



Full wwPDB EM Validation Report ⓘ

Dec 10, 2022 – 08:05 pm GMT

PDB ID : 6R0Y
EMDB ID : EMD-4700
Title : Thermus thermophilus V/A-type ATPase/synthase, rotational state 3
Authors : Zhou, L.; Sazanov, L.
Deposited on : 2019-03-13
Resolution : 3.90 Å(reported)
Based on initial models : 5Y5Y, 5Y5X

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 : 1.8.4, 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) : 2.31.3

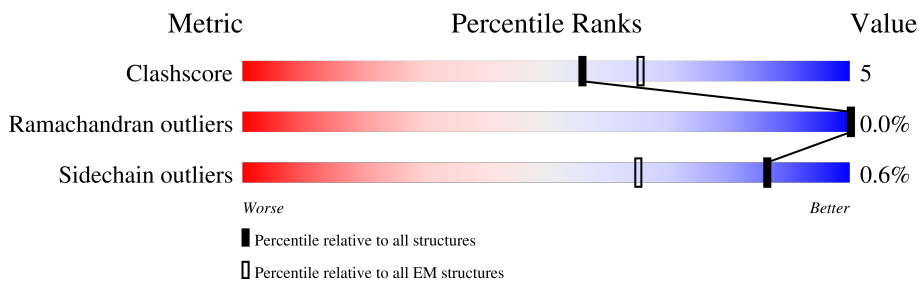
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.90 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	
1	B	578	
1	C	578	
2	D	478	
2	E	478	
2	F	478	
3	G	223	
4	H	104	

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Mol	Chain	Length	Quality of chain
5	I	120	
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 [i](#)

There are 11 unique types of molecules in this entry. The entry contains 40169 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
			Total	C	N	O	S		
1	A	577	Total 4472	C 2854	N 762	O 834	S 22	0	0
1	B	577	Total 4472	C 2854	N 762	O 834	S 22	0	0
1	C	577	Total 4472	C 2854	N 762	O 834	S 22	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	D	461	Total 3609	C 2285	N 625	O 689	S 10	0	0
2	E	462	Total 3618	C 2291	N 627	O 690	S 10	0	0
2	F	461	Total 3608	C 2286	N 624	O 688	S 10	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	G	206	Total 1619	C 1021	N 303	O 293	S 2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	H	104	Total 792	C 501	N 136	O 152	S 3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	103	Total	C	N	O	S	0	0
			808	501	150	156	1		
5	K	99	Total	C	N	O	S	0	0
			788	489	146	152	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
6	J	186	Total	C	N	O	0	0
			1437	894	270	273		
6	L	187	Total	C	N	O	0	0
			1441	896	271	274		

- 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
			1575	935	320	320		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
8	N	649	Total	C	N	O	0	0
			3190	1892	649	649		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
9	O	73	Total	C	N	O	0	0
			351	205	73	73		
9	P	73	Total	C	N	O	0	0
			351	205	73	73		
9	Q	74	Total	C	N	O	0	0
			356	208	74	74		
9	R	73	Total	C	N	O	0	0
			351	205	73	73		
9	S	73	Total	C	N	O	0	0
			351	205	73	73		
9	T	73	Total	C	N	O	0	0
			351	205	73	73		
9	U	73	Total	C	N	O	0	0
			351	205	73	73		

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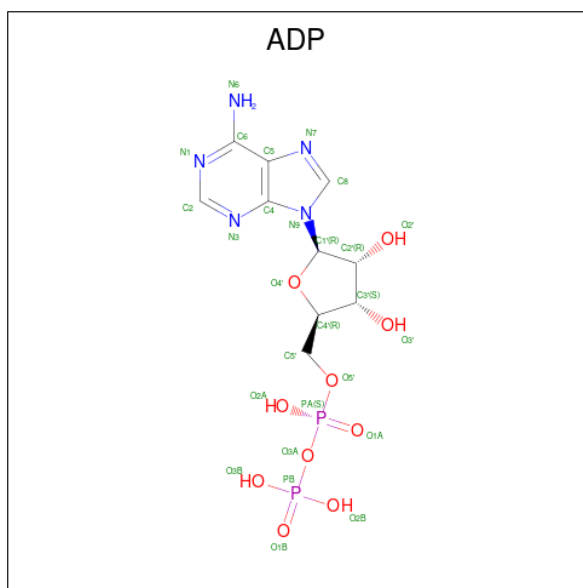
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Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
9	V	73	Total 351	C 205	N 73	O 73	0	0
9	W	73	Total 351	C 205	N 73	O 73	0	0
9	X	72	Total 347	C 203	N 72	O 72	0	0
9	Y	73	Total 351	C 205	N 73	O 73	0	0
9	Z	73	Total 351	C 205	N 73	O 73	0	0

- Molecule 10 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
10	B	1	Total 1	Mg 1	0

- Molecule 11 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).

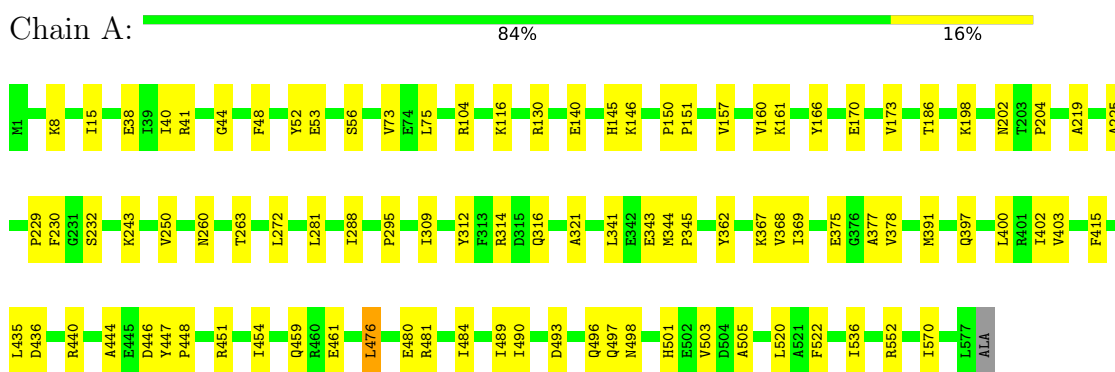


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
11	B	1	Total 27	C 10	N 5	O 10	P 2	0
11	D	1	Total 27	C 10	N 5	O 10	P 2	0

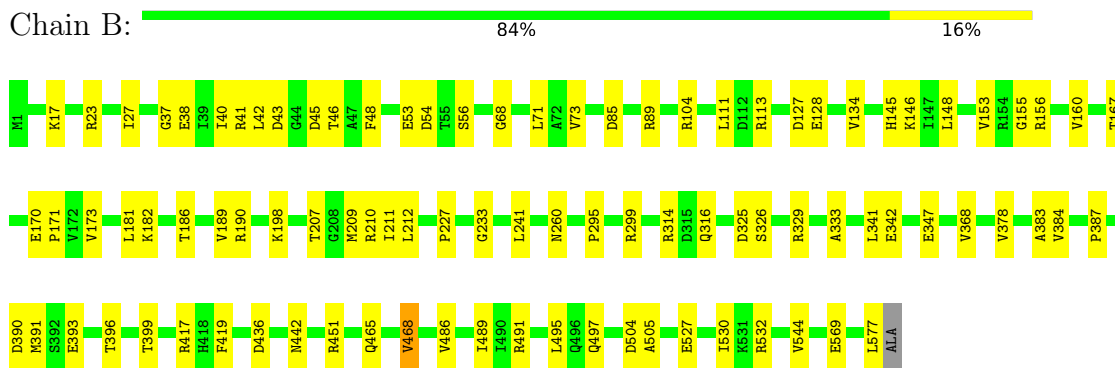
3 Residue-property plots [i](#)

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

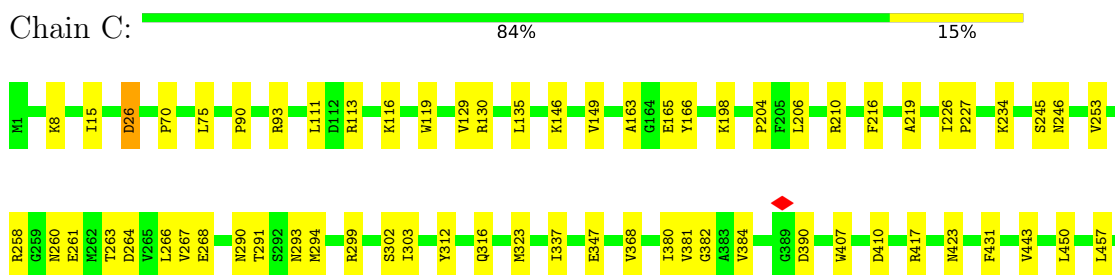
- Molecule 1: V-type ATP synthase alpha chain

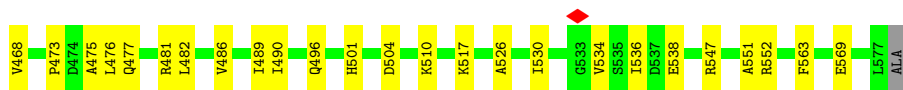


- Molecule 1: V-type ATP synthase alpha chain

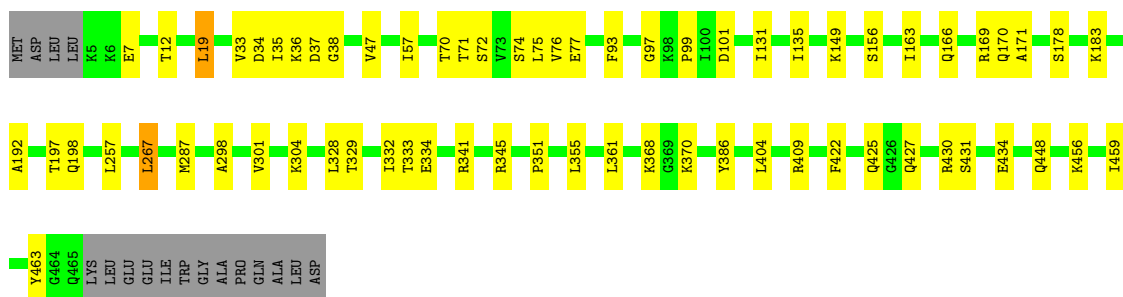
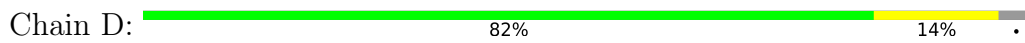


- Molecule 1: V-type ATP synthase alpha chain

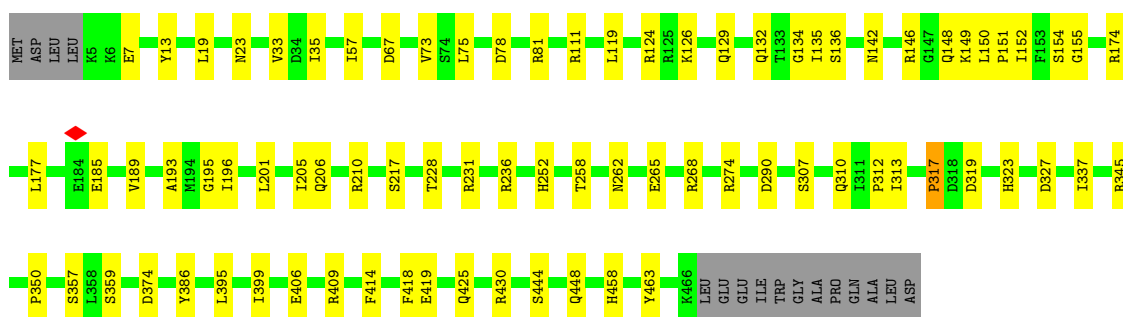
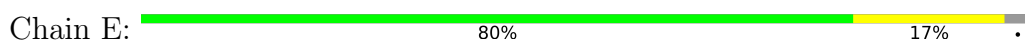




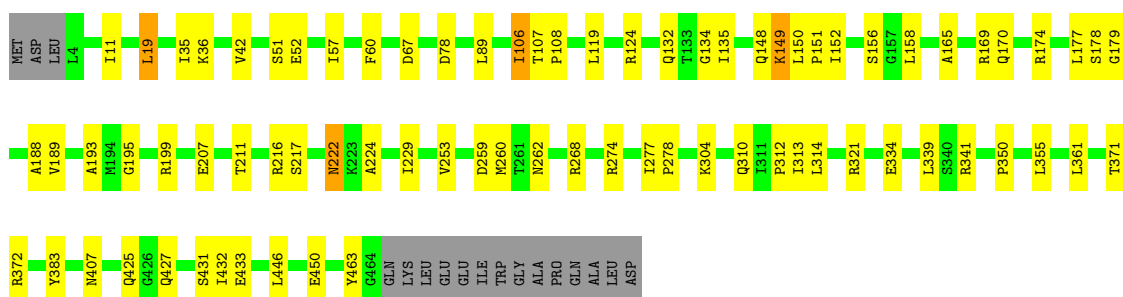
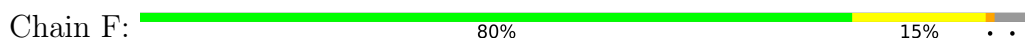
• Molecule 2: V-type ATP synthase beta chain



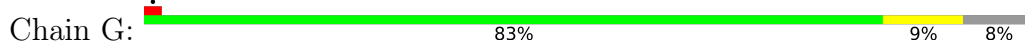
• Molecule 2: V-type ATP synthase beta chain

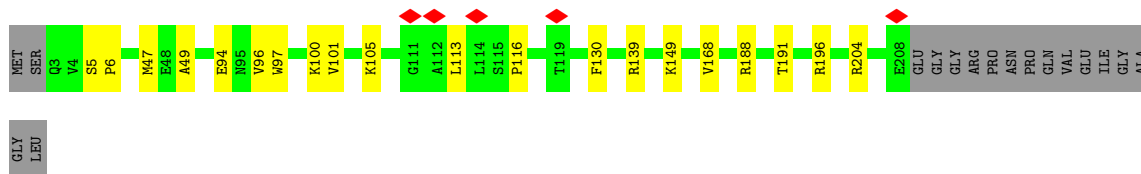


• Molecule 2: V-type ATP synthase beta chain

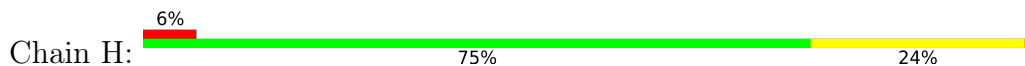


• Molecule 3: V-type ATP synthase subunit D

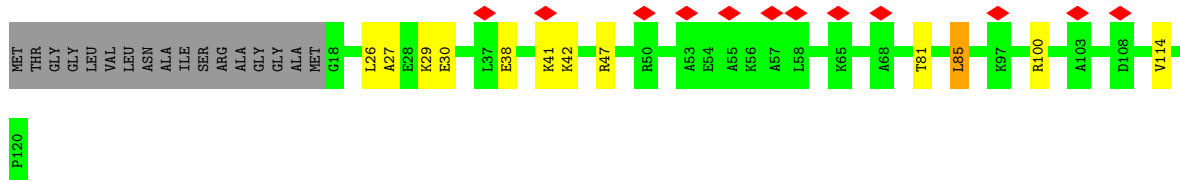
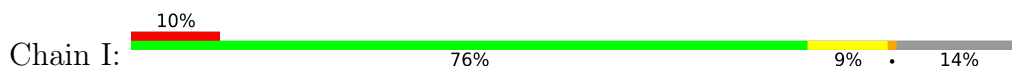




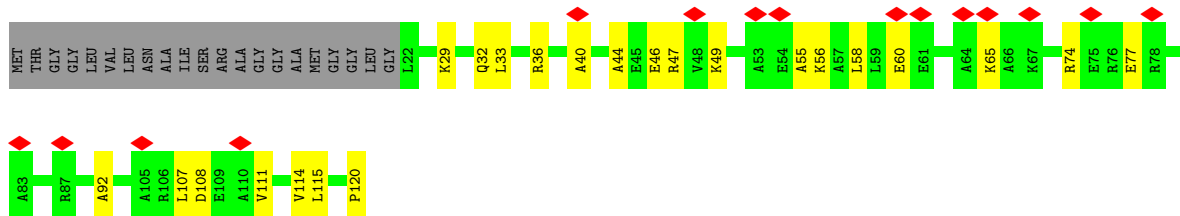
• Molecule 4: V-type ATP synthase subunit F



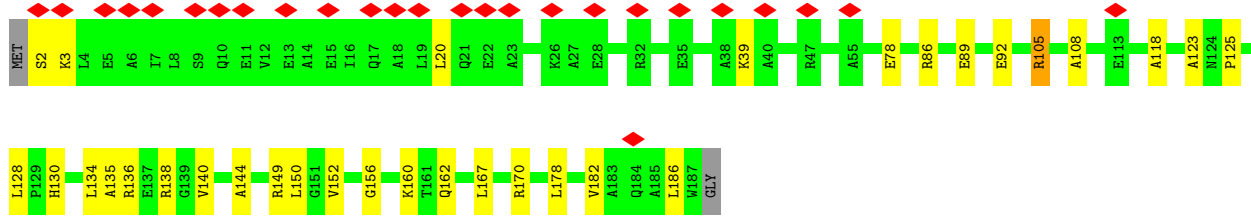
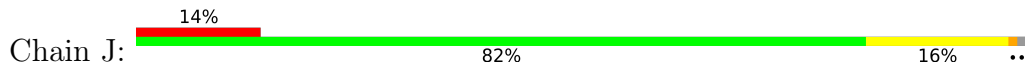
• Molecule 5: V-type ATP synthase, subunit (VAPC-THERM)



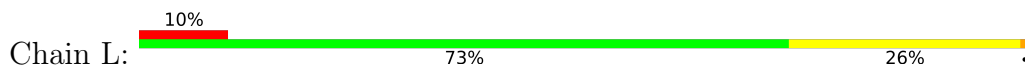
• Molecule 5: V-type ATP synthase, subunit (VAPC-THERM)

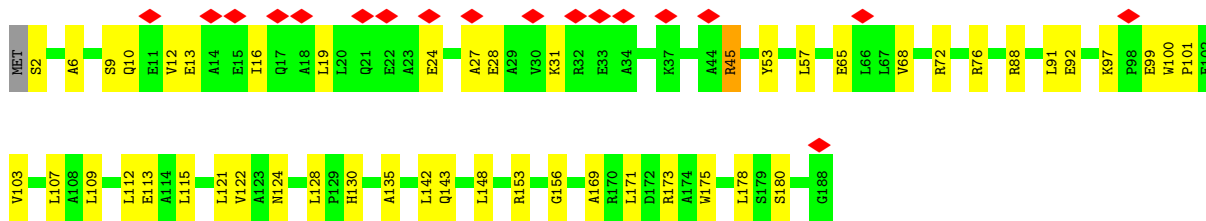


• Molecule 6: V-type ATP synthase subunit E

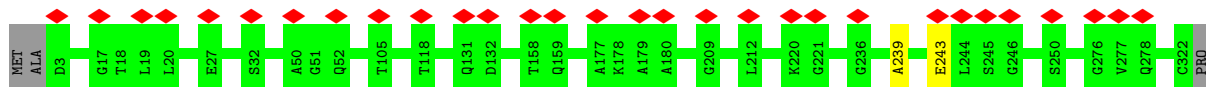


• Molecule 6: V-type ATP synthase subunit E

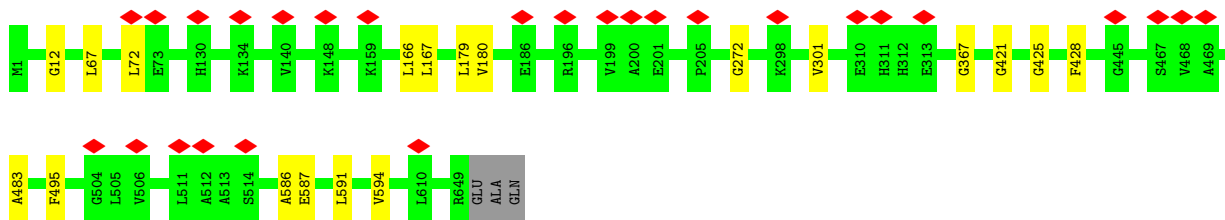




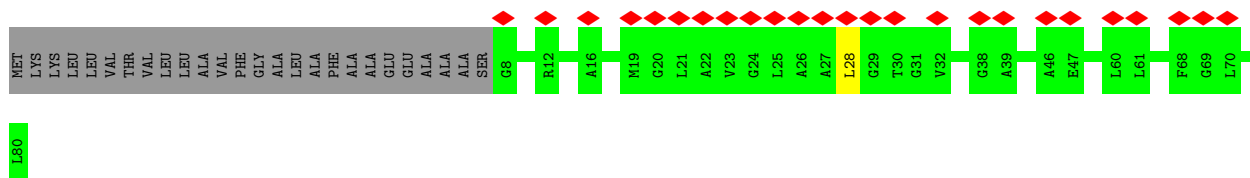
• Molecule 7: V-type ATP synthase subunit C



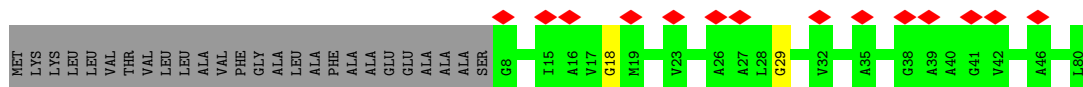
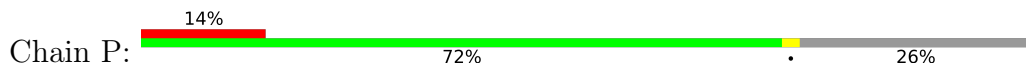
• Molecule 8: V-type ATP synthase subunit I



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

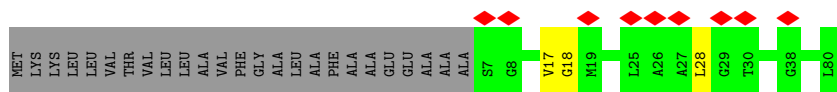


• Molecule 9: V-type ATP synthase, subunit K

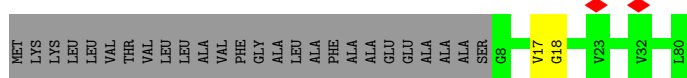


• Molecule 9: V-type ATP synthase, subunit K

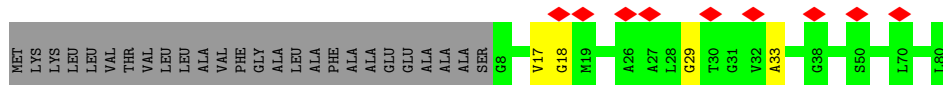




- Molecule 9: V-type ATP synthase, subunit K



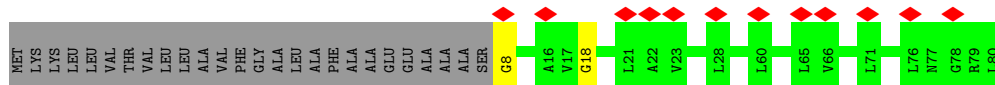
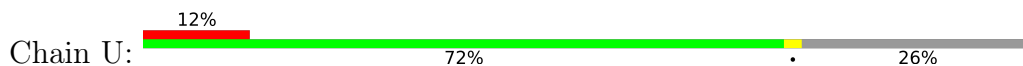
- Molecule 9: V-type ATP synthase, subunit K



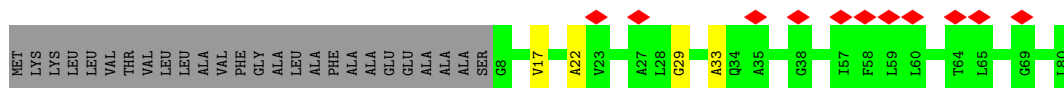
- Molecule 9: V-type ATP synthase, subunit K



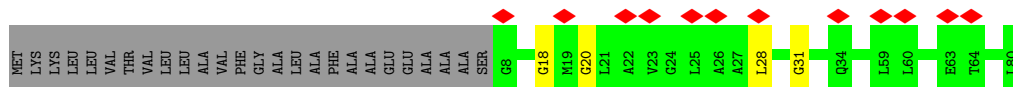
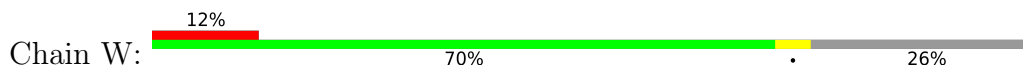
- Molecule 9: V-type ATP synthase, subunit K



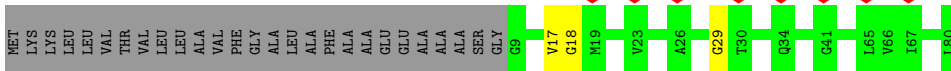
- Molecule 9: V-type ATP synthase, subunit K



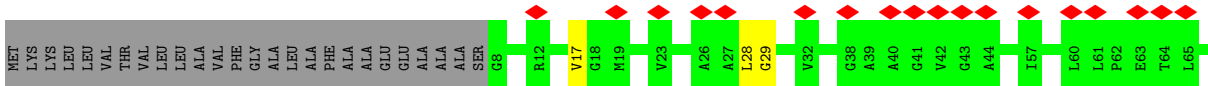
- Molecule 9: V-type ATP synthase, subunit K



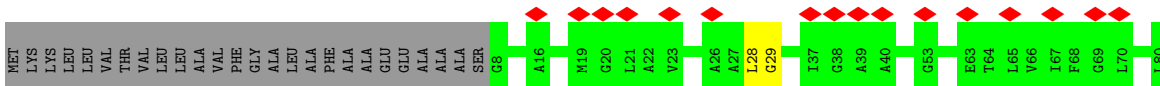
- Molecule 9: V-type ATP synthase, subunit K



• 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	23821	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1780	Depositor
Magnification	129032	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.255	Depositor
Minimum map value	-0.116	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.0233	Depositor
Map size (Å)	148.645, 146.475, 252.80501	wwPDB
Map dimensions	233, 135, 137	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.085, 1.085, 1.085	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	A	0.51	0/4568	0.65	0/6198
1	B	0.52	0/4568	0.65	0/6198
1	C	0.51	0/4568	0.66	3/6198 (0.0%)
2	D	0.50	0/3676	0.70	4/4977 (0.1%)
2	E	0.50	0/3685	0.69	3/4988 (0.1%)
2	F	0.49	0/3675	0.70	4/4976 (0.1%)
3	G	0.38	0/1639	0.60	0/2205
4	H	0.32	0/803	0.68	0/1084
5	I	0.33	0/810	0.59	1/1078 (0.1%)
5	K	0.34	0/790	0.58	0/1052
6	J	0.33	0/1451	0.60	0/1959
6	L	0.32	0/1455	0.63	0/1964
7	M	0.24	0/1574	0.37	0/2187
8	N	0.25	0/3189	0.44	0/4430
9	O	0.25	0/350	0.36	0/480
9	P	0.25	0/350	0.35	0/480
9	Q	0.26	0/355	0.38	0/487
9	R	0.25	0/350	0.36	0/480
9	S	0.25	0/350	0.34	0/480
9	T	0.25	0/350	0.36	0/480
9	U	0.25	0/350	0.35	0/480
9	V	0.25	0/350	0.36	0/480
9	W	0.24	0/350	0.39	0/480
9	X	0.25	0/346	0.35	0/475
9	Y	0.25	0/350	0.36	0/480
9	Z	0.25	0/350	0.38	0/480
All	All	0.43	0/40652	0.61	15/55256 (0.0%)

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

sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
2	D	0	1
2	E	0	1
3	G	0	1
4	H	0	2
8	N	0	1
All	All	0	9

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	450	LEU	CA-CB-CG	7.32	132.13	115.30
2	D	267	LEU	CA-CB-CG	6.85	131.06	115.30
2	D	361	LEU	CA-CB-CG	6.09	129.31	115.30
5	I	85	LEU	CA-CB-CG	5.95	128.97	115.30
2	F	150	LEU	CA-CB-CG	5.88	128.82	115.30
2	E	319	ASP	CB-CG-OD1	5.77	123.50	118.30
2	E	150	LEU	CA-CB-CG	5.69	128.38	115.30
2	E	19	LEU	CA-CB-CG	5.48	127.91	115.30
1	C	530	ILE	CB-CA-C	-5.46	100.67	111.60
2	F	19	LEU	CA-CB-CG	5.33	127.55	115.30
2	F	106	ILE	C-N-CA	5.30	134.96	121.70
2	D	19	LEU	CA-CB-CG	5.26	127.40	115.30
1	C	135	LEU	CA-CB-CG	5.25	127.38	115.30
2	D	75	LEU	CA-CB-CG	5.14	127.11	115.30
2	F	361	LEU	C-N-CA	5.04	134.29	121.70

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	476	LEU	Peptide
1	B	148	LEU	Peptide
1	C	26	ASP	Peptide
2	D	183	LYS	Peptide
2	E	345	ARG	Peptide
3	G	168	VAL	Peptide

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Mol	Chain	Res	Type	Group
4	H	83	GLY	Peptide
4	H	85	ASP	Peptide
8	N	301	VAL	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4472	0	4491	57	0
1	B	4472	0	4490	56	0
1	C	4472	0	4491	53	0
2	D	3609	0	3635	40	0
2	E	3618	0	3648	45	0
2	F	3608	0	3638	42	0
3	G	1619	0	1701	12	0
4	H	792	0	803	16	0
5	I	808	0	852	11	0
5	K	788	0	832	19	0
6	J	1437	0	1489	25	0
6	L	1441	0	1492	36	0
7	M	1575	0	775	1	0
8	N	3190	0	1547	10	0
9	O	351	0	194	1	0
9	P	351	0	194	2	0
9	Q	356	0	196	3	0
9	R	351	0	194	2	0
9	S	351	0	194	4	0
9	T	351	0	194	4	0
9	U	351	0	194	2	0
9	V	351	0	194	4	0
9	W	351	0	194	4	0
9	X	347	0	191	3	0
9	Y	351	0	194	3	0
9	Z	351	0	194	2	0
10	B	1	0	0	0	0
11	B	27	0	12	1	0
11	D	27	0	12	0	0
All	All	40169	0	36235	399	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 5.

All (399) 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)
1:B:40:ILE:O	1:B:48:PHE:HB3	1.80	0.81
2:D:36:LYS:O	2:D:71:THR:HA	1.81	0.79
6:L:135:ALA:HB1	6:L:142:LEU:HD21	1.72	0.71
2:F:193:ALA:O	2:F:222:ASN:HB2	1.89	0.71
6:L:171:LEU:O	6:L:175:TRP:HB2	1.91	0.70
2:F:189:VAL:O	2:F:217:SER:HA	1.93	0.69
3:G:94:GLU:O	3:G:100:LYS:HA	1.94	0.68
1:B:56:SER:H	1:B:104:ARG:HH12	1.41	0.68
2:F:119:LEU:HB2	2:F:124:ARG:HH21	1.59	0.66
1:C:517:LYS:HD2	1:C:563:PHE:HZ	1.61	0.66
6:J:135:ALA:HA	6:J:138:ARG:HD3	1.78	0.66
1:A:314:ARG:HH21	1:A:368:VAL:HG21	1.61	0.65
2:D:135:ILE:HA	2:D:425:GLN:HE22	1.62	0.65
6:L:97:LYS:HE2	6:L:99:GLU:HB2	1.78	0.64
2:D:131:ILE:HD11	2:D:171:ALA:HB1	1.80	0.64
1:A:116:LYS:HA	1:A:166:TYR:O	1.99	0.63
2:E:129:GLN:OE1	2:E:146:ARG:NH1	2.31	0.63
2:F:177:LEU:HD23	2:F:371:THR:HA	1.81	0.63
1:A:41:ARG:NH2	1:A:341:LEU:O	2.31	0.63
5:K:44:ALA:HB2	6:L:19:LEU:HD11	1.79	0.63
4:H:55:PRO:HB2	4:H:71:LEU:HD13	1.81	0.63
1:B:38:GLU:OE2	1:B:190:ARG:NH2	2.33	0.62
2:D:169:ARG:NH1	2:D:427:GLN:OE1	2.32	0.62
1:A:444:ALA:HB3	1:A:447:TYR:HB2	1.82	0.62
1:C:116:LYS:HA	1:C:166:TYR:O	1.99	0.62
6:J:105:ARG:HB3	6:J:130:HIS:HE1	1.64	0.62
1:A:272:LEU:HD22	1:A:281:LEU:HD22	1.81	0.61
2:E:149:LYS:HA	2:E:310:GLN:O	2.00	0.61
1:A:198:LYS:HG2	1:A:368:VAL:HG12	1.83	0.60
1:A:476:LEU:O	1:A:481:ARG:NH1	2.34	0.60
4:H:3:VAL:HG12	4:H:46:ALA:HB3	1.84	0.60
5:K:29:LYS:HA	5:K:32:GLN:HG2	1.84	0.60
8:N:586:ALA:HB1	8:N:594:VAL:HA	1.84	0.60
6:J:125:PRO:HB3	6:J:144:ALA:HB1	1.84	0.59
2:E:265:GLU:OE1	2:E:268:ARG:NH2	2.35	0.59
5:K:65:LYS:HB3	6:L:45:ARG:HH11	1.68	0.59
1:C:111:LEU:O	1:C:113:ARG:NH1	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:113:LEU:HB3	3:G:116:PRO:HB3	1.84	0.59
2:F:165:ALA:HB1	2:F:207:GLU:HG2	1.85	0.59
2:F:195:GLY:HA2	2:F:224:ALA:HB2	1.85	0.59
5:K:47:ARG:HD2	6:L:27:ALA:HB2	1.83	0.58
2:D:163:ILE:HD11	2:D:351:PRO:HD2	1.84	0.58
1:C:264:ASP:O	1:C:268:GLU:HB2	2.03	0.58
2:E:206:GLN:O	2:E:210:ARG:HB2	2.03	0.58
1:C:8:LYS:HD3	1:C:15:ILE:HD12	1.85	0.58
6:J:136:ARG:NH1	6:J:140:VAL:O	2.36	0.58
1:A:341:LEU:HD22	1:A:343:GLU:HG3	1.86	0.58
1:A:496:GLN:O	1:A:552:ARG:NH1	2.37	0.58
1:A:225:ALA:HB2	1:A:403:VAL:HG11	1.84	0.58
9:R:18:GLY:HA3	9:S:17:VAL:HA	1.85	0.58
2:D:33:VAL:HG21	2:D:57:ILE:HD13	1.85	0.57
5:K:115:LEU:HD11	6:L:91:LEU:HB3	1.87	0.57
2:F:149:LYS:HA	2:F:310:GLN:O	2.05	0.57
1:A:40:ILE:O	1:A:48:PHE:HB3	2.05	0.57
1:A:343:GLU:O	3:G:196:ARG:NH1	2.37	0.57
1:A:459:GLN:NE2	2:D:345:ARG:O	2.38	0.57
2:E:7:GLU:HB2	6:J:162:GLN:HG3	1.87	0.57
2:E:399:ILE:HG12	3:G:97:TRP:HE1	1.69	0.57
1:B:299:ARG:HD2	1:B:333:ALA:HB2	1.87	0.57
5:I:81:THR:O	5:I:85:LEU:HB2	2.05	0.56
6:L:2:SER:O	6:L:6:ALA:HB2	2.05	0.56
9:T:8:GLY:HA2	9:U:8:GLY:HA3	1.87	0.56
4:H:85:ASP:HB3	4:H:89:TYR:HB2	1.87	0.56
5:K:36:ARG:HB3	6:L:16:ILE:HD11	1.86	0.56
1:A:204:PRO:HA	1:A:219:ALA:HA	1.86	0.56
1:A:391:MET:O	1:A:397:GLN:NE2	2.35	0.56
9:W:18:GLY:HA3	9:X:17:VAL:HA	1.87	0.56
1:C:146:LYS:HB2	1:C:316:GLN:HG3	1.87	0.56
1:C:481:ARG:HG2	1:C:536:ILE:HG21	1.88	0.56
2:E:236:ARG:NH1	2:E:290:ASP:OD1	2.39	0.56
1:B:387:PRO:HD2	1:B:393:GLU:HG3	1.88	0.56
2:E:406:GLU:OE1	2:E:409:ARG:NH2	2.38	0.56
5:K:74:ARG:NH1	5:K:77:GLU:OE1	2.38	0.56
6:L:122:VAL:HG22	6:L:143:GLN:HB3	1.87	0.56
1:B:436:ASP:OD1	1:B:451:ARG:NH2	2.38	0.56
1:A:498:ASN:HD22	1:A:501:HIS:HB2	1.71	0.56
1:C:477:GLN:NE2	4:H:101:ASP:OD2	2.39	0.55
1:B:43:ASP:N	1:B:43:ASP:OD1	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:264:ASP:HA	1:C:267:VAL:HG12	1.88	0.55
2:D:149:LYS:O	2:D:333:THR:OG1	2.18	0.55
2:E:75:LEU:HD21	2:E:78:ASP:HB3	1.87	0.55
8:N:367:GLY:H	8:N:428:PHE:H	1.53	0.55
1:A:497:GLN:NE2	1:A:505:ALA:O	2.39	0.55
1:B:54:ASP:O	1:B:104:ARG:NH1	2.38	0.55
2:F:108:PRO:HG2	6:L:180:SER:HB2	1.87	0.55
2:D:34:ASP:OD1	2:D:74:SER:OG	2.23	0.55
2:F:156:SER:H	2:F:341:ARG:HH21	1.55	0.55
5:K:36:ARG:NH1	6:L:9:SER:OG	2.40	0.54
5:I:29:LYS:NZ	8:N:12:GLY:O	2.39	0.54
6:J:92:GLU:O	6:J:149:ARG:NH2	2.40	0.54
6:J:118:ALA:HA	6:J:156:GLY:HA2	1.88	0.54
1:A:8:LYS:HD3	1:A:15:ILE:HD12	1.89	0.54
1:B:23:ARG:NH2	1:B:68:GLY:O	2.39	0.54
2:D:448:GLN:NE2	2:D:463:TYR:OH	2.37	0.54
2:F:407:ASN:ND2	2:F:450:GLU:OE2	2.40	0.54
5:I:38:GLU:OE1	5:I:42:LYS:NZ	2.40	0.54
2:E:337:ILE:HA	2:E:357:SER:HB3	1.89	0.54
2:F:277:ILE:HD12	2:F:278:PRO:HD2	1.89	0.54
2:F:132:GLN:OE1	2:F:174:ARG:NE	2.35	0.54
1:C:75:LEU:HD13	1:C:312:TYR:HB2	1.90	0.54
1:C:204:PRO:HA	1:C:219:ALA:HA	1.90	0.54
2:E:174:ARG:HB3	2:E:177:LEU:HD23	1.89	0.54
1:B:134:VAL:HG11	1:B:146:LYS:HD3	1.89	0.54
2:D:149:LYS:HE3	2:D:298:ALA:HB3	1.90	0.54
2:D:197:THR:OG1	2:D:198:GLN:N	2.41	0.54
2:E:33:VAL:HG21	2:E:57:ILE:HD13	1.90	0.54
1:A:243:LYS:HA	1:A:281:LEU:HD21	1.89	0.53
2:F:372:ARG:NH1	2:F:433:GLU:OE1	2.39	0.53
1:B:198:LYS:HG2	1:B:368:VAL:HG12	1.90	0.53
1:C:227:PRO:HA	1:C:384:VAL:O	2.09	0.53
1:B:111:LEU:O	1:B:113:ARG:NH2	2.42	0.53
2:F:152:ILE:HB	2:F:313:ILE:HG12	1.89	0.53
2:E:228:THR:HG22	2:E:231:ARG:HH11	1.73	0.53
2:F:151:PRO:HA	2:F:312:PRO:O	2.09	0.53
1:A:146:LYS:O	1:A:316:GLN:NE2	2.42	0.53
5:I:38:GLU:HA	5:I:41:LYS:HG2	1.89	0.53
1:A:161:LYS:NZ	1:A:170:GLU:OE2	2.42	0.53
9:P:29:GLY:HA3	9:Q:28:LEU:HA	1.90	0.53
6:L:109:LEU:O	6:L:113:GLU:HB2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:160:VAL:HG22	1:B:173:VAL:HG22	1.92	0.52
2:F:355:LEU:HA	2:F:383:TYR:HE1	1.74	0.52
6:L:28:GLU:OE1	6:L:31:LYS:NZ	2.42	0.52
4:H:33:LEU:HD13	4:H:45:VAL:HG11	1.90	0.52
6:J:150:LEU:HD23	6:J:167:LEU:HD12	1.91	0.52
5:K:114:VAL:HG23	6:L:178:LEU:HD22	1.92	0.52
1:C:253:VAL:HG11	1:C:303:ILE:HA	1.90	0.52
2:E:193:ALA:HA	2:E:258:THR:HB	1.92	0.52
1:A:369:ILE:HG22	1:A:375:GLU:HB3	1.92	0.52
1:B:153:VAL:HG11	1:B:181:LEU:HD21	1.91	0.52
1:B:260:ASN:ND2	2:D:334:GLU:OE2	2.43	0.52
1:B:486:VAL:HA	1:B:489:ILE:HG12	1.90	0.52
5:I:100:ARG:NH2	6:J:78:GLU:OE1	2.38	0.52
2:E:151:PRO:HB3	2:E:312:PRO:HG2	1.91	0.52
6:L:65:GLU:HA	6:L:68:VAL:HG22	1.92	0.52
1:C:312:TYR:O	1:C:316:GLN:NE2	2.42	0.52
1:B:43:ASP:OD1	1:B:46:THR:OG1	2.28	0.52
2:F:169:ARG:NH1	2:F:427:GLN:OE1	2.43	0.52
1:C:501:HIS:HB3	1:C:504:ASP:HB3	1.92	0.52
2:E:135:ILE:HD12	2:E:350:PRO:HG3	1.92	0.52
9:V:22:ALA:HB2	9:W:20:GLY:HA2	1.92	0.52
1:A:75:LEU:HD13	1:A:312:TYR:HB2	1.93	0.51
2:D:7:GLU:HG2	2:D:74:SER:HB3	1.92	0.51
1:C:468:VAL:HG22	1:C:476:LEU:HD21	1.92	0.51
2:E:323:HIS:O	2:E:327:ASP:HB2	2.10	0.51
2:F:36:LYS:HB3	2:F:42:VAL:HG12	1.92	0.51
1:B:211:ILE:HD12	1:B:495:LEU:HD22	1.91	0.51
2:E:7:GLU:OE1	6:J:162:GLN:NE2	2.43	0.51
2:F:260:MET:HB2	2:F:314:LEU:HB3	1.92	0.51
5:K:120:PRO:HG3	6:L:107:LEU:HB3	1.93	0.51
9:V:29:GLY:HA3	9:W:28:LEU:HA	1.93	0.51
1:A:314:ARG:HD3	1:A:378:VAL:HG12	1.91	0.51
1:B:347:GLU:OE1	2:E:268:ARG:NH1	2.43	0.51
1:B:127:ASP:O	1:B:156:ARG:HA	2.10	0.51
2:E:136:SER:HB2	2:E:430:ARG:HD2	1.93	0.51
5:I:47:ARG:HH22	6:J:20:LEU:HB3	1.75	0.51
6:L:97:LYS:HG2	6:L:99:GLU:H	1.76	0.51
5:I:47:ARG:HH12	6:J:20:LEU:HB3	1.74	0.51
1:C:260:ASN:HA	1:C:263:THR:HG22	1.93	0.51
2:D:301:VAL:HG23	2:D:304:LYS:HB2	1.93	0.51
2:D:456:LYS:HA	2:D:459:ILE:HG22	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:268:GLU:OE2	2:E:126:LYS:NZ	2.37	0.51
2:E:119:LEU:HB2	2:E:124:ARG:HH21	1.76	0.51
9:U:18:GLY:HA3	9:V:17:VAL:HA	1.93	0.51
1:A:476:LEU:HB3	1:A:480:GLU:HB2	1.92	0.51
5:I:26:LEU:HD12	8:N:272:GLY:HA3	1.93	0.51
1:B:53:GLU:HA	1:B:295:PRO:HG2	1.93	0.50
9:Y:29:GLY:HA3	9:Z:28:LEU:HA	1.92	0.50
2:D:267:LEU:HD11	2:D:287:MET:HG3	1.93	0.50
1:C:245:SER:OG	1:C:246:ASN:N	2.44	0.50
1:B:73:VAL:O	1:B:186:THR:HA	2.10	0.50
2:E:252:HIS:ND1	2:E:307:SER:OG	2.38	0.50
6:J:123:ALA:HB2	6:J:152:VAL:HG23	1.94	0.50
1:A:454:ILE:HG23	1:A:490:ILE:HD11	1.94	0.50
1:B:43:ASP:HB3	2:E:13:TYR:HD1	1.77	0.50
2:D:355:LEU:HD13	2:D:386:TYR:HD2	1.77	0.50
6:L:2:SER:O	6:L:6:ALA:CB	2.59	0.50
1:A:522:PHE:HD1	1:A:570:ILE:HD11	1.77	0.50
6:J:86:ARG:NH1	6:J:89:GLU:OE1	2.45	0.50
9:X:18:GLY:HA3	9:Y:17:VAL:HA	1.93	0.50
6:L:124:ASN:ND2	6:L:148:LEU:O	2.45	0.50
2:D:404:LEU:HB2	2:D:409:ARG:HE	1.77	0.49
4:H:94:VAL:HG11	4:H:102:ILE:HG12	1.93	0.49
2:D:38:GLY:HA2	2:D:70:THR:HG21	1.94	0.49
2:E:35:ILE:HG12	2:E:73:VAL:HG12	1.93	0.49
6:J:108:ALA:HA	6:J:152:VAL:HG11	1.95	0.49
2:D:101:ASP:OD1	2:D:101:ASP:N	2.44	0.49
5:K:111:VAL:HA	5:K:114:VAL:HG12	1.93	0.49
6:J:89:GLU:HA	6:J:92:GLU:HG2	1.95	0.49
1:B:227:PRO:HA	1:B:384:VAL:O	2.13	0.49
1:A:489:ILE:O	1:A:493:ASP:HB3	2.13	0.49
1:B:465:GLN:HA	1:B:468:VAL:HG12	1.94	0.49
1:B:417:ARG:HG3	1:B:419:PHE:HE2	1.77	0.49
1:C:496:GLN:O	1:C:552:ARG:NH1	2.46	0.49
1:B:544:VAL:HG23	1:B:569:GLU:HG3	1.96	0.48
1:B:326:SER:HB3	1:B:329:ARG:HG2	1.95	0.48
2:E:154:SER:OG	2:E:155:GLY:N	2.47	0.48
1:A:160:VAL:HG22	1:A:173:VAL:HG22	1.95	0.48
1:C:486:VAL:HA	1:C:489:ILE:HG22	1.95	0.48
1:A:229:PRO:O	1:A:232:SER:OG	2.28	0.48
4:H:3:VAL:HA	4:H:46:ALA:O	2.14	0.48
2:F:148:GLN:HB2	2:F:334:GLU:HG3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:169:ARG:HB2	2:F:211:THR:HG21	1.96	0.48
1:B:325:ASP:HA	1:B:383:ALA:HB3	1.96	0.48
1:B:532:ARG:NH2	1:B:577:LEU:O	2.46	0.48
5:K:47:ARG:NH2	6:L:24:GLU:OE2	2.47	0.48
1:A:8:LYS:HB3	1:A:15:ILE:HB	1.96	0.48
1:B:54:ASP:OD1	1:B:54:ASP:N	2.46	0.48
2:D:156:SER:OG	2:D:341:ARG:NH2	2.43	0.48
5:K:40:ALA:HB2	6:L:16:ILE:HG12	1.95	0.48
8:N:167:LEU:HA	8:N:179:LEU:O	2.13	0.48
1:A:288:ILE:HD11	1:A:309:ILE:HD12	1.96	0.47
1:C:294:MET:O	1:C:299:ARG:NH1	2.47	0.47
1:A:56:SER:O	1:A:104:ARG:NH2	2.47	0.47
1:A:140:GLU:OE1	1:A:145:HIS:ND1	2.47	0.47
1:B:41:ARG:NH2	1:B:341:LEU:O	2.42	0.47
2:D:93:PHE:HA	2:D:99:PRO:HA	1.96	0.47
7:M:239:ALA:O	7:M:243:GLU:N	2.48	0.47
1:A:250:VAL:HG22	1:A:321:ALA:HB3	1.96	0.47
4:H:13:PHE:HD1	4:H:18:LEU:HD21	1.80	0.47
6:J:125:PRO:HA	6:J:128:LEU:HG	1.95	0.47
1:C:347:GLU:OE2	2:F:268:ARG:NH1	2.38	0.47
1:C:534:VAL:HB	1:C:538:GLU:HB2	1.95	0.47
3:G:130:PHE:HB3	4:H:16:ALA:HB2	1.96	0.47
6:L:112:LEU:HD11	6:L:121:LEU:HD21	1.96	0.47
1:C:290:ASN:OD1	1:C:302:SER:OG	2.31	0.47
5:I:114:VAL:HG13	6:J:178:LEU:HD13	1.97	0.47
2:F:11:ILE:HD12	2:F:19:LEU:HD13	1.96	0.47
2:F:51:SER:OG	2:F:52:GLU:N	2.47	0.47
1:C:8:LYS:HB3	1:C:15:ILE:HB	1.97	0.47
8:N:421:GLY:O	8:N:425:GLY:N	2.47	0.47
1:A:489:ILE:O	1:A:493:ASP:CB	2.63	0.46
9:S:18:GLY:HA3	9:T:17:VAL:HA	1.98	0.46
1:A:400:LEU:HG	2:D:156:SER:HB2	1.97	0.46
1:C:291:THR:OG1	1:C:293:ASN:OD1	2.27	0.46
5:K:107:LEU:HD23	5:K:108:ASP:HB2	1.96	0.46
1:A:44:GLY:N	2:D:12:THR:O	2.44	0.46
1:B:45:ASP:OD1	1:B:45:ASP:N	2.49	0.46
1:B:128:GLU:HA	1:B:155:GLY:O	2.15	0.46
1:A:260:ASN:HA	1:A:263:THR:HG22	1.97	0.46
2:D:7:GLU:HB3	2:D:72:SER:HB2	1.96	0.46
2:E:374:ASP:HB3	2:E:458:HIS:CD2	2.50	0.46
2:E:317:PRO:HG2	2:E:323:HIS:CD2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:410:ASP:OD2	1:C:423:ASN:ND2	2.49	0.46
2:E:23:ASN:HD21	6:J:160:LYS:HB2	1.81	0.46
5:K:92:ALA:HB2	6:L:68:VAL:HG12	1.97	0.46
1:B:71:LEU:HD23	1:B:189:VAL:HG21	1.99	0.45
1:B:85:ASP:OD2	1:B:89:ARG:NH2	2.49	0.45
2:D:333:THR:OG1	2:D:334:GLU:N	2.49	0.45
9:S:29:GLY:HA3	9:T:28:LEU:HA	1.98	0.45
1:A:73:VAL:O	1:A:186:THR:HA	2.15	0.45
1:B:23:ARG:HG2	2:E:67:ASP:HB3	1.98	0.45
1:B:145:HIS:CE1	1:B:316:GLN:HE22	2.34	0.45
2:E:195:GLY:O	2:E:262:ASN:ND2	2.49	0.45
3:G:47:MET:HG2	4:H:90:MET:HG3	1.97	0.45
6:L:100:TRP:HA	6:L:103:VAL:HG12	1.98	0.45
2:E:134:GLY:O	2:E:425:GLN:NE2	2.40	0.45
2:F:135:ILE:HA	2:F:425:GLN:HE22	1.81	0.45
5:I:27:ALA:HA	5:I:30:GLU:HG2	1.97	0.45
2:D:37:ASP:HA	2:D:71:THR:HG22	1.99	0.45
2:E:395:LEU:HD21	2:E:399:ILE:HD12	1.98	0.45
9:P:18:GLY:HA3	9:Q:17:VAL:HA	1.99	0.45
2:D:76:VAL:HG22	2:D:77:GLU:HG3	1.98	0.45
2:F:259:ASP:OD2	2:F:262:ASN:ND2	2.49	0.45
4:H:51:LEU:HG	4:H:52:LEU:HD12	1.99	0.45
6:J:128:LEU:HD21	6:J:144:ALA:HB2	1.98	0.45
6:L:122:VAL:HB	6:L:153:ARG:HB3	1.99	0.45
1:C:482:LEU:HD11	1:C:526:ALA:HB1	1.98	0.45
2:D:178:SER:OG	2:D:370:LYS:O	2.32	0.45
2:D:422:PHE:O	2:D:430:ARG:NH2	2.50	0.45
6:L:124:ASN:O	6:L:128:LEU:N	2.48	0.45
1:B:27:ILE:HA	1:B:37:GLY:O	2.17	0.45
1:C:226:ILE:HG22	1:C:407:TRP:HB2	1.98	0.45
1:A:436:ASP:OD1	1:A:451:ARG:NH2	2.49	0.44
6:L:72:ARG:HG2	6:L:76:ARG:HH11	1.82	0.44
1:A:501:HIS:CE1	1:A:503:VAL:HG12	2.52	0.44
8:N:166:LEU:O	8:N:180:VAL:HA	2.17	0.44
1:A:415:PHE:O	2:F:383:TYR:OH	2.35	0.44
9:Q:18:GLY:HA3	9:R:17:VAL:HA	1.99	0.44
2:E:196:ILE:HD11	2:E:201:LEU:HD12	1.98	0.44
2:F:431:SER:OG	2:F:432:ILE:N	2.50	0.44
1:A:38:GLU:OE1	1:A:52:TYR:OH	2.31	0.44
1:C:198:LYS:HA	1:C:368:VAL:HG23	2.00	0.44
1:C:475:ALA:HA	4:H:104:LEU:H	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:446:LEU:O	2:F:463:TYR:OH	2.29	0.44
1:A:344:MET:HA	1:A:345:PRO:HD3	1.85	0.44
1:B:497:GLN:NE2	1:B:504:ASP:O	2.50	0.44
1:C:258:ARG:HB2	1:C:261:GLU:HB3	2.00	0.44
1:C:337:ILE:HD13	1:C:337:ILE:HA	1.89	0.44
9:O:28:LEU:HA	9:Z:29:GLY:HA3	1.99	0.44
1:B:170:GLU:HA	1:B:171:PRO:HD3	1.88	0.44
2:F:35:ILE:HD11	2:F:57:ILE:HG21	2.00	0.44
6:J:182:VAL:O	6:J:186:LEU:CB	2.65	0.44
1:B:207:THR:HG23	1:B:241:LEU:HG	1.99	0.44
1:B:314:ARG:HB2	1:B:378:VAL:HG23	2.00	0.44
5:K:55:ALA:HA	5:K:58:LEU:HD12	2.00	0.44
1:C:26:ASP:HA	1:C:70:PRO:HA	2.00	0.44
2:E:148:GLN:NE2	2:E:359:SER:OG	2.38	0.43
1:C:431:PHE:CE1	2:F:199:ARG:HD3	2.53	0.43
1:C:473:PRO:HA	1:C:476:LEU:HD23	1.99	0.43
1:C:547:ARG:NH2	1:C:569:GLU:OE1	2.50	0.43
6:J:2:SER:OG	6:J:3:LYS:N	2.48	0.43
2:F:89:LEU:HD23	2:F:216:ARG:HA	2.00	0.43
5:K:33:LEU:HG	6:L:12:VAL:HG21	2.00	0.43
6:L:101:PRO:HB3	6:L:130:HIS:HB3	2.00	0.43
1:B:210:ARG:NH1	1:B:504:ASP:OD1	2.43	0.43
6:L:122:VAL:HA	6:L:143:GLN:O	2.18	0.43
1:B:497:GLN:NE2	1:B:505:ALA:O	2.52	0.43
2:E:132:GLN:OE1	2:E:174:ARG:NH2	2.50	0.43
6:L:115:LEU:HD21	6:L:156:GLY:HA3	1.99	0.43
8:N:587:GLU:HA	8:N:591:LEU:HA	1.99	0.43
1:B:233:GLY:N	11:B:602:ADP:O1B	2.50	0.43
1:C:206:LEU:H	1:C:246:ASN:HD22	1.66	0.43
6:L:13:GLU:HA	6:L:16:ILE:HD12	2.01	0.43
8:N:67:LEU:O	8:N:72:LEU:N	2.52	0.43
1:C:216:PHE:HB2	1:C:407:TRP:HE1	1.83	0.43
8:N:483:ALA:HA	8:N:495:PHE:HA	2.01	0.43
1:B:342:GLU:OE2	3:G:204:ARG:NH2	2.52	0.43
3:G:101:VAL:HG22	3:G:149:LYS:HZ3	1.83	0.43
4:H:1:MET:N	4:H:41:GLY:O	2.38	0.43
1:A:461:GLU:HG2	1:A:484:ILE:HD13	2.00	0.43
2:F:195:GLY:H	2:F:222:ASN:HB3	1.83	0.43
1:A:520:LEU:HD23	1:A:520:LEU:HA	1.86	0.42
1:C:116:LYS:HB3	1:C:165:GLU:HG2	2.01	0.42
1:C:457:LEU:HD22	1:C:490:ILE:HD12	1.99	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:189:VAL:O	2:E:217:SER:HA	2.18	0.42
2:F:60:PHE:HB3	2:F:229:ILE:HG21	2.01	0.42
1:B:391:MET:SD	1:B:391:MET:N	2.92	0.42
1:B:491:ARG:HG2	1:B:495:LEU:HD12	2.01	0.42
1:C:119:TRP:HD1	1:C:163:ALA:HA	1.83	0.42
1:A:230:PHE:HZ	2:F:321:ARG:HD3	1.85	0.42
2:D:166:GLN:HE21	2:D:170:GLN:NE2	2.17	0.42
2:F:158:LEU:HD22	2:F:339:LEU:HB3	2.01	0.42
2:D:328:LEU:O	2:D:332:ILE:HD12	2.20	0.42
2:D:329:THR:O	2:D:333:THR:HG22	2.20	0.42
2:E:448:GLN:HB2	2:E:463:TYR:CE2	2.54	0.42
2:F:134:GLY:HA3	2:F:170:GLN:NE2	2.34	0.42
1:C:547:ARG:O	1:C:551:ALA:HB2	2.20	0.42
6:J:134:LEU:O	6:J:138:ARG:NH1	2.52	0.42
1:B:113:ARG:O	1:B:167:THR:OG1	2.38	0.42
2:E:386:TYR:OH	2:E:419:GLU:OE1	2.35	0.42
2:F:106:ILE:HG23	2:F:107:THR:H	1.85	0.42
9:V:33:ALA:HB2	9:W:31:GLY:HA2	2.01	0.42
2:F:67:ASP:N	2:F:67:ASP:OD1	2.50	0.42
2:F:188:ALA:O	2:F:253:VAL:HA	2.20	0.42
6:L:169:ALA:O	6:L:173:ARG:HG2	2.20	0.42
3:G:49:ALA:HA	3:G:139:ARG:HH22	1.84	0.42
5:K:56:LYS:NZ	5:K:60:GLU:OE2	2.44	0.42
9:S:33:ALA:HA	9:T:35:ALA:HB2	2.01	0.42
5:K:46:GLU:HG2	5:K:49:LYS:HZ3	1.85	0.42
1:B:56:SER:O	1:B:104:ARG:NH2	2.43	0.41
2:D:431:SER:OG	2:D:434:GLU:OE1	2.29	0.41
2:E:81:ARG:HD3	2:E:111:ARG:HG3	2.02	0.41
2:F:178:SER:OG	2:F:179:GLY:N	2.52	0.41
1:A:150:PRO:HA	1:A:151:PRO:HD3	1.87	0.41
1:C:323:MET:HG2	1:C:381:VAL:HB	2.02	0.41
6:L:88:ARG:O	6:L:92:GLU:HB2	2.21	0.41
1:A:204:PRO:HB3	1:A:435:LEU:HD13	2.02	0.41
1:B:17:LYS:HA	1:B:46:THR:HA	2.03	0.41
1:C:443:VAL:O	1:C:510:LYS:NZ	2.38	0.41
6:J:20:LEU:HD23	6:J:20:LEU:HA	1.91	0.41
6:L:53:TYR:CZ	6:L:57:LEU:HD11	2.56	0.41
1:A:481:ARG:HH21	1:A:536:ILE:HG21	1.85	0.41
1:B:209:MET:HG3	1:B:212:LEU:HD12	2.01	0.41
2:E:444:SER:HA	2:E:463:TYR:CE1	2.55	0.41
1:B:396:THR:HA	1:B:399:THR:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:90:PRO:HG3	1:C:93:ARG:HH11	1.85	0.41
1:C:390:ASP:OD1	1:C:390:ASP:N	2.54	0.41
2:D:93:PHE:HB3	2:D:97:GLY:HA2	2.02	0.41
2:D:19:LEU:HD21	2:D:35:ILE:HD13	2.03	0.41
2:D:47:VAL:HG22	2:D:57:ILE:HG12	2.02	0.41
4:H:60:GLU:HA	4:H:64:ARG:HG2	2.01	0.41
1:C:129:VAL:HG11	1:C:149:VAL:HG11	2.03	0.41
2:D:192:ALA:HB3	2:D:257:LEU:HD23	2.03	0.41
2:E:185:GLU:H	2:E:185:GLU:HG3	1.73	0.41
2:E:414:PHE:O	2:E:418:PHE:HB2	2.20	0.41
4:H:2:ALA:O	4:H:45:VAL:HA	2.21	0.41
5:I:26:LEU:HD13	5:I:29:LYS:HE3	2.02	0.41
1:A:157:VAL:HG11	1:A:160:VAL:HG23	2.03	0.41
1:A:440:ARG:NH1	1:A:448:PRO:HG2	2.35	0.41
1:B:390:ASP:N	1:B:390:ASP:OD1	2.54	0.41
1:C:226:ILE:HD12	1:C:234:LYS:HE3	2.03	0.41
1:C:266:LEU:HD23	1:C:266:LEU:HA	1.93	0.41
1:C:380:ILE:HG22	1:C:382:GLY:H	1.86	0.41
3:G:96:VAL:HG12	3:G:149:LYS:HZ2	1.86	0.41
6:J:167:LEU:HD23	6:J:170:ARG:HD3	2.03	0.41
9:X:29:GLY:HA3	9:Y:28:LEU:HA	2.02	0.41
1:A:53:GLU:HA	1:A:295:PRO:HG2	2.03	0.41
1:A:367:LYS:HD2	1:A:377:ALA:HB2	2.01	0.41
2:E:142:ASN:N	2:E:142:ASN:OD1	2.52	0.41
3:G:188:ARG:HA	3:G:191:THR:HG22	2.03	0.41
1:B:527:GLU:HA	1:B:530:ILE:HG22	2.02	0.40
4:H:37:VAL:HG12	4:H:62:LEU:HD12	2.03	0.40
1:A:362:TYR:HB2	1:A:402:ILE:HD12	2.03	0.40
2:F:135:ILE:HD12	2:F:350:PRO:HG3	2.02	0.40
3:G:5:SER:HA	3:G:6:PRO:HD3	1.81	0.40
1:A:446:ASP:OD1	1:A:446:ASP:N	2.53	0.40
1:C:111:LEU:HB2	1:C:113:ARG:HH12	1.85	0.40
2:D:135:ILE:HA	2:D:425:GLN:NE2	2.33	0.40
2:E:152:ILE:HB	2:E:313:ILE:HG12	2.02	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%)	522 (91%)	53 (9%)	0	100	100
1	B	575/578 (100%)	541 (94%)	34 (6%)	0	100	100
1	C	575/578 (100%)	521 (91%)	54 (9%)	0	100	100
2	D	459/478 (96%)	420 (92%)	39 (8%)	0	100	100
2	E	460/478 (96%)	422 (92%)	37 (8%)	1 (0%)	47	79
2	F	459/478 (96%)	408 (89%)	50 (11%)	1 (0%)	47	79
3	G	204/223 (92%)	195 (96%)	9 (4%)	0	100	100
4	H	102/104 (98%)	90 (88%)	12 (12%)	0	100	100
5	I	101/120 (84%)	100 (99%)	1 (1%)	0	100	100
5	K	97/120 (81%)	95 (98%)	2 (2%)	0	100	100
6	J	184/188 (98%)	173 (94%)	11 (6%)	0	100	100
6	L	185/188 (98%)	175 (95%)	10 (5%)	0	100	100
7	M	318/323 (98%)	304 (96%)	14 (4%)	0	100	100
8	N	647/652 (99%)	583 (90%)	64 (10%)	0	100	100
9	O	71/99 (72%)	70 (99%)	1 (1%)	0	100	100
9	P	71/99 (72%)	70 (99%)	1 (1%)	0	100	100
9	Q	72/99 (73%)	70 (97%)	2 (3%)	0	100	100
9	R	71/99 (72%)	69 (97%)	2 (3%)	0	100	100
9	S	71/99 (72%)	68 (96%)	3 (4%)	0	100	100
9	T	71/99 (72%)	69 (97%)	2 (3%)	0	100	100
9	U	71/99 (72%)	69 (97%)	2 (3%)	0	100	100
9	V	71/99 (72%)	68 (96%)	3 (4%)	0	100	100
9	W	71/99 (72%)	68 (96%)	3 (4%)	0	100	100
9	X	70/99 (71%)	67 (96%)	3 (4%)	0	100	100
9	Y	71/99 (72%)	67 (94%)	4 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	Z	71/99 (72%)	67 (94%)	4 (6%)	0	100	100
All	All	5793/6274 (92%)	5371 (93%)	420 (7%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	78	ASP
2	E	317	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	468/468 (100%)	466 (100%)	2 (0%)	91	94
1	B	468/468 (100%)	464 (99%)	4 (1%)	78	87
1	C	468/468 (100%)	465 (99%)	3 (1%)	86	91
2	D	387/401 (96%)	386 (100%)	1 (0%)	92	95
2	E	388/401 (97%)	386 (100%)	2 (0%)	88	93
2	F	387/401 (96%)	383 (99%)	4 (1%)	76	86
3	G	164/176 (93%)	163 (99%)	1 (1%)	86	91
4	H	80/80 (100%)	80 (100%)	0	100	100
5	I	76/86 (88%)	76 (100%)	0	100	100
5	K	75/86 (87%)	75 (100%)	0	100	100
6	J	140/141 (99%)	138 (99%)	2 (1%)	67	81
6	L	140/141 (99%)	138 (99%)	2 (1%)	67	81
All	All	3241/3317 (98%)	3220 (99%)	21 (1%)	86	91

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	130	ARG

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Mol	Chain	Res	Type
1	A	202	ASN
1	B	42	LEU
1	B	182	LYS
1	B	442	ASN
1	B	468	VAL
1	C	130	ARG
1	C	210	ARG
1	C	417	ARG
2	D	368	LYS
2	E	205	ILE
2	E	274	ARG
2	F	149	LYS
2	F	222	ASN
2	F	274	ARG
2	F	304	LYS
3	G	105	LYS
6	J	39	LYS
6	J	105	ARG
6	L	10	GLN
6	L	45	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	238	GLN
1	A	316	GLN
1	A	498	ASN
1	B	145	HIS
1	B	316	GLN
1	B	442	ASN
1	B	459	GLN
1	B	496	GLN
2	D	170	GLN
2	D	323	HIS
2	D	448	GLN
2	E	310	GLN
2	E	458	HIS
2	F	170	GLN
2	F	198	GLN
2	F	249	HIS
2	F	252	HIS
2	F	262	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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
11	ADP	B	602	-	24,29,29	0.98	1 (4%)	29,45,45	1.44	4 (13%)
11	ADP	D	501	-	24,29,29	0.93	1 (4%)	29,45,45	1.35	4 (13%)

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
11	ADP	B	602	-	-	2/12/32/32	0/3/3/3
11	ADP	D	501	-	-	6/12/32/32	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	602	ADP	C5-C4	2.50	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	D	501	ADP	C5-C4	2.38	1.47	1.40

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	602	ADP	PA-O3A-PB	-4.15	118.58	132.83
11	B	602	ADP	N3-C2-N1	-3.16	123.74	128.68
11	D	501	ADP	C3'-C2'-C1'	3.10	105.64	100.98
11	D	501	ADP	C4-C5-N7	-3.08	106.19	109.40
11	D	501	ADP	N3-C2-N1	-2.65	124.54	128.68
11	B	602	ADP	C3'-C2'-C1'	2.43	104.64	100.98
11	D	501	ADP	C2-N1-C6	2.09	122.32	118.75
11	B	602	ADP	C4-C5-N7	-2.06	107.25	109.40

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	B	602	ADP	O4'-C4'-C5'-O5'
11	D	501	ADP	C5'-O5'-PA-O1A
11	D	501	ADP	C5'-O5'-PA-O2A
11	D	501	ADP	O4'-C4'-C5'-O5'
11	D	501	ADP	C3'-C4'-C5'-O5'
11	D	501	ADP	PB-O3A-PA-O5'
11	D	501	ADP	C5'-O5'-PA-O3A
11	B	602	ADP	C5'-O5'-PA-O1A

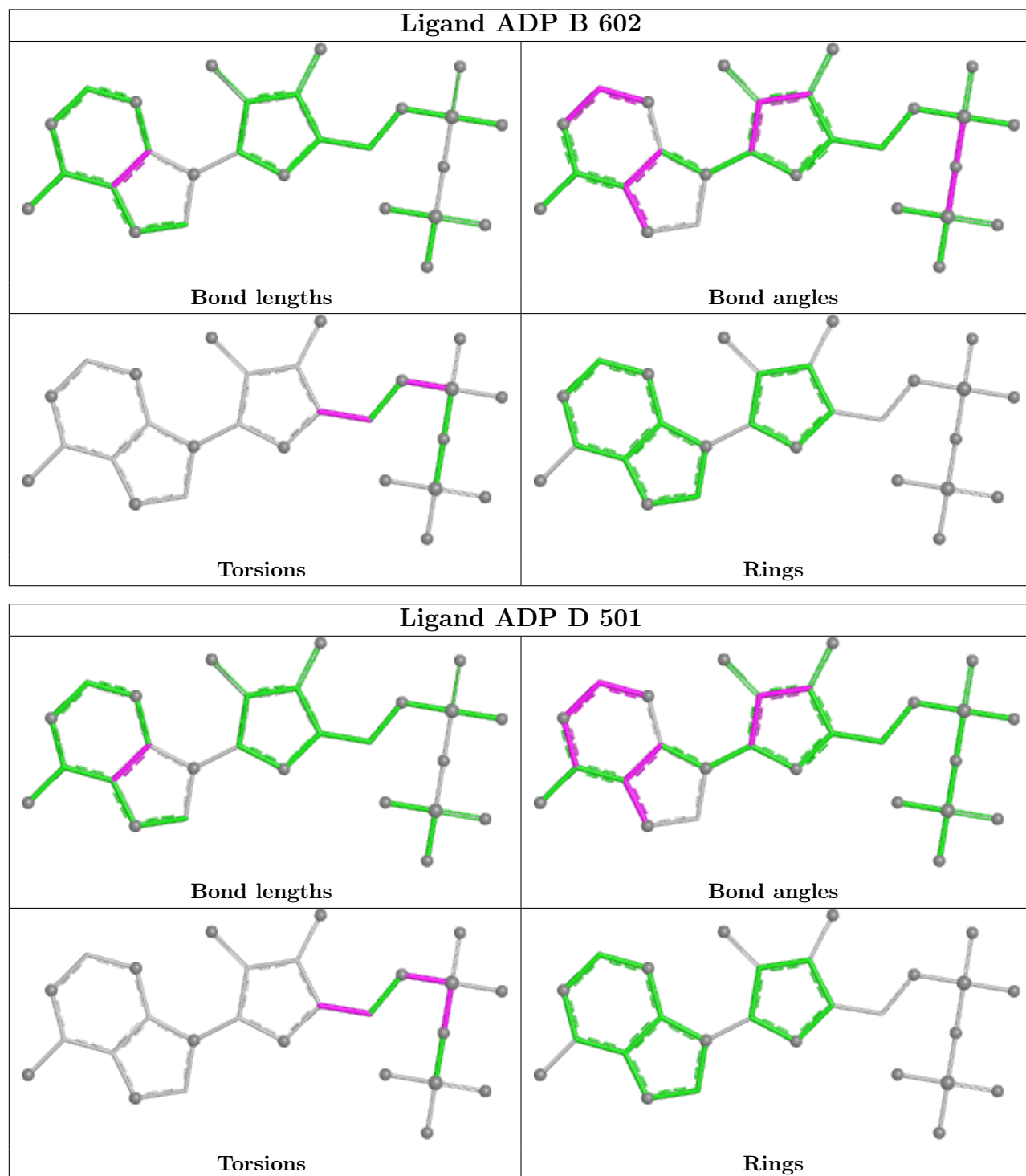
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	B	602	ADP	1	0

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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

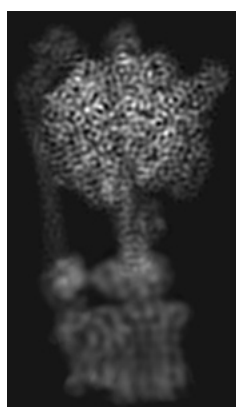
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4700. These allow visual inspection of the internal detail of the map and identification of artifacts.

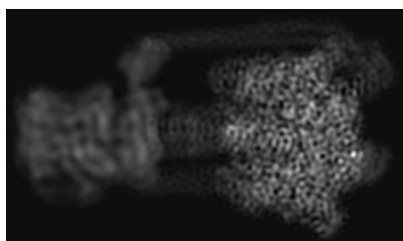
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

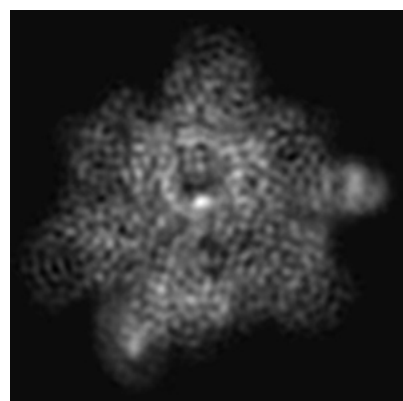
6.1.1 Primary map



X



Y



Z

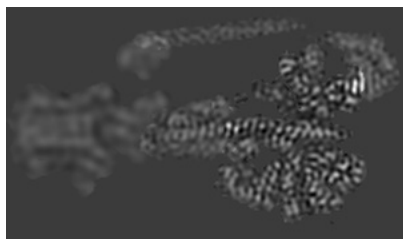
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

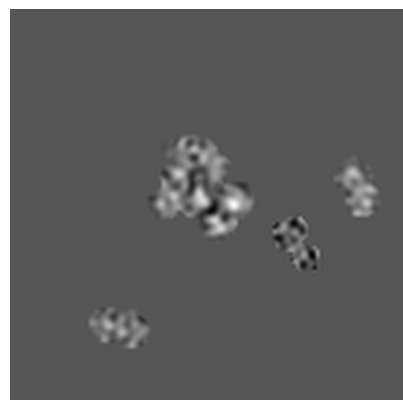
6.2.1 Primary map



X Index: 68



Y Index: 67



Z Index: 116

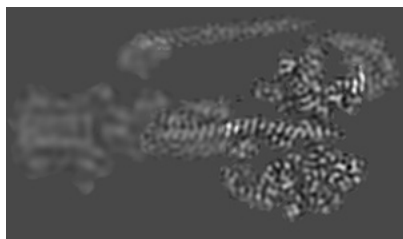
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

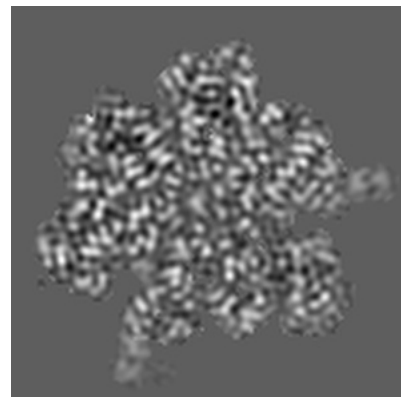
6.3.1 Primary map



X Index: 64



Y Index: 68



Z Index: 178

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

6.4 Orthogonal surface views [i](#)

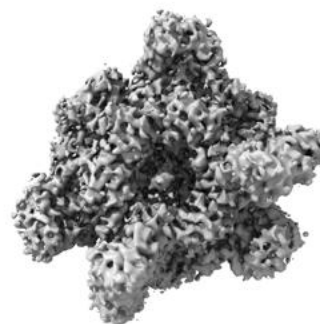
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0233. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

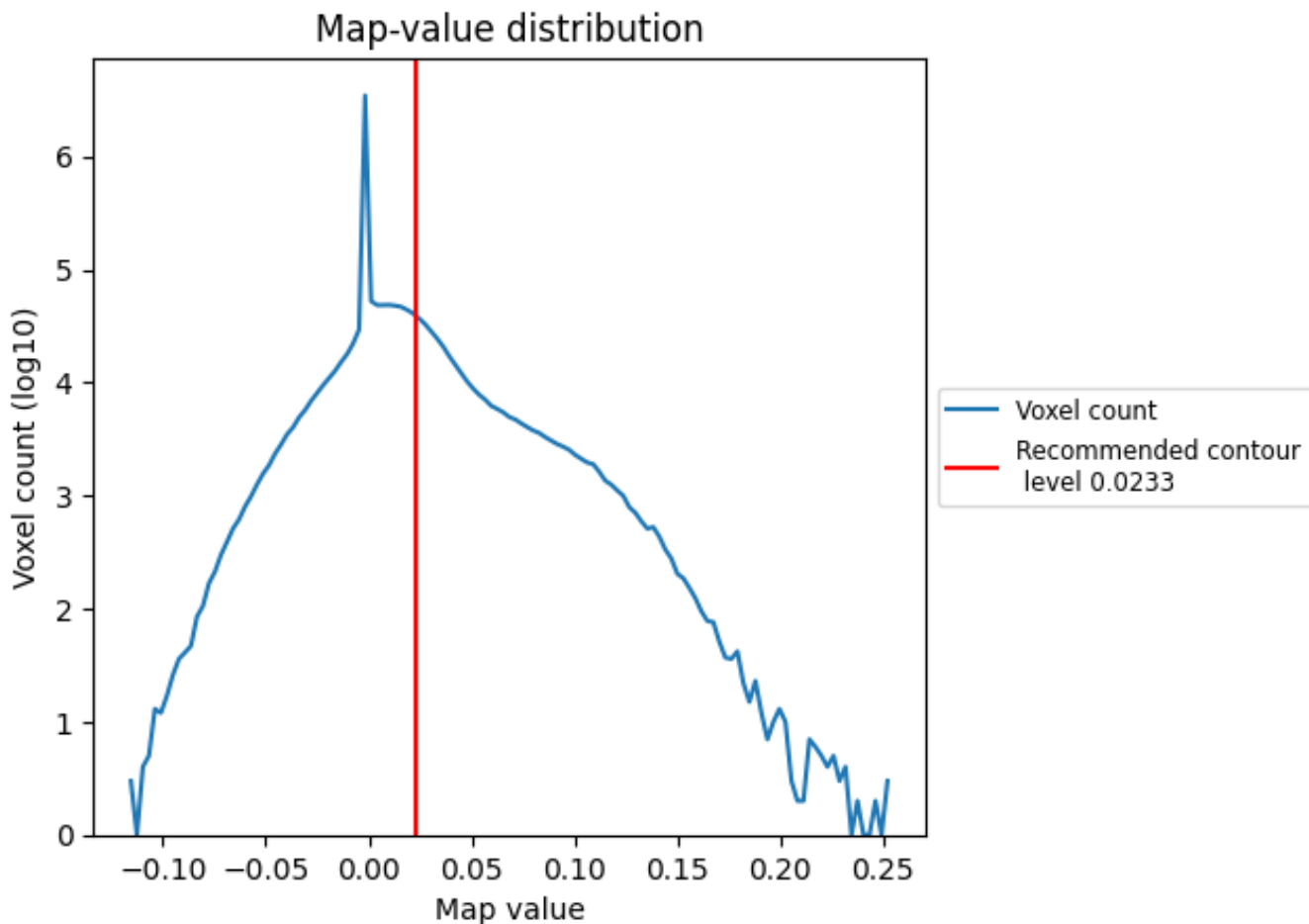
6.5 Mask visualisation

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

7 Map analysis [i](#)

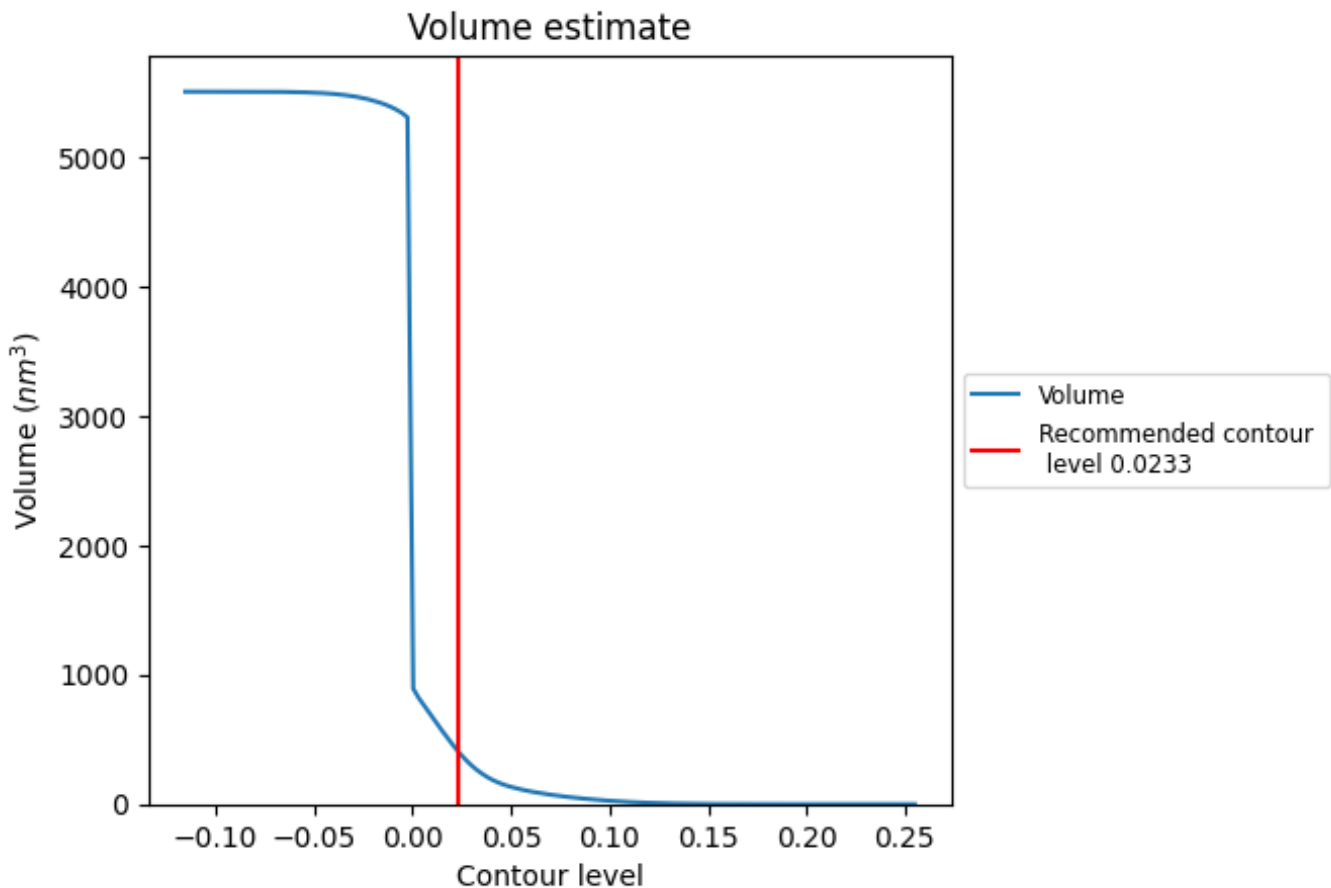
This section contains the results of statistical analysis of the map.

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 403 nm^3 ; this corresponds to an approximate mass of 364 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

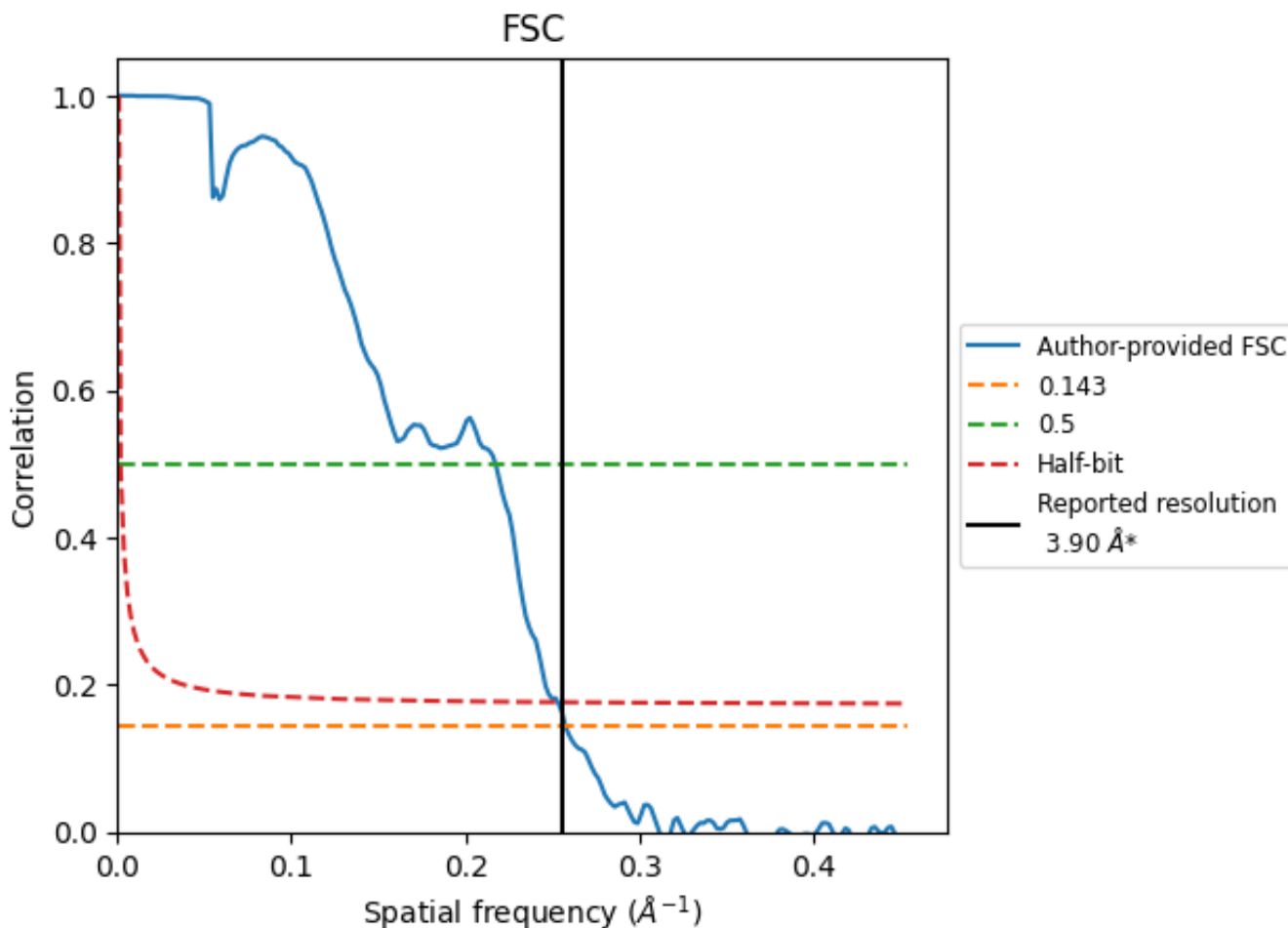
7.3 Rotationally averaged power spectrum [i](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

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 0.256 Å⁻¹

8.2 Resolution estimates [i](#)

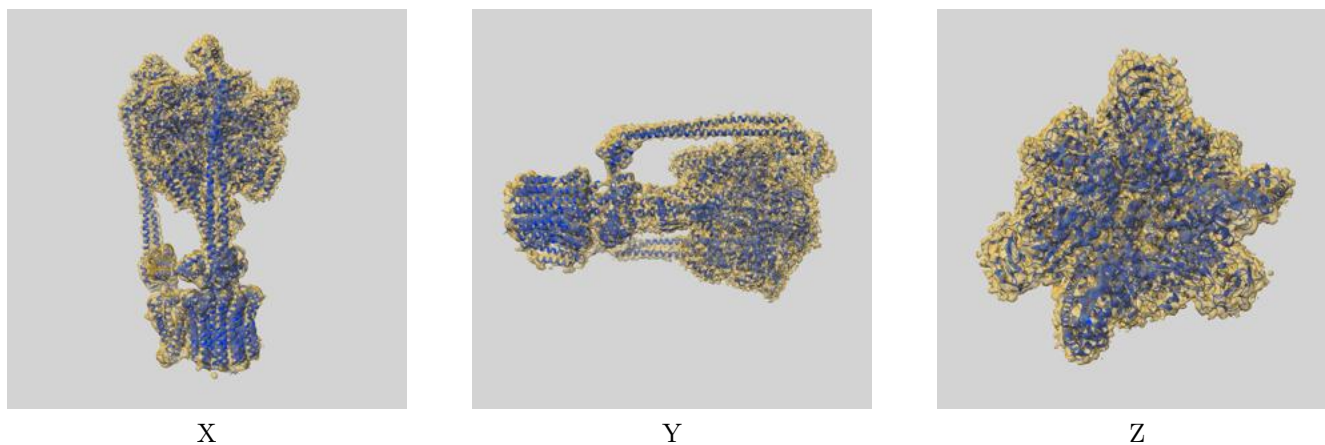
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	3.88	4.60	3.95
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

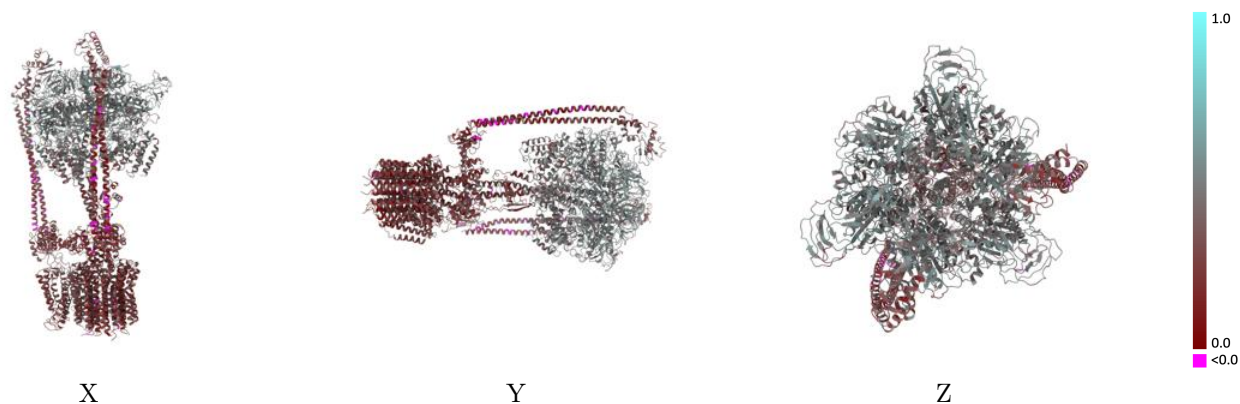
This section contains information regarding the fit between EMDB map EMD-4700 and PDB model 6R0Y. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)



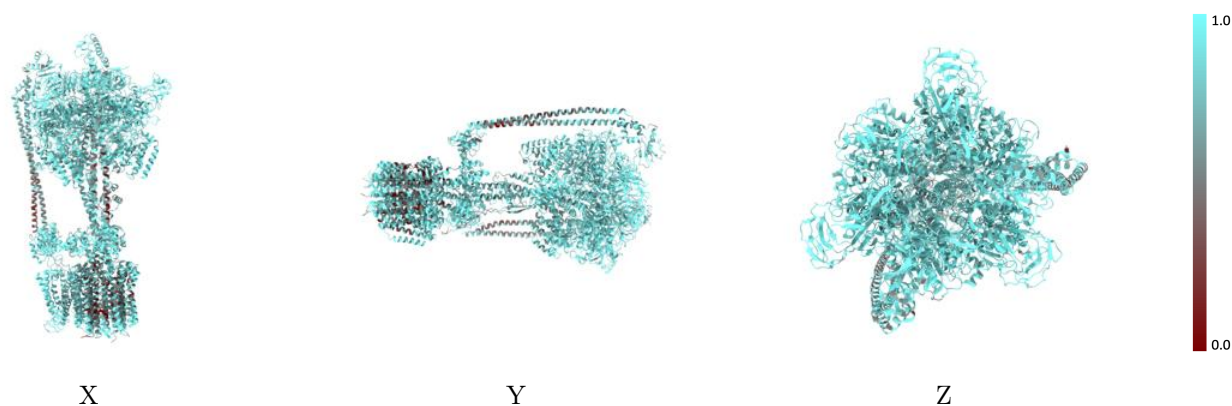
The images above show the 3D surface view of the map at the recommended contour level 0.0233 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



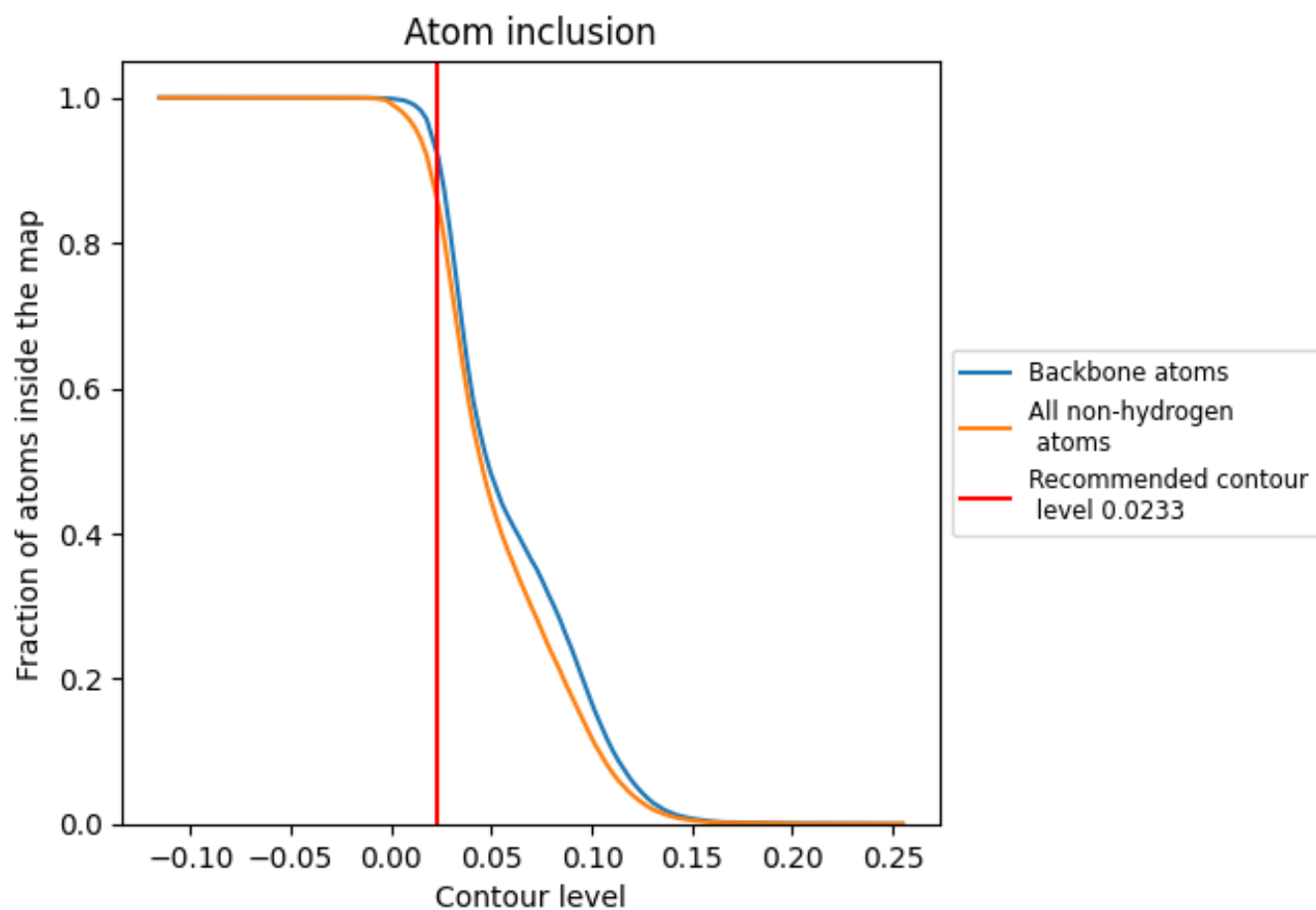
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0233).























































9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 85% 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 (0.0233) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8550	 0.3980
A	 0.9121	 0.4840
B	 0.9053	 0.4840
C	 0.9059	 0.4740
D	 0.9122	 0.4870
E	 0.9024	 0.4880
F	 0.8956	 0.4740
G	 0.7969	 0.3810
H	 0.7477	 0.2860
I	 0.6773	 0.2270
J	 0.7305	 0.2730
K	 0.6963	 0.2140
L	 0.7591	 0.2780
M	 0.8159	 0.2710
N	 0.8915	 0.2610
O	 0.6268	 0.2300
P	 0.6980	 0.2410
Q	 0.7416	 0.2500
R	 0.8234	 0.2600
S	 0.7635	 0.2480
T	 0.7151	 0.2500
U	 0.7521	 0.2380
V	 0.7521	 0.2390
W	 0.7550	 0.2330
X	 0.7608	 0.2350
Y	 0.7009	 0.2330
Z	 0.6895	 0.2400

