5825	3825	977	1005	18		

- Molecule 3 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	80	Total	C	N	O	S	0	0
			601	369	103	117	12		
3	c	80	Total	C	N	O	S	0	0
			601	369	103	117	12		

- Molecule 4 is a protein called Photosystem I reaction center subunit II, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	144	Total	C	N	O	S	0	0
			1135	725	201	202	7		
4	d	144	Total	C	N	O	S	0	0
			1135	725	201	202	7		

- Molecule 5 is a protein called Photosystem I reaction center subunit IV, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	63	Total	C	N	O	0	0
			497	316	87	94		
5	e	63	Total	C	N	O	0	0
			497	316	87	94		

- Molecule 6 is a protein called Photosystem I reaction center subunit III, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	165	Total	C	N	O	S	0	0
			1266	817	213	233	3		
6	f	165	Total	C	N	O	S	0	0
			1266	817	213	233	3		

- Molecule 7 is a protein called Photosystem I reaction center subunit V, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	G	74	Total	C	N	O	0	0
			550	354	94	102		
7	g	74	Total	C	N	O	0	0
			550	354	94	102		

- Molecule 8 is a protein called Photosystem I reaction center subunit VIII.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	37	Total	C	N	O	S	0	0
			282	195	39	47	1		
8	i	37	Total	C	N	O	S	0	0
			282	195	39	47	1		

- Molecule 9 is a protein called Photosystem I reaction center subunit IX.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	39	Total	C	N	O	S	0	0
			321	219	45	56	1		
9	j	39	Total	C	N	O	S	0	0
			321	219	45	56	1		

- Molecule 10 is a protein called Photosystem I reaction center subunit psaK, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	84	Total	C	N	O	S	0	0
			571	362	98	109	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	k	84	Total	C	N	O	S	0	0
			571	362	98	109	2		

- Molecule 11 is a protein called PSI subunit V.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	126	Total	C	N	O	S	0	0
			914	595	148	168	3		
11	l	126	Total	C	N	O	S	0	0
			914	595	148	168	3		

- Molecule 12 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	1	194	Total	C	N	O	S	0	0
			1445	941	240	261	3		
12	Z	194	Total	C	N	O	S	0	0
			1445	941	240	261	3		
12	p	194	Total	C	N	O	S	0	0
			1445	941	240	261	3		
12	z	194	Total	C	N	O	S	0	0
			1445	941	240	261	3		

- Molecule 13 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	3	219	Total	C	N	O	S	0	0
			1674	1092	270	304	8		
13	q	219	Total	C	N	O	S	0	0
			1674	1092	270	304	8		

- Molecule 14 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	7	213	Total	C	N	O	S	0	0
			1650	1072	274	298	6		
14	r	213	Total	C	N	O	S	0	0
			1650	1072	274	298	6		

- Molecule 15 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	8	217	Total	C	N	O	S	0	0
			1650	1073	280	293	4		
15	s	217	Total	C	N	O	S	0	0
			1650	1073	280	293	4		

- Molecule 16 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	4	210	Total	C	N	O	S	0	0
			1628	1068	262	293	5		
16	t	210	Total	C	N	O	S	0	0
			1628	1068	262	293	5		

- Molecule 17 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	5	227	Total	C	N	O	S	0	0
			1775	1154	297	316	8		
17	u	227	Total	C	N	O	S	0	0
			1775	1154	297	316	8		

- Molecule 18 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	6	229	Total	C	N	O	S	0	0
			1766	1164	292	304	6		
18	v	229	Total	C	N	O	S	0	0
			1766	1164	292	304	6		

- Molecule 19 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	2	198	Total	C	N	O	S	0	0
			1518	983	249	276	10		

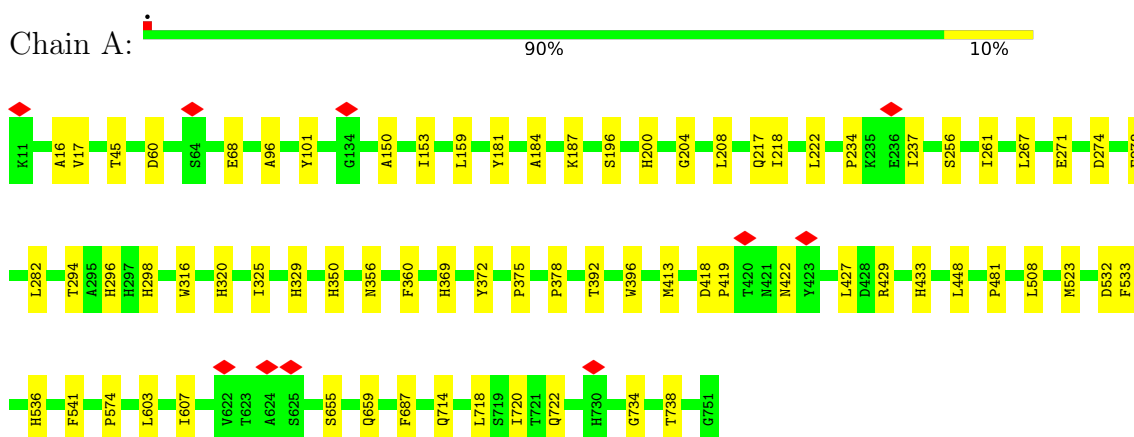
- Molecule 20 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	9	183	Total	C	N	O	S	0	0
			1406	910	235	254	7		

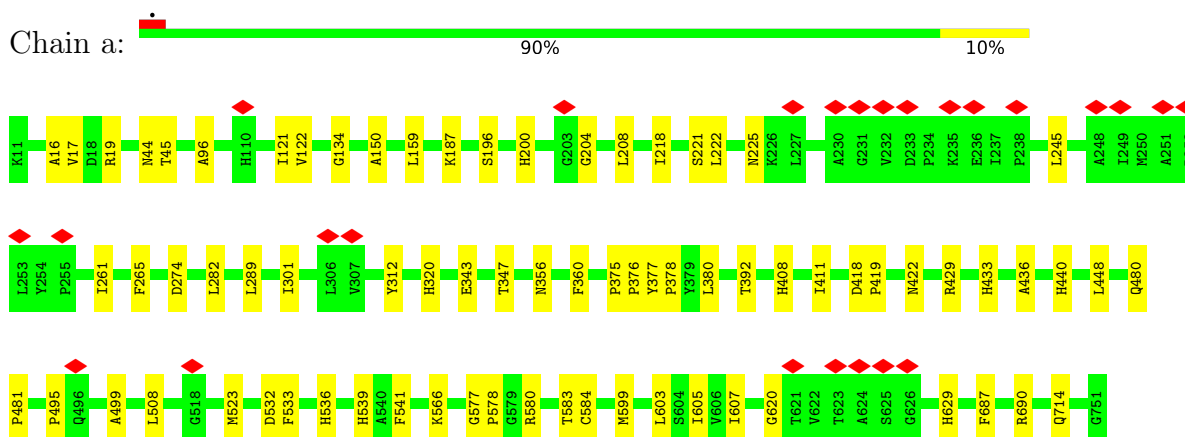
3 Residue-property plots

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.

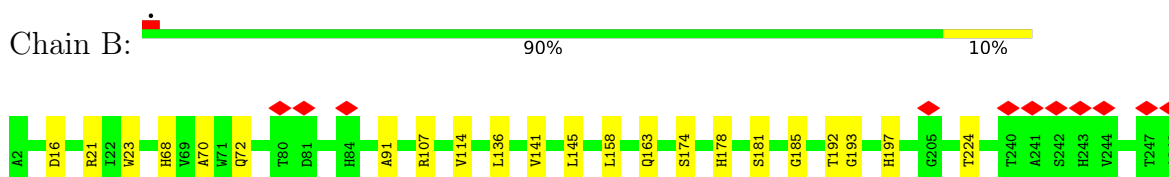
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

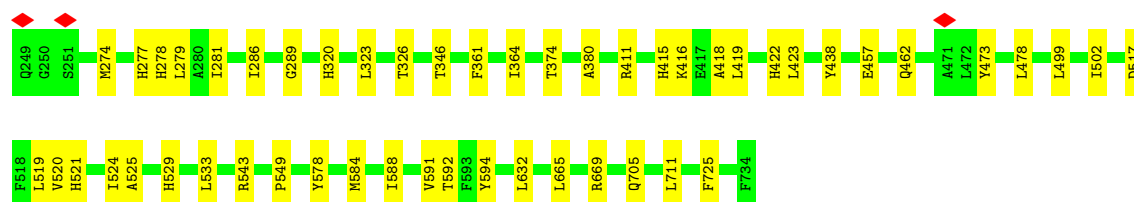


- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

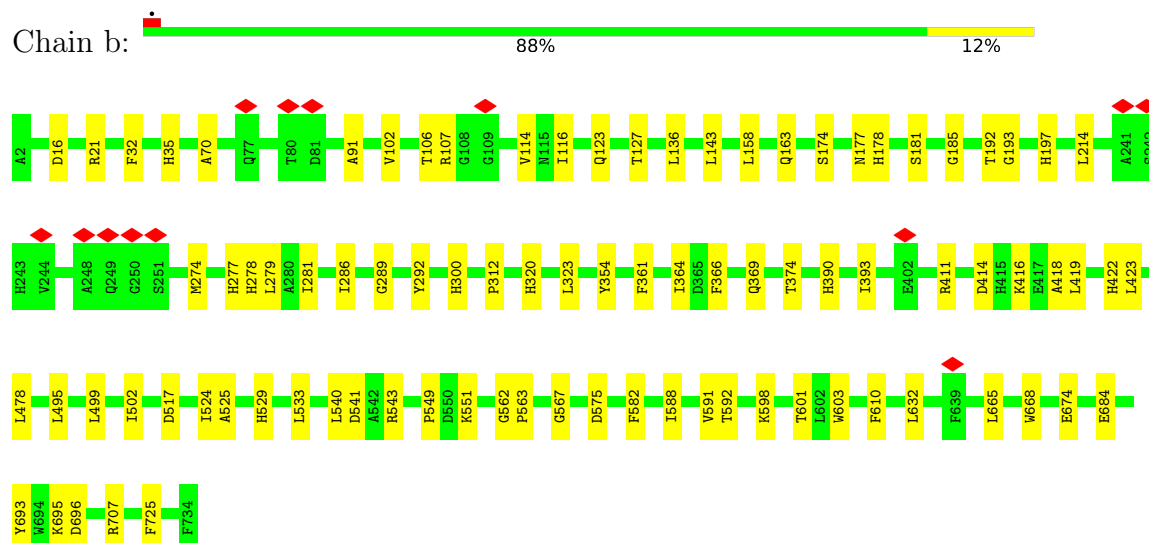


- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

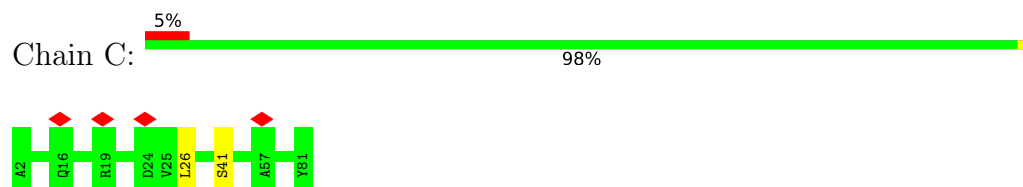




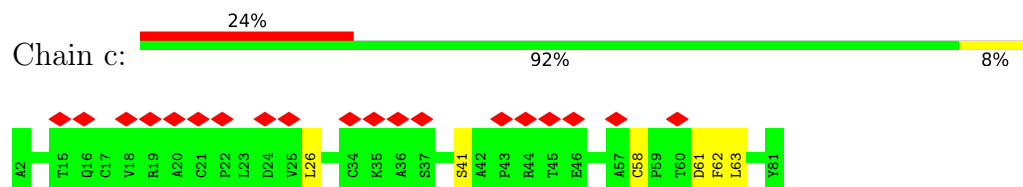
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2



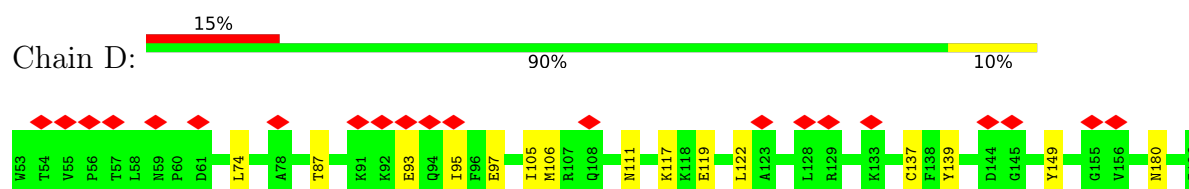
- Molecule 3: Photosystem I iron-sulfur center



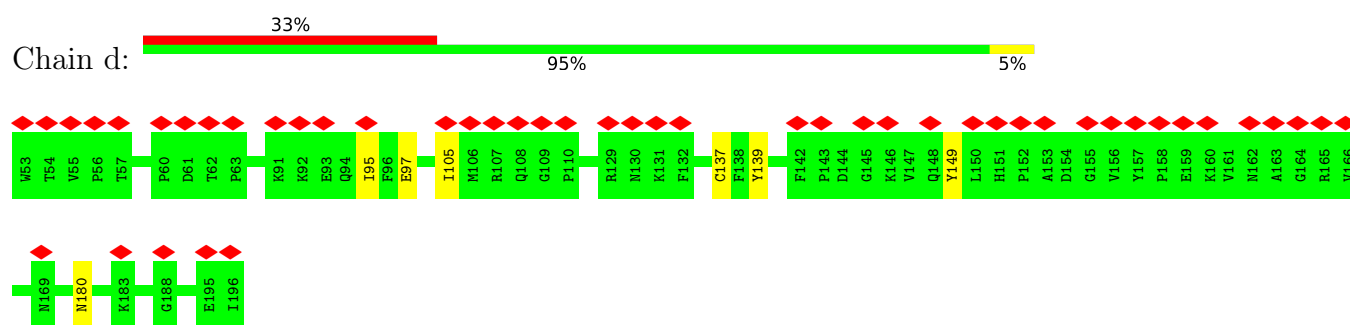
- Molecule 3: Photosystem I iron-sulfur center



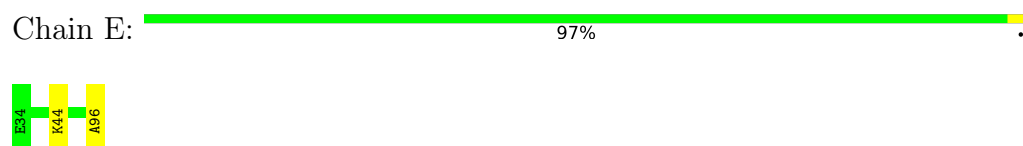
- Molecule 4: Photosystem I reaction center subunit II, chloroplastic



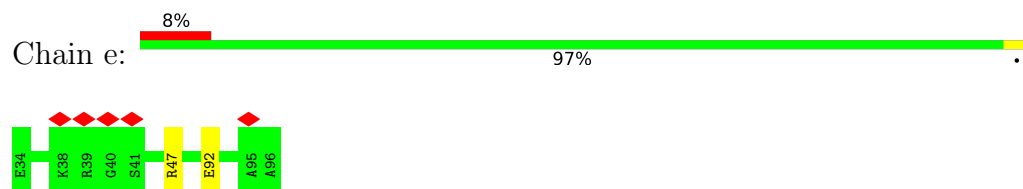
- Molecule 4: Photosystem I reaction center subunit II, chloroplastic



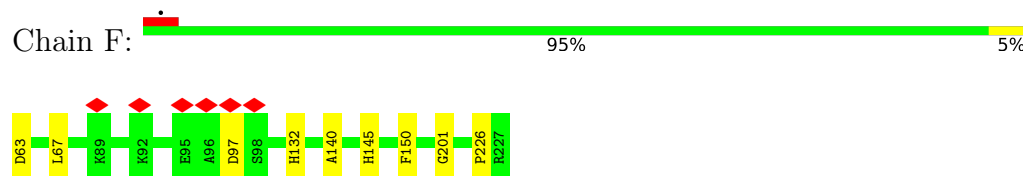
- Molecule 5: Photosystem I reaction center subunit IV, chloroplastic



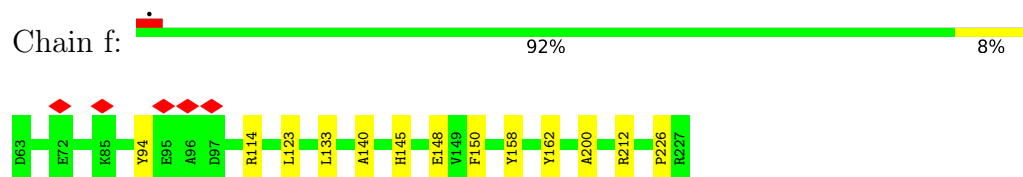
- Molecule 5: Photosystem I reaction center subunit IV, chloroplastic



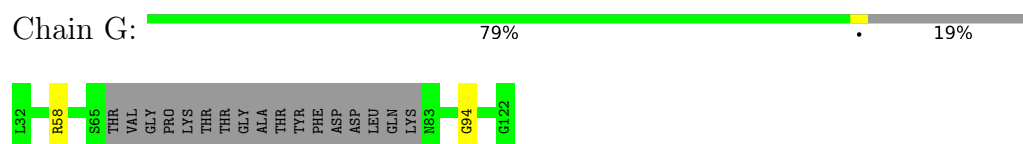
- Molecule 6: Photosystem I reaction center subunit III, chloroplastic



- Molecule 6: Photosystem I reaction center subunit III, chloroplastic

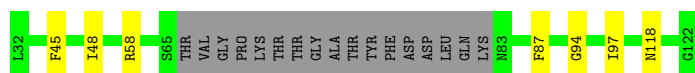


- Molecule 7: Photosystem I reaction center subunit V, chloroplastic



- Molecule 7: Photosystem I reaction center subunit V, chloroplastic

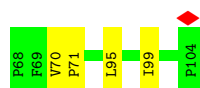




- Molecule 8: Photosystem I reaction center subunit VIII



- Molecule 8: Photosystem I reaction center subunit VIII

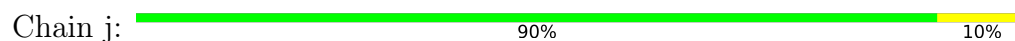


- Molecule 9: Photosystem I reaction center subunit IX



There are no outlier residues recorded for this chain.

- Molecule 9: Photosystem I reaction center subunit IX



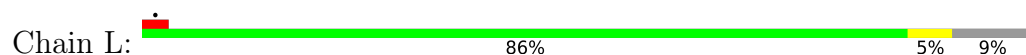
- Molecule 10: Photosystem I reaction center subunit psaK, chloroplastic

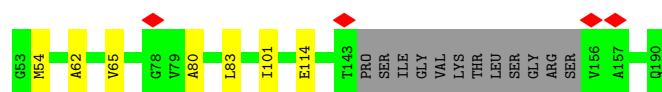


- Molecule 10: Photosystem I reaction center subunit psaK, chloroplastic

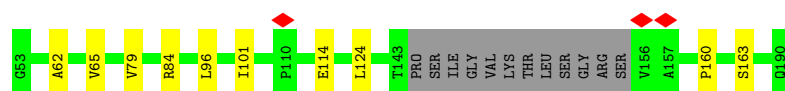
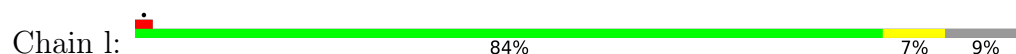


- Molecule 11: PSI subunit V

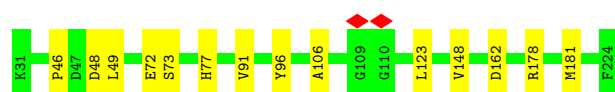




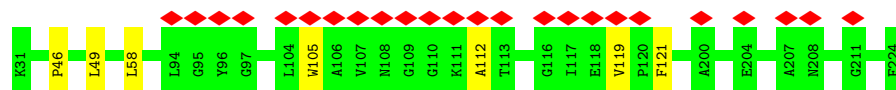
- Molecule 11: PSI subunit V



- Molecule 12: Chlorophyll a-b binding protein, chloroplastic



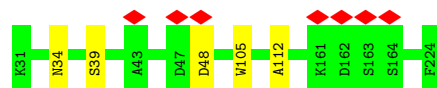
- Molecule 12: Chlorophyll a-b binding protein, chloroplastic



- Molecule 12: Chlorophyll a-b binding protein, chloroplastic



- Molecule 12: Chlorophyll a-b binding protein, chloroplastic



- Molecule 13: Chlorophyll a-b binding protein, chloroplastic

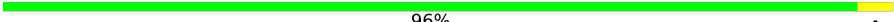


- Molecule 13: Chlorophyll a-b binding protein, chloroplastic

Chain q:  89% 11%



- Molecule 14: Chlorophyll a-b binding protein, chloroplastic

Chain 7:  96% .



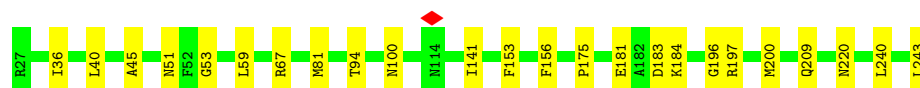
- Molecule 14: Chlorophyll a-b binding protein, chloroplastic

Chain r:  96% .



- Molecule 15: Chlorophyll a-b binding protein, chloroplastic

Chain 8:  89% 11%



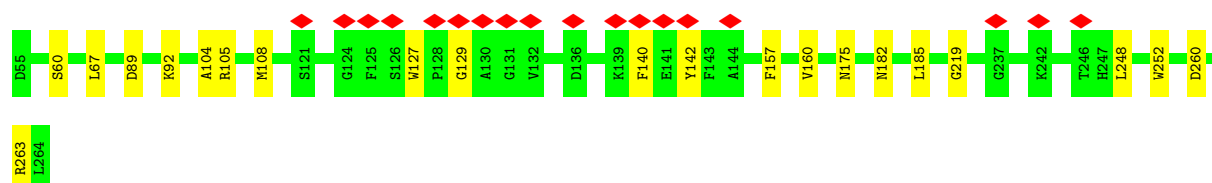
- Molecule 15: Chlorophyll a-b binding protein, chloroplastic

Chain s:  92% 8%



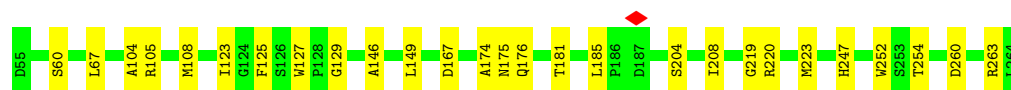
- Molecule 16: Chlorophyll a-b binding protein, chloroplastic

Chain 4:  9% 90% 10%



- Molecule 16: Chlorophyll a-b binding protein, chloroplastic

Chain t:  87% 13%



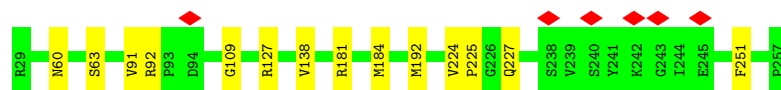
- Molecule 17: Chlorophyll a-b binding protein, chloroplastic



- Molecule 17: Chlorophyll a-b binding protein, chloroplastic



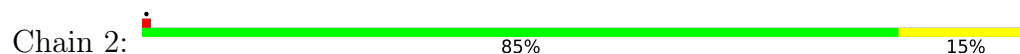
- Molecule 18: Chlorophyll a-b binding protein, chloroplastic



- Molecule 18: Chlorophyll a-b binding protein, chloroplastic



- Molecule 19: Chlorophyll a-b binding protein, chloroplastic



- Molecule 20: Chlorophyll a-b binding protein, chloroplastic



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	5707	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	46.8	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	165000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.094	Depositor
Minimum map value	-0.034	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.011	Depositor
Map size ($\text{\AA}$)	496.19998, 496.19998, 496.19998	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	2.481, 2.481, 2.481	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: SNC

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	0.22	0/6016	0.48	0/8201
1	a	0.24	0/6016	0.50	1/8201 (0.0%)
2	B	0.24	0/6037	0.50	1/8242 (0.0%)
2	b	0.24	0/6037	0.50	0/8242
3	C	0.17	0/611	0.47	0/826
3	c	0.21	0/611	0.48	0/826
4	D	0.17	0/1154	0.48	0/1556
4	d	0.21	0/1154	0.51	0/1556
5	E	0.14	0/507	0.36	0/689
5	e	0.18	0/507	0.39	0/689
6	F	0.20	0/1292	0.45	0/1747
6	f	0.23	0/1292	0.50	0/1747
7	G	0.17	0/561	0.42	0/760
7	g	0.18	0/561	0.44	0/760
8	I	0.28	0/294	0.58	0/406
8	i	0.27	0/294	0.58	0/406
9	J	0.23	0/332	0.42	0/454
9	j	0.27	0/332	0.47	0/454
10	K	0.15	0/576	0.40	0/779
10	k	0.21	0/576	0.47	0/779
11	L	0.19	0/935	0.42	0/1277
11	l	0.19	0/935	0.43	0/1277
12	1	0.18	0/1491	0.40	0/2028
12	Z	0.16	0/1491	0.38	0/2028
12	p	0.21	0/1491	0.44	0/2028
12	z	0.19	0/1491	0.42	0/2028
13	3	0.22	0/1722	0.48	0/2336
13	q	0.24	0/1722	0.48	0/2336
14	7	0.19	0/1702	0.46	0/2310
14	r	0.22	0/1702	0.44	0/2310
15	8	0.19	0/1701	0.42	0/2315
15	s	0.22	0/1701	0.46	0/2315

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	4	0.19	0/1683	0.43	0/2296
16	t	0.22	0/1683	0.46	0/2296
17	5	0.17	0/1830	0.38	0/2492
17	u	0.21	0/1830	0.45	0/2492
18	6	0.18	0/1828	0.40	0/2497
18	v	0.21	0/1828	0.44	0/2497
19	2	0.20	0/1556	0.50	0/2109
20	9	0.23	0/1447	0.52	0/1967
All	All	0.22	0/66529	0.47	2/90554 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	44	ASN	N-CA-C	-6.43	107.28	114.62
2	B	669	ARG	N-CA-C	5.36	117.55	111.02

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5820	0	5672	40	0
1	a	5820	0	5672	45	0
2	B	5825	0	5581	43	0
2	b	5825	0	5581	66	0
3	C	601	0	589	1	0
3	c	601	0	589	4	0
4	D	1135	0	1148	9	0
4	d	1135	0	1148	4	0
5	E	497	0	491	1	0
5	e	497	0	491	1	0
6	F	1266	0	1301	6	0
6	f	1266	0	1301	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	G	550	0	532	1	0
7	g	550	0	532	26	0
8	I	282	0	292	1	0
8	i	282	0	292	2	0
9	J	321	0	322	0	0
9	j	321	0	322	3	0
10	K	571	0	606	5	0
10	k	571	0	606	2	0
11	L	914	0	921	4	0
11	l	914	0	921	5	0
12	1	1445	0	1396	8	0
12	Z	1445	0	1396	4	0
12	p	1445	0	1396	9	0
12	z	1445	0	1396	3	0
13	3	1674	0	1633	8	0
13	q	1674	0	1633	17	0
14	7	1650	0	1589	6	0
14	r	1650	0	1589	7	0
15	8	1650	0	1629	14	0
15	s	1650	0	1629	11	0
16	4	1628	0	1576	12	0
16	t	1628	0	1576	15	0
17	5	1775	0	1746	5	0
17	u	1775	0	1746	10	0
18	6	1766	0	1765	8	0
18	v	1766	0	1765	12	0
19	2	1518	0	1512	53	0
20	9	1406	0	1386	13	0
All	All	64554	0	63268	416	0

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

All (416) 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)
19:2:187:GLN:HE22	2:b:214:LEU:C	1.37	1.30
19:2:148:MET:HB3	7:g:87:PHE:CE1	1.75	1.20
19:2:187:GLN:NE2	2:b:214:LEU:C	2.07	1.13
19:2:148:MET:HB3	7:g:87:PHE:HE1	0.92	1.05
19:2:148:MET:CB	7:g:87:PHE:HE1	1.72	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:2:146:MET:SD	7:g:97:ILE:CD1	2.49	1.00
19:2:146:MET:SD	7:g:97:ILE:HD13	2.06	0.95
19:2:187:GLN:NE2	2:b:214:LEU:O	2.04	0.90
19:2:117:VAL:O	19:2:121:LEU:HD13	1.73	0.87
19:2:190:LEU:HD12	2:b:214:LEU:CD1	2.05	0.87
19:2:146:MET:SD	7:g:97:ILE:HG12	2.15	0.86
19:2:190:LEU:HD12	2:b:214:LEU:HD12	1.63	0.80
19:2:190:LEU:CD1	2:b:214:LEU:CD1	2.59	0.80
19:2:146:MET:SD	7:g:97:ILE:CG1	2.71	0.79
19:2:146:MET:CG	7:g:97:ILE:HD13	2.16	0.76
19:2:148:MET:CB	7:g:87:PHE:CE1	2.57	0.75
19:2:146:MET:HG2	7:g:97:ILE:HD13	1.69	0.74
19:2:190:LEU:HD11	2:b:214:LEU:HD11	1.70	0.72
1:a:204:GLY:O	1:a:208:LEU:HB2	1.89	0.72
1:A:204:GLY:O	1:A:208:LEU:HB2	1.91	0.70
19:2:190:LEU:CD1	2:b:214:LEU:HD11	2.21	0.69
19:2:117:VAL:O	19:2:121:LEU:CD1	2.42	0.68
2:B:141:VAL:O	2:B:145:LEU:HD23	1.93	0.68
19:2:146:MET:HE2	7:g:97:ILE:HD13	1.79	0.65
19:2:146:MET:CE	7:g:97:ILE:HD13	2.26	0.65
15:8:181:GLU:OE1	15:8:184:LYS:NZ	2.30	0.64
2:b:174:SER:O	2:b:178:HIS:ND1	2.27	0.64
1:A:413:MET:HE1	1:A:427:LEU:HD11	1.80	0.64
19:2:146:MET:HG2	7:g:97:ILE:HB	1.80	0.62
13:3:65:ALA:HB1	13:3:191:GLY:HA3	1.82	0.62
12:p:46:PRO:HG2	12:p:49:LEU:HB2	1.81	0.61
6:f:123:LEU:HD21	9:j:38:VAL:HG11	1.81	0.61
19:2:190:LEU:CD1	2:b:214:LEU:HD12	2.26	0.60
12:p:210:TRP:HB3	15:s:117:ALA:HB2	1.82	0.60
16:4:104:ALA:HB1	16:4:219:GLY:HA3	1.84	0.60
1:a:448:LEU:HB3	1:a:541:PHE:HB2	1.83	0.60
13:q:142:MET:HE1	14:r:35:PRO:HB2	1.82	0.60
6:F:63:ASP:N	6:F:67:LEU:O	2.35	0.60
17:5:78:ALA:HB1	17:5:190:GLY:HA3	1.83	0.59
1:a:45:THR:HG22	1:a:714:GLN:HB2	1.84	0.59
19:2:146:MET:CE	7:g:97:ILE:CD1	2.81	0.59
2:b:107:ARG:NH1	2:b:114:VAL:O	2.36	0.58
13:q:31:LEU:HD22	13:q:58:GLN:HG3	1.84	0.58
16:t:104:ALA:HB1	16:t:219:GLY:HA3	1.83	0.58
2:b:181:SER:HB3	2:b:289:GLY:HA3	1.84	0.58
16:t:127:TRP:NE1	16:t:129:GLY:O	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:70:ALA:HB2	2:B:136:LEU:HB2	1.86	0.58
12:p:46:PRO:O	12:p:52:ASN:ND2	2.37	0.58
13:q:65:ALA:HB1	13:q:191:GLY:HA3	1.85	0.58
12:p:72:GLU:HB3	12:p:148:VAL:HG22	1.84	0.58
4:d:95:ILE:HG12	4:d:105:ILE:HG12	1.85	0.58
18:6:91:VAL:HG12	18:6:92:ARG:HG2	1.86	0.57
2:b:416:LYS:HA	2:b:419:LEU:HD12	1.86	0.57
2:b:70:ALA:HB2	2:b:136:LEU:HB2	1.86	0.57
1:a:436:ALA:O	1:a:440:HIS:ND1	2.28	0.57
1:A:196:SER:O	1:A:200:HIS:ND1	2.25	0.57
4:D:95:ILE:HG12	4:D:105:ILE:HG12	1.87	0.57
1:A:448:LEU:HB3	1:A:541:PHE:HB2	1.86	0.56
2:b:16:ASP:HB3	2:b:21:ARG:HB2	1.87	0.56
15:s:67:ARG:NH2	15:s:141:ILE:O	2.38	0.56
1:A:45:THR:HG22	1:A:714:GLN:HB2	1.87	0.56
16:4:127:TRP:NE1	16:4:129:GLY:O	2.39	0.56
17:u:78:ALA:HB1	17:u:190:GLY:HA3	1.86	0.56
2:B:418:ALA:O	2:B:422:HIS:ND1	2.33	0.55
7:g:58:ARG:NH2	7:g:94:GLY:O	2.39	0.55
1:A:508:LEU:HB2	1:A:523:MET:HG3	1.87	0.55
1:a:218:ILE:HA	1:a:222:LEU:HD12	1.89	0.55
19:2:146:MET:HE2	7:g:97:ILE:CD1	2.36	0.55
2:B:274:MET:O	2:B:278:HIS:ND1	2.40	0.55
20:9:126:ARG:HA	20:9:142:PHE:HZ	1.71	0.55
12:p:138:GLU:OE1	12:p:141:ARG:NH2	2.36	0.55
2:B:525:ALA:O	2:B:529:HIS:ND1	2.35	0.55
13:q:174:GLY:HA3	13:q:180:MET:HE2	1.88	0.54
6:F:201:GLY:HA3	15:8:59:LEU:HD21	1.89	0.54
16:4:260:ASP:OD1	16:4:263:ARG:NH2	2.40	0.54
12:1:46:PRO:HG2	12:1:49:LEU:HB2	1.89	0.54
19:2:148:MET:CE	7:g:97:ILE:HG21	2.38	0.54
2:b:21:ARG:NH2	2:b:696:ASP:OD2	2.39	0.54
17:u:142:ASN:ND2	18:v:35:GLY:O	2.36	0.54
2:B:192:THR:HG21	2:B:279:LEU:HB2	1.89	0.54
13:q:101:ILE:HG22	13:q:103:PRO:HD2	1.89	0.54
1:A:429:ARG:O	1:A:433:HIS:ND1	2.41	0.54
2:B:549:PRO:HB3	6:F:226:PRO:HG2	1.90	0.54
20:9:28:ARG:NH1	20:9:48:ASP:OD1	2.40	0.54
16:t:260:ASP:OD1	16:t:263:ARG:NH2	2.39	0.54
19:2:148:MET:HE1	7:g:97:ILE:HG21	1.90	0.53
2:B:457:GLU:OE1	6:F:132:HIS:ND1	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:4:60:SER:HB2	16:4:67:LEU:HD11	1.90	0.53
17:u:135:ARG:NH2	17:u:146:VAL:O	2.42	0.53
13:3:62:VAL:HG11	13:3:161:ALA:HB1	1.91	0.53
2:b:525:ALA:O	2:b:529:HIS:ND1	2.34	0.52
2:B:174:SER:O	2:B:178:HIS:ND1	2.26	0.52
17:u:191:ARG:HA	17:u:194:MET:HE3	1.92	0.52
2:B:361:PHE:HB3	2:B:364:ILE:HD11	1.92	0.52
1:a:429:ARG:O	1:a:433:HIS:ND1	2.42	0.52
1:a:495:PRO:HA	1:a:499:ALA:HB3	1.92	0.52
1:a:418:ASP:O	1:a:422:ASN:ND2	2.42	0.52
19:2:146:MET:HB3	7:g:97:ILE:HG21	1.92	0.52
16:t:252:TRP:HB3	18:v:109:GLY:H	1.75	0.52
1:A:734:GLY:O	1:A:738:THR:OG1	2.28	0.52
14:7:223:LEU:HD22	18:6:225:PRO:HB3	1.92	0.52
2:b:91:ALA:HA	2:b:114:VAL:HG12	1.92	0.52
19:2:146:MET:SD	7:g:97:ILE:HD11	2.48	0.51
16:t:175:ASN:HA	16:t:185:LEU:HD12	1.91	0.51
18:v:127:ARG:NH2	18:v:138:VAL:O	2.44	0.51
12:1:72:GLU:HB3	12:1:148:VAL:HG22	1.93	0.51
2:b:517:ASP:OD2	2:b:598:LYS:NZ	2.43	0.51
13:q:153:ILE:HD13	17:u:58:LEU:HA	1.91	0.51
10:k:93:GLY:O	10:k:97:HIS:ND1	2.43	0.51
6:F:140:ALA:HA	6:F:145:HIS:HB2	1.94	0.50
12:Z:46:PRO:HG2	12:Z:49:LEU:HB2	1.93	0.50
1:A:481:PRO:HG3	1:A:533:PHE:HB2	1.92	0.50
12:p:91:VAL:HG23	12:p:96:TYR:HB2	1.93	0.50
1:A:267:LEU:O	10:K:108:LYS:NZ	2.43	0.50
11:l:79:VAL:O	11:l:84:ARG:NH2	2.44	0.50
2:b:524:ILE:HG12	2:b:591:VAL:HG12	1.92	0.50
1:A:256:SER:OG	1:A:271:GLU:O	2.23	0.50
2:B:423:LEU:HD13	2:B:533:LEU:HA	1.92	0.50
1:A:218:ILE:HA	1:A:222:LEU:HD12	1.94	0.50
2:B:185:GLY:HA3	2:B:286:ILE:HG13	1.94	0.50
15:8:240:LEU:HD13	15:8:243:LEU:HD12	1.94	0.50
2:b:192:THR:HG21	2:b:279:LEU:HB2	1.93	0.50
14:r:44:ASP:OD1	14:r:44:ASP:N	2.43	0.50
16:t:123:ILE:HG13	16:t:125:PHE:H	1.75	0.50
2:B:416:LYS:HA	2:B:419:LEU:HD12	1.94	0.50
12:1:106:ALA:HB1	12:1:123:LEU:HD22	1.94	0.50
19:2:117:VAL:HG12	19:2:121:LEU:HD13	1.93	0.50
19:2:162:ARG:HA	19:2:165:MET:HE3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:577:GLY:HA2	2:b:563:PRO:HD3	1.93	0.50
2:b:549:PRO:HB3	6:f:226:PRO:HG2	1.93	0.50
19:2:46:LEU:O	19:2:67:ARG:NH2	2.42	0.50
13:q:81:LEU:HD22	13:q:86:LEU:HD12	1.94	0.50
18:v:152:HIS:ND1	18:v:153:GLU:O	2.44	0.50
5:E:44:LYS:HB2	5:E:96:ALA:HB3	1.94	0.49
2:b:320:HIS:HB3	2:b:323:LEU:HD12	1.94	0.49
17:5:135:ARG:NH2	17:5:146:VAL:O	2.45	0.49
19:2:33:PRO:O	20:9:128:GLN:NE2	2.41	0.49
1:a:481:PRO:HG3	1:a:533:PHE:HB2	1.94	0.49
2:b:390:HIS:HA	2:b:393:ILE:HD12	1.95	0.49
12:z:34:ASN:ND2	12:z:39:SER:O	2.37	0.49
15:8:67:ARG:NH2	15:8:141:ILE:O	2.43	0.49
19:2:75:ARG:NE	19:2:157:GLU:OE2	2.38	0.49
1:a:419:PRO:HG3	4:d:97:GLU:HB2	1.94	0.49
1:A:261:ILE:HD11	13:3:207:MET:HE1	1.95	0.49
19:2:28:ARG:NH2	19:2:41:LEU:O	2.41	0.49
6:f:212:ARG:NH1	15:s:62:ASP:OD2	2.42	0.49
2:B:588:ILE:HA	2:B:591:VAL:HG22	1.93	0.49
9:j:28:GLU:OE1	9:j:31:ARG:NH2	2.46	0.49
8:i:95:LEU:O	8:i:99:ILE:HG12	2.13	0.48
19:2:148:MET:HE1	7:g:97:ILE:HG12	1.95	0.48
1:a:392:THR:HG23	1:a:607:ILE:HG21	1.95	0.48
1:a:408:HIS:HA	1:a:411:ILE:HD12	1.94	0.48
7:g:45:PHE:HA	7:g:48:ILE:HG12	1.95	0.48
13:3:142:MET:HE1	14:7:35:PRO:HB2	1.96	0.48
14:7:147:ASP:OD1	14:7:147:ASP:N	2.43	0.48
1:a:196:SER:O	1:a:200:HIS:ND1	2.29	0.48
2:b:158:LEU:O	2:b:163:GLN:NE2	2.47	0.48
2:b:588:ILE:HA	2:b:591:VAL:HG22	1.95	0.48
7:G:58:ARG:NH2	7:G:94:GLY:O	2.47	0.48
13:3:27:LEU:HD21	13:3:43:LEU:HD12	1.95	0.48
19:2:117:VAL:C	19:2:121:LEU:HD13	2.38	0.48
3:c:58:CYS:HB3	3:c:63:LEU:HD22	1.96	0.48
1:a:150:ALA:HB2	1:a:378:PRO:HD2	1.95	0.48
1:a:274:ASP:OD1	1:a:274:ASP:N	2.41	0.48
2:B:224:THR:OG1	20:9:204:THR:O	2.31	0.48
12:Z:58:LEU:HD11	15:8:175:PRO:HB3	1.96	0.48
18:6:192:MET:HE1	18:6:251:PHE:HB3	1.95	0.48
4:D:87:THR:HA	4:D:111:ASN:O	2.14	0.48
13:3:153:ILE:HD13	17:5:58:LEU:HA	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:520:VAL:HG21	2:B:594:TYR:HB2	1.96	0.47
4:D:139:TYR:HD1	4:D:149:TYR:HA	1.79	0.47
19:2:187:GLN:HE22	2:b:214:LEU:CA	1.71	0.47
1:a:221:SER:O	1:a:225:ASN:HB2	2.13	0.47
1:a:508:LEU:HB2	1:a:523:MET:HG3	1.95	0.47
1:A:418:ASP:O	1:A:422:ASN:ND2	2.47	0.47
12:1:91:VAL:HG23	12:1:96:TYR:HB2	1.97	0.47
11:l:62:ALA:HB3	11:l:65:VAL:HG22	1.96	0.47
2:B:543:ARG:NH2	4:D:180:ASN:OD1	2.36	0.47
17:5:191:ARG:HA	17:5:194:MET:HE3	1.96	0.47
2:b:575:ASP:OD1	2:b:707:ARG:NH1	2.47	0.47
16:t:60:SER:HB2	16:t:67:LEU:HD11	1.95	0.47
1:a:19:ARG:NE	13:q:48:SER:O	2.47	0.47
2:b:423:LEU:HD13	2:b:533:LEU:HA	1.97	0.47
18:v:46:LEU:HD11	18:v:64:LEU:HD21	1.97	0.47
8:I:95:LEU:O	8:I:99:ILE:HG12	2.15	0.47
16:4:157:PHE:HA	16:4:160:VAL:HG22	1.95	0.47
13:q:126:GLN:O	13:q:130:LEU:HB2	2.13	0.47
16:t:105:ARG:HA	16:t:108:MET:HE3	1.96	0.47
1:a:16:ALA:HB1	1:a:187:LYS:HD3	1.96	0.47
2:b:684:GLU:OE2	2:b:693:TYR:OH	2.29	0.47
15:s:181:GLU:OE1	15:s:184:LYS:NZ	2.41	0.47
15:8:36:ILE:HD12	15:8:53:GLY:HA3	1.97	0.46
17:u:32:ARG:NH2	17:u:45:LEU:O	2.48	0.46
1:A:392:THR:HG23	1:A:607:ILE:HG21	1.98	0.46
2:B:524:ILE:HG12	2:B:591:VAL:HG12	1.97	0.46
20:9:163:ARG:HA	20:9:166:MET:HE3	1.97	0.46
1:a:289:LEU:HB2	1:a:376:PRO:HA	1.98	0.46
16:t:204:SER:HB2	16:t:208:ILE:HD13	1.98	0.46
1:A:282:LEU:HD21	1:A:375:PRO:HD2	1.98	0.46
2:B:193:GLY:O	2:B:197:HIS:HB2	2.15	0.46
6:F:97:ASP:OD1	6:F:97:ASP:N	2.48	0.46
2:B:438:TYR:CE1	2:B:519:LEU:HB3	2.51	0.46
1:A:96:ALA:HB2	1:A:159:LEU:HB2	1.96	0.46
1:A:274:ASP:OD1	1:A:274:ASP:N	2.41	0.46
19:2:41:LEU:HD11	19:2:52:ASP:HB2	1.98	0.46
7:g:118:ASN:OD1	12:p:124:ASN:ND2	2.48	0.46
2:B:181:SER:HB3	2:B:289:GLY:HA3	1.97	0.46
19:2:75:ARG:HA	19:2:78:MET:HE3	1.98	0.46
1:a:282:LEU:HD21	1:a:375:PRO:HD2	1.97	0.46
6:f:162:TYR:HE1	6:f:200:ALA:HA	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:2:42:ASP:N	19:2:42:ASP:OD1	2.47	0.46
11:l:96:LEU:HD21	11:l:124:LEU:HB3	1.97	0.46
12:z:48:ASP:OD1	12:z:48:ASP:N	2.49	0.46
2:B:107:ARG:NH1	2:B:114:VAL:O	2.45	0.46
15:s:153:PHE:HD2	15:s:156:PHE:HB3	1.80	0.46
5:e:47:ARG:NE	5:e:92:GLU:OE2	2.47	0.45
15:s:81:MET:HG3	15:s:196:GLY:HA2	1.98	0.45
1:a:508:LEU:HD12	1:a:523:MET:HB3	1.98	0.45
12:Z:119:VAL:HG12	12:Z:121:PHE:H	1.80	0.45
1:A:68:GLU:OE2	1:A:181:TYR:OH	2.29	0.45
2:B:374:THR:HG23	2:B:592:THR:HG21	1.98	0.45
2:B:578:TYR:HE1	2:B:711:LEU:HB2	1.82	0.45
18:6:127:ARG:NH2	18:6:138:VAL:O	2.50	0.45
1:a:580:ARG:HH11	1:a:583:THR:HG21	1.81	0.45
19:2:30:MET:HB3	19:2:35:ALA:HB3	1.99	0.45
2:b:177:ASN:ND2	2:b:292:TYR:O	2.49	0.45
2:b:543:ARG:NH2	4:d:180:ASN:OD1	2.49	0.45
15:s:240:LEU:HD13	15:s:243:LEU:HD12	1.99	0.45
1:A:278:PHE:HE1	1:A:296:HIS:HD2	1.65	0.45
2:B:16:ASP:HB3	2:B:21:ARG:HB2	1.98	0.45
18:6:60:ASN:HB3	18:6:63:SER:HB2	1.98	0.45
12:1:48:ASP:OD1	12:1:48:ASP:N	2.50	0.45
14:7:221:ASP:HB3	14:7:229:VAL:HG11	1.99	0.45
16:4:105:ARG:HA	16:4:108:MET:HE3	1.99	0.45
19:2:146:MET:CG	7:g:97:ILE:HB	2.46	0.45
18:v:69:GLU:HG2	18:v:132:LEU:HD12	1.98	0.45
2:b:541:ASP:O	2:b:551:LYS:NZ	2.40	0.45
10:k:49:ALA:HB1	10:k:56:THR:HG22	1.98	0.45
2:B:423:LEU:HB3	2:B:533:LEU:HB2	2.00	0.44
3:C:26:LEU:HA	3:C:41:SER:O	2.17	0.44
4:D:74:LEU:H	11:L:54:MET:HE1	1.81	0.44
18:v:168:ASP:HB3	18:v:171:GLU:HB3	1.98	0.44
6:f:114:ARG:NH1	9:j:35:ASP:OD2	2.48	0.44
11:l:101:ILE:HG12	11:l:114:GLU:HA	2.00	0.44
13:q:111:TRP:HB3	17:u:254:PRO:HB3	1.99	0.44
6:f:133:LEU:HD22	6:f:148:GLU:HB3	1.98	0.44
1:A:16:ALA:HB1	1:A:187:LYS:HD3	2.00	0.44
1:A:294:THR:O	1:A:298:HIS:ND1	2.51	0.44
2:b:193:GLY:O	2:b:197:HIS:HB2	2.18	0.44
16:t:175:ASN:HB3	16:t:185:LEU:HB2	1.98	0.44
15:8:153:PHE:HD2	15:8:156:PHE:HB3	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:9:62:ARG:NH2	20:9:66:TYR:OH	2.50	0.44
2:b:374:THR:HG23	2:b:592:THR:HG21	2.00	0.44
2:b:411:ARG:HA	2:b:414:ASP:HB2	2.00	0.44
12:z:105:TRP:CE2	12:z:112:ALA:HB2	2.53	0.44
1:a:599:MET:HG2	1:a:603:LEU:HD13	2.00	0.44
1:A:655:SER:O	1:A:659:GLN:HG2	2.18	0.44
1:a:566:LYS:NZ	2:b:674:GLU:OE2	2.41	0.44
19:2:148:MET:HB3	7:g:87:PHE:CD1	2.45	0.44
20:9:75:ARG:HA	20:9:78:MET:HE3	1.99	0.44
13:q:129:GLU:OE1	13:q:132:ARG:NH2	2.48	0.44
18:v:181:ARG:HA	18:v:184:MET:HE3	1.99	0.44
2:B:23:TRP:CG	2:B:705:GLN:HE22	2.36	0.44
12:Z:105:TRP:CE2	12:Z:112:ALA:HB2	2.53	0.44
1:a:356:ASN:O	1:a:360:PHE:HB2	2.18	0.44
15:s:197:ARG:HA	15:s:200:MET:HE3	2.00	0.44
1:A:17:VAL:HG11	1:A:184:ALA:HB1	1.99	0.43
15:8:81:MET:HG3	15:8:196:GLY:HA2	1.98	0.43
16:4:89:ASP:HB3	16:4:92:LYS:HB2	2.00	0.43
14:r:216:LEU:HD23	14:r:216:LEU:HA	1.85	0.43
4:D:93:GLU:HA	4:D:106:MET:O	2.18	0.43
18:v:75:SER:HB3	18:v:180:GLY:HA3	1.99	0.43
1:A:234:PRO:HA	1:A:237:ILE:HD12	2.00	0.43
19:2:28:ARG:NH1	19:2:42:ASP:O	2.51	0.43
19:2:107:ASN:HA	19:2:110:LEU:HD12	1.99	0.43
19:2:198:ILE:HG12	19:2:207:THR:HG21	2.00	0.43
1:a:17:VAL:H	13:q:47:ASN:HB3	1.82	0.43
2:b:277:HIS:CE1	2:b:281:ILE:HD13	2.53	0.43
2:b:361:PHE:HB3	2:b:364:ILE:HD11	1.99	0.43
2:b:418:ALA:O	2:b:422:HIS:ND1	2.30	0.43
14:r:221:ASP:HB3	14:r:229:VAL:HG11	1.99	0.43
1:A:718:LEU:HB3	1:A:722:GLN:HG2	2.01	0.43
19:2:128:ILE:HD13	19:2:136:GLY:HA3	2.00	0.43
16:t:167:ASP:HB2	16:t:174:ALA:HB3	1.99	0.43
2:B:91:ALA:HA	2:B:114:VAL:HG12	1.99	0.43
2:B:158:LEU:O	2:B:163:GLN:NE2	2.51	0.43
13:q:28:ASP:OD1	13:q:28:ASP:N	2.48	0.43
1:A:356:ASN:O	1:A:360:PHE:HB2	2.18	0.43
15:s:159:SER:HB3	15:s:172:PRO:HD3	2.00	0.43
2:B:578:TYR:CE1	2:B:711:LEU:HB2	2.53	0.43
15:8:183:ASP:N	15:8:183:ASP:OD1	2.50	0.43
1:a:690:ARG:HD3	2:b:567:GLY:HA3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:u:202:LEU:HD23	17:u:202:LEU:HA	1.84	0.43
1:A:60:ASP:OD2	1:A:350:HIS:NE2	2.45	0.43
10:K:72:ASN:OD1	10:K:72:ASN:N	2.52	0.43
12:1:178:ARG:HA	12:1:181:MET:HE3	2.01	0.43
2:b:123:GLN:O	2:b:127:THR:OG1	2.35	0.43
2:b:366:PHE:HB3	2:b:603:TRP:CZ3	2.53	0.43
2:b:499:LEU:HA	2:b:502:ILE:HG22	2.01	0.43
1:A:101:TYR:OH	1:A:153:ILE:O	2.30	0.43
2:b:107:ARG:HG3	2:b:116:ILE:HD11	2.00	0.43
2:b:292:TYR:HA	2:b:300:HIS:H	1.84	0.43
6:f:140:ALA:HA	6:f:145:HIS:HB2	2.01	0.43
12:p:178:ARG:HA	12:p:181:MET:HE3	2.01	0.43
2:B:517:ASP:O	2:B:521:HIS:ND1	2.42	0.42
20:9:124:ILE:HD12	20:9:124:ILE:HA	1.91	0.42
1:a:343:GLU:O	1:a:347:THR:OG1	2.28	0.42
1:a:377:TYR:HD2	1:a:380:LEU:HD22	1.84	0.42
14:7:156:GLU:OE2	14:7:168:ARG:NH1	2.52	0.42
1:a:532:ASP:O	1:a:536:HIS:ND1	2.31	0.42
2:b:274:MET:O	2:b:278:HIS:ND1	2.51	0.42
3:c:26:LEU:HA	3:c:41:SER:O	2.19	0.42
17:u:153:LYS:HA	17:u:153:LYS:HD3	1.83	0.42
2:B:411:ARG:O	2:B:415:HIS:ND1	2.45	0.42
11:L:62:ALA:HB3	11:L:65:VAL:HG22	2.01	0.42
20:9:203:LEU:HD23	20:9:203:LEU:HA	1.84	0.42
1:a:245:LEU:HD11	13:q:103:PRO:HB3	2.02	0.42
16:t:176:GLN:NE2	16:t:181:THR:O	2.52	0.42
1:A:687:PHE:CD1	2:B:665:LEU:HB3	2.54	0.42
2:b:354:TYR:HA	2:b:369:GLN:HE22	1.84	0.42
2:b:416:LYS:HD2	2:b:540:LEU:HB3	2.01	0.42
4:d:139:TYR:HD1	4:d:149:TYR:HA	1.84	0.42
14:r:175:LEU:HD21	18:v:57:LEU:HA	2.02	0.42
13:3:66:ARG:HA	13:3:69:MET:HE3	2.02	0.42
2:b:312:PRO:HB2	12:p:63:GLU:HG3	2.02	0.42
2:b:478:LEU:HD23	2:b:478:LEU:HA	1.86	0.42
14:r:195:ARG:HA	14:r:198:MET:HE3	2.01	0.42
1:a:312:TYR:HA	1:a:320:HIS:H	1.83	0.42
1:A:396:TRP:HA	1:A:603:LEU:HD23	2.01	0.42
18:6:181:ARG:HA	18:6:184:MET:HE3	2.01	0.42
20:9:105:ASP:OD1	20:9:105:ASP:N	2.52	0.42
20:9:140:ASN:OD1	20:9:140:ASN:N	2.53	0.42
1:a:134:GLY:HA2	6:f:94:TYR:HE1	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:q:117:ILE:H	13:q:117:ILE:HG13	1.68	0.42
16:t:146:ALA:HA	16:t:149:LEU:HD12	2.02	0.42
4:D:117:LYS:HE3	4:D:119:GLU:HB3	2.01	0.42
10:K:49:ALA:HB1	10:K:56:THR:HG22	2.02	0.42
13:q:62:VAL:HG11	13:q:161:ALA:HB1	2.01	0.42
1:a:96:ALA:HB2	1:a:159:LEU:HB2	2.01	0.42
11:l:160:PRO:O	11:l:163:SER:OG	2.36	0.42
16:t:220:ARG:HA	16:t:223:MET:HE3	2.01	0.41
18:v:125:GLU:OE2	18:v:128:ARG:NH2	2.43	0.41
12:1:73:SER:O	12:1:77:HIS:ND1	2.43	0.41
19:2:96:TRP:CD1	19:2:97:THR:HG23	2.55	0.41
1:A:150:ALA:HB2	1:A:378:PRO:HD2	2.01	0.41
2:B:323:LEU:HA	2:B:326:THR:HG22	2.02	0.41
16:4:175:ASN:HB3	16:4:185:LEU:HB2	2.02	0.41
2:b:185:GLY:HA3	2:b:286:ILE:HG13	2.02	0.41
1:A:532:ASP:O	1:A:536:HIS:ND1	2.37	0.41
1:A:574:PRO:HB3	1:A:720:ILE:HB	2.02	0.41
15:8:45:ALA:O	15:8:51:ASN:ND2	2.53	0.41
1:a:687:PHE:CD1	2:b:665:LEU:HB3	2.56	0.41
3:c:61:ASP:HA	3:c:62:PHE:HA	1.85	0.41
17:u:50:ALA:O	17:u:71:ARG:NH2	2.43	0.41
18:v:44:GLY:HA2	18:v:49:ASP:HB3	2.02	0.41
1:A:316:TRP:HB3	10:K:57:VAL:HG23	2.02	0.41
1:A:369:HIS:HA	1:A:372:TYR:CE2	2.56	0.41
2:B:277:HIS:CE1	2:B:281:ILE:HD13	2.56	0.41
12:1:162:ASP:OD1	12:1:162:ASP:N	2.49	0.41
2:b:601:THR:HG21	2:b:610:PHE:HB2	2.02	0.41
2:b:695:LYS:HD2	2:b:695:LYS:HA	1.94	0.41
11:L:80:ALA:HB3	11:L:83:LEU:HD23	2.03	0.41
13:3:27:LEU:HD23	13:3:27:LEU:HA	1.90	0.41
6:f:158:TYR:O	6:f:162:TYR:HB2	2.21	0.41
16:t:247:HIS:ND1	16:t:254:THR:O	2.45	0.41
15:8:94:THR:HG23	15:8:100:ASN:HA	2.03	0.41
19:2:146:MET:HB3	7:g:97:ILE:CG2	2.50	0.41
1:a:584:CYS:HB3	2:b:668:TRP:HE3	1.86	0.41
2:b:549:PRO:HD2	3:c:62:PHE:CZ	2.55	0.41
15:s:183:ASP:OD1	15:s:183:ASP:N	2.54	0.41
19:2:190:LEU:HD12	2:b:214:LEU:CG	2.49	0.41
1:a:480:GLN:HA	1:a:481:PRO:HD3	1.95	0.41
2:b:32:PHE:HA	2:b:35:HIS:CD2	2.56	0.41
2:b:102:VAL:O	2:b:106:THR:OG1	2.32	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:i:70:VAL:HA	8:i:71:PRO:HD3	1.93	0.41
2:B:320:HIS:HB3	2:B:323:LEU:HD12	2.02	0.41
2:B:632:LEU:HD22	2:B:725:PHE:HA	2.03	0.41
4:D:122:LEU:HD12	4:D:122:LEU:HA	1.85	0.41
14:7:42:HIS:NE2	14:7:54:ASP:OD2	2.47	0.41
16:4:182:ASN:OD1	16:4:182:ASN:N	2.53	0.41
1:a:121:ILE:HG13	1:a:122:VAL:HG13	2.01	0.41
13:q:27:LEU:HD21	13:q:43:LEU:HD12	2.02	0.41
1:A:217:GLN:OE1	1:A:298:HIS:ND1	2.54	0.41
1:A:325:ILE:O	1:A:329:HIS:ND1	2.48	0.41
2:b:632:LEU:HD22	2:b:725:PHE:HA	2.03	0.41
2:B:68:HIS:ND1	2:B:72:GLN:OE1	2.52	0.40
10:K:60:ASN:N	10:K:68:VAL:O	2.47	0.40
15:8:197:ARG:HA	15:8:200:MET:HE3	2.03	0.40
18:6:224:VAL:HG23	18:6:227:GLN:H	1.86	0.40
14:r:225:ASP:HB3	14:r:229:VAL:HG23	2.02	0.40
1:A:320:HIS:HB3	1:A:325:ILE:HD11	2.03	0.40
2:B:346:THR:HB	2:B:380:ALA:HB2	2.04	0.40
2:B:499:LEU:HA	2:B:502:ILE:HG22	2.02	0.40
15:8:40:LEU:HD23	15:8:40:LEU:HA	1.92	0.40
16:4:248:LEU:HD23	16:4:248:LEU:HA	1.96	0.40
16:4:252:TRP:HB3	18:6:109:GLY:H	1.87	0.40
17:5:153:LYS:HA	17:5:153:LYS:HD3	1.88	0.40
19:2:117:VAL:CG1	19:2:121:LEU:HD13	2.51	0.40
2:b:143:LEU:HD23	2:b:143:LEU:HA	1.90	0.40
1:A:419:PRO:HG3	4:D:97:GLU:HB2	2.04	0.40
2:B:478:LEU:HD23	2:B:478:LEU:HA	1.87	0.40
16:4:140:PHE:HB3	16:4:142:TYR:CE2	2.56	0.40
1:a:539:HIS:HE1	1:a:605:ILE:HG22	1.86	0.40
2:b:582:PHE:HZ	2:b:665:LEU:HD21	1.85	0.40
2:B:462:GLN:HG2	2:B:473:TYR:CZ	2.56	0.40
11:L:101:ILE:HG12	11:L:114:GLU:HA	2.03	0.40
15:8:209:GLN:HB3	15:8:220:ASN:ND2	2.36	0.40
20:9:32:LEU:HD12	20:9:32:LEU:HA	1.88	0.40
20:9:133:THR:HG23	20:9:135:THR:HG22	2.03	0.40
1:a:301:ILE:HD13	1:a:301:ILE:HA	1.84	0.40
1:a:620:GLY:HA3	1:a:629:HIS:HA	2.04	0.40
15:s:114:ASN:OD1	15:s:114:ASN:N	2.53	0.40
2:B:584:MET:HE3	2:B:584:MET:HB3	2.01	0.40
1:a:261:ILE:HD12	1:a:265:PHE:HE2	1.87	0.40
1:a:578:PRO:HD3	2:b:562:GLY:HA2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:495:LEU:HD23	2:b:495:LEU:HA	1.84	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	739/741 (100%)	720 (97%)	19 (3%)	0	100	100
1	a	739/741 (100%)	717 (97%)	22 (3%)	0	100	100
2	B	731/733 (100%)	707 (97%)	24 (3%)	0	100	100
2	b	731/733 (100%)	706 (97%)	25 (3%)	0	100	100
3	C	78/80 (98%)	75 (96%)	3 (4%)	0	100	100
3	c	78/80 (98%)	76 (97%)	2 (3%)	0	100	100
4	D	141/144 (98%)	135 (96%)	6 (4%)	0	100	100
4	d	141/144 (98%)	136 (96%)	5 (4%)	0	100	100
5	E	61/63 (97%)	57 (93%)	4 (7%)	0	100	100
5	e	61/63 (97%)	57 (93%)	4 (7%)	0	100	100
6	F	163/165 (99%)	158 (97%)	4 (2%)	1 (1%)	21	59
6	f	163/165 (99%)	157 (96%)	5 (3%)	1 (1%)	21	59
7	G	70/91 (77%)	70 (100%)	0	0	100	100
7	g	70/91 (77%)	70 (100%)	0	0	100	100
8	I	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
8	i	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
9	J	37/39 (95%)	36 (97%)	1 (3%)	0	100	100
9	j	37/39 (95%)	36 (97%)	1 (3%)	0	100	100
10	K	82/84 (98%)	81 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	k	82/84 (98%)	80 (98%)	2 (2%)	0	100	100
11	L	122/138 (88%)	119 (98%)	3 (2%)	0	100	100
11	l	122/138 (88%)	119 (98%)	3 (2%)	0	100	100
12	1	192/194 (99%)	185 (96%)	7 (4%)	0	100	100
12	Z	192/194 (99%)	187 (97%)	5 (3%)	0	100	100
12	p	192/194 (99%)	182 (95%)	10 (5%)	0	100	100
12	z	192/194 (99%)	189 (98%)	3 (2%)	0	100	100
13	3	217/219 (99%)	209 (96%)	8 (4%)	0	100	100
13	q	217/219 (99%)	209 (96%)	8 (4%)	0	100	100
14	7	211/213 (99%)	203 (96%)	8 (4%)	0	100	100
14	r	211/213 (99%)	205 (97%)	6 (3%)	0	100	100
15	8	215/217 (99%)	210 (98%)	5 (2%)	0	100	100
15	s	215/217 (99%)	208 (97%)	7 (3%)	0	100	100
16	4	208/210 (99%)	199 (96%)	9 (4%)	0	100	100
16	t	208/210 (99%)	198 (95%)	10 (5%)	0	100	100
17	5	225/227 (99%)	221 (98%)	3 (1%)	1 (0%)	30	67
17	u	225/227 (99%)	221 (98%)	4 (2%)	0	100	100
18	6	227/229 (99%)	223 (98%)	4 (2%)	0	100	100
18	v	227/229 (99%)	222 (98%)	5 (2%)	0	100	100
19	2	196/198 (99%)	187 (95%)	8 (4%)	1 (0%)	24	63
20	9	181/183 (99%)	170 (94%)	10 (6%)	1 (1%)	21	59
All	All	8269/8417 (98%)	8008 (97%)	256 (3%)	5 (0%)	49	83

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	150	PHE
6	f	150	PHE
17	5	243	GLN
19	2	180	LYS
20	9	139	ILE

5.3.2 Protein sidechains ⓘ

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	A	601/601 (100%)	601 (100%)	0	100	100
1	a	601/601 (100%)	601 (100%)	0	100	100
2	B	596/596 (100%)	596 (100%)	0	100	100
2	b	596/596 (100%)	596 (100%)	0	100	100
3	C	69/69 (100%)	69 (100%)	0	100	100
3	c	69/69 (100%)	69 (100%)	0	100	100
4	D	120/120 (100%)	120 (100%)	0	100	100
4	d	120/120 (100%)	120 (100%)	0	100	100
5	E	54/54 (100%)	54 (100%)	0	100	100
5	e	54/54 (100%)	54 (100%)	0	100	100
6	F	127/127 (100%)	127 (100%)	0	100	100
6	f	127/127 (100%)	127 (100%)	0	100	100
7	G	54/68 (79%)	54 (100%)	0	100	100
7	g	54/68 (79%)	54 (100%)	0	100	100
8	I	31/31 (100%)	31 (100%)	0	100	100
8	i	31/31 (100%)	31 (100%)	0	100	100
9	J	35/35 (100%)	35 (100%)	0	100	100
9	j	35/35 (100%)	35 (100%)	0	100	100
10	K	58/58 (100%)	58 (100%)	0	100	100
10	k	58/58 (100%)	58 (100%)	0	100	100
11	L	92/102 (90%)	92 (100%)	0	100	100
11	l	92/102 (90%)	92 (100%)	0	100	100
12	1	137/137 (100%)	137 (100%)	0	100	100
12	Z	137/137 (100%)	137 (100%)	0	100	100
12	p	137/137 (100%)	137 (100%)	0	100	100
12	z	137/137 (100%)	137 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	3	167/167 (100%)	167 (100%)	0	100	100
13	q	167/167 (100%)	167 (100%)	0	100	100
14	7	164/164 (100%)	164 (100%)	0	100	100
14	r	164/164 (100%)	164 (100%)	0	100	100
15	8	163/163 (100%)	163 (100%)	0	100	100
15	s	163/163 (100%)	163 (100%)	0	100	100
16	4	164/165 (99%)	164 (100%)	0	100	100
16	t	164/165 (99%)	164 (100%)	0	100	100
17	5	184/184 (100%)	184 (100%)	0	100	100
17	u	184/184 (100%)	184 (100%)	0	100	100
18	6	183/183 (100%)	183 (100%)	0	100	100
18	v	183/183 (100%)	183 (100%)	0	100	100
19	2	154/156 (99%)	154 (100%)	0	100	100
20	9	141/141 (100%)	141 (100%)	0	100	100
All	All	6567/6619 (99%)	6567 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (69) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	ASN
1	A	94	HIS
1	A	225	ASN
1	A	296	HIS
1	A	425	ASN
1	A	637	GLN
2	B	54	GLN
2	B	179	HIS
2	B	197	HIS
2	B	376	HIS
2	B	453	GLN
2	B	505	ASN
2	B	586	ASN
2	B	628	ASN
2	B	705	GLN
4	D	108	GLN

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Mol	Chain	Res	Type
6	F	198	GLN
12	1	140	GLN
12	1	191	HIS
12	Z	191	HIS
13	3	47	ASN
13	3	145	GLN
13	3	204	GLN
13	3	215	ASN
13	3	225	ASN
13	3	226	ASN
14	7	207	GLN
14	7	218	ASN
15	8	230	HIS
16	4	175	ASN
16	4	232	GLN
16	4	243	ASN
17	5	230	ASN
18	6	206	GLN
19	2	59	ASN
20	9	109	GLN
1	a	20	ASN
1	a	80	GLN
1	a	219	HIS
1	a	539	HIS
1	a	637	GLN
1	a	705	ASN
2	b	54	GLN
2	b	115	ASN
2	b	352	HIS
2	b	491	GLN
2	b	504	ASN
2	b	586	ASN
4	d	108	GLN
4	d	127	GLN
4	d	162	ASN
5	e	64	GLN
6	f	198	GLN
9	j	30	ASN
10	k	35	ASN
12	p	52	ASN
12	p	140	GLN
12	z	52	ASN

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Mol	Chain	Res	Type
13	q	225	ASN
13	q	231	ASN
14	r	162	ASN
14	r	207	GLN
14	r	218	ASN
15	s	139	GLN
16	t	258	GLN
17	u	108	ASN
17	u	225	ASN
17	u	230	ASN
18	v	140	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	SNC	D	137	4	4,7,8	1.07	0	2,7,9	2.28	1 (50%)
4	SNC	d	137	4	4,7,8	1.01	0	2,7,9	2.07	1 (50%)

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
4	SNC	D	137	4	-	0/0/6/8	-
4	SNC	d	137	4	-	0/0/6/8	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	137	SNC	CA-CB-SG	-3.17	105.24	112.49
4	d	137	SNC	CA-CB-SG	-2.84	105.97	112.49

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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](#)

There are no chain breaks in this entry.

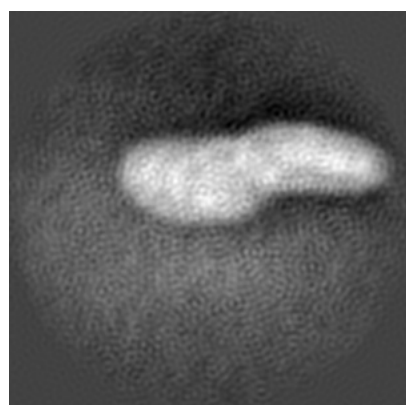
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12672. These allow visual inspection of the internal detail of the map and identification of artifacts.

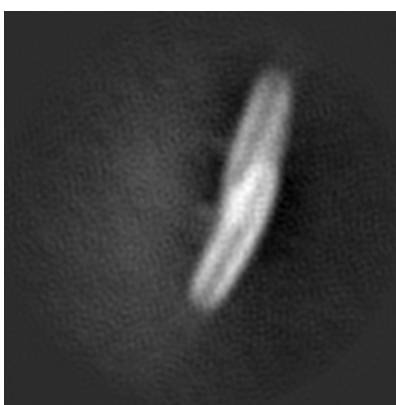
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

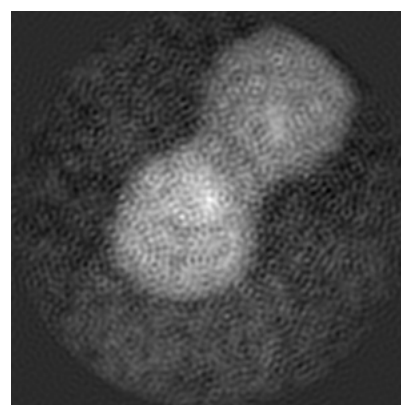
6.1.1 Primary map



X



Y

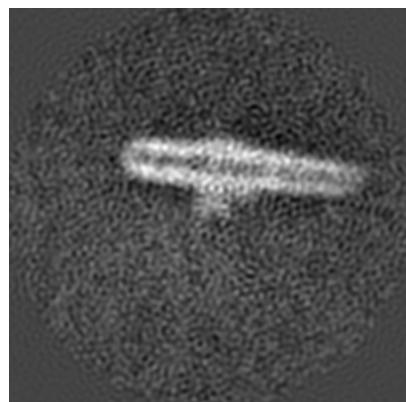


Z

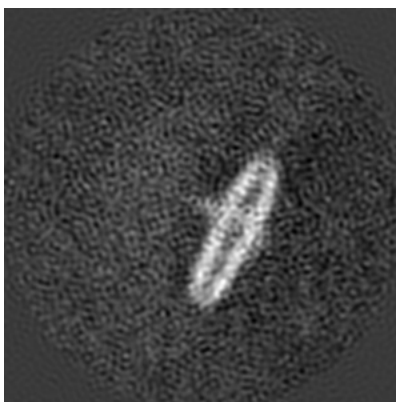
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

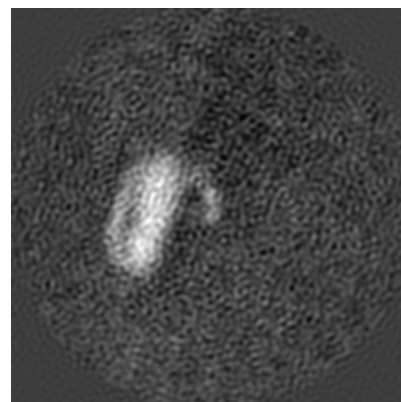
6.2.1 Primary map



X Index: 100



Y Index: 100

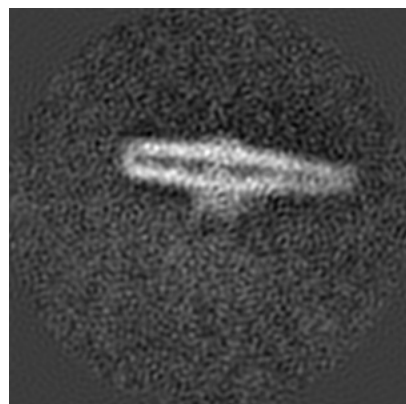


Z Index: 100

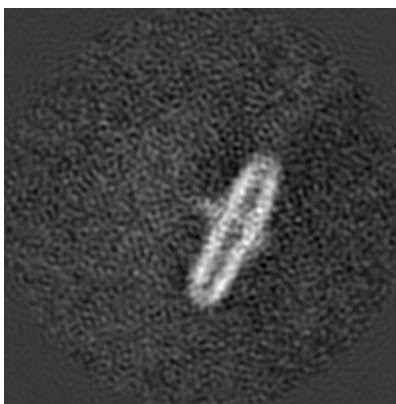
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

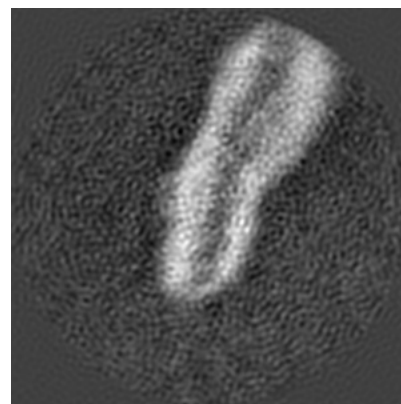
6.3.1 Primary map



X Index: 98



Y Index: 99

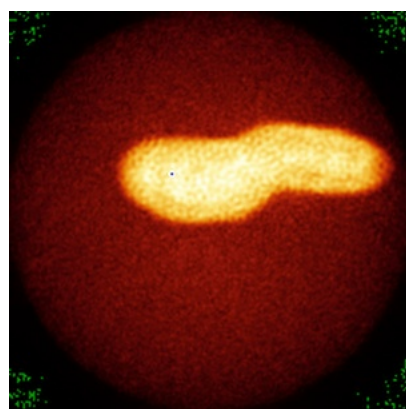


Z Index: 123

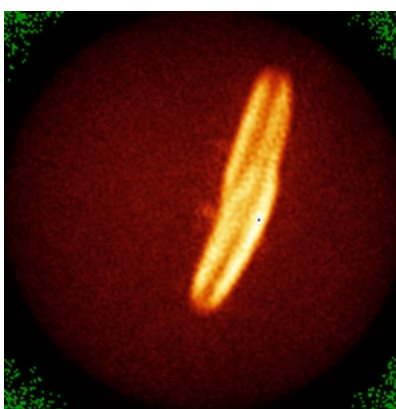
The images above show the largest variance slices of the map in three orthogonal directions.

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

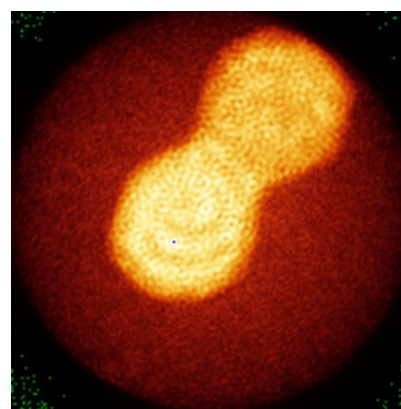
6.4.1 Primary map



X



Y

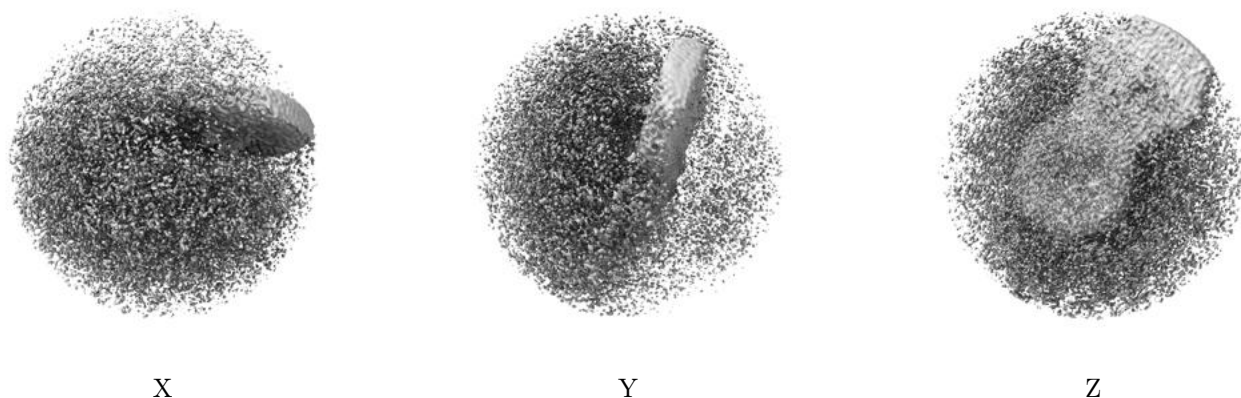


Z

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

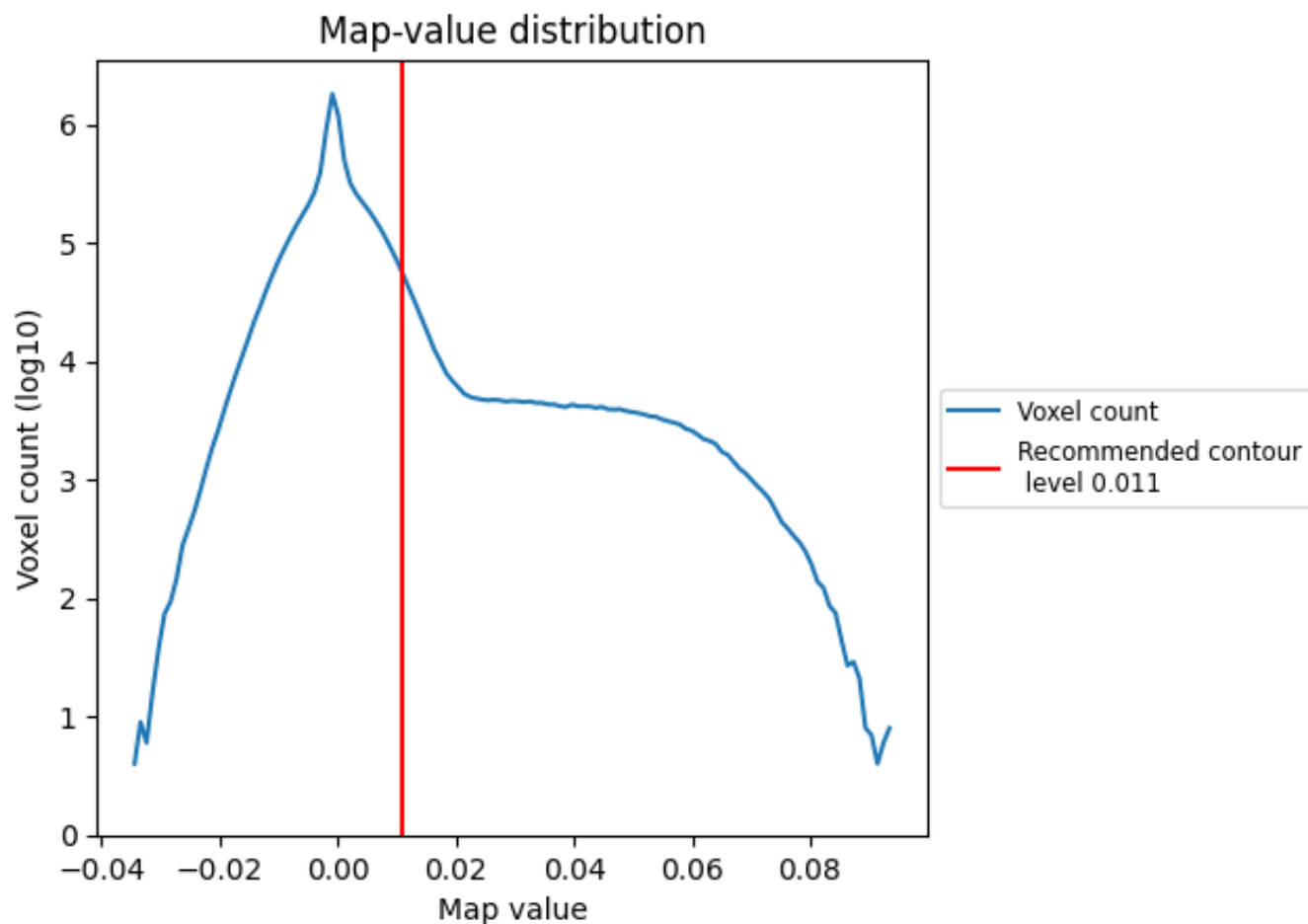
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

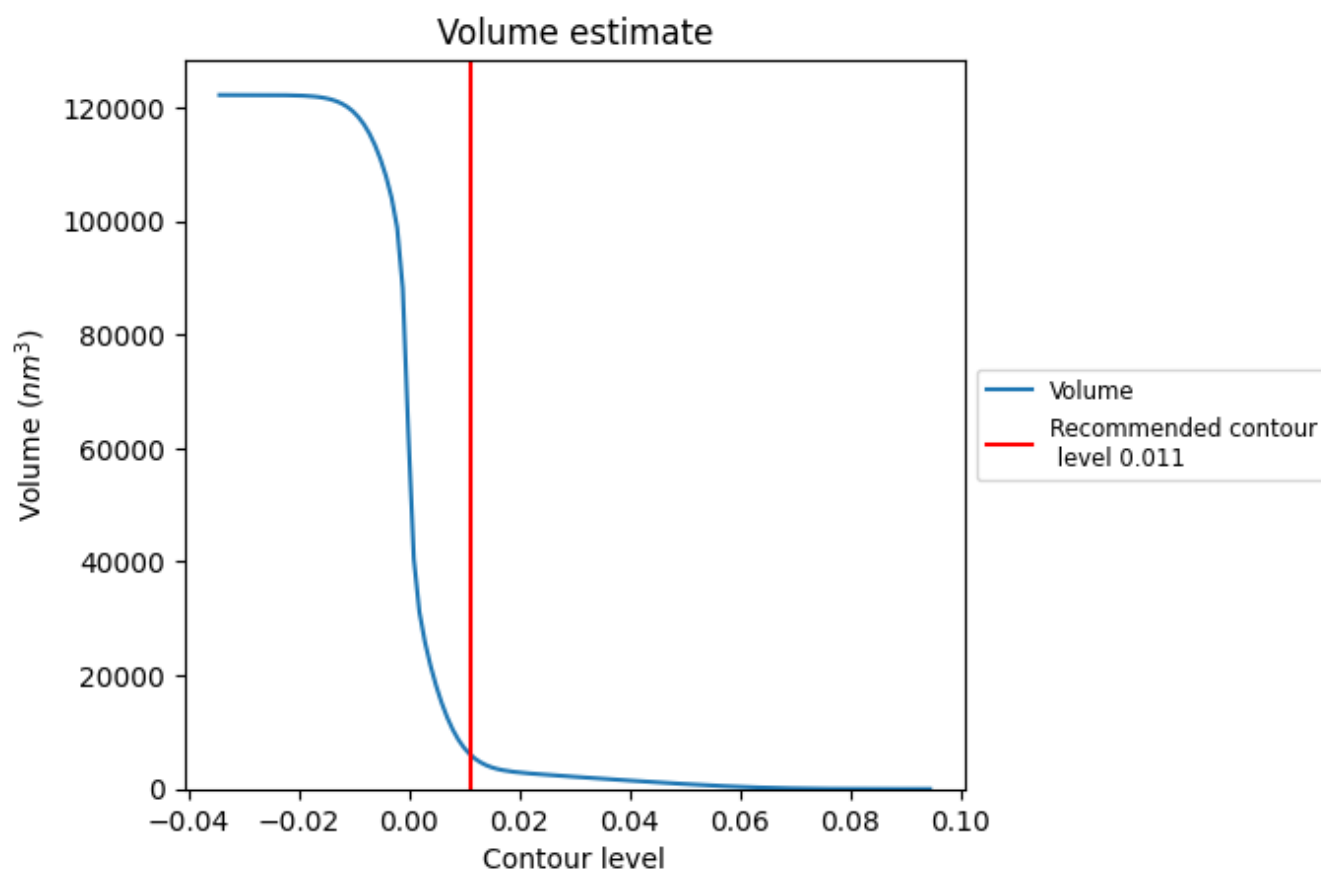
This section contains the results of statistical analysis of the map.

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.

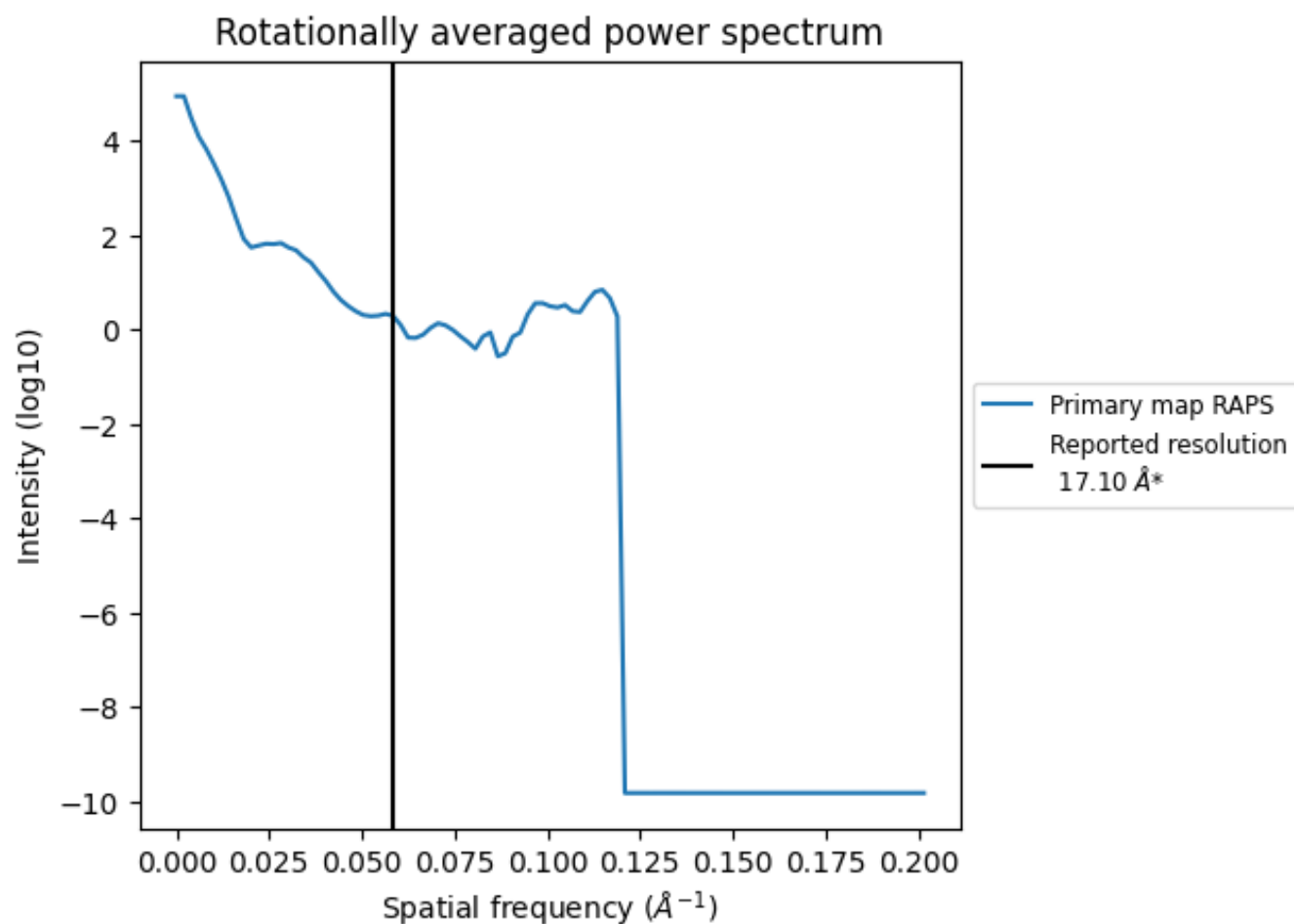
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 6120 nm^3 ; this corresponds to an approximate mass of 5529 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 ⓘ

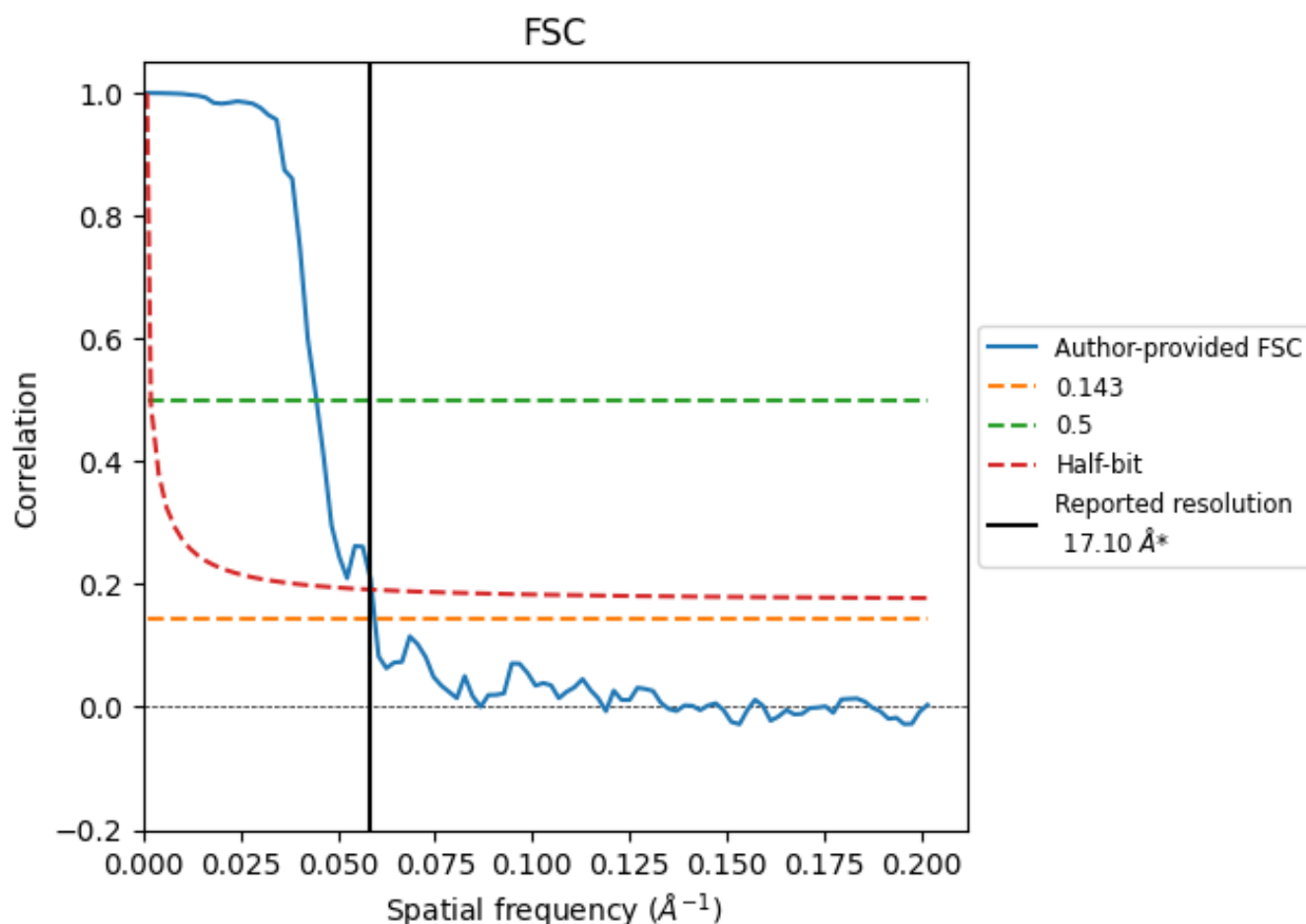


*Reported resolution corresponds to spatial frequency of 0.058 Å⁻¹

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 0.058 Å⁻¹

8.2 Resolution estimates [i](#)

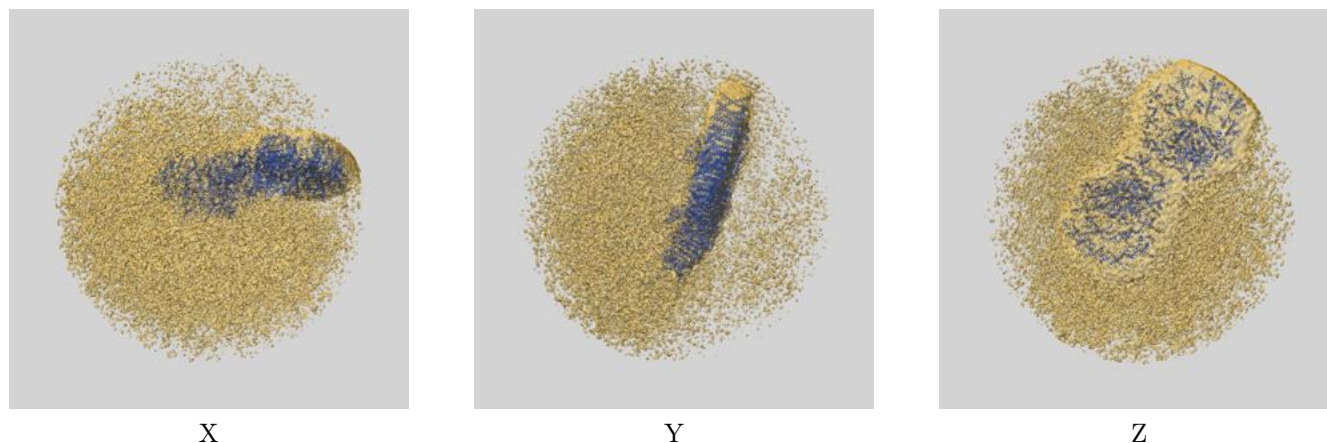
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	17.10	-	-
Author-provided FSC curve	16.81	22.47	17.04
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

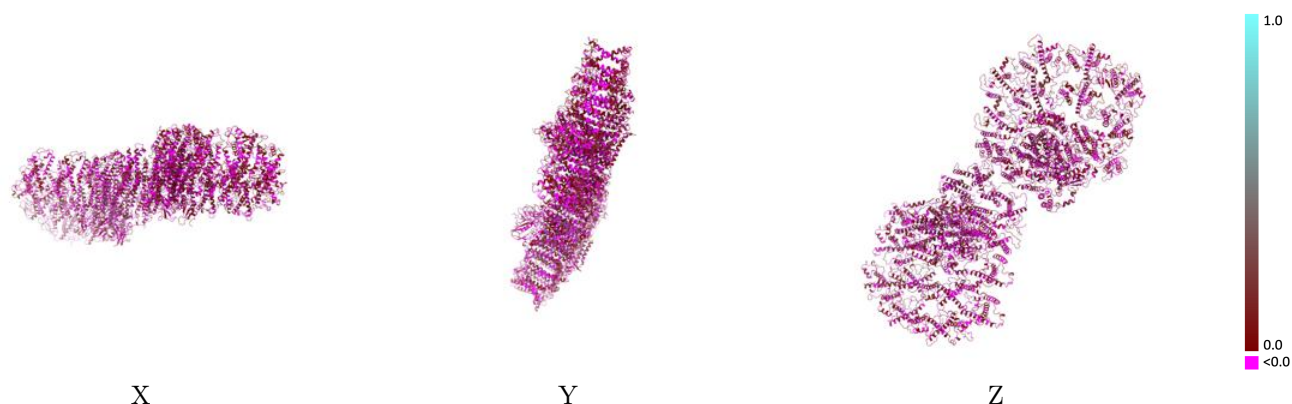
This section contains information regarding the fit between EMDB map EMD-12672 and PDB model 7O01. Per-residue inclusion information can be found in section [3](#) on page [9](#).

9.1 Map-model overlay [i](#)



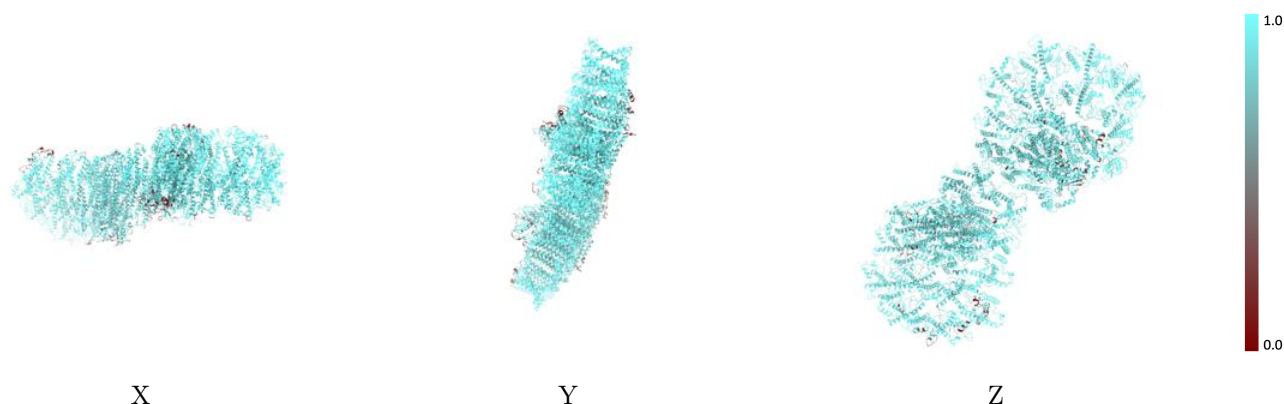
The images above show the 3D surface view of the map at the recommended contour level 0.011 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



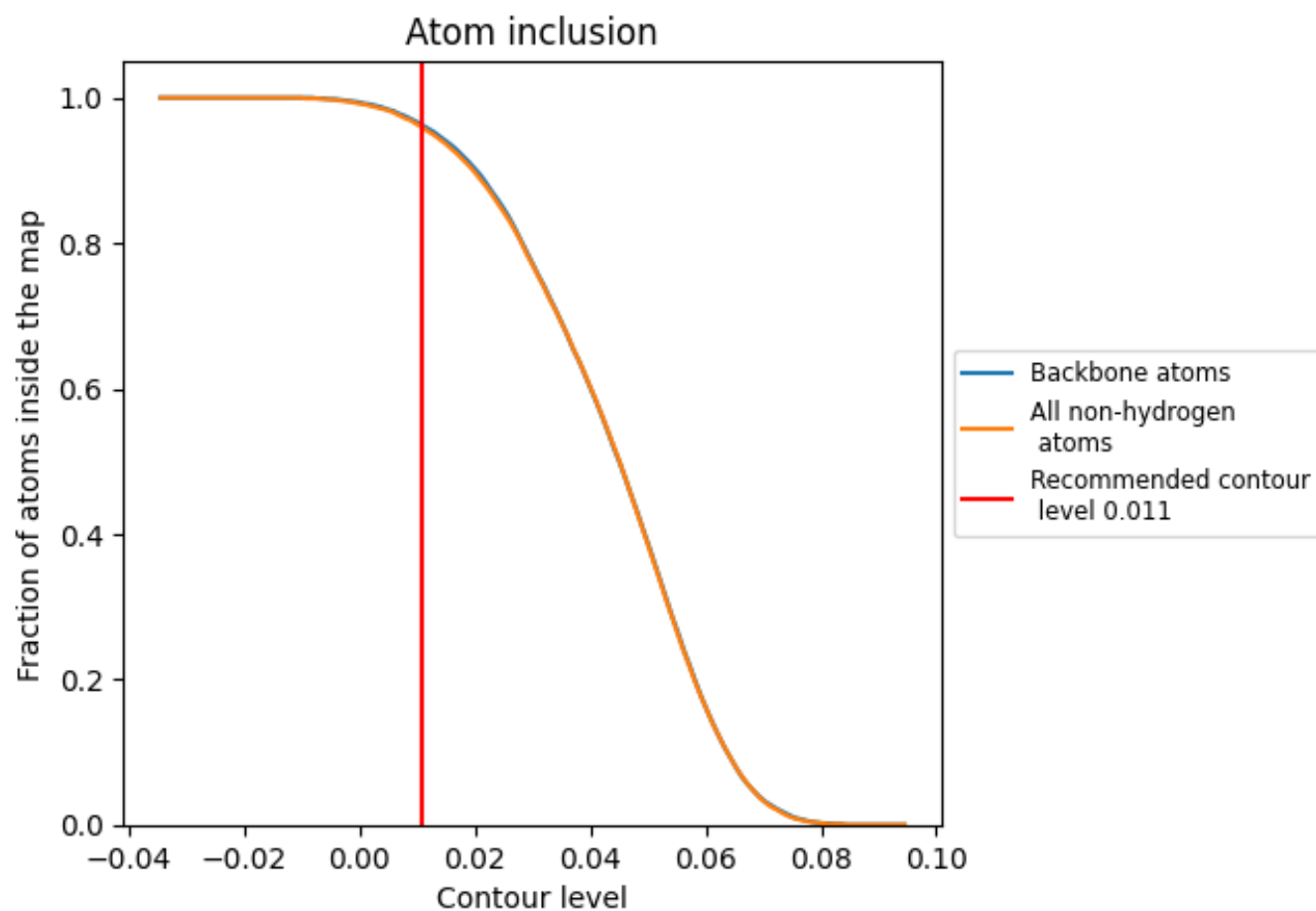
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.011).

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 96% 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 (0.011) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9590	 0.0360
1	 0.9860	 0.0350
2	 0.9870	 0.0500
3	 0.9470	 0.0180
4	 0.9060	 0.0240
5	 0.9710	 0.0460
6	 0.9670	 0.0370
7	 0.9960	 0.0500
8	 0.9830	 0.0320
9	 0.9740	 0.0380
A	 0.9800	 0.0340
B	 0.9770	 0.0230
C	 0.9050	 -0.0090
D	 0.7990	 0.0210
E	 0.9810	 0.0240
F	 0.9390	 0.0300
G	 0.9960	 0.0270
I	 0.9820	 0.0380
J	 1.0000	 0.0610
K	 0.8820	 -0.0110
L	 0.9610	 0.0090
Z	 0.8740	 0.0260
a	 0.9600	 0.0400
b	 0.9780	 0.0280
c	 0.7210	 -0.0380
d	 0.6350	 0.0210
e	 0.8970	 0.0470
f	 0.9480	 0.0410
g	 1.0000	 0.0370
i	 0.9710	 0.0500
j	 1.0000	 0.0550
k	 0.9950	 0.0290
l	 0.9690	 0.0440
p	 0.9830	 0.0690
q	 0.9950	 0.0620



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Chain	Atom inclusion	Q-score
r	 0.9890	 0.0490
s	 0.9930	 0.0550
t	 0.9890	 0.0590
u	 0.9770	 0.0510
v	 0.9930	 0.0450
z	 0.9620	 0.0580