



Full wwPDB EM Validation Report ⓘ

Sep 2, 2026 – 06:28 PM EDT

PDB ID : 36QX / pdb_000036qx
EMDB ID : EMD-77789
Title : Arabidopsis thaliana V-type ATPase, State 1 bound to OXR5, Backbone model
Authors : Khamina, M.; Rubinstein, J.L.
Deposited on : 2026-06-26
Resolution : 4.30 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:

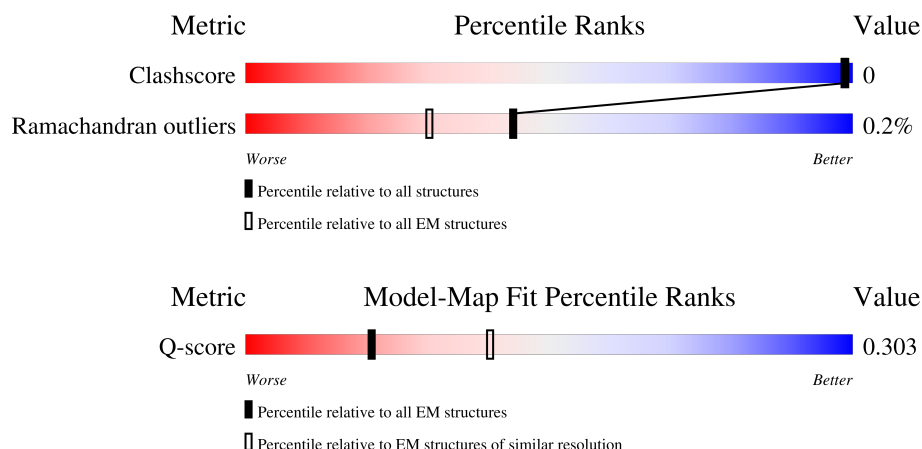
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

1 Overall quality at a glance

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

The reported resolution of this entry is 4.30 Å.

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



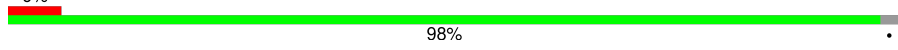
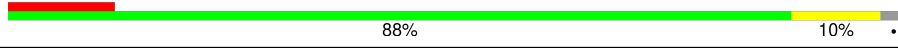
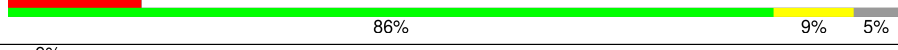
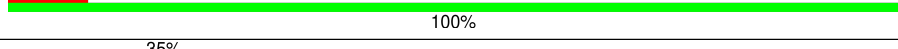
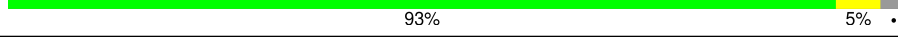
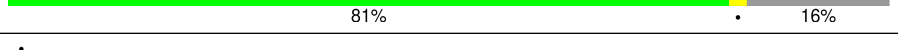
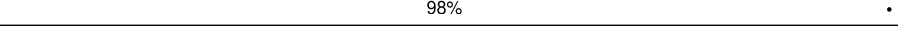
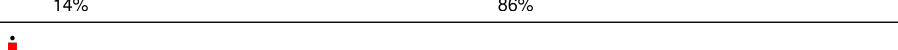
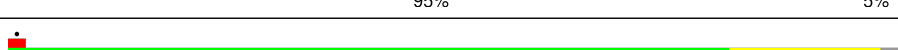
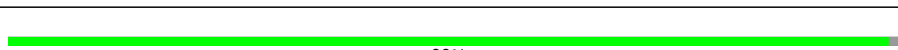
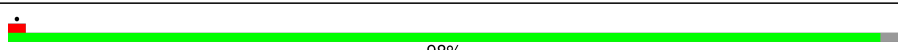
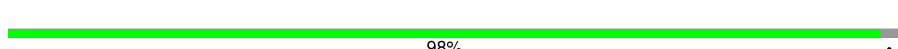
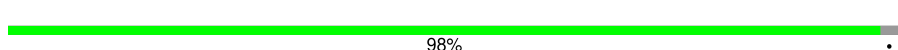
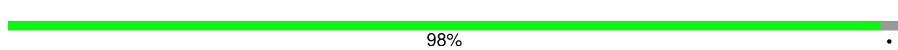
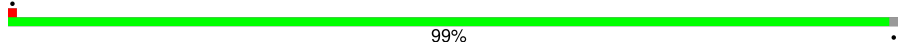
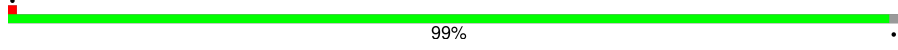
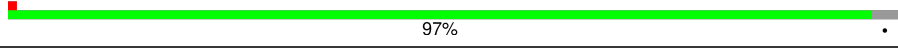
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Q-score	-	25397	4585 (3.80 - 4.80)

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	T	542	
2	a	817	
3	B	486	
3	D	486	
3	F	486	

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Mol	Chain	Length	Quality of chain
4	G	230	
4	I	230	
4	K	230	
5	H	110	
5	J	110	
5	L	110	
6	M	261	
7	N	128	
8	P	441	
9	b	321	
10	c	180	
11	d	351	
12	e	70	
13	g	164	
13	h	164	
13	i	164	
13	j	164	
13	k	164	
13	l	164	
13	m	164	
13	n	164	
13	o	164	
14	r	364	
15	A	623	
15	C	623	

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Mol	Chain	Length	Quality of chain
15	E	623	86% 13%
16	O	375	18% 92% 8%

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 34440 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 TLD-domain containing nucleolar protein OXR5.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	T	518	Total	C	N	O	0	0
			2073	1036	518	519		

- Molecule 2 is a protein called V-type proton ATPase subunit a1.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	a	717	Total	C	N	O	0	0
			2869	1434	717	718		

- Molecule 3 is a protein called V-type proton ATPase subunit B1.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	F	456	Total	C	N	O	0	0
			1824	912	456	456		
3	D	454	Total	C	N	O	0	0
			1816	908	454	454		
3	B	458	Total	C	N	O	0	0
			1832	916	458	458		

- Molecule 4 is a protein called V-type proton ATPase subunit E1.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	G	213	Total	C	N	O	0	0
			852	426	213	213		
4	I	226	Total	C	N	O	0	0
			904	452	226	226		
4	K	224	Total	C	N	O	0	0
			896	448	224	224		

- Molecule 5 is a protein called V-type proton ATPase subunit G1.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	H	105	Total	C	N	O	0	0
			420	210	105	105		
5	J	110	Total	C	N	O	0	0
			441	220	110	111		
5	L	107	Total	C	N	O	0	0
			429	215	107	107		

- Molecule 6 is a protein called V-type proton ATPase subunit D.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	M	218	Total	C	N	O	0	0
			872	436	218	218		

- Molecule 7 is a protein called V-type proton ATPase subunit F.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	N	101	Total	C	N	O	0	0
			404	202	101	101		

- Molecule 8 is a protein called V-type proton ATPase subunit H.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	P	433	Total	C	N	O	0	0
			1732	866	433	433		

- Molecule 9 is a protein called V-type proton ATPase subunit AP1 fragment.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	b	44	Total	C	N	O	0	0
			176	88	44	44		

- Molecule 10 is a protein called V-type proton ATPase subunit c'1.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	c	171	Total	C	N	O	0	0
			685	342	171	172		

- Molecule 11 is a protein called V-type proton ATPase subunit d1.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	d	342	Total	C	N	O	0	0
			1369	684	342	343		

- Molecule 12 is a protein called V-type proton ATPase subunit e2.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	e	54	Total	C	N	O	0	0
			224	116	54	54		

- Molecule 13 is a protein called V-type proton ATPase subunit c1.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	g	162	Total	C	N	O	0	0
			648	324	162	162		
13	h	162	Total	C	N	O	0	0
			648	324	162	162		
13	i	161	Total	C	N	O	0	0
			644	322	161	161		
13	j	161	Total	C	N	O	0	0
			644	322	161	161		
13	k	161	Total	C	N	O	0	0
			644	322	161	161		
13	l	161	Total	C	N	O	0	0
			644	322	161	161		
13	m	162	Total	C	N	O	0	0
			648	324	162	162		
13	n	162	Total	C	N	O	0	0
			648	324	162	162		
13	o	159	Total	C	N	O	0	0
			636	318	159	159		

- Molecule 14 is a protein called V-type proton ATPase subunit AP2 fragment.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	r	48	Total	C	N	O	0	0
			192	96	48	48		

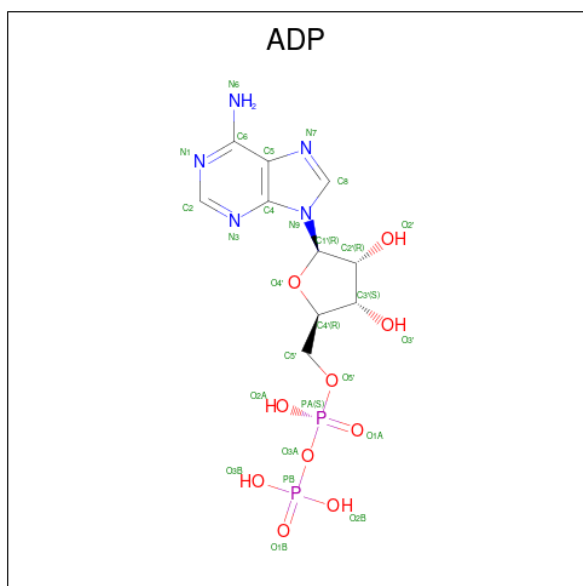
- Molecule 15 is a protein called V-type proton ATPase catalytic subunit A.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	C	610	Total	C	N	O	0	0
			2440	1220	610	610		
15	E	616	Total	C	N	O	0	0
			2465	1232	616	617		
15	A	577	Total	C	N	O	0	0
			2308	1154	577	577		

- Molecule 16 is a protein called V-type proton ATPase subunit C.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	O	346	Total	C	N	O	0	0
			1385	693	346	346		

- Molecule 17 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



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

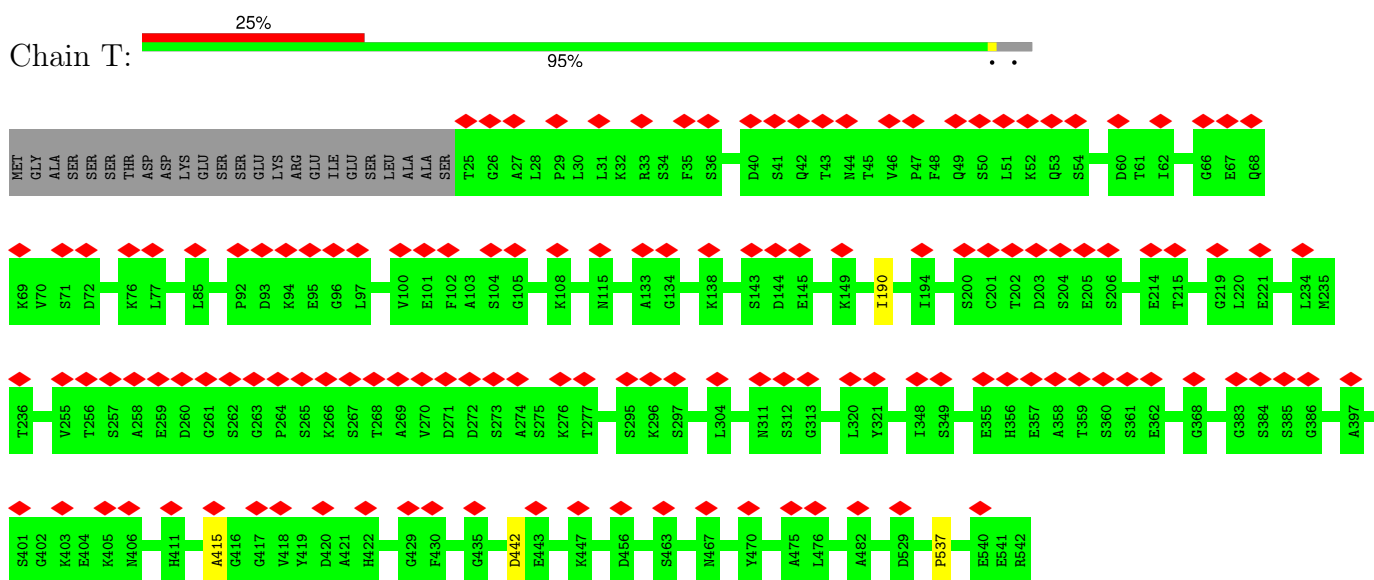
- Molecule 18 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
18	E	1	Total	Mg	0
			1	1	

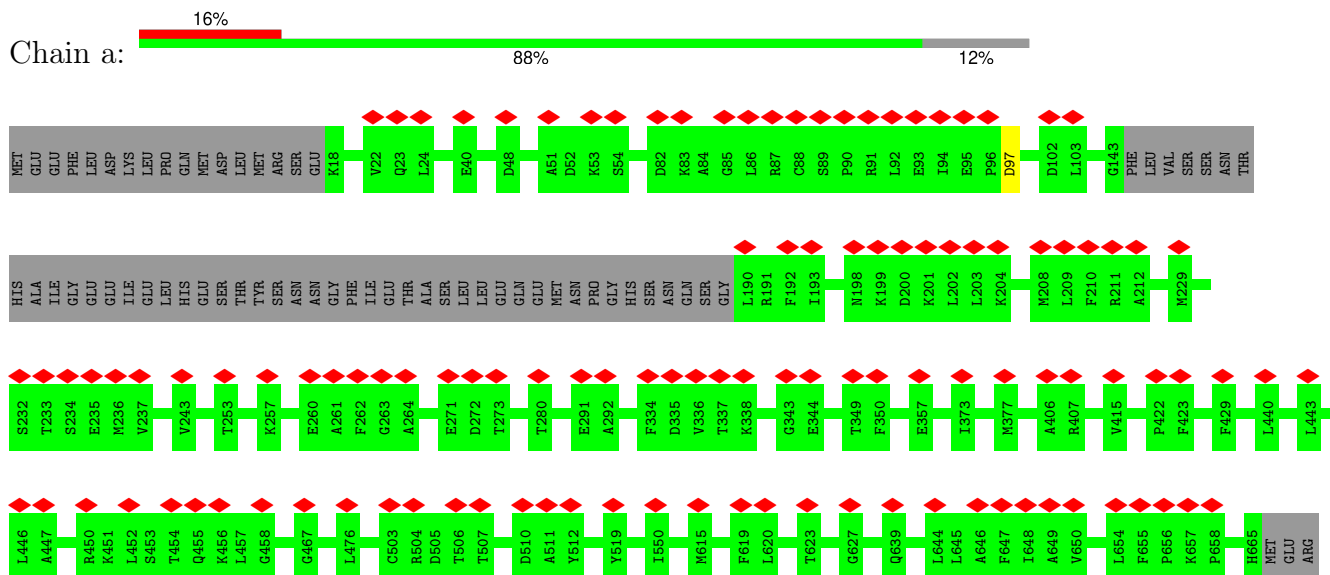
3 Residue-property plots [i](#)

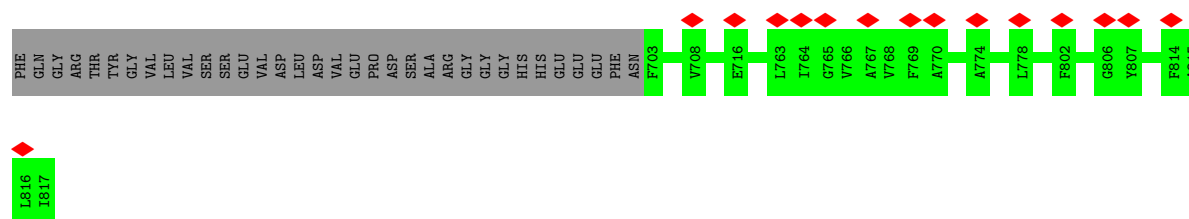
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: TLD-domain containing nucleolar protein OXR5



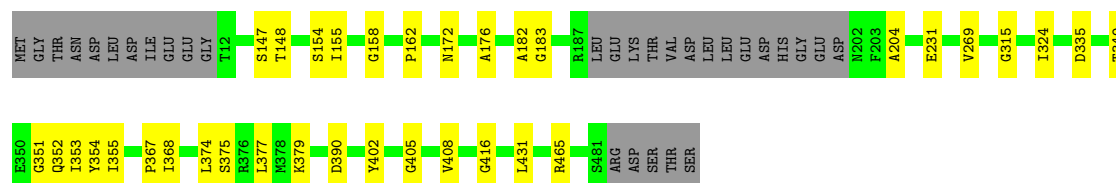
- Molecule 2: V-type proton ATPase subunit a1





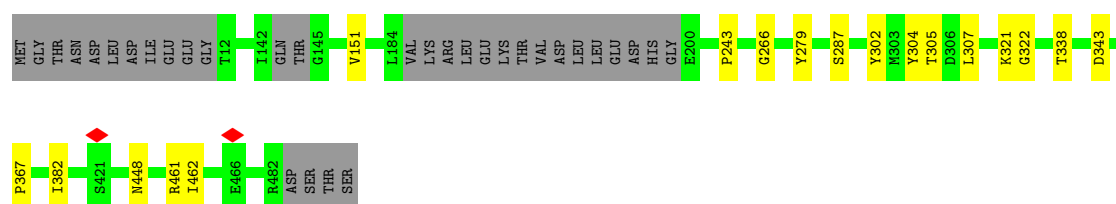
- Molecule 3: V-type proton ATPase subunit B1

Chain F: 87% 7% 6%



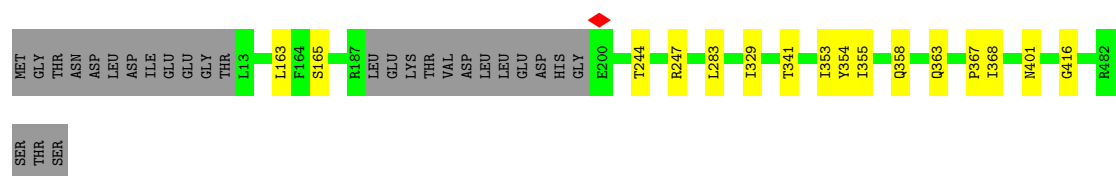
- Molecule 3: V-type proton ATPase subunit B1

Chain D: 90% 7%



- Molecule 3: V-type proton ATPase subunit B1

Chain B: 91% 6%



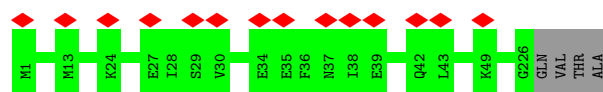
- Molecule 4: V-type proton ATPase subunit E1

Chain G: 88% 7%

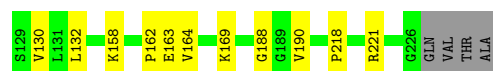
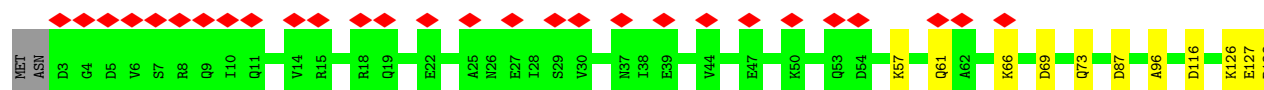
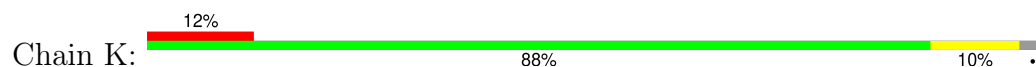


- Molecule 4: V-type proton ATPase subunit E1

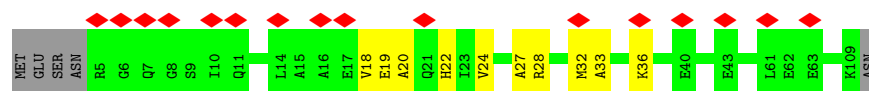
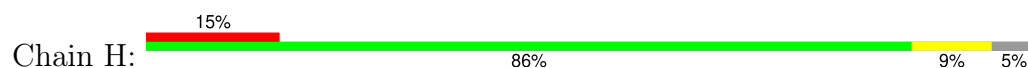
Chain I: 98% 6%



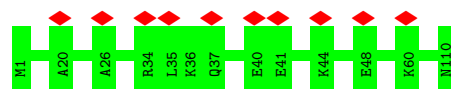
- Molecule 4: V-type proton ATPase subunit E1



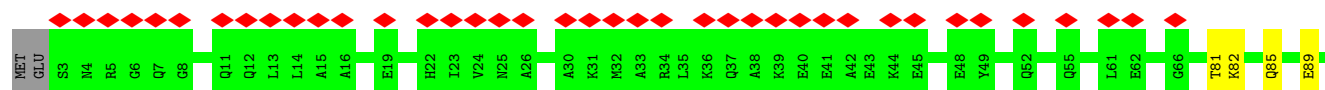
- Molecule 5: V-type proton ATPase subunit G1



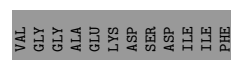
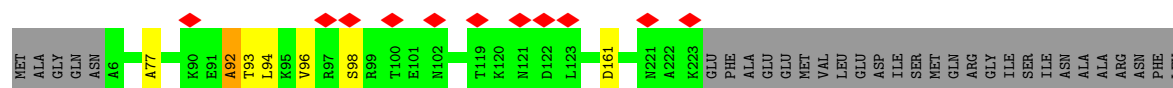
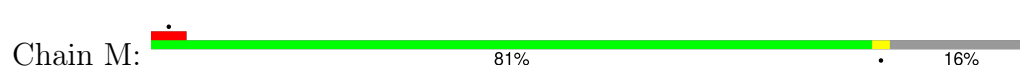
- Molecule 5: V-type proton ATPase subunit G1



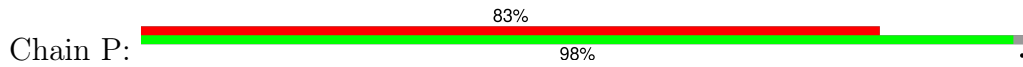
- Molecule 5: V-type proton ATPase subunit G1



- Molecule 6: V-type proton ATPase subunit D



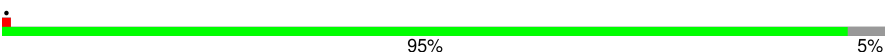
Chain N: 75% 21%



SER PHE LYS ASP HIS LEU LEU ALA ARG THR ARG LYS GLU GLY THR THR ASP LEU VAL LEU CYS SER GLU GLY SER GLU SER ASN SER GLN ALA GLY GLN SER HIS SER ASP ARG ARG SER PHE LEU LEU VAL SER VAL SER VAL GLN SER GLY SER LYS THR THR ALA

LEU TYR VAL SER ASP PRO TYR TRP THR THR LYS LEU GLN ARG PHE THR LEU ALA GLU VAL THR ALA LYS SER GLY ASN THR PRO GLU SER ILE ALA THR GLN ALA GLY C275 P313 GLN ASP SER

- Molecule 10: V-type proton ATPase subunit c'1

Chain c:  95% 5%

MET SER GLY VAL ALA LEU GLY HIS A10 G157 K180

- Molecule 11: V-type proton ATPase subunit d1

Chain d:  81% 17%

M1 A31 N41 A51 N60 S63 P64 C74 K77 L78 V79 D80 Y82 G103 H104 M105 G115 V122 G133 D136 S137 I138 L141 A142 V143 A144 Q145 N146 E149 P162 C167 E171 D172 L173 D174 D175 A188 E191 F193

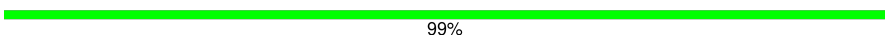
D210 L211 F214 E215 A220 G245 L246 G251 E254 L255 A256 I257 V264 R265 G266 S279 LYS MET SER TYR GLY SER GLN MET L289 D290 K291 E295 E296 E297 F314 F315 W330 I331 C334 V335 H344 Y349 M350 F351

- Molecule 12: V-type proton ATPase subunit e2

Chain e:  29% 77% 23%

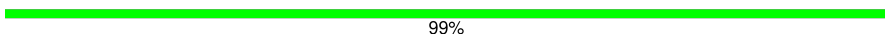
MET ALA F3 V4 S7 L8 A11 V12 V13 G14 N26 K27 L36 V39 T41 A42 T43 V44 C45 C46 W47 M48 M49 Y54 I55 A56 GLN MET ASN PRO LEU ILE VAL PRO ILE LEU SER GLU VAL GLU

- Molecule 13: V-type proton ATPase subunit c1

Chain g:  99%

MET S2 A163 GLU

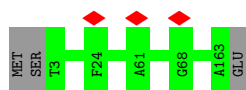
- Molecule 13: V-type proton ATPase subunit c1

Chain h:  99%

MET S2 A163 GLU

- Molecule 13: V-type proton ATPase subunit c1

Chain i:  98%



- Molecule 13: V-type proton ATPase subunit c1

Chain j: 98%



- Molecule 13: V-type proton ATPase subunit c1

Chain k: 98%



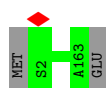
- Molecule 13: V-type proton ATPase subunit c1

Chain l: 98%



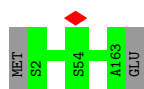
- Molecule 13: V-type proton ATPase subunit c1

Chain m: 99%



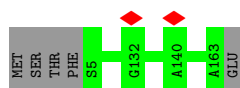
- Molecule 13: V-type proton ATPase subunit c1

Chain n: 99%



- Molecule 13: V-type proton ATPase subunit c1

Chain o: 97%

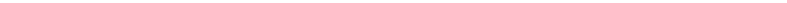


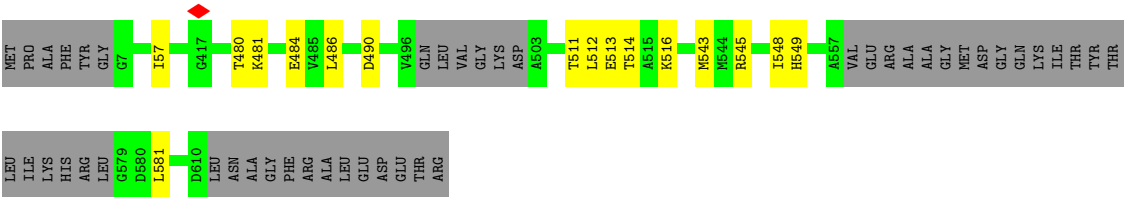
- Molecule 14: V-type proton ATPase subunit AP2 fragment

[illegible]

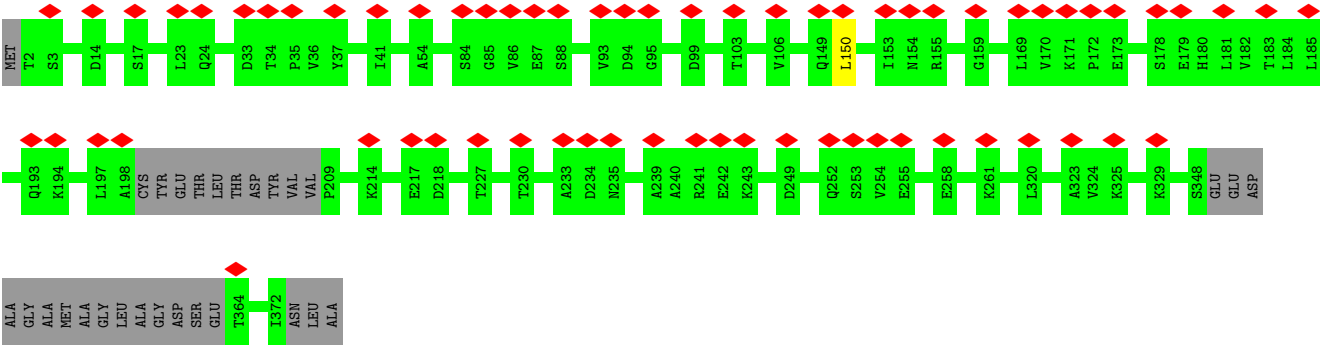
N546	N549	R560	ALA	GLY	MET	ASP	GLY	GLN	R568	L585	Q588	E621	THR	ARG	M349	M350	T354	S355	A358	R362	F368	G400	V407	T408	I409	P423	T425	S426	A427	T428	V432	Q433	Y457	Y460	I478	R479	E484	V485	L486	Q487	A505	E506	G507	D508	K509	I510	T514	L517	N526	Y538	W542	M349	M350	T354	S355	A358	R362	F368	G400	V407	T408	I409	P423	T425	S426	A427	T428	V432	Q433	Y457	Y460	I478	R479	E484	V485	L486	Q487	A505	E506	G507	D508	K509	I510	T514	L517	N526	Y538	W542	MET	PRO	ALA	PHE	Y5	Y21	F30	V31	V32	V33	V46	R47	V48	G49	N52	L53	I54	G55	A65	I66	I67	Q68	V69	Y70	P81	W82	P228	G232	Q233	R234	V235	L239	G246	T247	Q263	A264	V274	V275	V276	V277	G278	G279	G280	T313	P322
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L454	M298	MET
Y468	S307	PRO
1476	K310	ALA
G563	R326	PHE
MET	A337	Y5
ASP	F340	G6
GLY	Y345	S19
Q567	N346	E20
R623	V347	Y21
	S348	G22
	M349	Y23
	S353	F30
	E359	V31
	I364	V32
	Y380	V33
	L381	G36
	A382	E44
	F388	L45
	V396	V46
	R403	R47
	N404	I54
	G405	G55
	S406	E56
	V407	A65
	T408	T66
	I409	I67
	V410	Q68
	G411	P81
	A412	V82
	V413	S90
	G418	G104
	S426	P218
	A427	V219
	V432	A225
	Q433	G245
	V434	G246
	F435	T247
	V436	C248
	G437	S262
	L438	Q263
	D439	A264
	A443	L265
		S266
		S271

Chain A:  90% • 7%



• Molecule 16: V-type proton ATPase subunit C



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	5323	Depositor
Resolution determination method	DIFFRACTION PATTERN/LAYERLINES	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	130000	Depositor
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	1.136	Depositor
Minimum map value	-0.258	Depositor
Average map value	0.016	Depositor
Map value standard deviation	0.047	Depositor
Recommended contour level	0.194	Depositor
Map size (Å)	476.16, 476.16, 476.16	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.93, 0.93, 0.93	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 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	T	0.86	0/2072	1.50	3/2587 (0.1%)
2	a	0.70	0/2866	1.34	0/3576
3	B	0.95	2/1830 (0.1%)	1.24	24/2284 (1.1%)
3	D	0.92	2/1813 (0.1%)	1.49	22/2261 (1.0%)
3	F	1.24	5/1822 (0.3%)	1.71	65/2274 (2.9%)
4	G	0.85	0/851	1.20	20/1062 (1.9%)
4	I	0.21	0/903	0.41	0/1127
4	K	1.54	1/895 (0.1%)	2.05	41/1117 (3.7%)
5	H	1.18	0/419	1.58	20/522 (3.8%)
5	J	0.20	0/440	0.42	0/547
5	L	1.19	0/428	1.54	10/534 (1.9%)
6	M	0.81	0/871	1.47	4/1087 (0.4%)
7	N	0.94	0/403	1.69	2/502 (0.4%)
8	P	0.17	0/1731	0.37	0/2162
9	b	0.17	0/175	0.30	0/217
10	c	0.20	0/684	0.37	0/852
11	d	1.77	3/1367 (0.2%)	2.34	108/1704 (6.3%)
12	e	0.17	0/223	0.48	0/283
13	g	0.19	0/647	0.32	0/807
13	h	0.18	0/647	0.33	0/807
13	i	0.17	0/643	0.33	0/802
13	j	0.18	0/643	0.35	0/802
13	k	0.18	0/643	0.38	0/802
13	l	0.20	0/643	0.35	0/802
13	m	0.20	0/647	0.34	0/807
13	n	0.19	0/647	0.35	0/807
13	o	0.20	0/635	0.34	0/792
14	r	0.14	0/191	0.28	0/237
15	A	0.83	0/2305	1.19	32/2876 (1.1%)
15	C	1.45	6/2438 (0.2%)	1.97	134/3044 (4.4%)
15	E	1.46	8/2463 (0.3%)	2.05	143/3074 (4.7%)
16	O	0.26	0/1382	0.52	2/1723 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.94	27/34367 (0.1%)	1.37	630/42880 (1.5%)

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	E	55	GLY	N-CA	-7.91	1.37	1.45
15	E	405	GLY	N-CA	-7.79	1.37	1.44
15	C	55	GLY	N-CA	-7.75	1.37	1.45
3	D	322	GLY	N-CA	-6.99	1.37	1.45
15	E	246	GLY	N-CA	-6.74	1.37	1.45
15	E	22	GLY	N-CA	-6.53	1.37	1.45
3	F	416	GLY	N-CA	-6.48	1.38	1.45
11	d	266	GLY	N-CA	-6.22	1.37	1.45
3	F	405	GLY	N-CA	-6.20	1.38	1.45
4	K	188	GLY	N-CA	-6.04	1.37	1.44
11	d	103	GLY	N-CA	-6.03	1.38	1.45
3	F	183	GLY	N-CA	-5.85	1.38	1.45
15	C	246	GLY	N-CA	-5.80	1.37	1.45
3	B	416	GLY	N-CA	-5.73	1.38	1.45
3	B	341	THR	N-CA	-5.71	1.42	1.46
3	F	351	GLY	N-CA	-5.70	1.37	1.44
15	C	280	GLY	N-CA	-5.47	1.38	1.46
15	E	245	GLY	N-CA	-5.46	1.37	1.45
15	C	278	GLY	N-CA	-5.43	1.37	1.45
11	d	245	GLY	N-CA	-5.28	1.37	1.44
15	E	418	GLY	N-CA	-5.28	1.37	1.45
15	E	36	GLY	N-CA	-5.28	1.37	1.45
15	E	411	GLY	N-CA	-5.27	1.37	1.45
15	C	49	GLY	N-CA	-5.20	1.37	1.45
3	D	266	GLY	N-CA	-5.14	1.38	1.45
15	C	55	GLY	CA-C	-5.13	1.47	1.52
3	F	158	GLY	N-CA	-5.12	1.38	1.45

All (630) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	511	THR	CA-C-N	8.42	131.91	120.38
15	A	511	THR	C-N-CA	8.42	131.91	120.38
15	C	54	ILE	CA-C-N	7.62	129.56	121.48
15	C	54	ILE	C-N-CA	7.62	129.56	121.48
15	E	468	TYR	CA-C-N	7.10	130.12	120.54
15	E	468	TYR	C-N-CA	7.10	130.12	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	461	ARG	CA-C-N	7.09	134.74	121.97
3	D	461	ARG	C-N-CA	7.09	134.74	121.97
15	E	435	PHE	CA-C-N	7.03	132.21	122.79
15	E	435	PHE	C-N-CA	7.03	132.21	122.79
15	E	47	ARG	CA-C-N	6.89	131.62	122.93
15	E	47	ARG	C-N-CA	6.89	131.62	122.93
15	E	31	VAL	CA-C-N	6.89	132.56	123.06
15	E	31	VAL	C-N-CA	6.89	132.56	123.06
15	C	68	GLN	CA-C-N	6.77	130.84	122.37
15	C	68	GLN	C-N-CA	6.77	130.84	122.37
15	C	47	ARG	CA-C-N	6.77	131.46	122.93
15	C	47	ARG	C-N-CA	6.77	131.46	122.93
3	B	354	TYR	CA-C-N	6.76	131.56	122.90
3	B	354	TYR	C-N-CA	6.76	131.56	122.90
15	E	66	THR	CA-C-N	6.68	132.27	122.99
15	E	66	THR	C-N-CA	6.68	132.27	122.99
15	E	395	VAL	CA-C-N	6.57	131.15	122.42
15	E	395	VAL	C-N-CA	6.57	131.15	122.42
3	F	354	TYR	CA-C-N	6.52	130.52	122.37
3	F	354	TYR	C-N-CA	6.52	130.52	122.37
15	C	322	PRO	CA-C-N	6.50	128.88	120.56
15	C	322	PRO	C-N-CA	6.50	128.88	120.56
15	E	406	SER	CA-C-N	6.49	131.65	123.14
15	E	406	SER	C-N-CA	6.49	131.65	123.14
3	F	352	GLN	CA-C-N	6.46	130.57	122.43
3	F	352	GLN	C-N-CA	6.46	130.57	122.43
15	C	276	TYR	CA-C-N	6.46	130.56	122.48
15	C	276	TYR	C-N-CA	6.46	130.56	122.48
15	E	68	GLN	CA-C-N	6.45	131.16	122.90
15	E	68	GLN	C-N-CA	6.45	131.16	122.90
11	d	256	ALA	CA-C-N	6.43	129.82	122.36
11	d	256	ALA	C-N-CA	6.43	129.82	122.36
15	C	409	ILE	CA-C-N	6.40	131.82	123.11
15	C	409	ILE	C-N-CA	6.40	131.82	123.11
15	E	349	MET	CA-C-N	6.40	130.93	122.30
15	E	349	MET	C-N-CA	6.40	130.93	122.30
15	E	404	ASN	CA-C-N	6.38	129.58	122.69
15	E	404	ASN	C-N-CA	6.38	129.58	122.69
11	d	145	GLN	CA-C-N	6.38	132.38	123.07
11	d	145	GLN	C-N-CA	6.38	132.38	123.07
15	E	82	VAL	CA-C-N	6.36	131.50	122.72
15	E	82	VAL	C-N-CA	6.36	131.50	122.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	E	439	ASP	CA-C-N	6.35	128.79	120.28
15	E	439	ASP	C-N-CA	6.35	128.79	120.28
15	C	66	THR	CA-C-N	6.35	131.81	122.99
15	C	66	THR	C-N-CA	6.35	131.81	122.99
15	C	232	GLY	CA-C-N	6.35	130.87	122.30
15	C	232	GLY	C-N-CA	6.35	130.87	122.30
15	E	407	VAL	CA-C-N	6.34	132.11	123.11
15	E	407	VAL	C-N-CA	6.34	132.11	123.11
15	C	408	THR	CA-C-N	6.32	130.27	122.37
15	C	408	THR	C-N-CA	6.32	130.27	122.37
15	C	31	VAL	CA-C-N	6.27	133.20	122.67
15	C	31	VAL	C-N-CA	6.27	133.20	122.67
3	B	163	LEU	CA-C-N	6.26	131.09	122.77
3	B	163	LEU	C-N-CA	6.26	131.09	122.77
15	C	30	PRO	CA-C-N	6.24	130.88	122.90
15	C	30	PRO	C-N-CA	6.24	130.88	122.90
4	K	158	LYS	CA-C-N	6.21	130.65	122.51
4	K	158	LYS	C-N-CA	6.21	130.65	122.51
7	N	60	LYS	CA-C-N	6.20	129.41	120.79
7	N	60	LYS	C-N-CA	6.20	129.41	120.79
3	F	367	PRO	CA-C-N	6.18	130.82	122.90
3	F	367	PRO	C-N-CA	6.18	130.82	122.90
15	A	548	ILE	CA-C-N	6.17	128.46	120.44
15	A	548	ILE	C-N-CA	6.17	128.46	120.44
3	F	390	ASP	CA-C-N	6.16	129.68	120.31
3	F	390	ASP	C-N-CA	6.16	129.68	120.31
16	O	150	LEU	CA-C-N	6.11	129.60	120.31
16	O	150	LEU	C-N-CA	6.11	129.60	120.31
15	E	30	PRO	CA-C-N	6.11	130.76	123.19
15	E	30	PRO	C-N-CA	6.11	130.76	123.19
15	E	434	VAL	CA-C-N	6.11	131.99	123.07
15	E	434	VAL	C-N-CA	6.11	131.99	123.07
11	d	192	ASP	CA-C-N	6.10	128.37	120.44
11	d	192	ASP	C-N-CA	6.10	128.37	120.44
15	E	81	PRO	CA-C-N	6.08	131.19	123.10
15	E	81	PRO	C-N-CA	6.08	131.19	123.10
15	C	239	LEU	CA-C-N	6.08	130.51	123.15
15	C	239	LEU	C-N-CA	6.08	130.51	123.15
3	F	353	ILE	CA-C-N	6.04	130.70	122.84
3	F	353	ILE	C-N-CA	6.04	130.70	122.84
3	F	368	ILE	CA-C-N	6.04	130.46	122.30
3	F	368	ILE	C-N-CA	6.04	130.46	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	K	169	LYS	CA-C-N	6.04	131.13	123.10
4	K	169	LYS	C-N-CA	6.04	131.13	123.10
15	A	512	LEU	CA-C-N	6.04	128.37	120.28
15	A	512	LEU	C-N-CA	6.04	128.37	120.28
11	d	78	LEU	CA-C-N	6.03	128.15	120.56
11	d	78	LEU	C-N-CA	6.03	128.15	120.56
15	E	433	GLN	CA-C-N	6.02	131.36	122.99
15	E	433	GLN	C-N-CA	6.02	131.36	122.99
15	C	33	VAL	CA-C-N	5.99	131.26	123.00
15	C	33	VAL	C-N-CA	5.99	131.26	123.00
15	E	90	SER	CA-C-N	5.99	130.62	123.19
15	E	90	SER	C-N-CA	5.99	130.62	123.19
15	C	457	TYR	CA-C-N	5.98	131.24	122.39
15	C	457	TYR	C-N-CA	5.98	131.24	122.39
15	E	225	ALA	CA-C-N	5.98	132.95	121.54
15	E	225	ALA	C-N-CA	5.98	132.95	121.54
5	H	36	LYS	CA-C-N	5.97	128.28	120.28
5	H	36	LYS	C-N-CA	5.97	128.28	120.28
15	C	354	THR	CA-C-N	5.96	128.59	120.54
15	C	354	THR	C-N-CA	5.96	128.59	120.54
4	G	59	GLU	CA-C-N	5.94	128.24	120.28
4	G	59	GLU	C-N-CA	5.94	128.24	120.28
15	E	20	GLU	CA-C-N	5.94	131.37	123.00
15	E	20	GLU	C-N-CA	5.94	131.37	123.00
3	D	343	ASP	CA-C-N	5.93	128.82	120.28
3	D	343	ASP	C-N-CA	5.93	128.82	120.28
3	B	329	ILE	CA-C-N	5.93	131.13	122.77
3	B	329	ILE	C-N-CA	5.93	131.13	122.77
15	C	349	MET	CA-C-N	5.92	131.51	123.11
15	C	349	MET	C-N-CA	5.92	131.51	123.11
15	E	54	ILE	CA-C-N	5.90	129.58	122.03
15	E	54	ILE	C-N-CA	5.90	129.58	122.03
3	F	324	ILE	CA-C-N	5.89	131.29	123.05
3	F	324	ILE	C-N-CA	5.89	131.29	123.05
15	C	407	VAL	CA-C-N	5.89	131.47	123.11
15	C	407	VAL	C-N-CA	5.89	131.47	123.11
3	D	321	LYS	CA-C-N	5.89	128.10	122.27
3	D	321	LYS	C-N-CA	5.89	128.10	122.27
3	F	465	ARG	N-CA-C	5.88	117.36	111.07
3	F	269	VAL	CA-C-N	5.86	131.42	123.11
3	F	269	VAL	C-N-CA	5.86	131.42	123.11
5	H	28	ARG	CA-C-N	5.85	128.04	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	28	ARG	C-N-CA	5.85	128.04	120.44
11	d	149	GLU	CA-C-N	5.84	128.43	120.54
11	d	149	GLU	C-N-CA	5.84	128.43	120.54
6	M	96	VAL	CA-C-O	-5.84	116.06	120.96
11	d	245	GLY	N-CA-C	5.83	119.25	110.97
11	d	193	PHE	CA-C-N	5.83	128.02	120.44
11	d	193	PHE	C-N-CA	5.83	128.02	120.44
6	M	93	THR	CA-C-N	5.82	132.66	121.54
6	M	93	THR	C-N-CA	5.82	132.66	121.54
3	F	315	GLY	CA-C-N	5.82	131.36	122.93
3	F	315	GLY	C-N-CA	5.82	131.36	122.93
3	F	355	ILE	CA-C-N	5.80	130.73	122.72
3	F	355	ILE	C-N-CA	5.80	130.73	122.72
15	E	409	ILE	CA-C-N	5.80	130.99	123.10
15	E	409	ILE	C-N-CA	5.80	130.99	123.10
5	H	18	VAL	CA-C-N	5.80	128.05	120.28
5	H	18	VAL	C-N-CA	5.80	128.05	120.28
15	E	298	MET	CA-C-N	5.79	130.12	122.30
15	E	298	MET	C-N-CA	5.79	130.12	122.30
4	K	69	ASP	CA-C-N	5.79	127.96	120.44
4	K	69	ASP	C-N-CA	5.79	127.96	120.44
15	E	346	ASN	CA-C-N	5.77	131.03	123.06
15	E	346	ASN	C-N-CA	5.77	131.03	123.06
4	K	218	PRO	CA-C-N	5.77	128.37	120.46
4	K	218	PRO	C-N-CA	5.77	128.37	120.46
4	K	57	LYS	CA-C-N	5.77	128.26	120.65
4	K	57	LYS	C-N-CA	5.77	128.26	120.65
11	d	335	VAL	CA-C-N	5.76	127.93	120.44
11	d	335	VAL	C-N-CA	5.76	127.93	120.44
15	E	403	ARG	CA-C-N	5.76	130.95	123.00
15	E	403	ARG	C-N-CA	5.76	130.95	123.00
11	d	141	LEU	CA-C-N	5.76	128.00	120.28
11	d	141	LEU	C-N-CA	5.76	128.00	120.28
4	K	130	VAL	CA-C-N	5.74	132.39	122.64
4	K	130	VAL	C-N-CA	5.74	132.39	122.64
11	d	64	PRO	CA-C-N	5.74	129.62	121.42
11	d	64	PRO	C-N-CA	5.74	129.62	121.42
3	D	338	THR	CA-C-N	5.73	128.82	120.51
3	D	338	THR	C-N-CA	5.73	128.82	120.51
15	C	46	VAL	CA-C-N	5.71	131.21	123.11
15	C	46	VAL	C-N-CA	5.71	131.21	123.11
15	A	484	GLU	CA-C-N	5.71	127.75	120.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	484	GLU	C-N-CA	5.71	127.75	120.56
15	C	484	GLU	CA-C-N	5.70	127.75	120.56
15	C	484	GLU	C-N-CA	5.70	127.75	120.56
5	H	32	MET	CA-C-N	5.70	127.85	120.44
5	H	32	MET	C-N-CA	5.70	127.85	120.44
15	C	514	THR	CA-C-N	5.69	127.84	120.44
15	C	514	THR	C-N-CA	5.69	127.84	120.44
15	E	218	PRO	CA-C-N	5.69	130.77	122.69
15	E	218	PRO	C-N-CA	5.69	130.77	122.69
11	d	314	PHE	CA-C-N	5.68	128.22	120.54
11	d	314	PHE	C-N-CA	5.68	128.22	120.54
15	C	65	ALA	CA-C-N	5.68	130.20	122.19
15	C	65	ALA	C-N-CA	5.68	130.20	122.19
15	E	23	TYR	CA-C-N	5.68	129.06	120.77
15	E	23	TYR	C-N-CA	5.68	129.06	120.77
11	d	115	GLY	CA-C-N	5.67	128.16	120.44
11	d	115	GLY	C-N-CA	5.67	128.16	120.44
11	d	167	CYS	N-CA-C	5.67	119.46	112.03
15	A	513	GLU	CA-C-N	5.67	128.34	120.29
15	A	513	GLU	C-N-CA	5.67	128.34	120.29
4	K	188	GLY	N-CA-C	5.67	118.87	110.60
11	d	142	ALA	CA-C-N	5.66	127.69	120.56
11	d	142	ALA	C-N-CA	5.66	127.69	120.56
15	C	233	GLN	CA-C-N	5.65	127.78	120.44
15	C	233	GLN	C-N-CA	5.65	127.78	120.44
15	E	45	LEU	CA-C-N	5.64	130.70	122.69
15	E	45	LEU	C-N-CA	5.64	130.70	122.69
3	B	368	ILE	CA-C-N	5.64	130.71	122.41
3	B	368	ILE	C-N-CA	5.64	130.71	122.41
11	d	188	ALA	CA-C-N	5.64	127.77	120.44
11	d	188	ALA	C-N-CA	5.64	127.77	120.44
15	E	408	THR	CA-C-N	5.64	129.65	122.37
15	E	408	THR	C-N-CA	5.64	129.65	122.37
15	C	478	ILE	CA-C-N	5.64	127.77	120.44
15	C	478	ILE	C-N-CA	5.64	127.77	120.44
15	A	516	LYS	CA-C-N	5.63	127.76	120.44
15	A	516	LYS	C-N-CA	5.63	127.76	120.44
15	E	33	VAL	CA-C-N	5.63	130.93	123.05
15	E	33	VAL	C-N-CA	5.63	130.93	123.05
15	E	345	TYR	CA-C-N	5.63	130.26	122.77
15	E	345	TYR	C-N-CA	5.63	130.26	122.77
15	E	413	VAL	CA-C-N	5.63	130.60	123.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	E	413	VAL	C-N-CA	5.63	130.60	123.34
11	d	215	GLU	CA-C-N	5.62	127.75	120.44
11	d	215	GLU	C-N-CA	5.62	127.75	120.44
3	B	283	LEU	CA-C-N	5.62	128.12	120.54
3	B	283	LEU	C-N-CA	5.62	128.12	120.54
15	E	65	ALA	CA-C-N	5.61	130.46	122.72
15	E	65	ALA	C-N-CA	5.61	130.46	122.72
4	K	221	ARG	CA-C-N	5.59	127.78	120.28
4	K	221	ARG	C-N-CA	5.59	127.78	120.28
15	C	70	TYR	CA-C-N	5.59	131.31	122.36
15	C	70	TYR	C-N-CA	5.59	131.31	122.36
3	B	363	GLN	CA-C-N	5.59	129.63	121.80
3	B	363	GLN	C-N-CA	5.59	129.63	121.80
5	L	82	LYS	CA-C-N	5.59	127.61	120.56
5	L	82	LYS	C-N-CA	5.59	127.61	120.56
11	d	315	PHE	CA-C-N	5.58	127.70	120.44
11	d	315	PHE	C-N-CA	5.58	127.70	120.44
3	F	162	PRO	CA-C-N	5.58	130.61	122.41
3	F	162	PRO	C-N-CA	5.58	130.61	122.41
11	d	122	VAL	CA-C-N	5.58	127.75	120.28
11	d	122	VAL	C-N-CA	5.58	127.75	120.28
15	E	246	GLY	CA-C-N	5.57	131.20	123.07
15	E	246	GLY	C-N-CA	5.57	131.20	123.07
3	D	304	TYR	CA-C-N	5.56	127.67	120.44
3	D	304	TYR	C-N-CA	5.56	127.67	120.44
4	K	164	VAL	CA-C-N	5.55	130.57	122.85
4	K	164	VAL	C-N-CA	5.55	130.57	122.85
3	F	172	ASN	CA-C-N	5.55	127.66	120.44
3	F	172	ASN	C-N-CA	5.55	127.66	120.44
15	C	588	GLN	CA-C-N	5.55	132.15	121.54
15	C	588	GLN	C-N-CA	5.55	132.15	121.54
4	K	162	PRO	CA-C-N	5.54	129.75	121.72
4	K	162	PRO	C-N-CA	5.54	129.75	121.72
3	F	154	SER	CA-C-N	5.53	129.90	122.93
3	F	154	SER	C-N-CA	5.53	129.90	122.93
3	B	355	ILE	CA-C-N	5.53	130.80	123.05
3	B	355	ILE	C-N-CA	5.53	130.80	123.05
3	B	367	PRO	CA-C-N	5.52	129.53	121.80
3	B	367	PRO	C-N-CA	5.52	129.53	121.80
11	d	296	GLU	CA-C-N	5.52	127.99	120.54
11	d	296	GLU	C-N-CA	5.52	127.99	120.54
5	H	22	HIS	CA-C-N	5.51	127.59	120.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	22	HIS	C-N-CA	5.51	127.59	120.70
4	G	29	SER	CA-C-N	5.51	127.61	120.56
4	G	29	SER	C-N-CA	5.51	127.61	120.56
15	E	437	GLY	CA-C-N	5.50	129.29	121.42
15	E	437	GLY	C-N-CA	5.50	129.29	121.42
4	G	63	ASP	CA-C-N	5.50	127.48	120.56
4	G	63	ASP	C-N-CA	5.50	127.48	120.56
15	C	510	ILE	CA-C-N	5.50	127.59	120.44
15	C	510	ILE	C-N-CA	5.50	127.59	120.44
5	H	20	ALA	CA-C-N	5.49	127.58	120.44
5	H	20	ALA	C-N-CA	5.49	127.58	120.44
15	E	307	SER	CA-C-N	5.49	127.98	120.46
15	E	307	SER	C-N-CA	5.49	127.98	120.46
15	E	464	LEU	CA-C-N	5.49	127.57	120.44
15	E	464	LEU	C-N-CA	5.49	127.57	120.44
5	H	27	ALA	CA-C-N	5.47	128.40	120.79
5	H	27	ALA	C-N-CA	5.47	128.40	120.79
11	d	105	MET	CA-C-N	5.46	127.44	120.56
11	d	105	MET	C-N-CA	5.46	127.44	120.56
6	M	92	ALA	N-CA-C	5.46	122.43	110.80
15	E	266	SER	CA-C-N	5.46	127.86	120.44
15	E	266	SER	C-N-CA	5.46	127.86	120.44
3	B	353	ILE	CA-C-N	5.45	129.88	122.19
3	B	353	ILE	C-N-CA	5.45	129.88	122.19
4	G	51	ILE	CA-C-N	5.44	127.52	120.44
4	G	51	ILE	C-N-CA	5.44	127.52	120.44
15	C	228	PRO	CA-C-N	5.44	130.41	122.41
15	C	228	PRO	C-N-CA	5.44	130.41	122.41
15	C	274	VAL	CA-C-N	5.43	130.32	123.10
15	C	274	VAL	C-N-CA	5.43	130.32	123.10
4	K	61	GLN	CA-C-N	5.43	127.50	120.44
4	K	61	GLN	C-N-CA	5.43	127.50	120.44
15	E	438	LEU	CA-C-N	5.43	130.65	123.05
15	E	438	LEU	C-N-CA	5.43	130.65	123.05
15	E	56	GLU	CA-C-N	5.43	128.45	120.91
15	E	56	GLU	C-N-CA	5.43	128.45	120.91
15	E	426	SER	CA-C-N	5.42	127.55	120.28
15	E	426	SER	C-N-CA	5.42	127.55	120.28
15	E	21	TYR	CA-C-N	5.42	128.22	121.83
15	E	21	TYR	C-N-CA	5.42	128.22	121.83
3	F	204	ALA	CA-C-N	5.41	130.29	123.10
3	F	204	ALA	C-N-CA	5.41	130.29	123.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	E	353	SER	CA-C-N	5.40	129.32	120.63
15	E	353	SER	C-N-CA	5.40	129.32	120.63
15	C	313	THR	CA-C-N	5.39	130.44	123.00
15	C	313	THR	C-N-CA	5.39	130.44	123.00
15	E	347	VAL	CA-C-N	5.39	130.75	122.93
15	E	347	VAL	C-N-CA	5.39	130.75	122.93
3	D	279	TYR	CA-C-N	5.39	127.50	120.28
3	D	279	TYR	C-N-CA	5.39	127.50	120.28
15	C	487	GLN	CA-C-N	5.39	127.76	120.38
15	C	487	GLN	C-N-CA	5.39	127.76	120.38
4	K	66	LYS	CA-C-N	5.38	127.80	120.54
4	K	66	LYS	C-N-CA	5.38	127.80	120.54
15	C	549	HIS	CA-C-N	5.37	127.79	120.54
15	C	549	HIS	C-N-CA	5.37	127.79	120.54
15	E	247	THR	CA-C-N	5.36	130.99	122.94
15	E	247	THR	C-N-CA	5.36	130.99	122.94
15	E	364	ILE	CA-C-N	5.36	127.46	120.28
15	E	364	ILE	C-N-CA	5.36	127.46	120.28
15	E	443	ALA	CA-C-N	5.36	127.46	120.28
15	E	443	ALA	C-N-CA	5.36	127.46	120.28
4	G	52	ARG	CA-C-N	5.36	127.46	120.28
4	G	52	ARG	C-N-CA	5.36	127.46	120.28
15	E	326	ARG	CA-C-N	5.36	127.77	120.54
15	E	326	ARG	C-N-CA	5.36	127.77	120.54
15	A	490	ASP	CA-C-N	5.36	127.91	120.63
15	A	490	ASP	C-N-CA	5.36	127.91	120.63
4	G	35	GLU	CA-C-N	5.35	127.45	120.28
4	G	35	GLU	C-N-CA	5.35	127.45	120.28
15	E	46	VAL	CA-C-N	5.34	130.87	123.07
15	E	46	VAL	C-N-CA	5.34	130.87	123.07
15	E	432	VAL	CA-C-N	5.34	131.16	121.92
15	E	432	VAL	C-N-CA	5.34	131.16	121.92
3	F	377	LEU	CA-C-N	5.34	127.38	120.44
3	F	377	LEU	C-N-CA	5.34	127.38	120.44
15	E	427	ALA	CA-C-N	5.34	127.38	120.44
15	E	427	ALA	C-N-CA	5.34	127.38	120.44
15	C	526	ASN	CA-C-N	5.33	129.13	120.60
15	C	526	ASN	C-N-CA	5.33	129.13	120.60
3	F	375	SER	CA-C-N	5.33	127.37	120.44
3	F	375	SER	C-N-CA	5.33	127.37	120.44
15	A	514	THR	CA-C-N	5.33	127.42	120.28
15	A	514	THR	C-N-CA	5.33	127.42	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	335	ASP	CA-C-N	5.33	130.25	122.85
3	F	335	ASP	C-N-CA	5.33	130.25	122.85
4	K	87	ASP	CA-C-N	5.32	127.46	120.60
4	K	87	ASP	C-N-CA	5.32	127.46	120.60
11	d	220	ALA	CA-C-N	5.32	127.46	120.60
11	d	220	ALA	C-N-CA	5.32	127.46	120.60
3	F	402	TYR	CA-C-N	5.32	127.86	120.63
3	F	402	TYR	C-N-CA	5.32	127.86	120.63
3	F	431	LEU	CA-C-N	5.31	127.67	120.65
3	F	431	LEU	C-N-CA	5.31	127.67	120.65
15	E	104	GLY	CA-C-N	5.31	128.85	122.26
15	E	104	GLY	C-N-CA	5.31	128.85	122.26
11	d	162	PRO	CA-C-N	5.31	127.35	120.44
11	d	162	PRO	C-N-CA	5.31	127.35	120.44
15	C	278	GLY	CA-C-N	5.31	128.39	120.95
15	C	278	GLY	C-N-CA	5.31	128.39	120.95
11	d	210	ASP	CA-C-N	5.31	127.34	120.44
11	d	210	ASP	C-N-CA	5.31	127.34	120.44
11	d	291	LYS	CA-C-N	5.31	127.34	120.44
11	d	291	LYS	C-N-CA	5.31	127.34	120.44
4	G	48	LYS	CA-C-N	5.30	127.38	120.28
4	G	48	LYS	C-N-CA	5.30	127.38	120.28
5	H	19	GLU	CA-C-N	5.30	127.81	120.29
5	H	19	GLU	C-N-CA	5.30	127.81	120.29
15	C	82	VAL	CA-C-N	5.30	130.03	122.72
15	C	82	VAL	C-N-CA	5.30	130.03	122.72
5	L	89	GLU	CA-C-N	5.29	127.32	120.44
5	L	89	GLU	C-N-CA	5.29	127.32	120.44
4	K	73	GLN	CA-C-N	5.28	127.61	120.38
4	K	73	GLN	C-N-CA	5.28	127.61	120.38
15	C	235	VAL	CA-C-N	5.28	127.61	120.65
15	C	235	VAL	C-N-CA	5.28	127.61	120.65
11	d	295	GLU	CA-C-N	5.27	127.30	120.44
11	d	295	GLU	C-N-CA	5.27	127.30	120.44
15	E	271	SER	CA-C-N	5.27	127.77	120.29
15	E	271	SER	C-N-CA	5.27	127.77	120.29
15	C	509	LYS	CA-C-N	5.27	127.39	120.60
15	C	509	LYS	C-N-CA	5.27	127.39	120.60
15	C	424	VAL	CA-C-N	5.27	127.28	120.44
15	C	424	VAL	C-N-CA	5.27	127.28	120.44
15	A	543	MET	CA-C-N	5.27	127.29	120.44
15	A	543	MET	C-N-CA	5.27	127.29	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	d	330	TRP	CA-C-N	5.26	127.19	120.56
11	d	330	TRP	C-N-CA	5.26	127.19	120.56
15	C	81	PRO	CA-C-N	5.25	130.72	122.84
15	C	81	PRO	C-N-CA	5.25	130.72	122.84
15	E	337	ALA	CA-C-N	5.25	127.27	120.44
15	E	337	ALA	C-N-CA	5.25	127.27	120.44
3	F	374	LEU	CA-C-N	5.25	130.35	122.47
3	F	374	LEU	C-N-CA	5.25	130.35	122.47
11	d	175	ASP	CA-C-N	5.25	128.30	120.95
11	d	175	ASP	C-N-CA	5.25	128.30	120.95
15	C	538	TYR	CA-C-N	5.25	127.27	120.44
15	C	538	TYR	C-N-CA	5.25	127.27	120.44
3	F	351	GLY	N-CA-C	5.25	117.97	110.46
15	C	546	ASN	CA-C-N	5.25	127.17	120.56
15	C	546	ASN	C-N-CA	5.25	127.17	120.56
15	E	381	LEU	CA-C-N	5.24	127.26	120.44
15	E	381	LEU	C-N-CA	5.24	127.26	120.44
15	E	44	GLU	CA-C-N	5.24	128.31	120.87
15	E	44	GLU	C-N-CA	5.24	128.31	120.87
11	d	31	ALA	CA-C-N	5.24	127.25	120.44
11	d	31	ALA	C-N-CA	5.24	127.25	120.44
11	d	191	GLU	CA-C-N	5.24	127.25	120.44
11	d	191	GLU	C-N-CA	5.24	127.25	120.44
15	E	19	SER	CA-C-N	5.23	129.53	120.58
15	E	19	SER	C-N-CA	5.23	129.53	120.58
1	T	537	PRO	CA-C-N	5.23	130.53	121.64
1	T	537	PRO	C-N-CA	5.23	130.53	121.64
11	d	137	SER	CA-C-N	5.23	127.62	120.46
11	d	137	SER	C-N-CA	5.23	127.62	120.46
15	E	340	PHE	CA-C-N	5.22	127.59	120.54
15	E	340	PHE	C-N-CA	5.22	127.59	120.54
15	C	358	ALA	CA-C-N	5.22	127.28	120.28
15	C	358	ALA	C-N-CA	5.22	127.28	120.28
3	F	182	ALA	CA-C-N	5.22	130.70	121.05
3	F	182	ALA	C-N-CA	5.22	130.70	121.05
5	L	100	MET	CA-C-N	5.21	127.22	120.44
5	L	100	MET	C-N-CA	5.21	127.22	120.44
11	d	103	GLY	CA-C-N	5.21	127.27	120.28
11	d	103	GLY	C-N-CA	5.21	127.27	120.28
11	d	82	TYR	CA-C-N	5.21	127.21	120.44
11	d	82	TYR	C-N-CA	5.21	127.21	120.44
15	C	275	VAL	CA-C-N	5.21	130.50	123.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	C	275	VAL	C-N-CA	5.21	130.50	123.11
15	E	219	VAL	CA-C-N	5.21	127.52	120.44
15	E	219	VAL	C-N-CA	5.21	127.52	120.44
4	K	116	ASP	CA-C-N	5.20	127.20	120.44
4	K	116	ASP	C-N-CA	5.20	127.20	120.44
15	C	246	GLY	CA-C-N	5.20	129.73	121.72
15	C	246	GLY	C-N-CA	5.20	129.73	121.72
15	E	297	THR	CA-C-N	5.20	131.06	122.33
15	E	297	THR	C-N-CA	5.20	131.06	122.33
3	D	243	PRO	CA-C-N	5.20	128.21	120.31
3	D	243	PRO	C-N-CA	5.20	128.21	120.31
15	C	52	ASN	CA-C-N	5.19	128.14	120.82
15	C	52	ASN	C-N-CA	5.19	128.14	120.82
15	E	388	PHE	CA-C-N	5.19	127.24	120.28
15	E	388	PHE	C-N-CA	5.19	127.24	120.28
15	C	350	MET	CA-C-N	5.18	130.81	123.14
15	C	350	MET	C-N-CA	5.18	130.81	123.14
15	E	265	LEU	CA-C-N	5.18	127.23	120.28
15	E	265	LEU	C-N-CA	5.18	127.23	120.28
15	C	460	TYR	CA-C-N	5.18	127.53	120.54
15	C	460	TYR	C-N-CA	5.18	127.53	120.54
3	F	148	THR	CA-C-N	5.18	127.56	120.77
3	F	148	THR	C-N-CA	5.18	127.56	120.77
4	G	21	ALA	CA-C-N	5.18	128.18	120.31
4	G	21	ALA	C-N-CA	5.18	128.18	120.31
11	d	334	CYS	CA-C-N	5.18	128.46	122.35
11	d	334	CYS	C-N-CA	5.18	128.46	122.35
3	F	231	GLU	CA-C-N	5.17	130.48	122.26
3	F	231	GLU	C-N-CA	5.17	130.48	122.26
4	K	128	PRO	CA-C-N	5.17	130.70	122.74
4	K	128	PRO	C-N-CA	5.17	130.70	122.74
15	E	359	GLU	CA-C-N	5.17	127.16	120.44
15	E	359	GLU	C-N-CA	5.17	127.16	120.44
15	A	57	ILE	CA-C-N	5.16	128.00	121.85
15	A	57	ILE	C-N-CA	5.16	128.00	121.85
15	E	310	LYS	CA-C-N	5.16	130.31	122.37
15	E	310	LYS	C-N-CA	5.16	130.31	122.37
11	d	344	HIS	CA-C-N	5.16	127.61	120.29
11	d	344	HIS	C-N-CA	5.16	127.61	120.29
4	G	43	LEU	CA-C-N	5.15	127.74	120.42
4	G	43	LEU	C-N-CA	5.15	127.74	120.42
15	C	21	TYR	CA-C-N	5.15	131.51	121.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	C	21	TYR	C-N-CA	5.15	131.51	121.41
15	C	263	GLN	CA-C-N	5.15	127.14	120.44
15	C	263	GLN	C-N-CA	5.15	127.14	120.44
15	C	517	LEU	CA-C-N	5.15	127.49	120.54
15	C	517	LEU	C-N-CA	5.15	127.49	120.54
15	C	388	PHE	CA-C-N	5.14	127.17	120.28
15	C	388	PHE	C-N-CA	5.14	127.17	120.28
15	E	382	ALA	CA-C-N	5.14	127.12	120.44
15	E	382	ALA	C-N-CA	5.14	127.12	120.44
3	B	401	ASN	CA-C-N	5.14	127.12	120.44
3	B	401	ASN	C-N-CA	5.14	127.12	120.44
4	K	163	GLU	CA-C-N	5.14	130.20	123.11
4	K	163	GLU	C-N-CA	5.14	130.20	123.11
15	C	507	GLY	CA-C-N	5.14	127.16	120.28
15	C	507	GLY	C-N-CA	5.14	127.16	120.28
11	d	211	LEU	CA-C-N	5.13	127.58	120.29
11	d	211	LEU	C-N-CA	5.13	127.58	120.29
15	C	355	SER	CA-C-N	5.13	127.16	120.28
15	C	355	SER	C-N-CA	5.13	127.16	120.28
15	C	428	THR	CA-C-N	5.13	127.67	120.28
15	C	428	THR	C-N-CA	5.13	127.67	120.28
3	D	302	TYR	CA-C-N	5.13	127.16	120.28
3	D	302	TYR	C-N-CA	5.13	127.16	120.28
3	F	405	GLY	CA-C-N	5.13	127.15	120.28
3	F	405	GLY	C-N-CA	5.13	127.15	120.28
15	C	433	GLN	CA-C-N	5.12	130.11	122.99
15	C	433	GLN	C-N-CA	5.12	130.11	122.99
11	d	133	GLY	CA-C-N	5.12	128.74	121.42
11	d	133	GLY	C-N-CA	5.12	128.74	121.42
4	K	96	ALA	CA-C-N	5.12	127.09	120.44
4	K	96	ALA	C-N-CA	5.12	127.09	120.44
11	d	143	VAL	CA-C-N	5.12	127.59	120.63
11	d	143	VAL	C-N-CA	5.12	127.59	120.63
15	E	262	SER	CA-C-N	5.12	127.55	120.29
15	E	262	SER	C-N-CA	5.12	127.55	120.29
3	F	379	LYS	CA-C-N	5.11	130.52	122.49
3	F	379	LYS	C-N-CA	5.11	130.52	122.49
15	E	55	GLY	N-CA-C	5.11	118.74	111.12
15	A	480	THR	CA-C-N	5.11	127.13	120.28
15	A	480	THR	C-N-CA	5.11	127.13	120.28
5	L	85	GLN	CA-C-N	5.11	127.09	120.44
5	L	85	GLN	C-N-CA	5.11	127.09	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	C	247	THR	CA-C-N	5.11	130.84	122.81
15	C	247	THR	C-N-CA	5.11	130.84	122.81
15	E	476	ILE	CA-C-N	5.11	127.13	120.28
15	E	476	ILE	C-N-CA	5.11	127.13	120.28
3	F	183	GLY	CA-C-N	5.11	128.72	121.42
3	F	183	GLY	C-N-CA	5.11	128.72	121.42
15	A	481	LYS	CA-C-N	5.11	127.08	120.44
15	A	481	LYS	C-N-CA	5.11	127.08	120.44
15	A	549	HIS	CA-C-N	5.11	127.12	120.28
15	A	549	HIS	C-N-CA	5.11	127.12	120.28
11	d	146	ASN	CA-C-N	5.10	127.43	120.54
11	d	146	ASN	C-N-CA	5.10	127.43	120.54
15	C	485	VAL	CA-C-N	5.10	127.12	120.28
15	C	485	VAL	C-N-CA	5.10	127.12	120.28
15	A	486	LEU	CA-C-N	5.10	127.12	120.28
15	A	486	LEU	C-N-CA	5.10	127.12	120.28
5	L	81	THR	CA-C-N	5.10	127.07	120.44
5	L	81	THR	C-N-CA	5.10	127.07	120.44
11	d	79	VAL	CA-C-N	5.10	127.07	120.44
11	d	79	VAL	C-N-CA	5.10	127.07	120.44
11	d	173	LEU	CA-C-N	5.10	127.37	120.44
11	d	173	LEU	C-N-CA	5.10	127.37	120.44
15	E	248	CYS	CA-C-N	5.09	130.57	122.94
15	E	248	CYS	C-N-CA	5.09	130.57	122.94
11	d	41	ASN	CA-C-N	5.08	127.60	120.28
11	d	41	ASN	C-N-CA	5.08	127.60	120.28
5	H	24	VAL	CA-C-N	5.08	127.50	120.29
5	H	24	VAL	C-N-CA	5.08	127.50	120.29
15	C	505	ALA	CA-C-N	5.08	127.09	120.28
15	C	505	ALA	C-N-CA	5.08	127.09	120.28
4	K	127	GLU	CA-C-N	5.08	124.57	119.19
4	K	127	GLU	C-N-CA	5.08	124.57	119.19
11	d	257	ILE	CA-C-N	5.08	128.08	120.87
11	d	257	ILE	C-N-CA	5.08	128.08	120.87
15	C	362	ARG	CA-C-N	5.08	127.04	120.44
15	C	362	ARG	C-N-CA	5.08	127.04	120.44
3	F	183	GLY	N-CA-C	5.07	118.98	110.56
15	C	432	VAL	CA-C-N	5.07	129.31	120.68
15	C	432	VAL	C-N-CA	5.07	129.31	120.68
4	K	190	VAL	CA-C-N	5.07	130.18	122.98
4	K	190	VAL	C-N-CA	5.07	130.18	122.98
4	K	132	LEU	CA-C-N	5.07	130.55	122.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	K	132	LEU	C-N-CA	5.07	130.55	122.74
11	d	77	LYS	CA-C-N	5.07	127.03	120.44
11	d	77	LYS	C-N-CA	5.07	127.03	120.44
11	d	331	ILE	CA-C-N	5.07	127.07	120.28
11	d	331	ILE	C-N-CA	5.07	127.07	120.28
15	C	427	ALA	CA-C-N	5.07	127.34	120.65
15	C	427	ALA	C-N-CA	5.07	127.34	120.65
11	d	214	PHE	CA-C-N	5.06	127.37	120.54
11	d	214	PHE	C-N-CA	5.06	127.37	120.54
3	B	358	GLN	CA-C-N	5.06	127.02	120.44
3	B	358	GLN	C-N-CA	5.06	127.02	120.44
3	F	408	VAL	CA-C-N	5.06	127.31	120.38
3	F	408	VAL	C-N-CA	5.06	127.31	120.38
15	C	234	ARG	CA-C-N	5.06	127.12	120.60
15	C	234	ARG	C-N-CA	5.06	127.12	120.60
3	B	165	SER	CA-C-N	5.06	130.40	122.21
3	B	165	SER	C-N-CA	5.06	130.40	122.21
11	d	349	TYR	CA-C-N	5.06	128.65	121.42
11	d	349	TYR	C-N-CA	5.06	128.65	121.42
15	A	581	LEU	CA-C-N	5.05	127.75	120.38
15	A	581	LEU	C-N-CA	5.05	127.75	120.38
11	d	74	CYS	CA-C-N	5.05	127.05	120.28
11	d	74	CYS	C-N-CA	5.05	127.05	120.28
3	D	305	THR	CA-C-N	5.05	127.31	120.65
3	D	305	THR	C-N-CA	5.05	127.31	120.65
3	D	287	SER	CA-C-N	5.04	127.35	120.54
3	D	287	SER	C-N-CA	5.04	127.35	120.54
3	F	155	ILE	CA-C-N	5.04	130.99	122.87
3	F	155	ILE	C-N-CA	5.04	130.99	122.87
11	d	171	GLU	CA-C-N	5.04	127.45	120.29
11	d	171	GLU	C-N-CA	5.04	127.45	120.29
11	d	264	VAL	CA-C-N	5.04	127.04	120.28
11	d	264	VAL	C-N-CA	5.04	127.04	120.28
15	E	380	TYR	CA-C-N	5.04	127.80	120.79
15	E	380	TYR	C-N-CA	5.04	127.80	120.79
11	d	246	LEU	CA-C-N	5.04	130.46	122.60
11	d	246	LEU	C-N-CA	5.04	130.46	122.60
15	C	426	SER	CA-C-N	5.04	127.28	120.38
15	C	426	SER	C-N-CA	5.04	127.28	120.38
11	d	81	ASP	CA-C-N	5.03	126.98	120.44
11	d	81	ASP	C-N-CA	5.03	126.98	120.44
11	d	251	GLY	CA-C-N	5.03	126.98	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	d	251	GLY	C-N-CA	5.03	126.98	120.44
11	d	254	GLU	CA-C-N	5.03	127.43	120.29
11	d	254	GLU	C-N-CA	5.03	127.43	120.29
15	C	479	ARG	CA-C-N	5.03	127.33	120.54
15	C	479	ARG	C-N-CA	5.03	127.33	120.54
3	D	307	LEU	CA-C-N	5.03	126.98	120.44
3	D	307	LEU	C-N-CA	5.03	126.98	120.44
4	G	46	ALA	CA-C-N	5.03	127.29	120.65
4	G	46	ALA	C-N-CA	5.03	127.29	120.65
15	E	32	VAL	CA-C-N	5.03	129.78	123.10
15	E	32	VAL	C-N-CA	5.03	129.78	123.10
3	F	176	ALA	CA-C-N	5.03	127.01	120.28
3	F	176	ALA	C-N-CA	5.03	127.01	120.28
5	H	33	ALA	CA-C-N	5.02	127.32	120.54
5	H	33	ALA	C-N-CA	5.02	127.32	120.54
15	E	263	GLN	CA-C-N	5.02	126.97	120.44
15	E	263	GLN	C-N-CA	5.02	126.97	120.44
1	T	442	ASP	N-CA-C	5.01	117.27	110.35
11	d	138	ILE	CA-C-N	5.01	126.99	120.28
11	d	138	ILE	C-N-CA	5.01	126.99	120.28
15	C	423	PRO	CA-C-N	5.01	126.87	120.56
15	C	423	PRO	C-N-CA	5.01	126.87	120.56
3	F	349	THR	CA-C-N	5.01	130.96	122.65
3	F	349	THR	C-N-CA	5.01	130.96	122.65
15	C	542	TRP	CA-C-N	5.01	127.49	120.28
15	C	542	TRP	C-N-CA	5.01	127.49	120.28
11	d	297	GLU	CA-C-N	5.00	127.32	120.46
11	d	297	GLU	C-N-CA	5.00	127.32	120.46
15	C	264	ALA	CA-C-N	5.00	127.30	120.54
15	C	264	ALA	C-N-CA	5.00	127.30	120.54
15	A	545	ARG	CA-C-N	5.00	127.25	120.44
15	A	545	ARG	C-N-CA	5.00	127.25	120.44
3	F	147	SER	CA-C-N	5.00	127.29	120.54
3	F	147	SER	C-N-CA	5.00	127.29	120.54
15	C	585	LEU	CA-C-N	5.00	128.37	120.47
15	C	585	LEU	C-N-CA	5.00	128.37	120.47

There are no chirality outliers.

There are no planarity outliers.

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	T	2073	0	576	0	0
2	a	2869	0	774	0	0
3	B	1832	0	504	1	0
3	D	1816	0	499	0	0
3	F	1824	0	502	0	0
4	G	852	0	218	0	0
4	I	904	0	236	0	0
4	K	896	0	231	0	0
5	H	420	0	112	0	0
5	J	441	0	120	0	0
5	L	429	0	115	0	0
6	M	872	0	238	0	0
7	N	404	0	101	0	0
8	P	1732	0	450	0	0
9	b	176	0	49	0	0
10	c	685	0	202	0	0
11	d	1369	0	364	1	0
12	e	224	0	67	0	0
13	g	648	0	204	0	0
13	h	648	0	204	0	0
13	i	644	0	203	0	0
13	j	644	0	203	0	0
13	k	644	0	203	0	0
13	l	644	0	203	0	0
13	m	648	0	204	0	0
13	n	648	0	204	0	0
13	o	636	0	201	0	0
14	r	192	0	50	0	0
15	A	2308	0	635	0	0
15	C	2440	0	675	0	0
15	E	2465	0	683	0	0
16	O	1385	0	352	0	0
17	E	27	0	11	0	0
18	E	1	0	0	0	0
All	All	34440	0	9593	2	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 0.

All (2) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:244:THR:O	3:B:247:ARG:N	2.53	0.41
11:d:350:MET:O	11:d:351:PHE:C	2.65	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	T	516/542 (95%)	483 (94%)	31 (6%)	2 (0%)	30	66
2	a	711/817 (87%)	700 (98%)	10 (1%)	1 (0%)	48	83
3	B	454/486 (93%)	437 (96%)	17 (4%)	0	100	100
3	D	448/486 (92%)	415 (93%)	28 (6%)	5 (1%)	11	45
3	F	452/486 (93%)	432 (96%)	20 (4%)	0	100	100
4	G	211/230 (92%)	207 (98%)	4 (2%)	0	100	100
4	I	224/230 (97%)	221 (99%)	3 (1%)	0	100	100
4	K	222/230 (96%)	218 (98%)	3 (1%)	1 (0%)	24	62
5	H	103/110 (94%)	102 (99%)	1 (1%)	0	100	100
5	J	108/110 (98%)	101 (94%)	7 (6%)	0	100	100
5	L	105/110 (96%)	103 (98%)	2 (2%)	0	100	100
6	M	216/261 (83%)	196 (91%)	15 (7%)	5 (2%)	5	28
7	N	99/128 (77%)	87 (88%)	8 (8%)	4 (4%)	2	18
8	P	431/441 (98%)	423 (98%)	8 (2%)	0	100	100
9	b	42/321 (13%)	42 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	c	169/180 (94%)	168 (99%)	1 (1%)	0	100	100
11	d	338/351 (96%)	324 (96%)	14 (4%)	0	100	100
12	e	52/70 (74%)	50 (96%)	2 (4%)	0	100	100
13	g	160/164 (98%)	158 (99%)	2 (1%)	0	100	100
13	h	160/164 (98%)	158 (99%)	2 (1%)	0	100	100
13	i	159/164 (97%)	158 (99%)	1 (1%)	0	100	100
13	j	159/164 (97%)	157 (99%)	2 (1%)	0	100	100
13	k	159/164 (97%)	157 (99%)	2 (1%)	0	100	100
13	l	159/164 (97%)	155 (98%)	4 (2%)	0	100	100
13	m	160/164 (98%)	157 (98%)	3 (2%)	0	100	100
13	n	160/164 (98%)	157 (98%)	3 (2%)	0	100	100
13	o	157/164 (96%)	156 (99%)	1 (1%)	0	100	100
14	r	46/364 (13%)	45 (98%)	1 (2%)	0	100	100
15	A	571/623 (92%)	553 (97%)	18 (3%)	0	100	100
15	C	606/623 (97%)	587 (97%)	18 (3%)	1 (0%)	43	77
15	E	612/623 (98%)	575 (94%)	37 (6%)	0	100	100
16	O	340/375 (91%)	322 (95%)	18 (5%)	0	100	100
All	All	8509/9673 (88%)	8204 (96%)	286 (3%)	19 (0%)	44	77

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	M	92	ALA
3	D	448	ASN
3	D	462	ILE
2	a	97	ASP
6	M	161	ASP
3	D	382	ILE
6	M	77	ALA
7	N	40	LYS
1	T	415	ALA
4	K	126	LYS
6	M	94	LEU
7	N	31	GLY
7	N	35	VAL
6	M	98	SER

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Mol	Chain	Res	Type
7	N	87	SER
15	C	419	ASP
3	D	151	VAL
1	T	190	ILE
3	D	367	PRO

5.3.2 Protein sidechains [i](#)

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

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
17	ADP	E	701	18	28,29,29	3.01	10 (35%)	43,45,45	2.29	10 (23%)

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
17	ADP	E	701	18	-	3/16/32/32	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	E	701	ADP	O4'-C1'	8.55	1.61	1.42
17	E	701	ADP	C2'-C1'	-7.26	1.30	1.53
17	E	701	ADP	O4'-C4'	-6.30	1.31	1.45
17	E	701	ADP	PA-O3A	4.55	1.64	1.59
17	E	701	ADP	C6-N6	4.25	1.45	1.34
17	E	701	ADP	O3'-C3'	-2.95	1.35	1.43
17	E	701	ADP	C5-N7	-2.81	1.34	1.39
17	E	701	ADP	C5-C4	-2.71	1.34	1.39
17	E	701	ADP	O2'-C2'	2.42	1.49	1.43
17	E	701	ADP	C8-N9	-2.13	1.33	1.37

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	E	701	ADP	N6-C6-N1	-7.28	102.17	118.38
17	E	701	ADP	C5-C6-N6	5.79	137.61	123.29
17	E	701	ADP	C5-C4-N3	-5.50	119.15	126.72
17	E	701	ADP	N3-C2-N1	-5.07	120.90	128.58
17	E	701	ADP	N3-C4-N9	3.70	133.47	127.17
17	E	701	ADP	N9-C8-N7	-3.67	108.73	113.94
17	E	701	ADP	C2-N3-C4	3.27	119.83	111.83
17	E	701	ADP	C5-N7-C8	2.64	107.60	103.45
17	E	701	ADP	C6-C5-C4	2.52	120.61	117.18
17	E	701	ADP	O4'-C1'-N9	2.38	112.67	108.09

There are no chirality outliers.

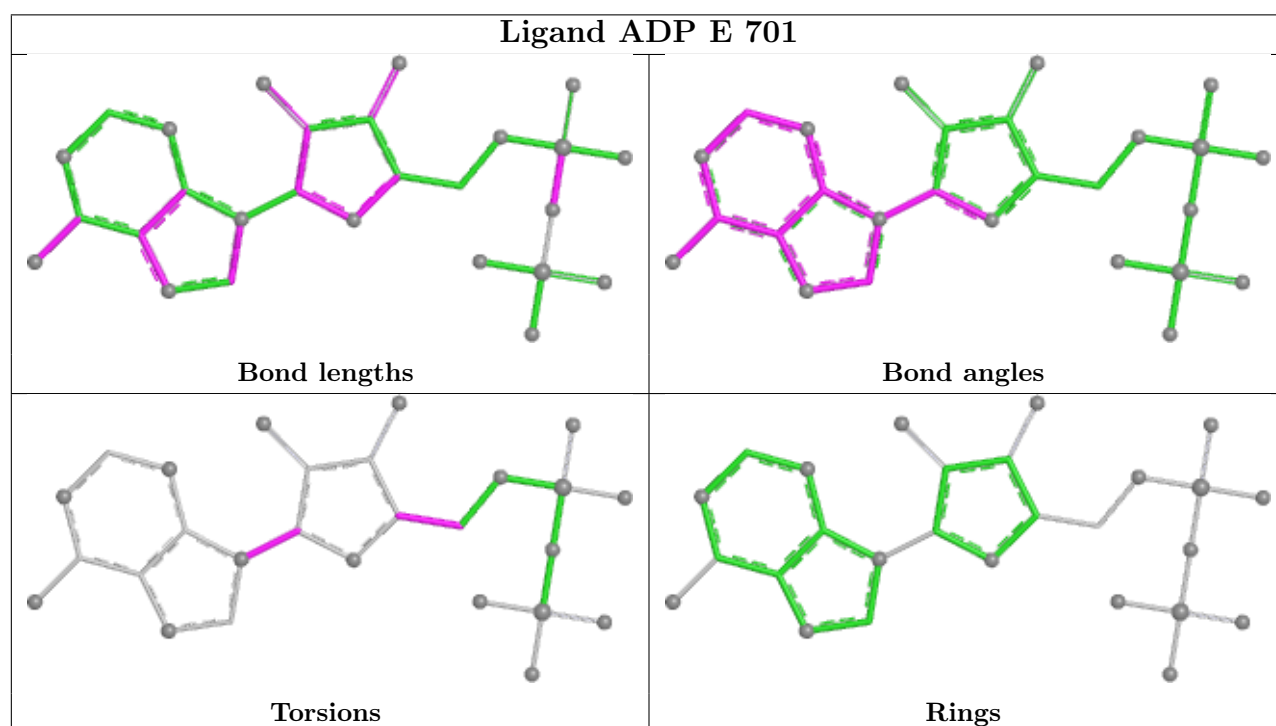
All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	E	701	ADP	O4'-C1'-N9-C8
17	E	701	ADP	O4'-C1'-N9-C4
17	E	701	ADP	O4'-C4'-C5'-O5'

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.

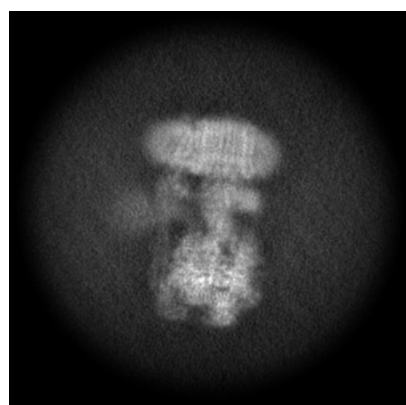
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-77789. These allow visual inspection of the internal detail of the map and identification of artifacts.

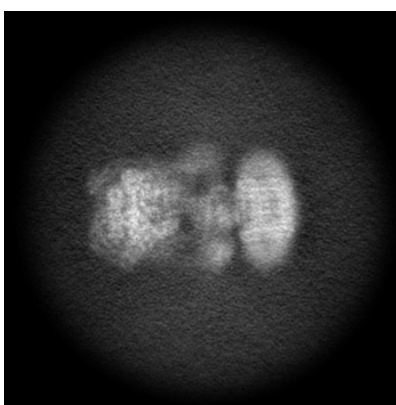
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

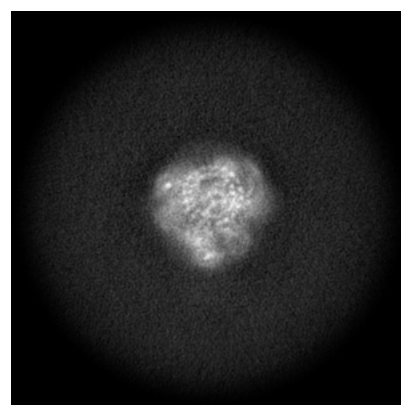
6.1.1 Primary map



X



Y

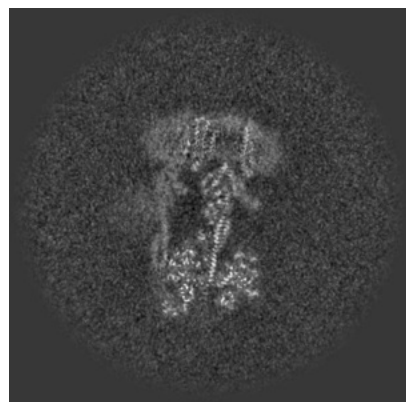


Z

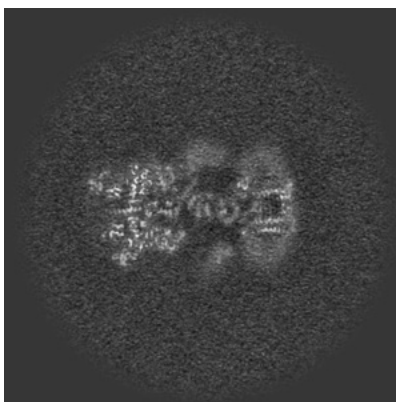
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

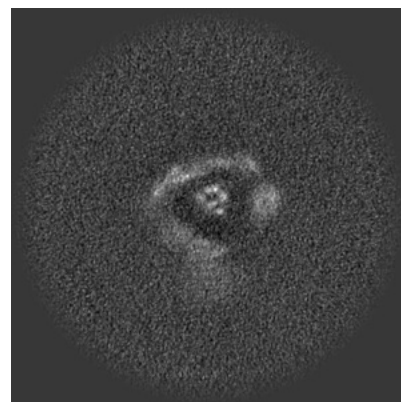
6.2.1 Primary map



X Index: 256



Y Index: 256

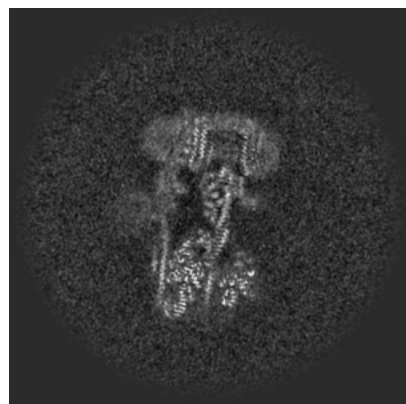


Z Index: 256

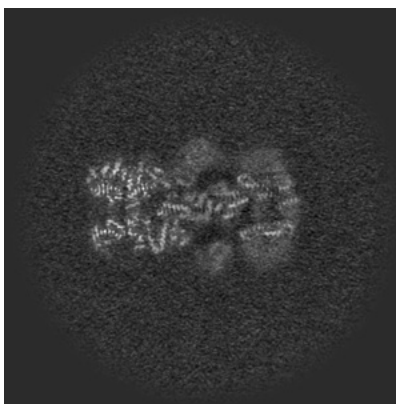
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

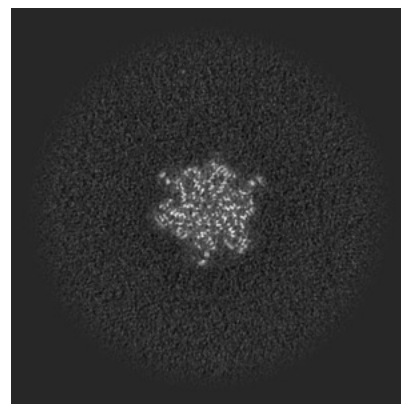
6.3.1 Primary map



X Index: 252



Y Index: 267

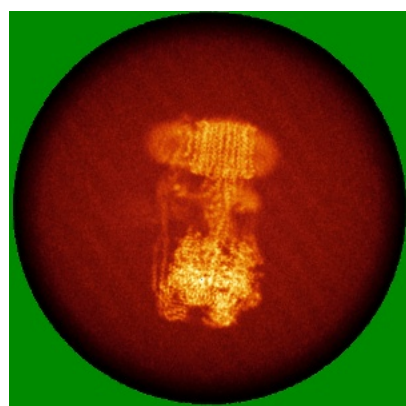


Z Index: 167

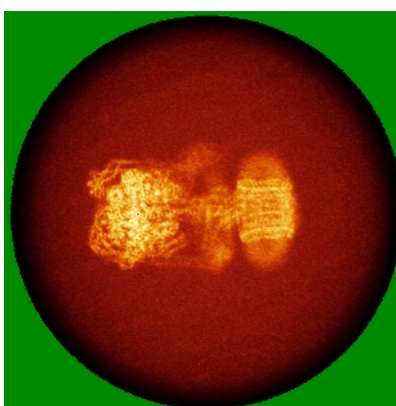
The images above show the largest variance slices of the map in three orthogonal directions.

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

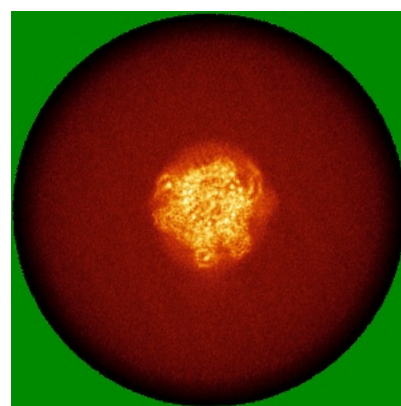
6.4.1 Primary map



X



Y



Z

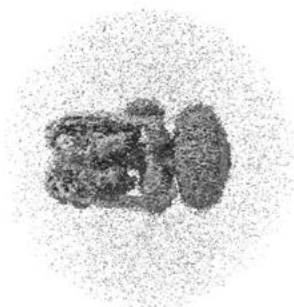
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

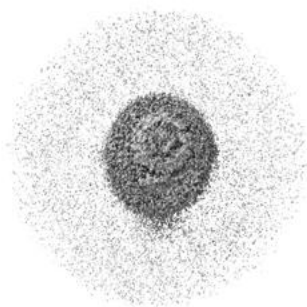
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.194. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

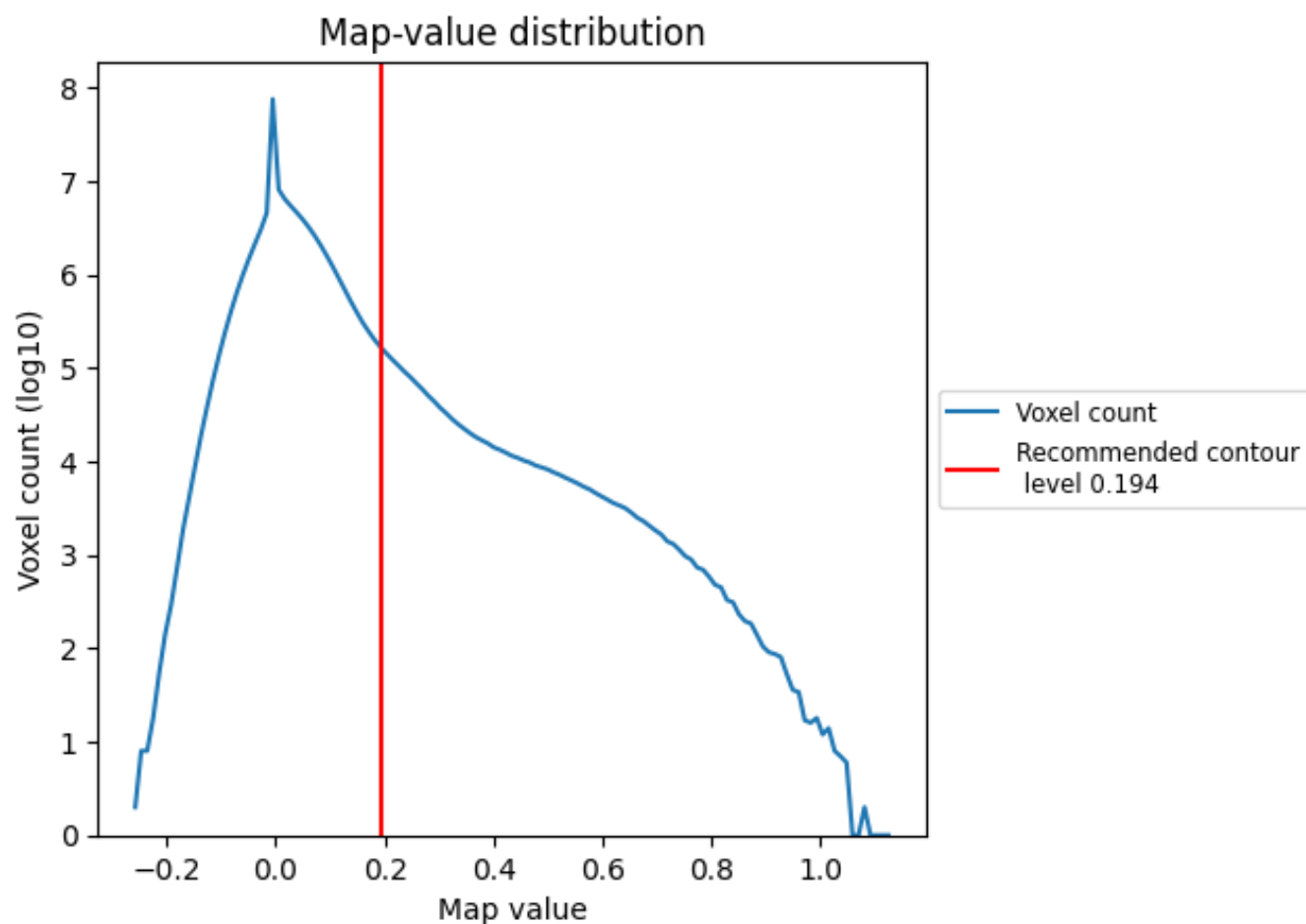
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

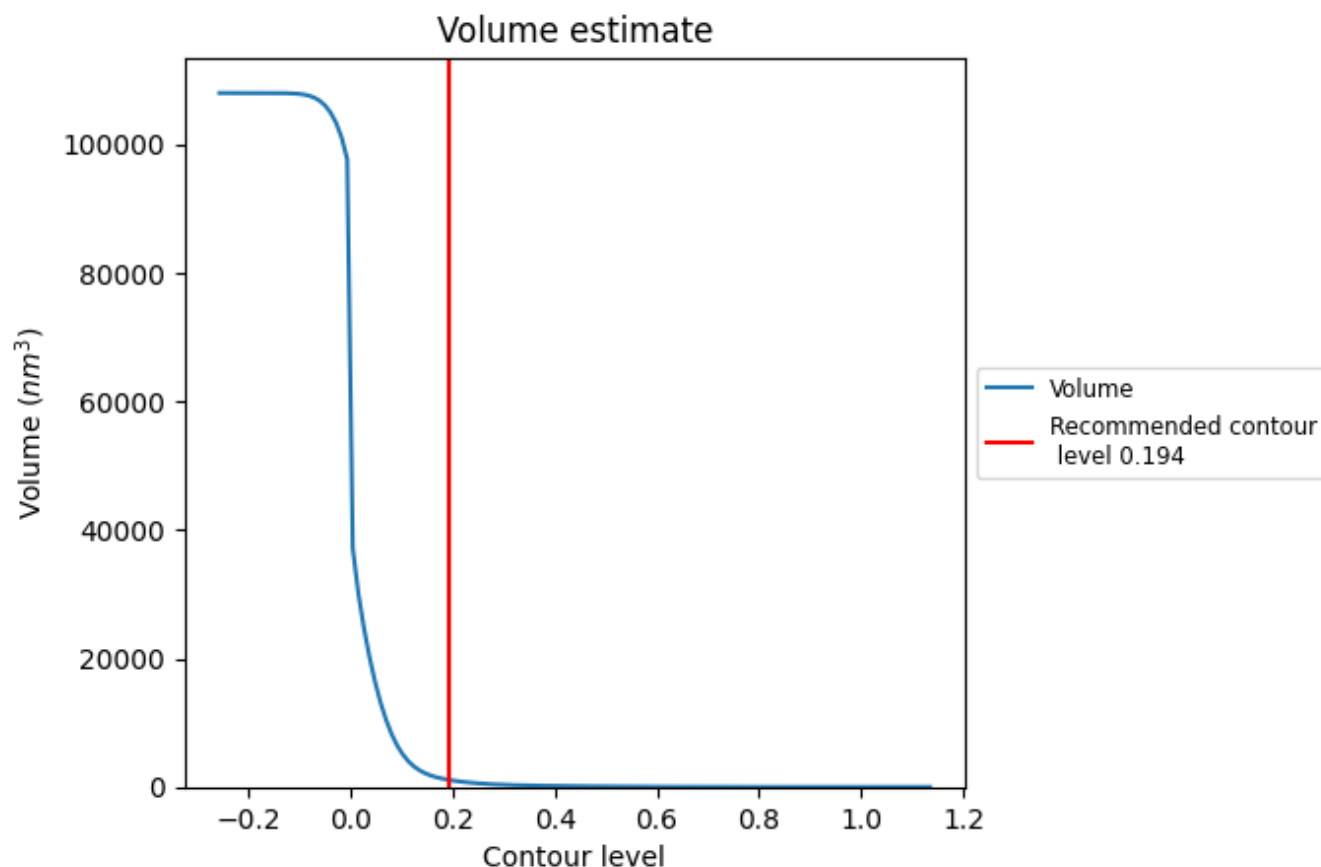
This section contains the results of statistical analysis of the map.

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.

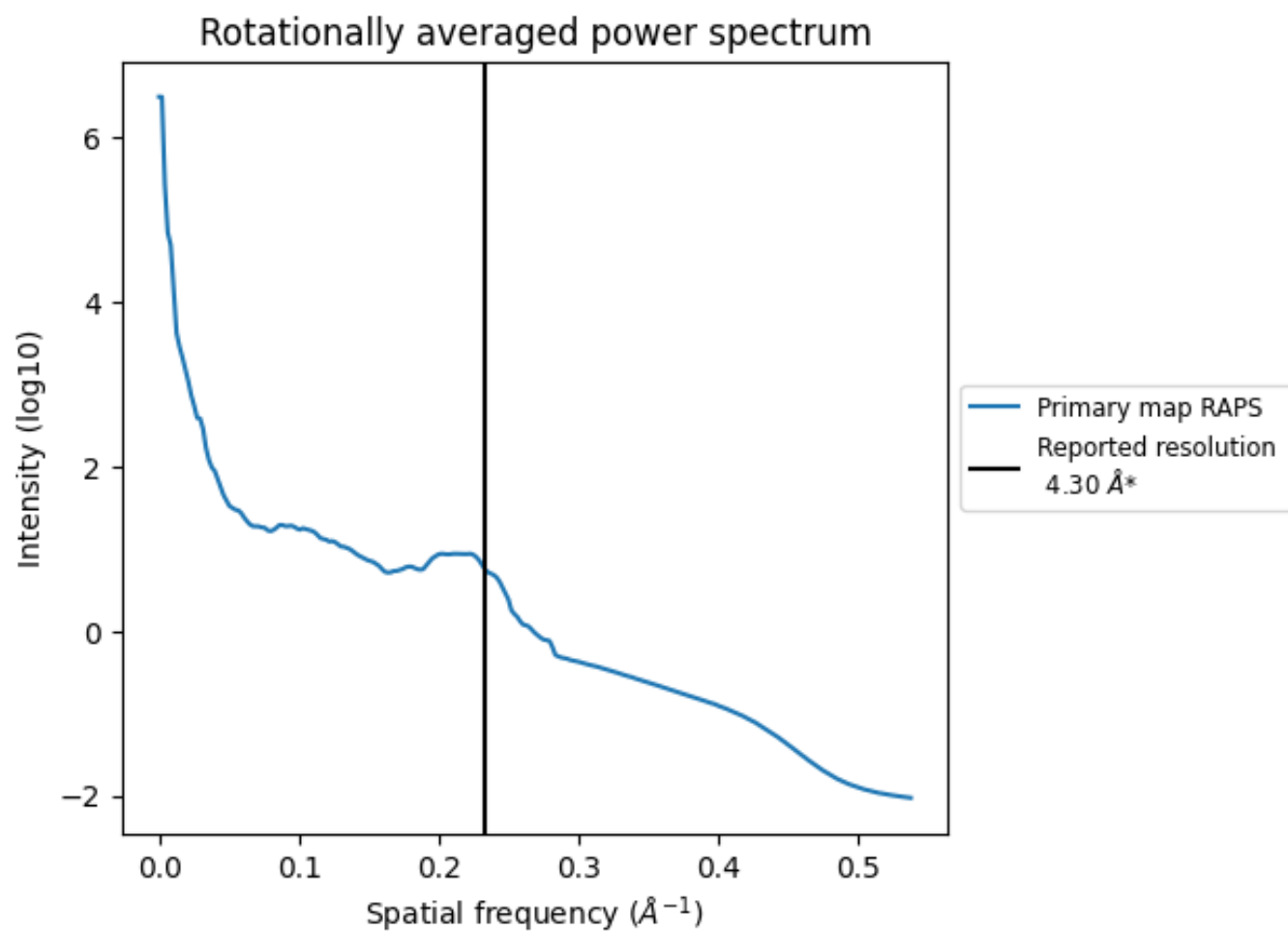
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1072 nm^3 ; this corresponds to an approximate mass of 968 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 0.233 Å⁻¹

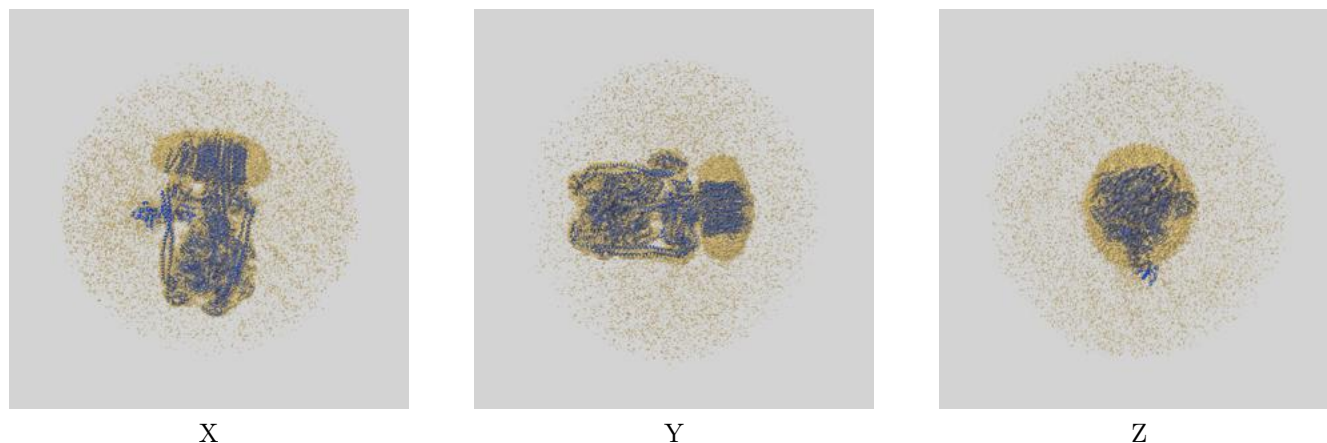
8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

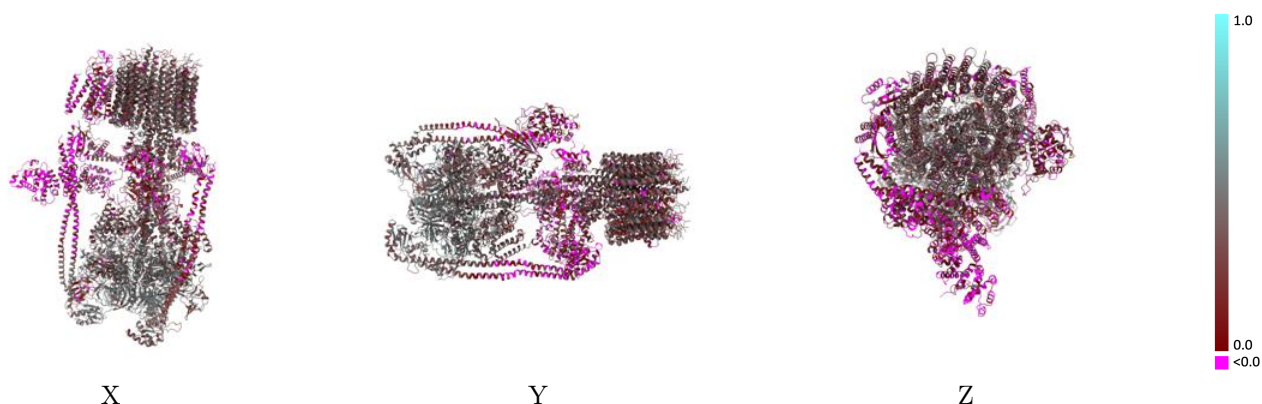
This section contains information regarding the fit between EMDB map EMD-77789 and PDB model 36QX. Per-residue inclusion information can be found in section [3](#) on page [9](#).

9.1 Map-model overlay [i](#)



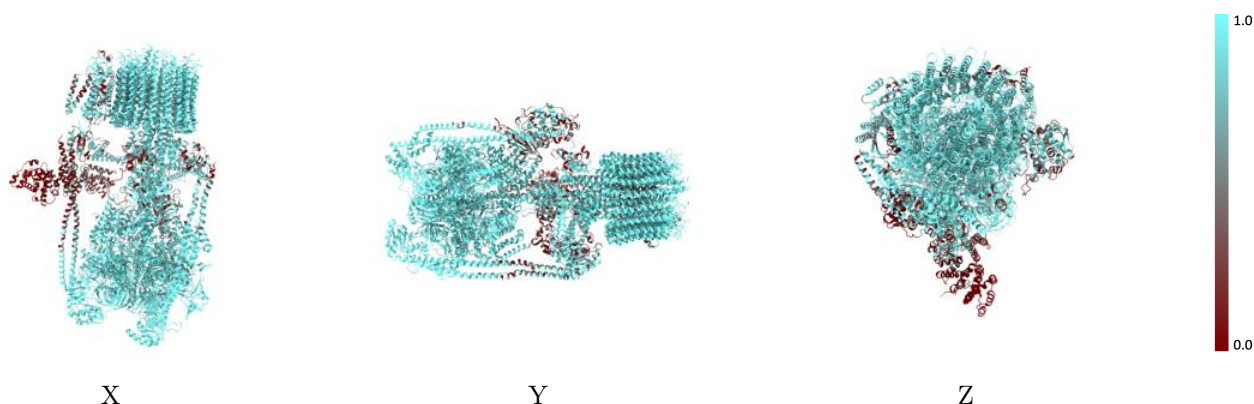
The images above show the 3D surface view of the map at the recommended contour level 0.194 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



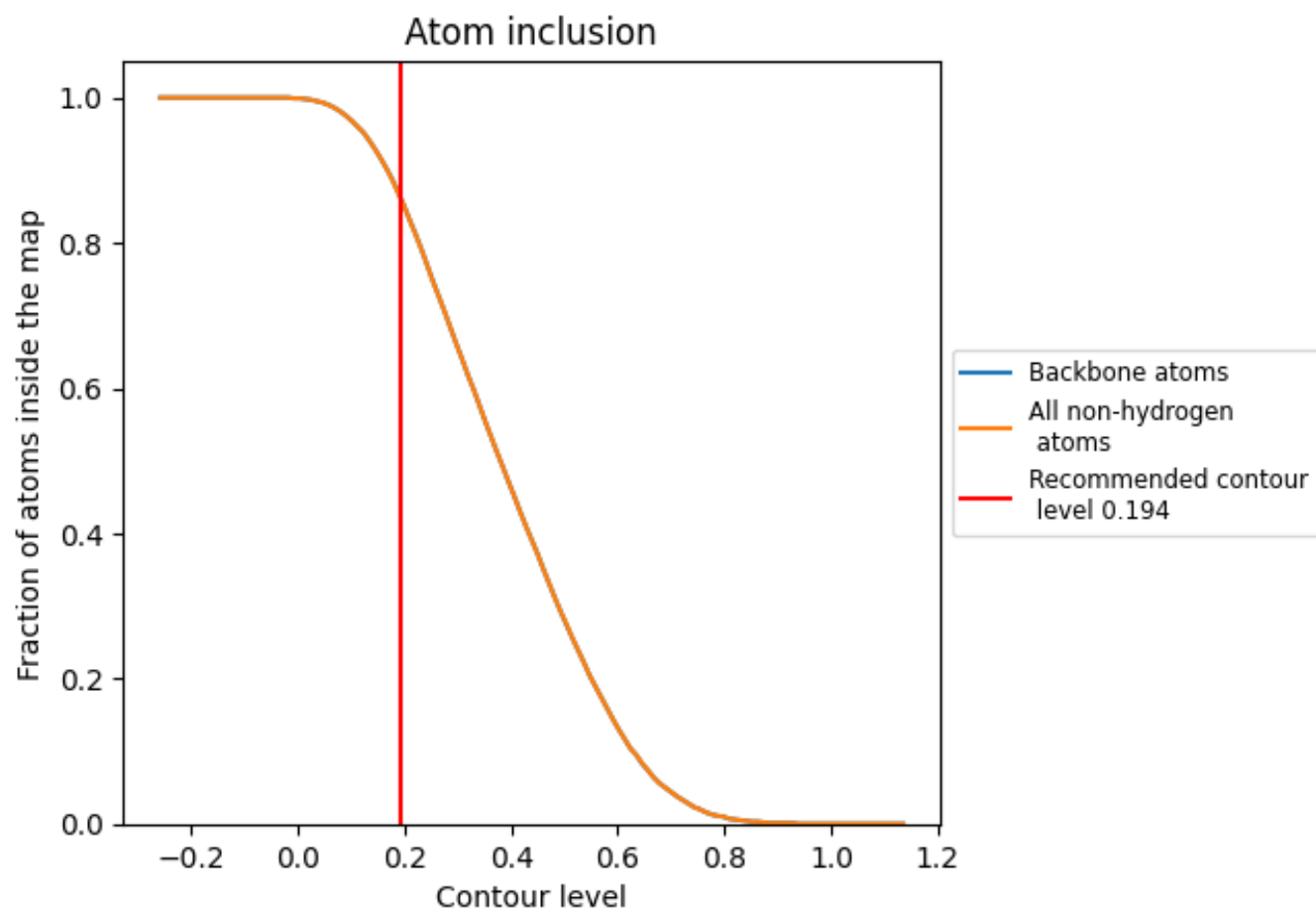
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.194).

9.4 Atom inclusion ⓘ



At the recommended contour level, 86% of all backbone atoms, 86% 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 (0.194) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8600	 0.3030
A	 0.9850	 0.4050
B	 0.9890	 0.4500
C	 0.9740	 0.4100
D	 0.9800	 0.4430
E	 0.9680	 0.3650
F	 0.9840	 0.4290
G	 0.9570	 0.3130
H	 0.8140	 0.1900
I	 0.9180	 0.3280
J	 0.8230	 0.1840
K	 0.8390	 0.3000
L	 0.5800	 0.1460
M	 0.9290	 0.3490
N	 0.9460	 0.3030
O	 0.7160	 0.1010
P	 0.1420	 0.0230
T	 0.6310	 0.2210
a	 0.7310	 0.1200
b	 0.9200	 0.3410
c	 0.9640	 0.3390
d	 0.9550	 0.3320
e	 0.5310	 -0.0070
g	 0.9660	 0.3380
h	 0.9610	 0.3230
i	 0.9350	 0.3130
j	 0.9630	 0.3260
k	 0.9490	 0.3360
l	 0.9800	 0.3440
m	 0.9610	 0.3170
n	 0.9320	 0.2960
o	 0.9560	 0.3350
r	 0.9270	 0.3720

