



Full wwPDB EM Validation Report ⓘ

Nov 8, 2022 – 05:57 AM JST

PDB ID : 5Y5Z
EMDB ID : EMD-6812
Title : V/A-type ATPase/synthase from *Thermus thermophilus*, rotational state 2
Authors : Nakanishi, A.; Kishikawa, J.; Tamakoshi, M.; Mitsuoka, K.; Yokoyama, K.
Deposited on : 2017-08-10
Resolution : 6.70 Å(reported)

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:

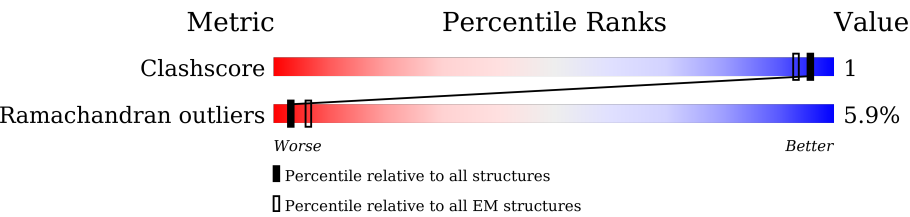
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

1 Overall quality at a glance i

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

The reported resolution of this entry is 6.70 Å.

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



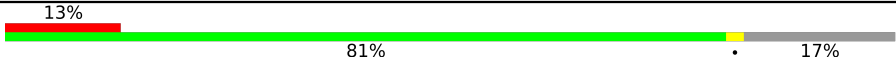
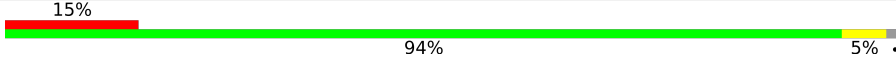
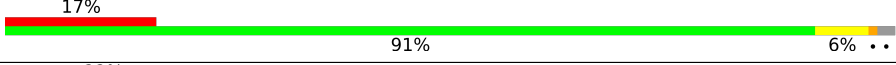
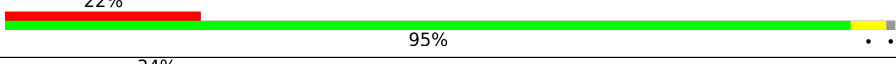
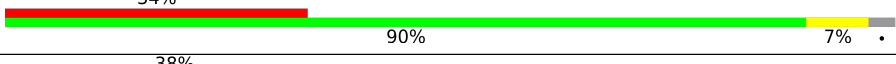

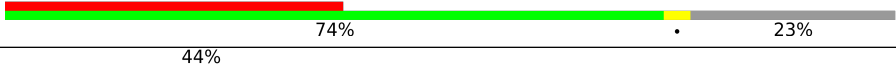

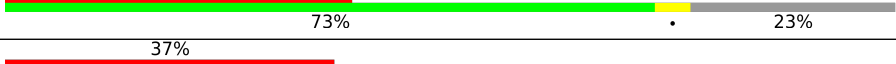


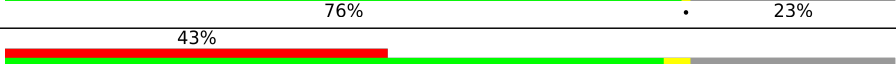

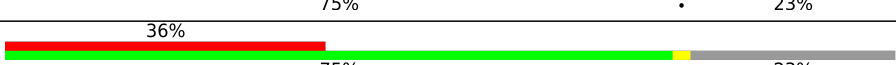

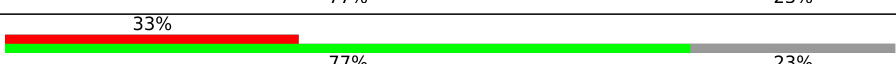
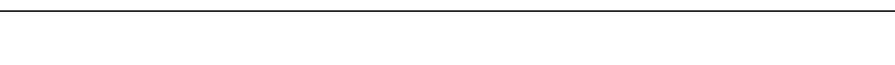
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023

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	578	<div><div>7%</div><div>89%</div><div>11%</div></div>
1	B	578	<div><div>89%</div><div>10%</div><div></div></div>
1	C	578	<div><div>88%</div><div>12%</div><div></div></div>
2	D	478	<div><div>7%</div><div>84%</div><div>12%</div><div></div></div>
2	E	478	<div><div>5%</div><div>83%</div><div>13%</div><div></div></div>
2	F	478	<div><div>81%</div><div>15%</div><div></div></div>
3	G	223	<div><div>14%</div><div>78%</div><div>15%</div><div>6%</div></div>
4	H	104	<div><div>18%</div><div>84%</div><div>8%</div><div>5%</div></div>
5	I	120	<div><div>22%</div><div>82%</div><div></div><div>17%</div></div>

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Mol	Chain	Length	Quality of chain
5	K	120	
6	J	188	
6	L	188	
7	M	323	
8	N	652	
9	O	99	
9	P	99	
9	Q	99	
9	R	99	
9	S	99	
9	T	99	
9	U	99	
9	V	99	
9	W	99	
9	X	99	
9	Y	99	
9	Z	99	

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 23433 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 V-type ATP synthase alpha chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	577	Total	C	N	O	0	0
			2307	1154	577	576		
1	B	577	Total	C	N	O	0	0
			2307	1154	577	576		
1	C	577	Total	C	N	O	0	0
			2307	1154	577	576		

- Molecule 2 is a protein called V-type ATP synthase beta chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	D	459	Total	C	N	O	0	0
			1835	918	459	458		
2	E	459	Total	C	N	O	0	0
			1835	918	459	458		
2	F	459	Total	C	N	O	0	0
			1835	918	459	458		

- Molecule 3 is a protein called V-type ATP synthase subunit D.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	G	210	Total	C	N	O	0	0
			839	420	210	209		

- Molecule 4 is a protein called V-type ATP synthase subunit F.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	H	100	Total	C	N	O	0	0
			399	200	100	99		

- Molecule 5 is a protein called V-type ATP synthase, subunit (VAPC-THERM).

Mol	Chain	Residues	Atoms				AltConf	Trace
5	I	100	Total	C	N	O	0	0
			399	200	100	99		
5	K	100	Total	C	N	O	0	0
			399	200	100	99		

- Molecule 6 is a protein called V-type ATP synthase subunit E.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	J	185	Total	C	N	O	0	0
			738	370	185	183		
6	L	185	Total	C	N	O	0	0
			738	370	185	183		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	134	MET	LEU	conflict	UNP P74901
J	171	MET	LEU	conflict	UNP P74901
J	178	MET	LEU	conflict	UNP P74901
L	134	MET	LEU	conflict	UNP P74901
L	171	MET	LEU	conflict	UNP P74901
L	178	MET	LEU	conflict	UNP P74901

- Molecule 7 is a protein called V-type ATP synthase subunit C.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	M	320	Total	C	N	O	0	0
			1279	640	320	319		

- Molecule 8 is a protein called V-type ATP synthase subunit I.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	N	632	Total	C	N	O	0	0
			2526	1264	632	630		

- Molecule 9 is a protein called V-type ATP synthase, subunit K.

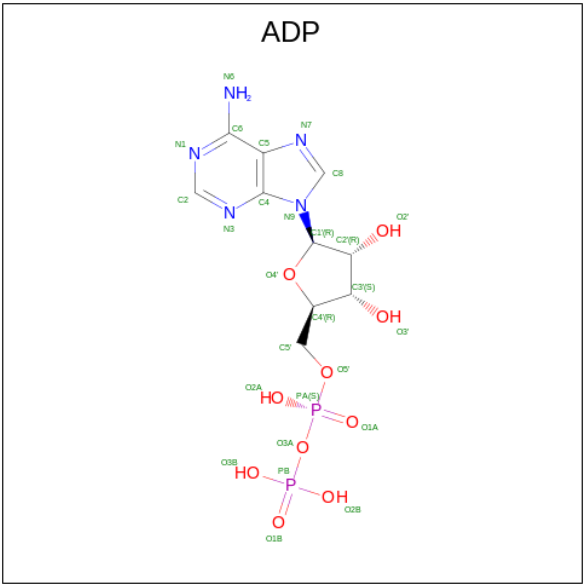
Mol	Chain	Residues	Atoms				AltConf	Trace
9	O	76	Total	C	N	O	0	0
			303	152	76	75		
9	P	76	Total	C	N	O	0	0
			303	152	76	75		

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Mol	Chain	Residues	Atoms				AltConf	Trace
9	Q	76	Total	C	N	O	0	0
			303	152	76	75		
9	R	76	Total	C	N	O	0	0
			303	152	76	75		
9	S	76	Total	C	N	O	0	0
			303	152	76	75		
9	T	76	Total	C	N	O	0	0
			303	152	76	75		
9	U	76	Total	C	N	O	0	0
			303	152	76	75		
9	V	76	Total	C	N	O	0	0
			303	152	76	75		
9	W	76	Total	C	N	O	0	0
			303	152	76	75		
9	X	76	Total	C	N	O	0	0
			303	152	76	75		
9	Y	76	Total	C	N	O	0	0
			303	152	76	75		
9	Z	76	Total	C	N	O	0	0
			303	152	76	75		

- Molecule 10 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms				AltConf
10	B	1	Total	C	N	O	P
			27	10	5	10	2

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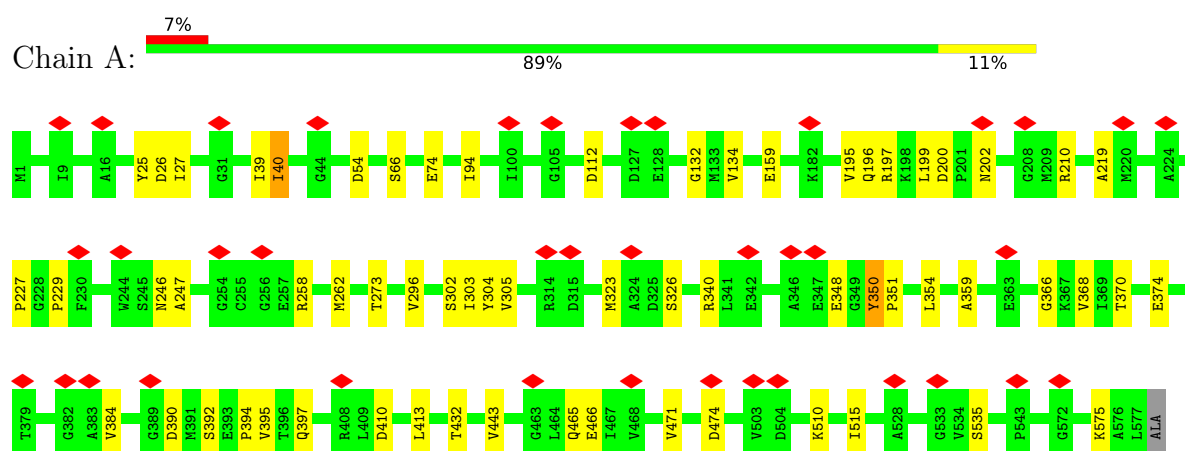
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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
10	C	1	27	10	5	10	2	0

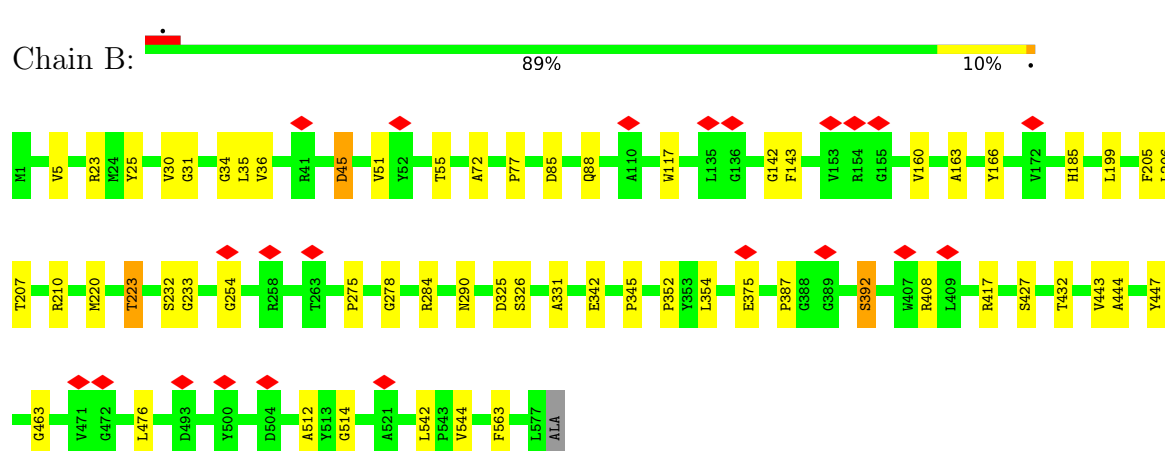
3 Residue-property plots

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.

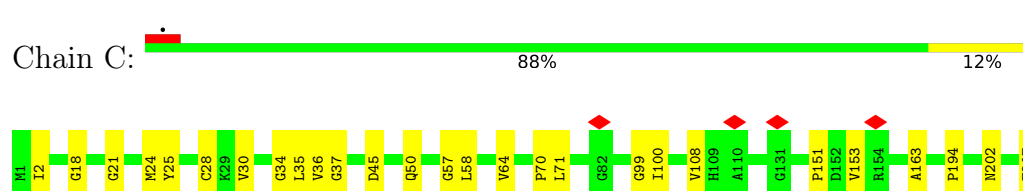
- Molecule 1: V-type ATP synthase alpha chain

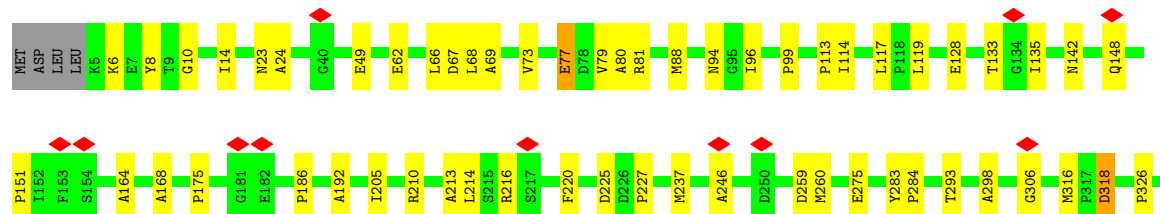


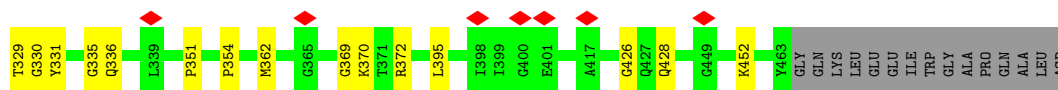
- Molecule 1: V-type ATP synthase alpha chain



- Molecule 1: V-type ATP synthase alpha chain

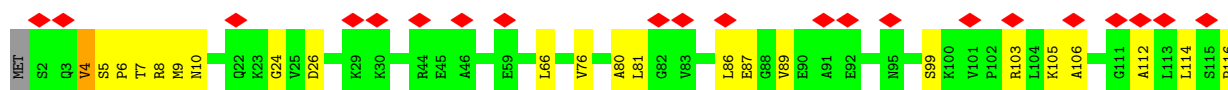






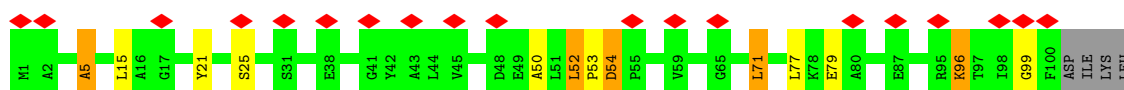
- Molecule 3: V-type ATP synthase subunit D

Chain G: 14% 78% 15% 6%



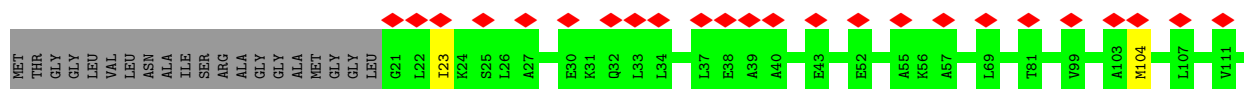
- Molecule 4: V-type ATP synthase subunit F

Chain H: 18% 84% 8% 5%



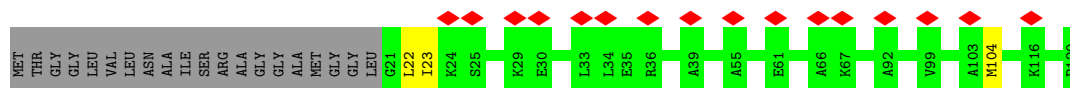
- Molecule 5: V-type ATP synthase, subunit (VAPC-THERM)

Chain I: 22% 82% 17%



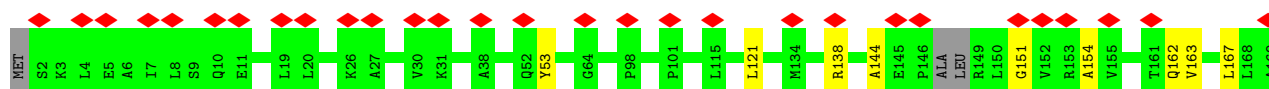
- Molecule 5: V-type ATP synthase, subunit (VAPC-THERM)

Chain K: 13% 81% 17%



- Molecule 6: V-type ATP synthase subunit E

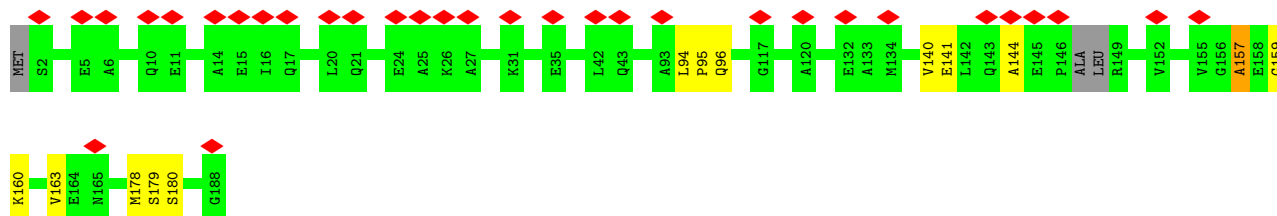
Chain J: 15% 94% 5%





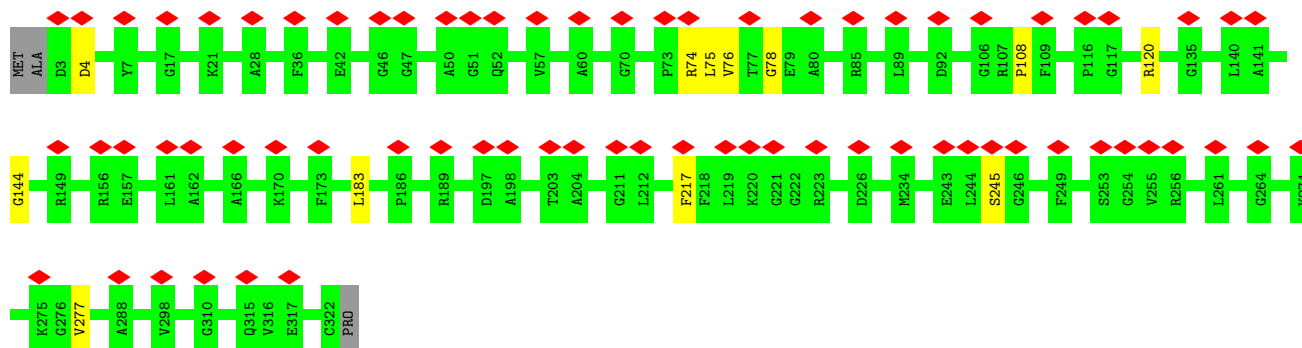
- Molecule 6: V-type ATP synthase subunit E

Chain L: 17% 91% 6% ..



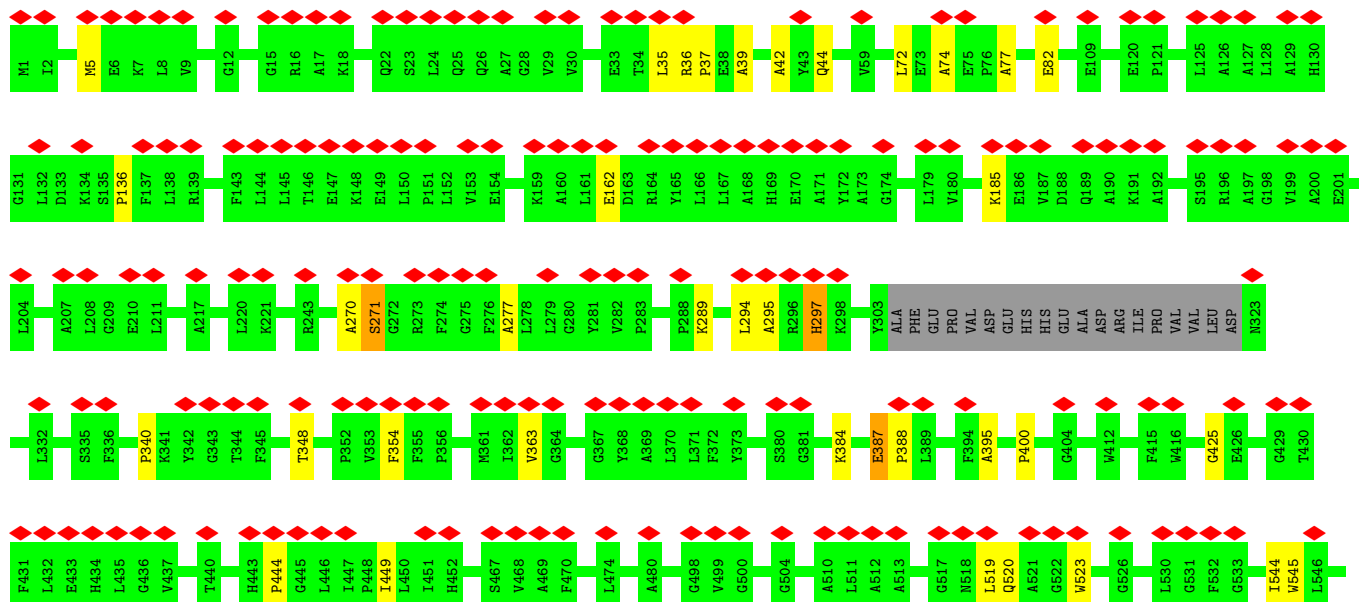
- Molecule 7: V-type ATP synthase subunit C

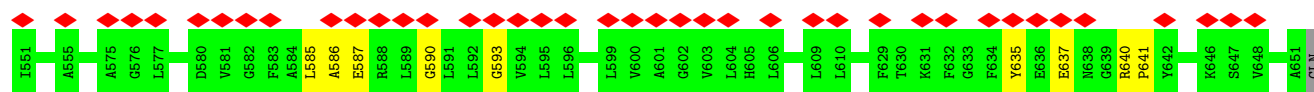
Chain M: 22% 95% ..



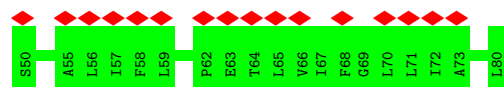
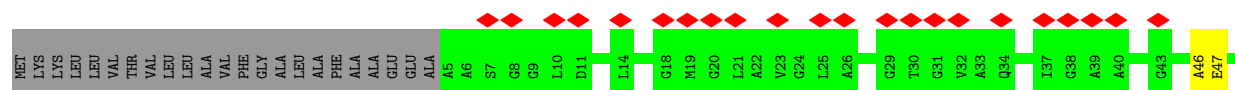
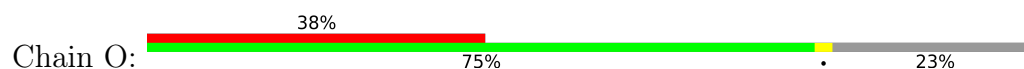
- Molecule 8: V-type ATP synthase subunit I

Chain N: 34% 90% 7% .

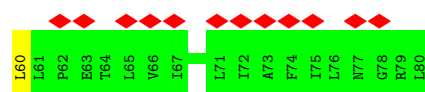
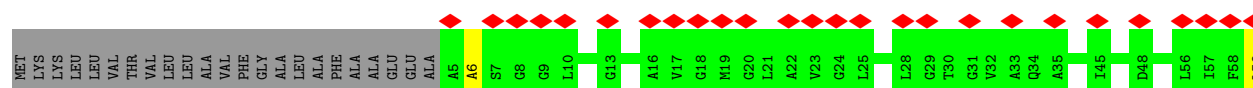
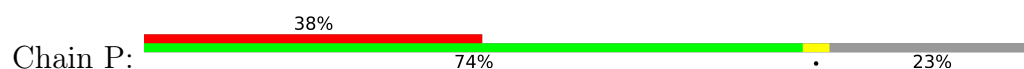




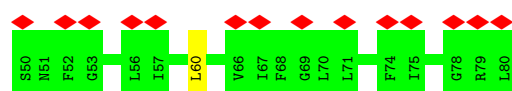
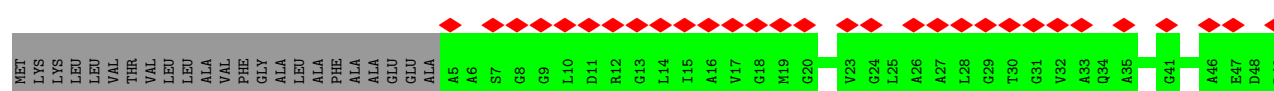
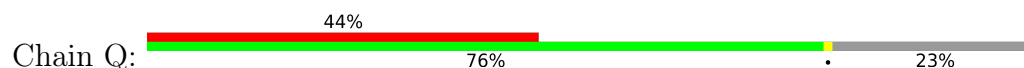
• Molecule 9: V-type ATP synthase, subunit K



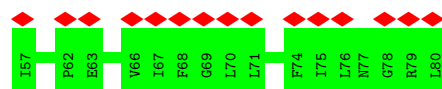
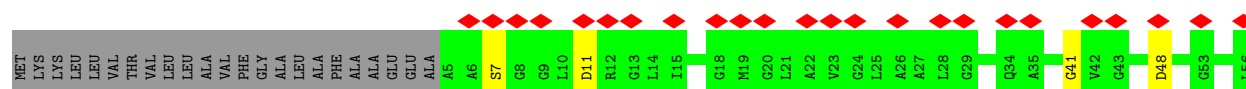
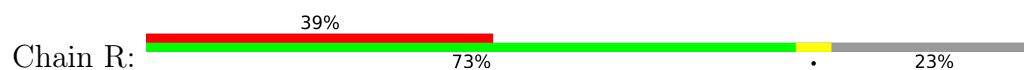
• Molecule 9: V-type ATP synthase, subunit K



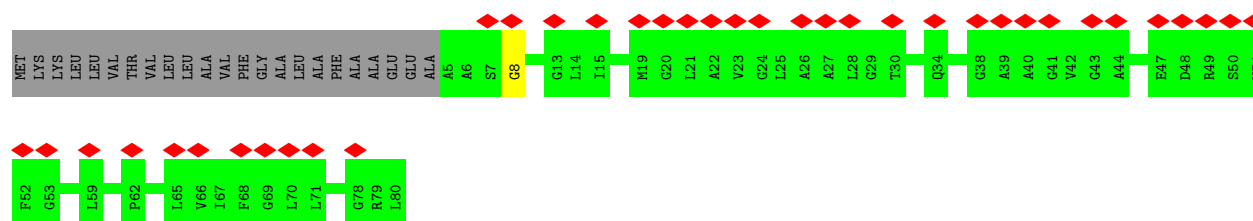
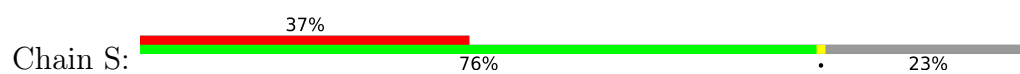
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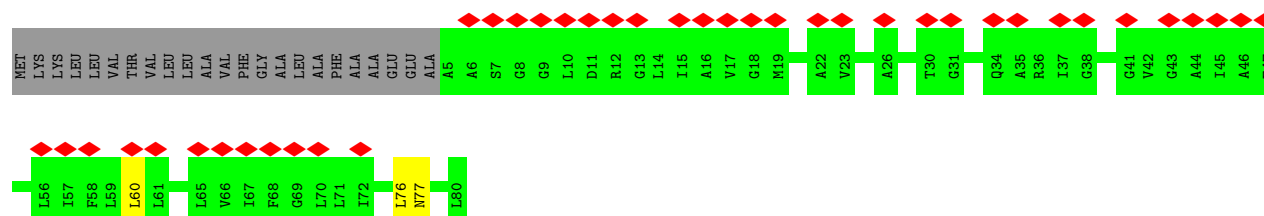
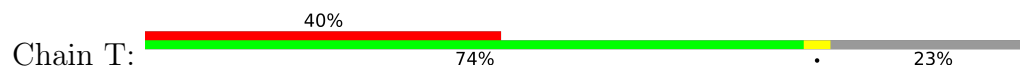
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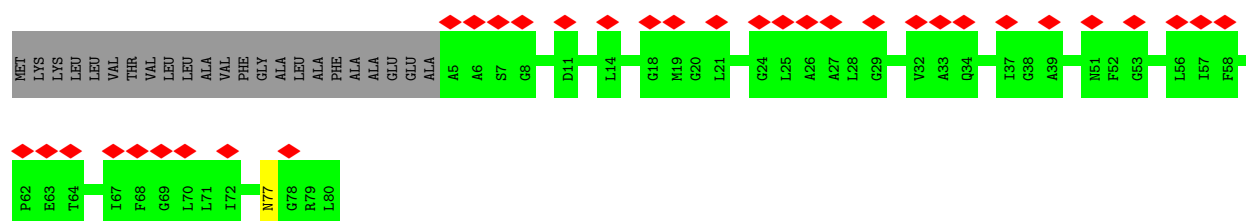
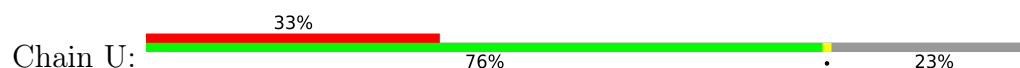
• Molecule 9: V-type ATP synthase, subunit K



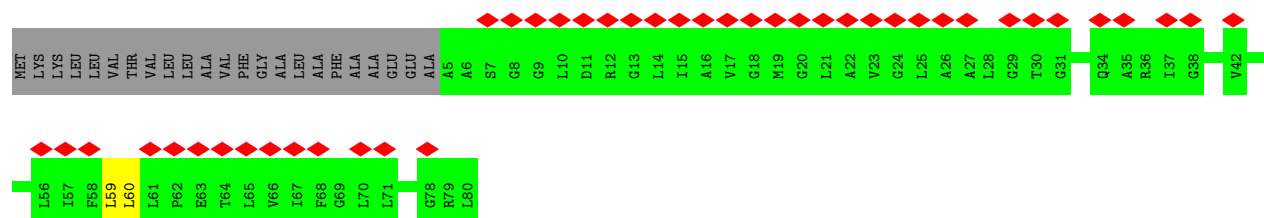
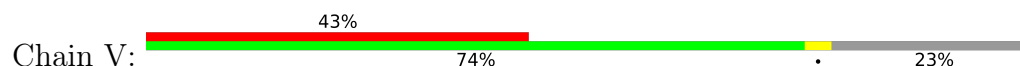
- Molecule 9: V-type ATP synthase, subunit K



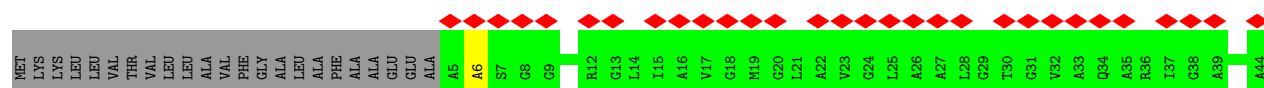
- Molecule 9: V-type ATP synthase, subunit K

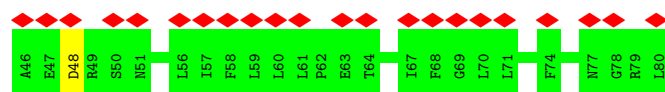


- Molecule 9: V-type ATP synthase, subunit K

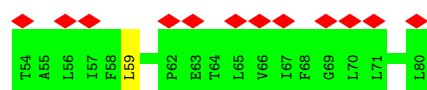
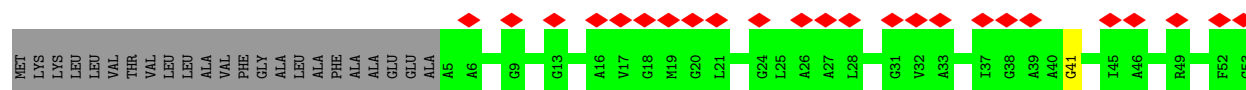
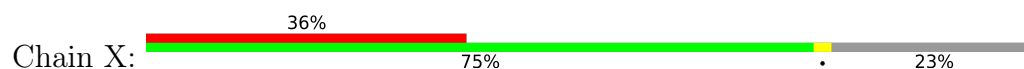


- Molecule 9: V-type ATP synthase, subunit K

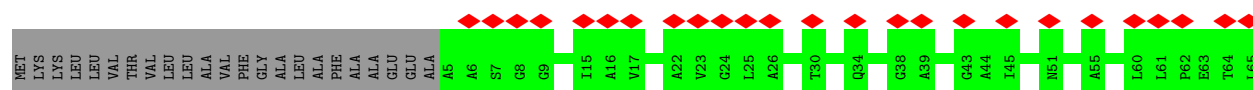
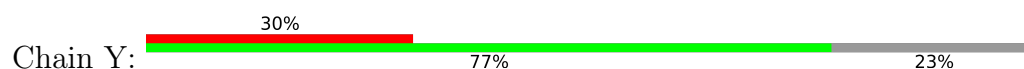




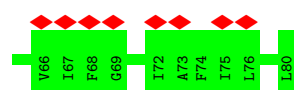
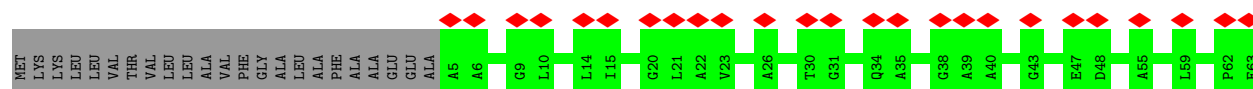
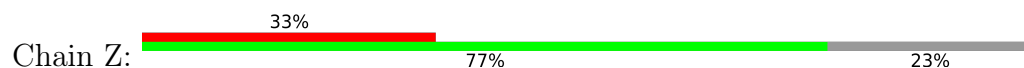
- Molecule 9: V-type ATP synthase, subunit K



- Molecule 9: V-type ATP synthase, subunit K



- Molecule 9: V-type ATP synthase, subunit K



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	30802	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 ($e^-/\text{\AA}^2$)	26	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.518	Depositor
Minimum map value	-0.322	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.026	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	330.4, 330.4, 330.4	wwPDB
Map dimensions	236, 236, 236	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.4, 1.4, 1.4	Depositor

5 Model quality

5.1 Standard geometry

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

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	1.33	0/2306	1.25	3/2881 (0.1%)
1	B	1.39	0/2306	1.25	7/2881 (0.2%)
1	C	1.36	0/2306	1.21	3/2881 (0.1%)
2	D	1.32	0/1834	1.27	2/2291 (0.1%)
2	E	1.40	0/1834	1.24	4/2291 (0.2%)
2	F	1.42	0/1834	1.28	7/2291 (0.3%)
3	G	1.31	0/838	1.30	4/1046 (0.4%)
4	H	1.18	0/398	1.21	0/496
5	I	0.91	0/398	0.96	0/496
5	K	1.03	0/398	1.00	1/496 (0.2%)
6	J	1.06	0/736	1.04	1/917 (0.1%)
6	L	1.08	0/736	1.03	0/917
7	M	1.06	0/1278	0.93	0/1596
8	N	1.05	0/2524	1.09	0/3152
9	O	0.86	0/302	0.96	0/376
9	P	0.86	0/302	1.05	0/376
9	Q	0.85	0/302	0.96	0/376
9	R	0.85	0/302	0.97	0/376
9	S	0.85	0/302	1.00	0/376
9	T	0.80	0/302	1.00	0/376
9	U	0.83	0/302	1.00	0/376
9	V	0.80	0/302	0.95	0/376
9	W	0.81	0/302	1.07	0/376
9	X	0.84	0/302	1.03	0/376
9	Y	0.84	0/302	0.97	0/376
9	Z	0.87	0/302	0.93	0/376
All	All	1.21	0/23350	1.16	32/29144 (0.1%)

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

sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	14
1	B	0	15
1	C	0	21
2	D	0	10
2	E	0	17
2	F	0	16
3	G	0	7
4	H	0	5
6	J	0	1
6	L	0	6
7	M	0	4
8	N	0	14
9	O	0	2
9	P	0	2
9	Q	0	1
9	R	0	2
9	T	0	2
9	V	0	3
9	X	0	2
All	All	0	144

There are no bond length outliers.

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	185	HIS	C-N-CA	7.83	141.27	121.70
1	A	465	GLN	C-N-CA	6.30	137.46	121.70
1	B	232	SER	C-N-CA	6.23	135.39	122.30
3	G	4	VAL	N-CA-C	-6.21	94.23	111.00
3	G	105	LYS	N-CA-C	-6.17	94.34	111.00
2	F	335	GLY	N-CA-C	-6.04	98.00	113.10
1	C	99	GLY	N-CA-C	-6.02	98.05	113.10
2	E	256	ILE	N-CA-C	-5.91	95.04	111.00
1	B	72	ALA	N-CA-C	-5.88	95.13	111.00
6	J	53	TYR	N-CA-C	-5.72	95.54	111.00
2	D	451	LEU	N-CA-C	-5.69	95.64	111.00
1	B	160	VAL	N-CA-C	-5.68	95.65	111.00
2	F	260	MET	C-N-CA	5.61	135.72	121.70
2	F	142	ASN	N-CA-C	-5.56	95.99	111.00
2	F	220	PHE	N-CA-C	-5.51	96.12	111.00
2	E	140	VAL	N-CA-C	-5.49	96.19	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	273	THR	N-CA-C	-5.41	96.39	111.00
2	E	255	VAL	N-CA-C	-5.40	96.42	111.00
2	D	136	SER	C-N-CA	5.38	135.14	121.70
1	B	447	TYR	N-CA-C	-5.36	96.52	111.00
2	E	21	VAL	N-CA-C	-5.34	96.59	111.00
1	A	410	ASP	C-N-CA	5.33	135.02	121.70
1	B	205	PHE	N-CA-C	-5.28	96.73	111.00
1	C	2	ILE	N-CA-C	-5.24	96.85	111.00
1	B	143	PHE	C-N-CA	5.23	134.77	121.70
3	G	9	MET	C-N-CA	5.19	134.69	121.70
1	C	419	PHE	N-CA-C	-5.12	97.19	111.00
2	F	428	GLN	N-CA-C	-5.09	97.25	111.00
2	F	77	GLU	C-N-CA	5.09	134.41	121.70
5	K	22	LEU	C-N-CA	5.05	134.32	121.70
2	F	77	GLU	CA-C-N	-5.02	106.17	117.20
3	G	103	ARG	N-CA-C	-5.01	97.47	111.00

There are no chirality outliers.

All (144) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	112	ASP	Peptide
1	A	200	ASP	Peptide
1	A	258	ARG	Peptide
1	A	262	MET	Peptide
1	A	323	MET	Peptide
1	A	326	SER	Peptide
1	A	350	TYR	Peptide
1	A	366	GLY	Peptide
1	A	368	VAL	Peptide
1	A	384	VAL	Peptide
1	A	392	SER	Peptide
1	A	40	ILE	Peptide
1	A	575	LYS	Peptide
1	A	94	ILE	Peptide
1	B	142	GLY	Peptide
1	B	199	LEU	Peptide
1	B	206	LEU	Peptide
1	B	220	MET	Peptide
1	B	223	THR	Peptide
1	B	254	GLY	Peptide
1	B	290	ASN	Peptide

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Mol	Chain	Res	Type	Group
1	B	31	GLY	Peptide
1	B	325	ASP	Peptide
1	B	34	GLY	Peptide
1	B	345	PRO	Peptide
1	B	352	PRO	Peptide
1	B	392	SER	Peptide
1	B	45	ASP	Peptide
1	B	55	THR	Peptide
1	C	108	VAL	Peptide
1	C	18	GLY	Peptide
1	C	209	MET	Peptide
1	C	213	ASP	Peptide
1	C	237	THR	Peptide
1	C	238	GLN	Peptide
1	C	254	GLY	Peptide
1	C	272	LEU	Peptide
1	C	291	THR	Peptide
1	C	318	PHE	Peptide
1	C	320	VAL	Peptide
1	C	34	GLY	Peptide
1	C	351	PRO	Peptide
1	C	391	MET	Peptide
1	C	415	PHE	Peptide
1	C	417	ARG	Peptide
1	C	436	ASP	Peptide
1	C	441	GLU	Peptide
1	C	477	GLN	Peptide
1	C	50	GLN	Peptide
1	C	506	TYR	Peptide
2	D	129	GLN	Peptide
2	D	145	VAL	Peptide
2	D	153	PHE	Peptide
2	D	160	ALA	Peptide
2	D	25	LYS	Peptide
2	D	286	TYR	Peptide
2	D	319	ASP	Peptide
2	D	404	LEU	Peptide
2	D	59	VAL	Peptide
2	D	8	TYR	Peptide
2	E	158	LEU	Peptide
2	E	160	ALA	Peptide
2	E	175	PRO	Peptide

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Mol	Chain	Res	Type	Group
2	E	214	LEU	Peptide
2	E	228	THR	Peptide
2	E	241	VAL	Peptide
2	E	25	LYS	Peptide
2	E	257	LEU	Peptide
2	E	271	GLY	Peptide
2	E	272	ALA	Peptide
2	E	319	ASP	Peptide
2	E	335	GLY	Peptide
2	E	346	LYS	Peptide
2	E	400	GLY	Peptide
2	E	401	GLU	Peptide
2	E	63	THR	Peptide
2	E	70	THR	Peptide
2	F	135	ILE	Peptide
2	F	14	ILE	Peptide
2	F	186	PRO	Peptide
2	F	192	ALA	Peptide
2	F	213	ALA	Peptide
2	F	214	LEU	Peptide
2	F	216	ARG	Peptide
2	F	225	ASP	Peptide
2	F	283	TYR	Peptide
2	F	316	MET	Peptide
2	F	318	ASP	Peptide
2	F	369	GLY	Peptide
2	F	426	GLY	Peptide
2	F	6	LYS	Peptide
2	F	81	ARG	Peptide
2	F	94	ASN	Peptide
3	G	106	ALA	Peptide
3	G	119	THR	Peptide
3	G	120	PRO	Peptide
3	G	24	GLY	Peptide
3	G	26	ASP	Peptide
3	G	5	SER	Peptide
3	G	76	VAL	Peptide
4	H	5	ALA	Peptide
4	H	54	ASP	Peptide
4	H	71	LEU	Peptide
4	H	96	LYS	Peptide
4	H	99	GLY	Peptide

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Mol	Chain	Res	Type	Group
6	J	162	GLN	Peptide
6	L	141	GLU	Peptide
6	L	144	ALA	Peptide
6	L	157	ALA	Peptide
6	L	159	GLY	Peptide
6	L	178	MET	Peptide
6	L	94	LEU	Peptide
7	M	120	ARG	Peptide
7	M	183	LEU	Peptide
7	M	74	ARG	Peptide
7	M	75	LEU	Peptide
8	N	271	SER	Peptide
8	N	289	LYS	Peptide
8	N	297	HIS	Peptide
8	N	340	PRO	Peptide
8	N	354	PHE	Peptide
8	N	384	LYS	Peptide
8	N	387	GLU	Peptide
8	N	44	GLN	Peptide
8	N	449	ILE	Peptide
8	N	5	MET	Peptide
8	N	587	GLU	Peptide
8	N	635	TYR	Peptide
8	N	641	PRO	Peptide
8	N	82	GLU	Peptide
9	O	46	ALA	Peptide
9	O	47	GLU	Peptide
9	P	59	LEU	Peptide
9	P	60	LEU	Peptide
9	Q	60	LEU	Peptide
9	R	41	GLY	Peptide
9	R	48	ASP	Peptide
9	T	60	LEU	Peptide
9	T	76	LEU	Peptide
9	V	48	ASP	Peptide
9	V	59	LEU	Peptide
9	V	60	LEU	Peptide
9	X	41	GLY	Peptide
9	X	59	LEU	Peptide

5.2 Too-close contacts ⓘ

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	2307	0	654	3	0
1	B	2307	0	654	3	0
1	C	2307	0	654	7	0
2	D	1835	0	512	4	0
2	E	1835	0	512	1	0
2	F	1835	0	512	5	0
3	G	839	0	230	1	0
4	H	399	0	119	1	0
5	I	399	0	100	0	0
5	K	399	0	100	0	0
6	J	738	0	192	2	0
6	L	738	0	192	0	0
7	M	1279	0	357	0	0
8	N	2526	0	709	1	0
9	O	303	0	102	0	0
9	P	303	0	102	0	0
9	Q	303	0	102	0	0
9	R	303	0	102	1	0
9	S	303	0	102	1	0
9	T	303	0	102	0	0
9	U	303	0	102	0	0
9	V	303	0	102	0	0
9	W	303	0	102	0	0
9	X	303	0	102	0	0
9	Y	303	0	102	0	0
9	Z	303	0	102	0	0
10	B	27	0	12	0	0
10	C	27	0	12	0	0
All	All	23433	0	6745	26	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 1.

All (26) 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)
2:D:95:GLY:H	2:D:221:LEU:H	1.38	0.69
1:A:26:ASP:H	1:A:39:ILE:H	1.44	0.65
1:C:30:VAL:H	1:C:35:LEU:H	1.49	0.59
6:J:151:GLY:HA2	6:J:167:LEU:H	1.67	0.58
1:B:30:VAL:H	1:B:35:LEU:H	1.52	0.58
6:J:151:GLY:CA	6:J:167:LEU:H	2.23	0.52
3:G:8:ARG:C	3:G:10:ASN:H	2.15	0.50
2:D:90:GLY:H	2:D:217:SER:H	1.61	0.49
9:R:11:ASP:H	9:S:8:GLY:HA2	1.78	0.49
1:C:21:GLY:HA2	2:F:68:LEU:H	1.77	0.48
1:C:24:MET:H	2:F:66:LEU:N	2.12	0.47
1:C:30:VAL:H	1:C:35:LEU:N	2.11	0.47
1:C:58:LEU:H	2:E:29:TYR:H	1.63	0.46
2:F:8:TYR:H	2:F:73:VAL:H	1.65	0.45
1:C:151:PRO:C	1:C:153:VAL:H	2.21	0.44
1:A:370:THR:H	1:A:374:GLU:H	1.65	0.43
2:D:299:GLY:H	2:D:308:VAL:H	1.66	0.43
2:F:329:THR:C	2:F:331:TYR:H	2.23	0.42
1:C:28:CYS:H	1:C:37:GLY:H	1.65	0.42
8:N:363:VAL:C	8:N:425:GLY:HA2	2.40	0.42
1:B:117:TRP:H	1:B:166:TYR:H	1.68	0.41
2:F:246:ALA:O	2:F:306:GLY:HA3	2.20	0.41
1:A:348:GLU:C	1:A:350:TYR:H	2.24	0.41
1:B:542:LEU:C	1:B:544:VAL:H	2.24	0.41
2:D:341:ARG:C	2:D:343:LEU:H	2.24	0.41
4:H:50:ALA:C	4:H:52:LEU:H	2.23	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	575/578 (100%)	443 (77%)	90 (16%)	42 (7%)	1 14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	575/578 (100%)	456 (79%)	84 (15%)	35 (6%)	1	17
1	C	575/578 (100%)	453 (79%)	86 (15%)	36 (6%)	1	17
2	D	457/478 (96%)	323 (71%)	96 (21%)	38 (8%)	1	12
2	E	457/478 (96%)	357 (78%)	56 (12%)	44 (10%)	0	10
2	F	457/478 (96%)	336 (74%)	77 (17%)	44 (10%)	0	10
3	G	208/223 (93%)	149 (72%)	35 (17%)	24 (12%)	0	6
4	H	98/104 (94%)	74 (76%)	13 (13%)	11 (11%)	0	7
5	I	98/120 (82%)	93 (95%)	3 (3%)	2 (2%)	7	38
5	K	98/120 (82%)	95 (97%)	1 (1%)	2 (2%)	7	38
6	J	181/188 (96%)	159 (88%)	17 (9%)	5 (3%)	5	30
6	L	181/188 (96%)	155 (86%)	18 (10%)	8 (4%)	2	22
7	M	318/323 (98%)	299 (94%)	11 (4%)	8 (2%)	5	32
8	N	628/652 (96%)	550 (88%)	44 (7%)	34 (5%)	2	19
9	O	74/99 (75%)	71 (96%)	3 (4%)	0	100	100
9	P	74/99 (75%)	72 (97%)	1 (1%)	1 (1%)	11	46
9	Q	74/99 (75%)	73 (99%)	1 (1%)	0	100	100
9	R	74/99 (75%)	71 (96%)	2 (3%)	1 (1%)	11	46
9	S	74/99 (75%)	70 (95%)	4 (5%)	0	100	100
9	T	74/99 (75%)	72 (97%)	1 (1%)	1 (1%)	11	46
9	U	74/99 (75%)	70 (95%)	3 (4%)	1 (1%)	11	46
9	V	74/99 (75%)	71 (96%)	3 (4%)	0	100	100
9	W	74/99 (75%)	71 (96%)	1 (1%)	2 (3%)	5	31
9	X	74/99 (75%)	73 (99%)	1 (1%)	0	100	100
9	Y	74/99 (75%)	72 (97%)	2 (3%)	0	100	100
9	Z	74/99 (75%)	73 (99%)	1 (1%)	0	100	100
All	All	5794/6274 (92%)	4801 (83%)	654 (11%)	339 (6%)	3	17

All (339) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	74	GLU
1	A	134	VAL
1	A	159	GLU

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Mol	Chain	Res	Type
1	A	197	ARG
1	A	202	ASN
1	A	210	ARG
1	A	247	ALA
1	A	303	ILE
1	A	304	TYR
1	A	305	VAL
1	A	351	PRO
1	A	466	GLU
1	A	535	SER
1	B	45	ASP
1	B	77	PRO
1	B	207	THR
1	B	223	THR
1	B	233	GLY
1	B	342	GLU
1	B	427	SER
1	B	432	THR
1	B	444	ALA
1	B	476	LEU
1	C	163	ALA
1	C	405	ALA
1	C	416	ARG
1	C	471	VAL
1	C	480	GLU
2	D	7	GLU
2	D	18	LEU
2	D	26	ASP
2	D	101	ASP
2	D	137	THR
2	D	216	ARG
2	D	307	SER
2	D	355	LEU
2	D	357	SER
2	D	419	GLU
2	E	15	SER
2	E	25	LYS
2	E	128	GLU
2	E	139	ASP
2	E	145	VAL
2	E	151	PRO
2	E	159	PRO

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Mol	Chain	Res	Type
2	E	196	ILE
2	E	327	ASP
2	E	428	GLN
2	F	49	GLU
2	F	67	ASP
2	F	113	PRO
2	F	151	PRO
2	F	210	ARG
2	F	284	PRO
2	F	298	ALA
2	F	318	ASP
2	F	354	PRO
2	F	362	MET
2	F	395	LEU
3	G	7	THR
3	G	80	ALA
3	G	81	LEU
3	G	117	VAL
3	G	167	VAL
4	H	53	PRO
4	H	79	GLU
5	I	23	ILE
6	J	163	VAL
5	K	23	ILE
6	L	180	SER
7	M	4	ASP
7	M	108	PRO
8	N	37	PRO
8	N	39	ALA
8	N	72	LEU
8	N	294	LEU
8	N	348	THR
8	N	388	PRO
8	N	523	TRP
8	N	544	ILE
9	T	77	ASN
1	A	132	GLY
1	A	195	VAL
1	A	196	GLN
1	A	199	LEU
1	A	227	PRO
1	A	229	PRO

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Mol	Chain	Res	Type
1	A	340	ARG
1	A	354	LEU
1	A	413	LEU
1	A	443	VAL
1	A	471	VAL
1	A	510	LYS
1	B	85	ASP
1	B	163	ALA
1	B	210	ARG
1	B	275	PRO
1	B	392	SER
1	B	463	GLY
1	B	512	ALA
1	C	25	TYR
1	C	64	VAL
1	C	194	PRO
1	C	202	ASN
1	C	227	PRO
1	C	245	SER
1	C	326	SER
2	D	128	GLU
2	D	215	SER
2	D	239	LEU
2	D	256	ILE
2	D	298	ALA
2	D	332	ILE
2	D	336	GLN
2	D	399	ILE
2	E	30	GLY
2	E	53	GLU
2	E	71	THR
2	E	101	ASP
2	E	140	VAL
2	E	178	SER
2	E	194	MET
2	E	354	PRO
2	E	360	ARG
2	E	375	HIS
2	E	389	GLY
2	E	436	LEU
2	F	79	VAL
2	F	114	ILE

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Mol	Chain	Res	Type
2	F	148	GLN
2	F	237	MET
2	F	293	THR
2	F	330	GLY
2	F	351	PRO
2	F	370	LYS
3	G	4	VAL
3	G	66	LEU
3	G	87	GLU
3	G	89	VAL
3	G	99	SER
3	G	112	ALA
3	G	114	LEU
3	G	119	THR
3	G	134	ALA
3	G	168	VAL
3	G	174	ALA
4	H	15	LEU
4	H	21	TYR
6	J	121	LEU
6	J	154	ALA
6	L	140	VAL
8	N	77	ALA
8	N	185	LYS
8	N	277	ALA
8	N	395	ALA
8	N	520	GLN
8	N	586	ALA
8	N	593	GLY
8	N	637	GLU
9	W	6	ALA
1	A	246	ASN
1	A	302	SER
1	A	397	GLN
1	A	474	ASP
1	B	23	ARG
1	B	88	GLN
1	B	278	GLY
1	B	354	LEU
1	B	375	GLU
1	B	387	PRO
1	B	443	VAL

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Mol	Chain	Res	Type
1	C	45	ASP
1	C	57	GLY
1	C	207	THR
1	C	234	LYS
1	C	243	LYS
1	C	282	MET
1	C	302	SER
1	C	352	PRO
1	C	392	SER
1	C	510	LYS
2	D	10	GLY
2	D	64	THR
2	D	67	ASP
2	D	159	PRO
2	D	166	GLN
2	D	240	THR
2	E	215	SER
2	E	276	GLU
2	E	336	GLN
2	E	356	PRO
2	E	390	VAL
2	F	24	ALA
2	F	62	GLU
2	F	77	GLU
2	F	80	ALA
2	F	119	LEU
2	F	128	GLU
2	F	164	ALA
2	F	168	ALA
3	G	116	PRO
3	G	180	GLN
4	H	25	SER
4	H	77	LEU
6	J	138	ARG
6	L	96	GLN
6	L	160	LYS
7	M	245	SER
8	N	35	LEU
8	N	42	ALA
8	N	74	ALA
8	N	271	SER
8	N	387	GLU

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Mol	Chain	Res	Type
8	N	400	PRO
8	N	519	LEU
9	U	77	ASN
1	A	25	TYR
1	A	390	ASP
1	B	25	TYR
1	B	408	ARG
1	C	36	VAL
1	C	304	TYR
1	C	473	PRO
1	C	484	ILE
2	D	96	ILE
2	D	343	LEU
2	D	351	PRO
2	D	354	PRO
2	D	435	SER
2	E	17	PRO
2	E	275	GLU
2	E	278	PRO
2	E	383	TYR
2	E	415	ALA
2	E	429	ASN
2	E	434	GLU
2	F	88	MET
2	F	133	THR
2	F	227	PRO
2	F	275	GLU
2	F	326	PRO
2	F	336	GLN
2	F	452	LYS
4	H	52	LEU
4	H	71	LEU
4	H	96	LYS
5	I	104	MET
6	L	95	PRO
6	L	157	ALA
6	L	179	SER
7	M	144	GLY
8	N	36	ARG
8	N	136	PRO
8	N	162	GLU
8	N	270	ALA

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Mol	Chain	Res	Type
8	N	590	GLY
8	N	640	ARG
9	R	7	SER
1	A	66	SER
1	A	219	ALA
1	A	359	ALA
1	A	395	VAL
1	B	36	VAL
1	B	284	ARG
1	B	331	ALA
1	B	417	ARG
1	B	563	PHE
1	C	70	PRO
1	C	71	LEU
1	C	100	ILE
1	C	247	ALA
2	D	17	PRO
2	D	23	ASN
2	D	190	VAL
2	D	191	PHE
2	D	270	ILE
2	D	457	ASP
2	E	243	GLU
2	E	362	MET
2	E	437	GLN
2	F	99	PRO
2	F	175	PRO
2	F	259	ASP
2	F	372	ARG
3	G	6	PRO
3	G	123	THR
3	G	153	GLU
4	H	5	ALA
4	H	54	ASP
6	J	144	ALA
7	M	76	VAL
7	M	217	PHE
8	N	295	ALA
9	W	48	ASP
1	A	54	ASP
1	A	432	THR
1	B	326	SER

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Mol	Chain	Res	Type
1	C	486	VAL
2	D	340	SER
2	E	106	ILE
2	E	222	ASN
2	E	263	TYR
2	E	355	LEU
2	E	430	ARG
2	E	435	SER
2	F	23	ASN
2	F	69	ALA
3	G	86	LEU
5	K	104	MET
7	M	277	VAL
8	N	297	HIS
8	N	545	TRP
8	N	585	LEU
9	P	6	ALA
1	A	296	VAL
2	D	235	PRO
2	F	96	ILE
1	A	394	PRO
1	B	51	VAL
2	F	205	ILE
3	G	154	ILE
3	G	179	ILE
1	A	27	ILE
1	B	5	VAL
1	C	211	ILE
1	C	443	VAL
2	F	117	LEU
6	L	163	VAL
1	A	40	ILE
1	C	345	PRO
1	C	402	ILE
1	C	560	PRO
2	D	356	PRO
2	F	10	GLY
8	N	444	PRO
1	A	515	ILE
1	B	514	GLY
2	E	324	PRO
7	M	78	GLY

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
10	ADP	B	600	-	24,29,29	1.02	1 (4%)	29,45,45	2.00	3 (10%)
10	ADP	C	600	-	24,29,29	1.18	2 (8%)	29,45,45	1.48	3 (10%)

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
10	ADP	B	600	-	-	3/12/32/32	0/3/3/3
10	ADP	C	600	-	-	8/12/32/32	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	C	600	ADP	C8-N7	-2.93	1.29	1.34
10	C	600	ADP	C2'-C1'	-2.57	1.49	1.53
10	B	600	ADP	C8-N7	-2.36	1.30	1.34

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	600	ADP	PA-O3A-PB	9.07	163.95	132.83
10	C	600	ADP	PA-O3A-PB	4.93	149.73	132.83
10	C	600	ADP	N6-C6-N1	3.97	126.81	118.57
10	B	600	ADP	N6-C6-N1	3.26	125.33	118.57
10	B	600	ADP	C5-C6-N1	-2.14	115.50	120.35
10	C	600	ADP	C5-C6-N1	-2.05	115.70	120.35

There are no chirality outliers.

All (11) torsion outliers are listed below:

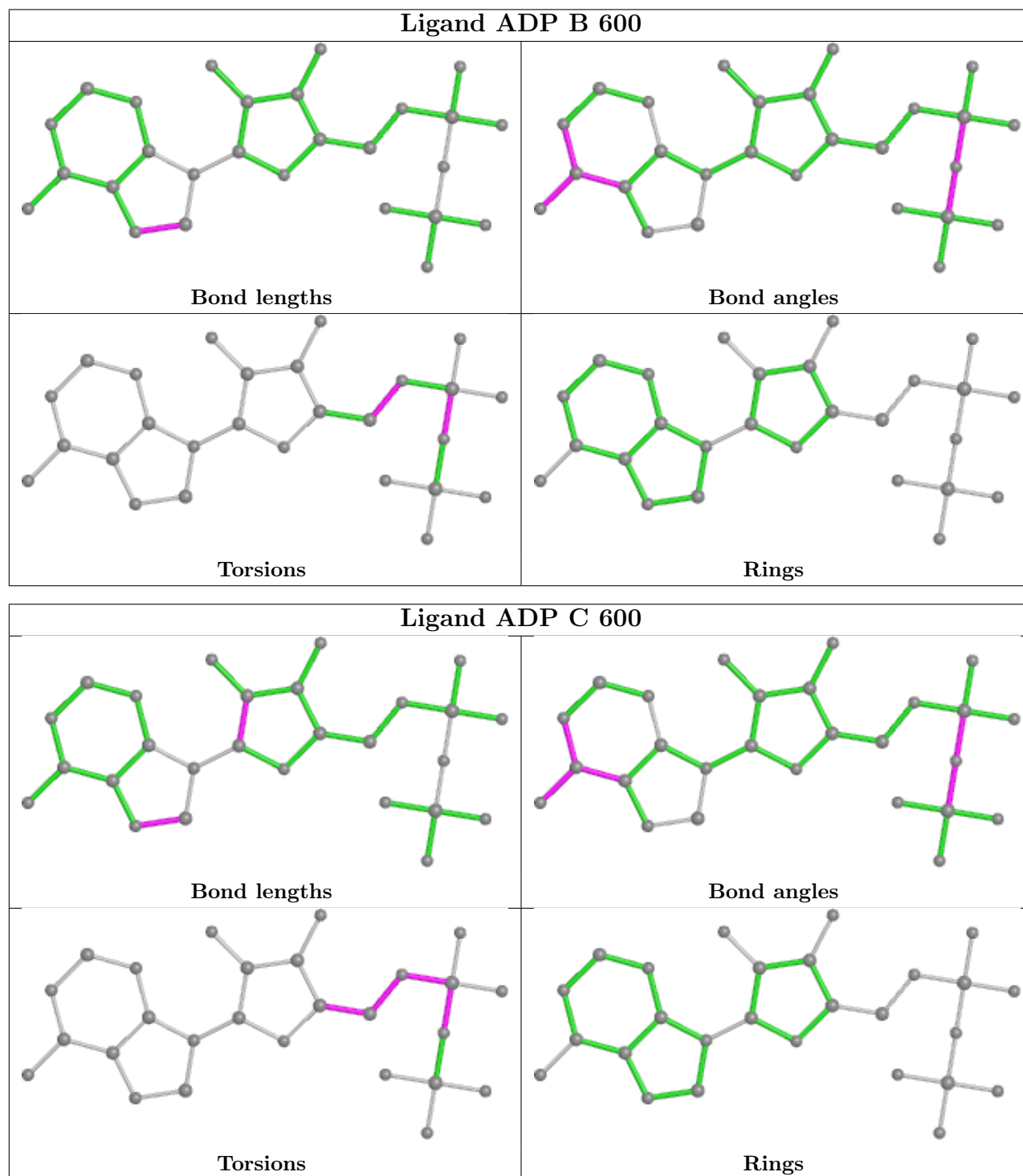
Mol	Chain	Res	Type	Atoms
10	B	600	ADP	PB-O3A-PA-O5'
10	C	600	ADP	C5'-O5'-PA-O1A
10	C	600	ADP	C5'-O5'-PA-O2A
10	C	600	ADP	C5'-O5'-PA-O3A
10	C	600	ADP	O4'-C4'-C5'-O5'
10	C	600	ADP	C3'-C4'-C5'-O5'
10	C	600	ADP	PB-O3A-PA-O2A
10	C	600	ADP	C4'-C5'-O5'-PA
10	B	600	ADP	C4'-C5'-O5'-PA
10	B	600	ADP	PB-O3A-PA-O1A
10	C	600	ADP	PB-O3A-PA-O1A

There are no ring outliers.

No monomer is involved in short contacts.

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

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



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.

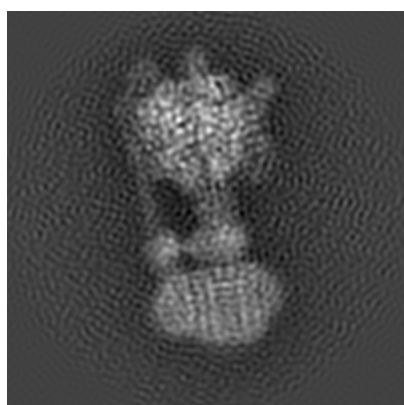
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6812. These allow visual inspection of the internal detail of the map and identification of artifacts.

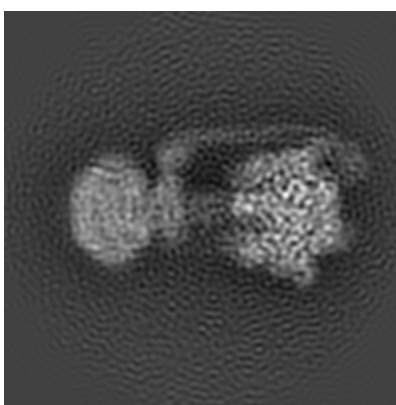
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

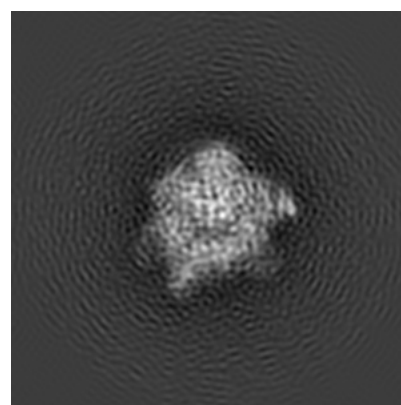
6.1.1 Primary map



X



Y

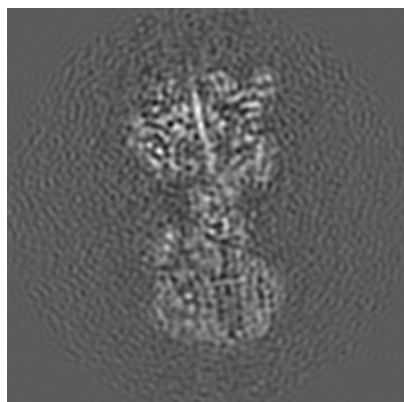


Z

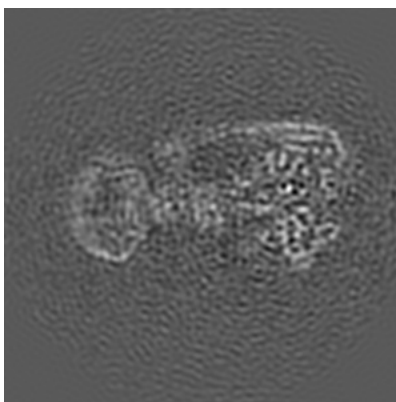
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

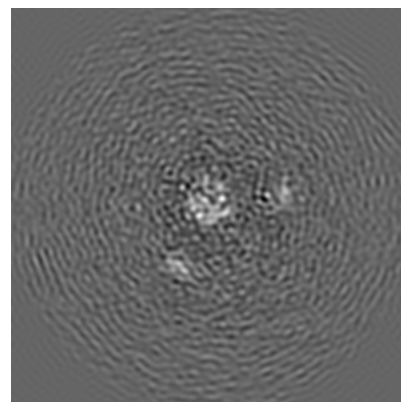
6.2.1 Primary map



X Index: 118



Y Index: 118



Z Index: 118

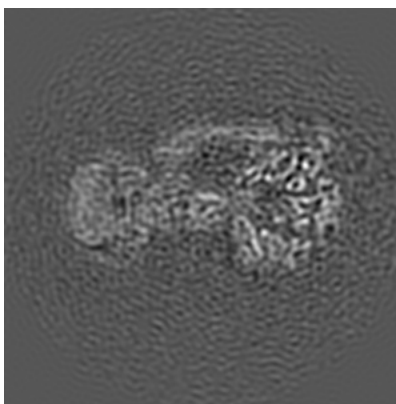
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

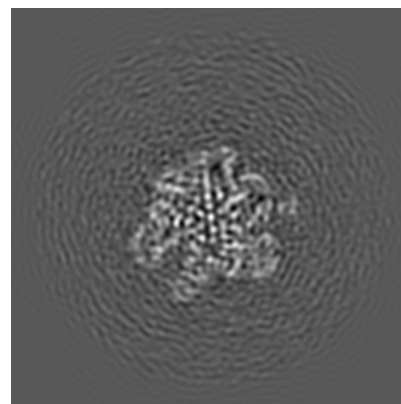
6.3.1 Primary map



X Index: 118



Y Index: 123



Z Index: 175

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

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

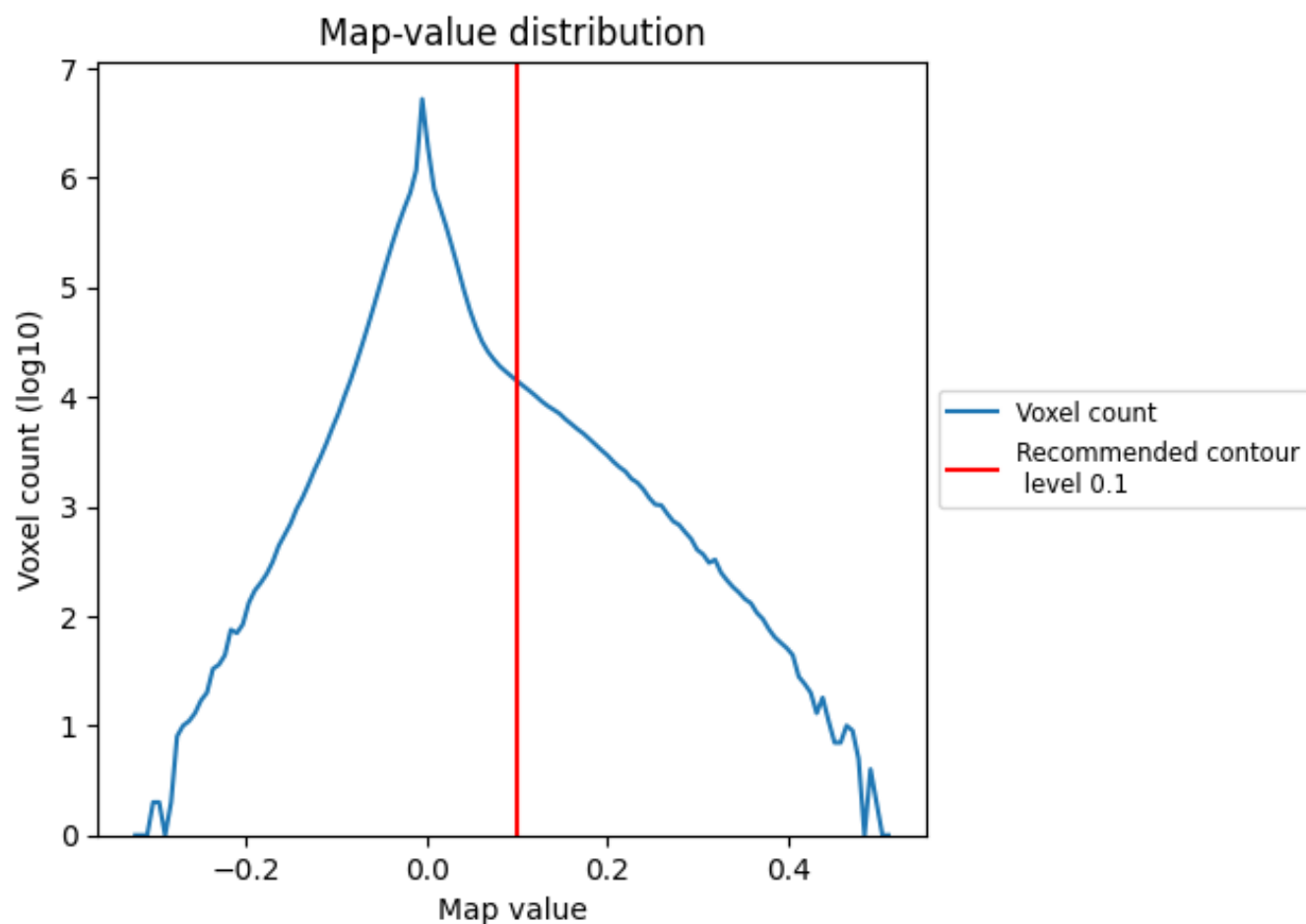
6.5 Mask visualisation

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

7 Map analysis [i](#)

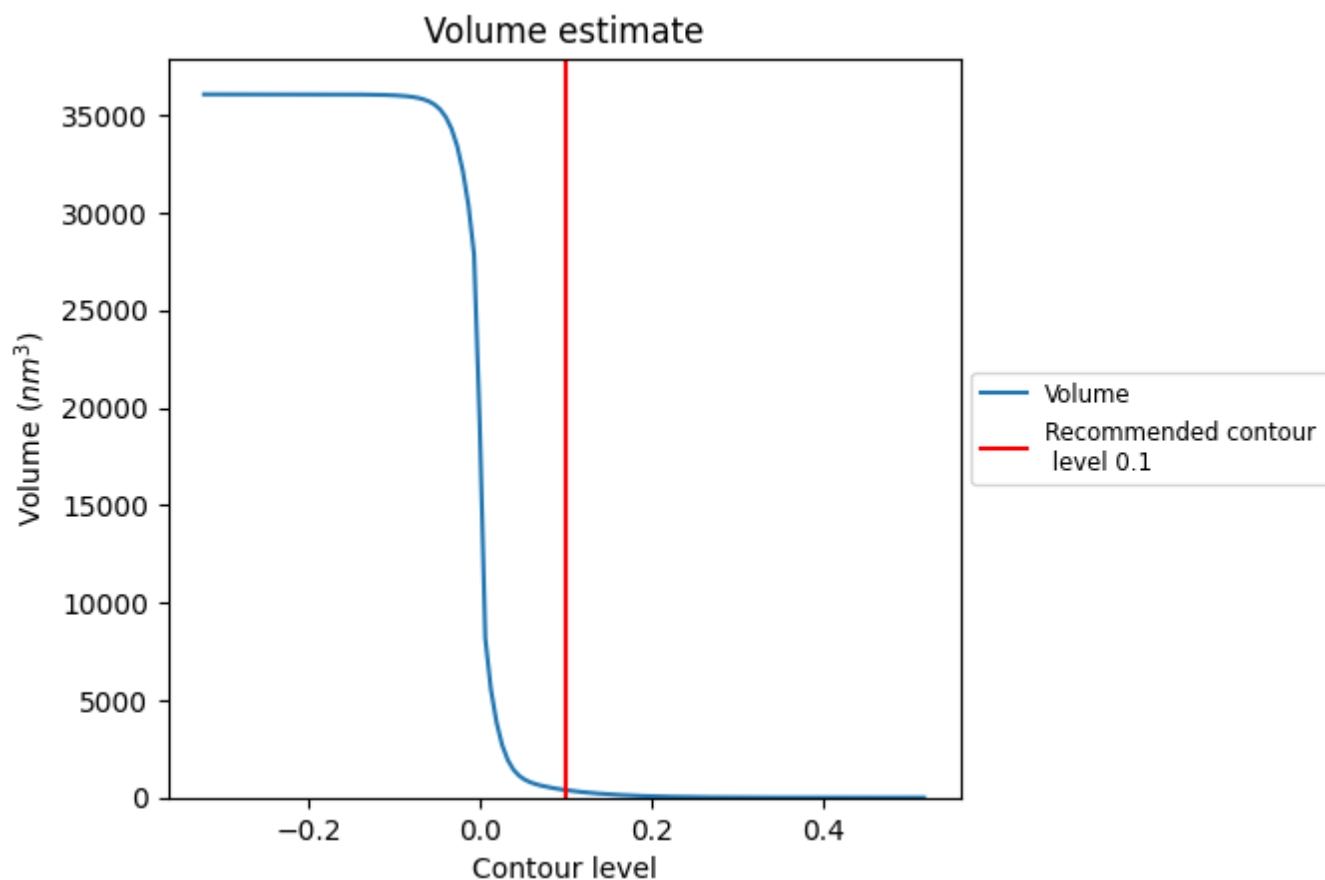
This section contains the results of statistical analysis of the map.

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.

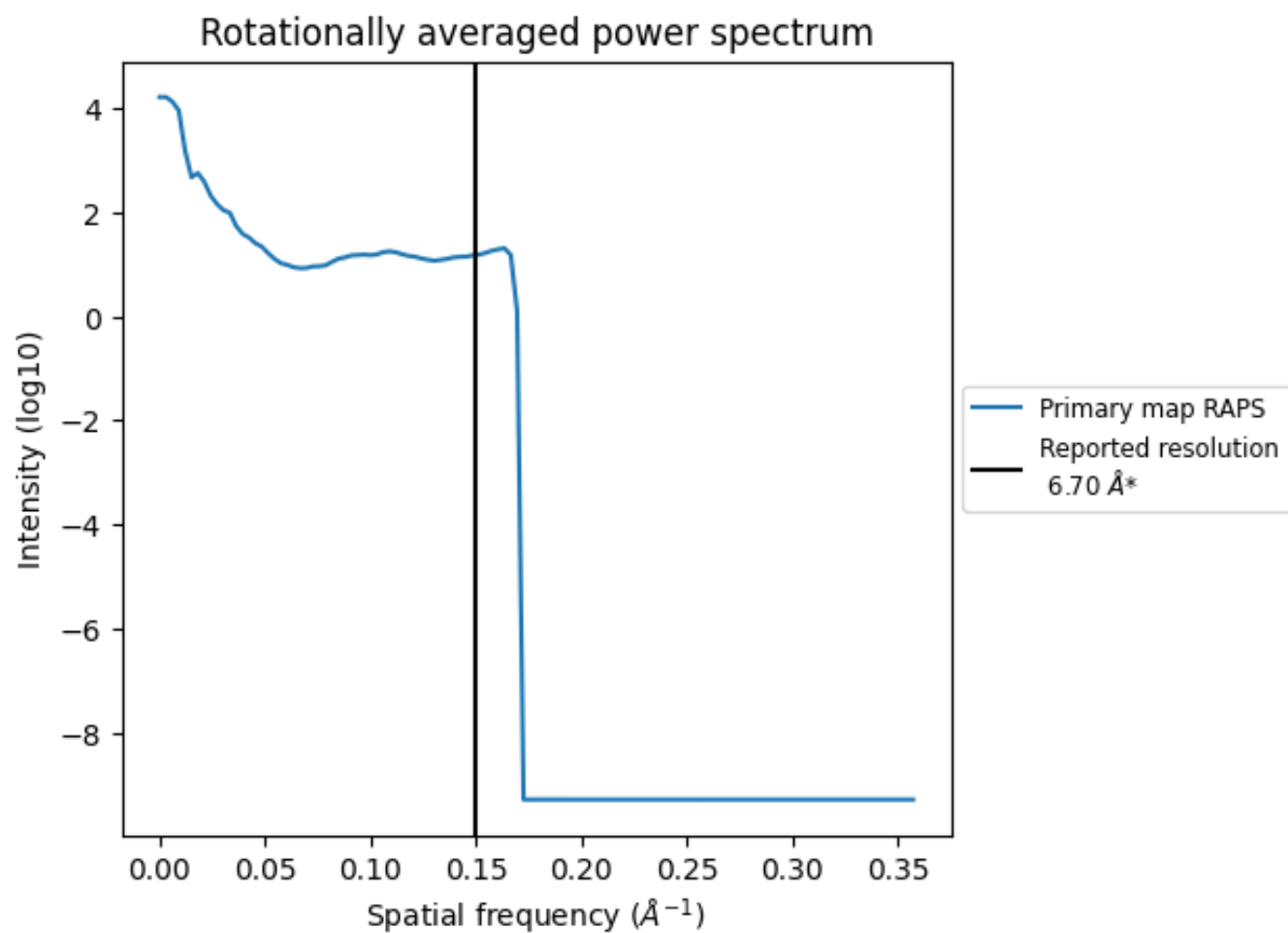
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 382 nm³; this corresponds to an approximate mass of 345 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 ⓘ

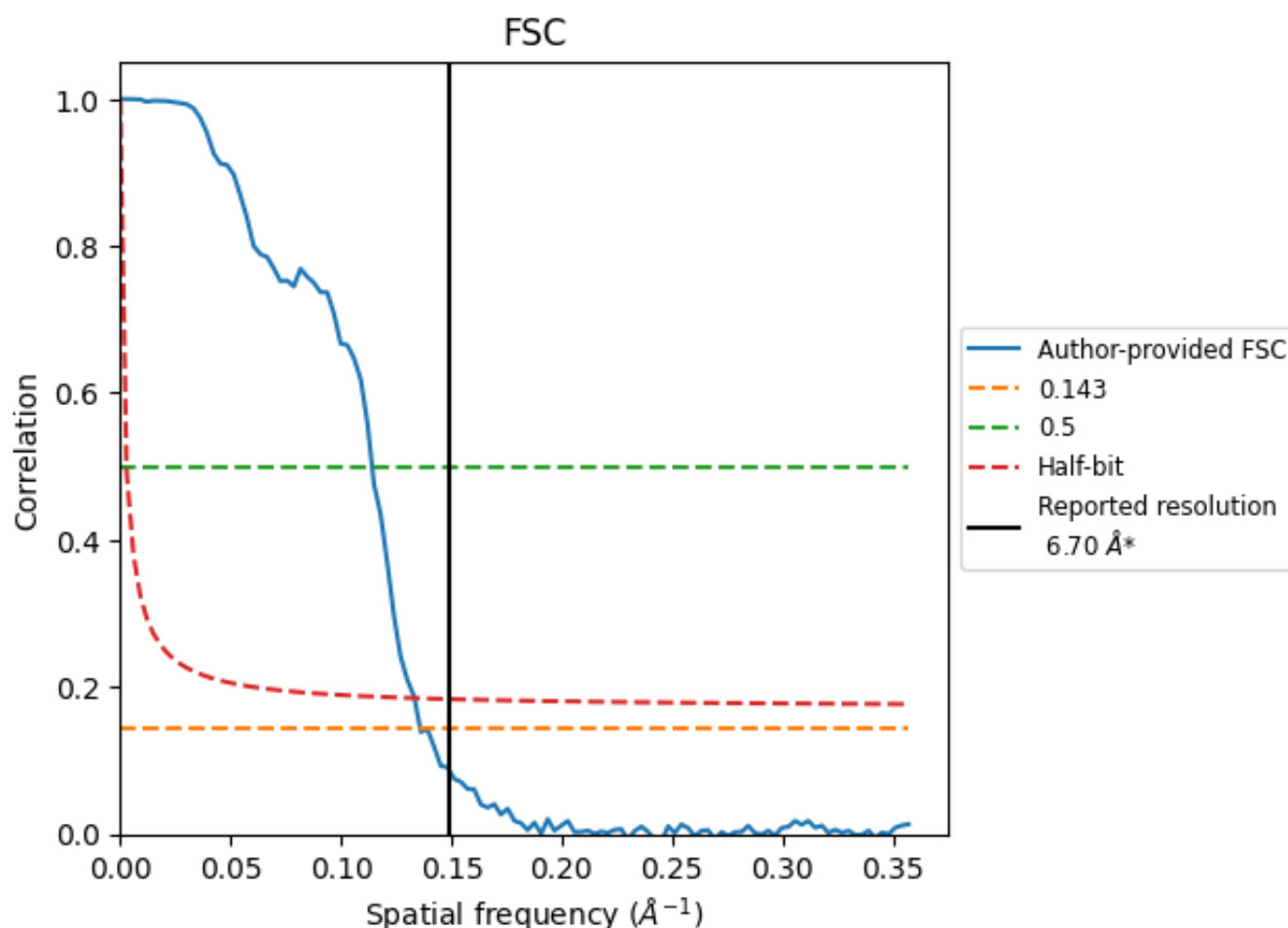


*Reported resolution corresponds to spatial frequency of 0.149 Å⁻¹

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 0.149 \AA^{-1}

8.2 Resolution estimates [i](#)

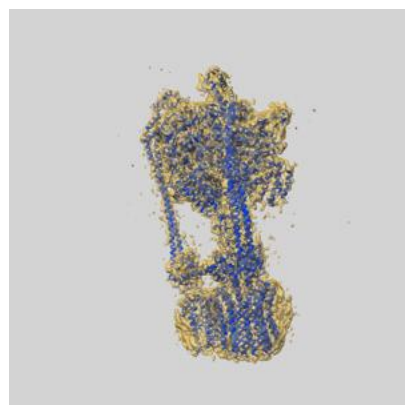
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.70	-	-
Author-provided FSC curve	7.36	8.76	7.50
Unmasked-calculated*	-	-	-

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

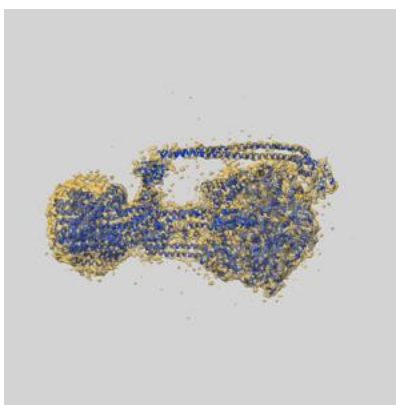
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-6812 and PDB model 5Y5Z. Per-residue inclusion information can be found in section [3](#) on page [8](#).

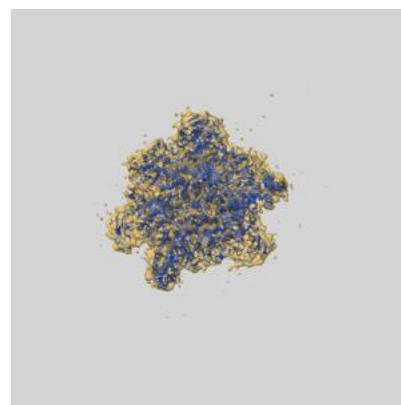
9.1 Map-model overlay [i](#)



X



Y



Z

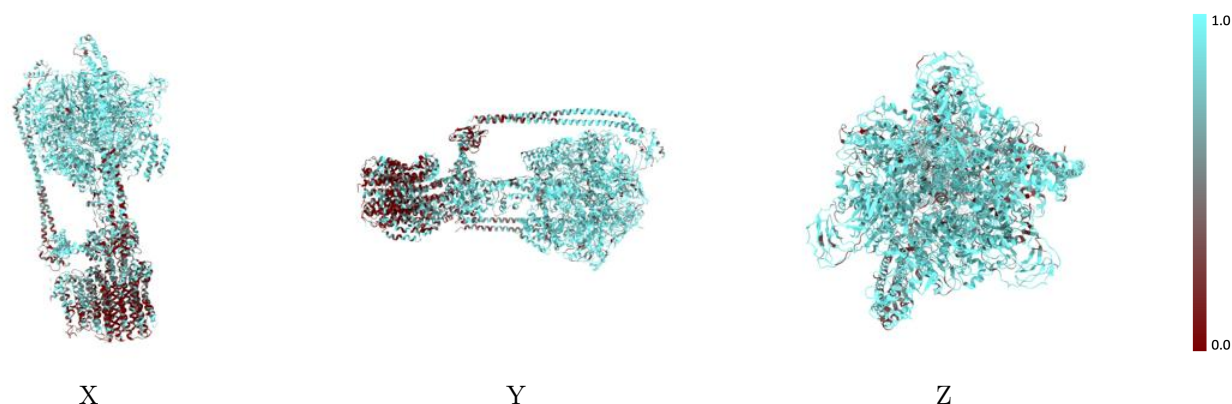
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



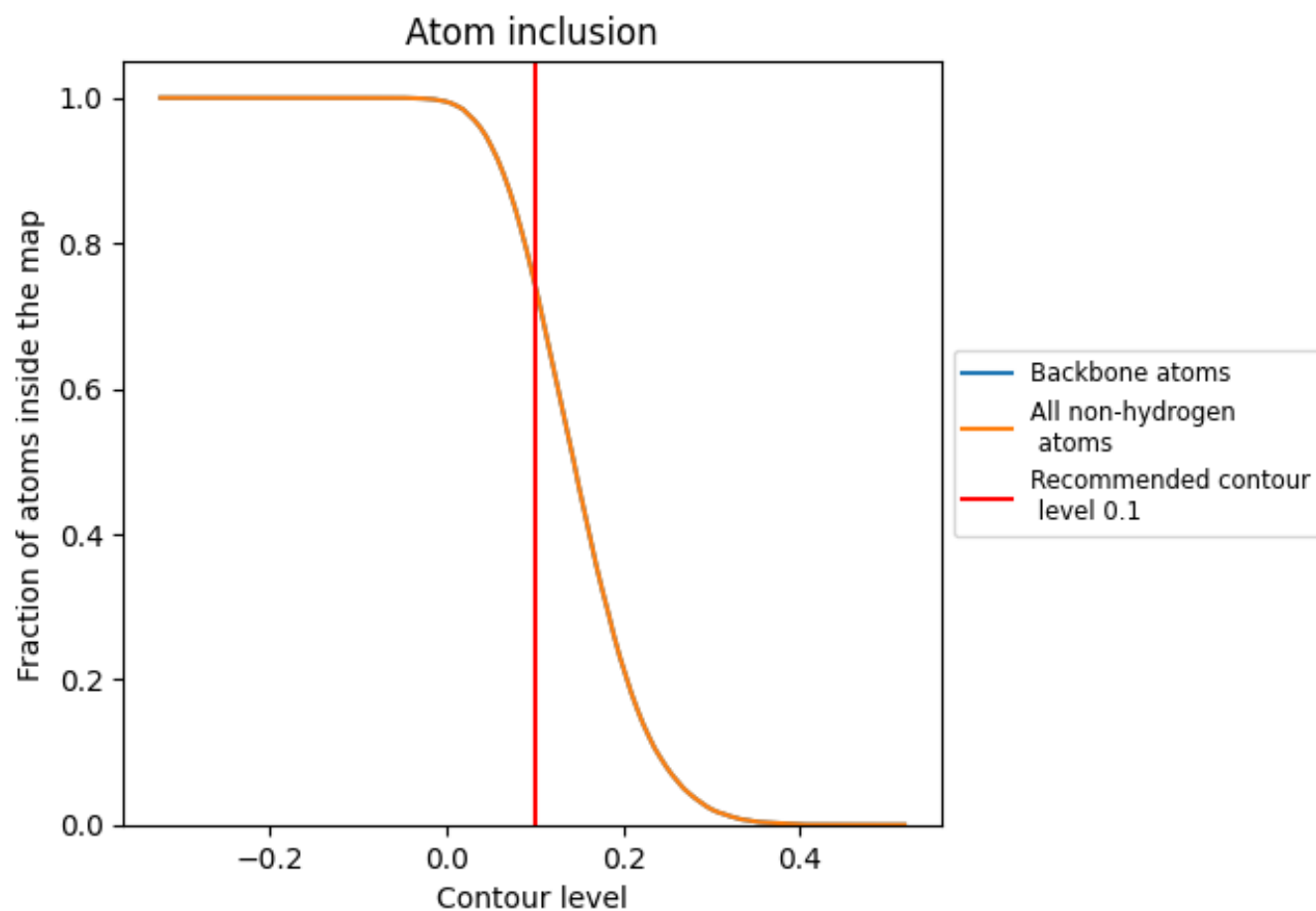
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).























































9.4 Atom inclusion [i](#)



At the recommended contour level, 75% of all backbone atoms, 75% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7460	 0.2370
A	 0.8669	 0.2730
B	 0.9040	 0.2900
C	 0.8770	 0.2870
D	 0.8545	 0.2730
E	 0.8916	 0.2970
F	 0.8894	 0.2930
G	 0.7998	 0.2580
H	 0.7719	 0.2460
I	 0.6316	 0.2000
J	 0.7615	 0.2210
K	 0.7594	 0.2140
L	 0.7520	 0.2230
M	 0.6708	 0.2040
N	 0.5808	 0.1750
O	 0.4191	 0.1400
P	 0.4224	 0.1550
Q	 0.3267	 0.1020
R	 0.4092	 0.1420
S	 0.4488	 0.1150
T	 0.4224	 0.1040
U	 0.4719	 0.1320
V	 0.3762	 0.1220
W	 0.2574	 0.0640
X	 0.4455	 0.1430
Y	 0.5149	 0.1720
Z	 0.4785	 0.1810

