



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 06:31 PM UTC

PDB ID : 5FWK / pdb_00005fwk
EMDB ID : EMD-3337
Title : Atomic cryoEM structure of Hsp90-Cdc37-Cdk4 complex
Authors : Verba, K.A.; Wang, R.Y.R.; Arakawa, A.; Liu, Y.; Yokoyama, S.; Agard, D.A.
Deposited on : 2016-02-17
Resolution : 3.90 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:

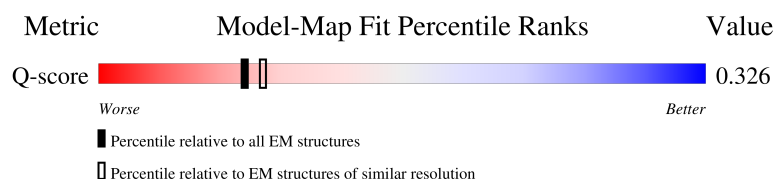
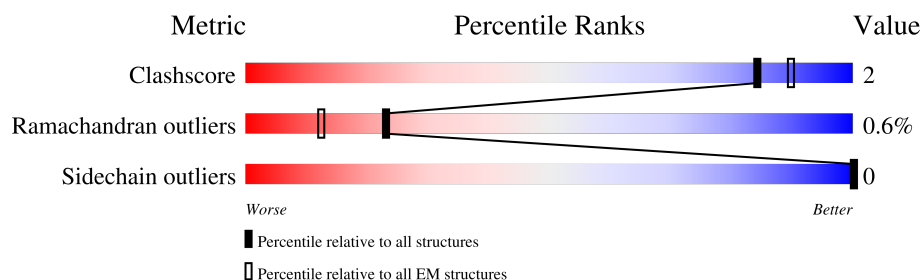
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	8855 (3.40 - 4.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	727	10% 82% 6% 12%
1	B	727	9% 82% 5% 13%
2	E	378	15% 33% 65%
3	K	310	56% 57% 9% 32%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 26225 atoms, of which 13113 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 HEAT SHOCK PROTEIN HSP 90 BETA.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	639	Total	C	H	N	O	S	0	1
			10400	3280	5226	871	1000	23		
1	B	631	Total	C	H	N	O	S	0	1
			10243	3235	5139	857	989	23		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP P08238
A	-1	GLY	-	expression tag	UNP P08238
A	0	PHE	-	expression tag	UNP P08238
B	-2	GLY	-	expression tag	UNP P08238
B	-1	GLY	-	expression tag	UNP P08238
B	0	PHE	-	expression tag	UNP P08238

- Molecule 2 is a protein called HSP90 CO-CHAPERONE CDC37.

Mol	Chain	Residues	Atoms							AltConf	Trace
2	E	132	Total	C	H	N	O	P	S	0	1
			2174	672	1070	204	220	1	7		

- Molecule 3 is a protein called CYCLIN-DEPENDENT KINASE 4.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	K	210	Total	C	H	N	O	S	0	1
			3344	1077	1678	285	295	9		

There are 7 discrepancies between the modelled and reference sequences:

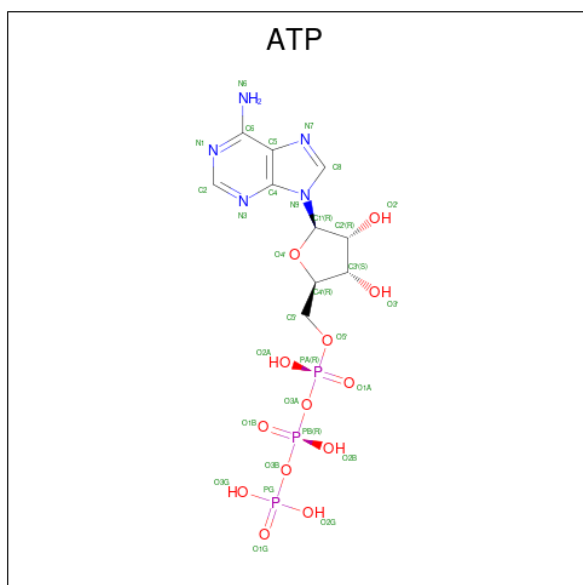
Chain	Residue	Modelled	Actual	Comment	Reference
K	-6	GLY	-	expression tag	UNP P11802
K	-5	ALA	-	expression tag	UNP P11802
K	-4	MET	-	expression tag	UNP P11802

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Chain	Residue	Modelled	Actual	Comment	Reference
K	-3	ASP	-	expression tag	UNP P11802
K	-2	PRO	-	expression tag	UNP P11802
K	-1	GLU	-	expression tag	UNP P11802
K	0	PHE	-	expression tag	UNP P11802

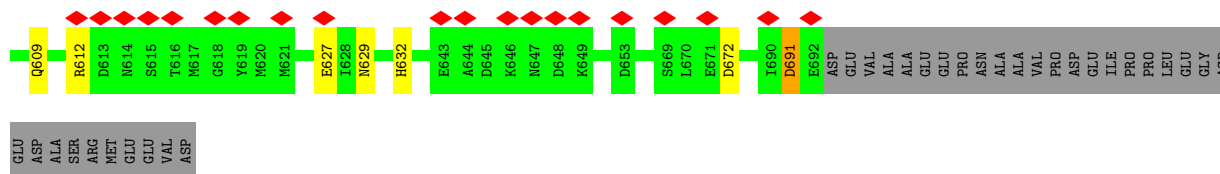
- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



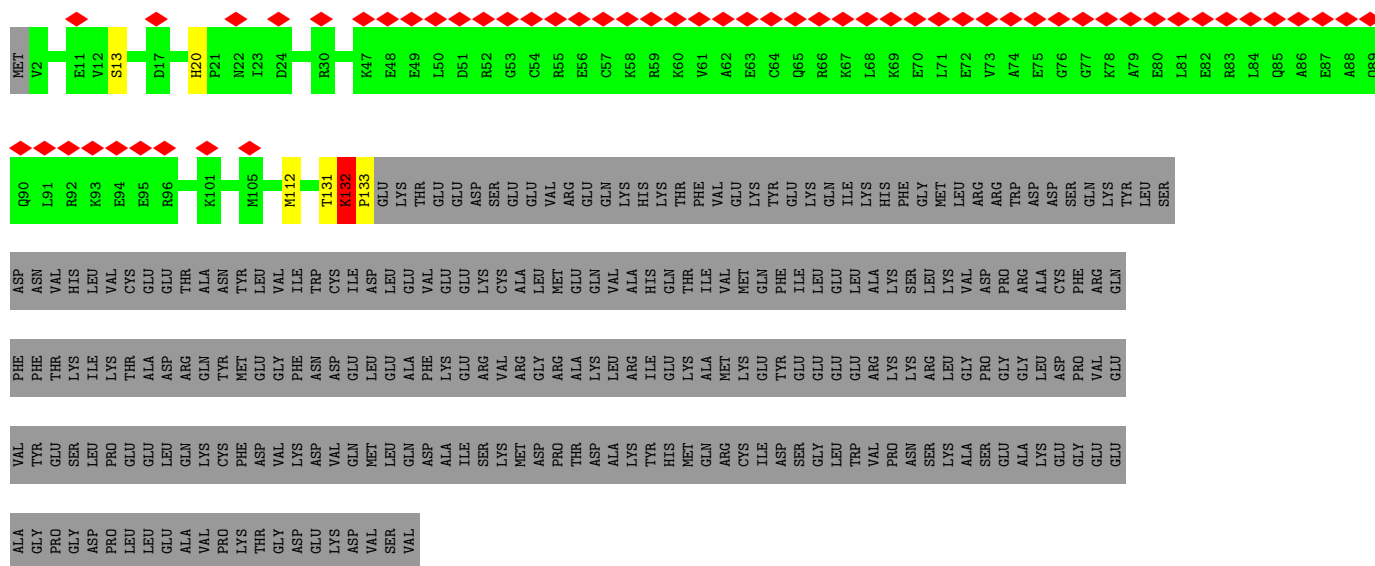
Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	B	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

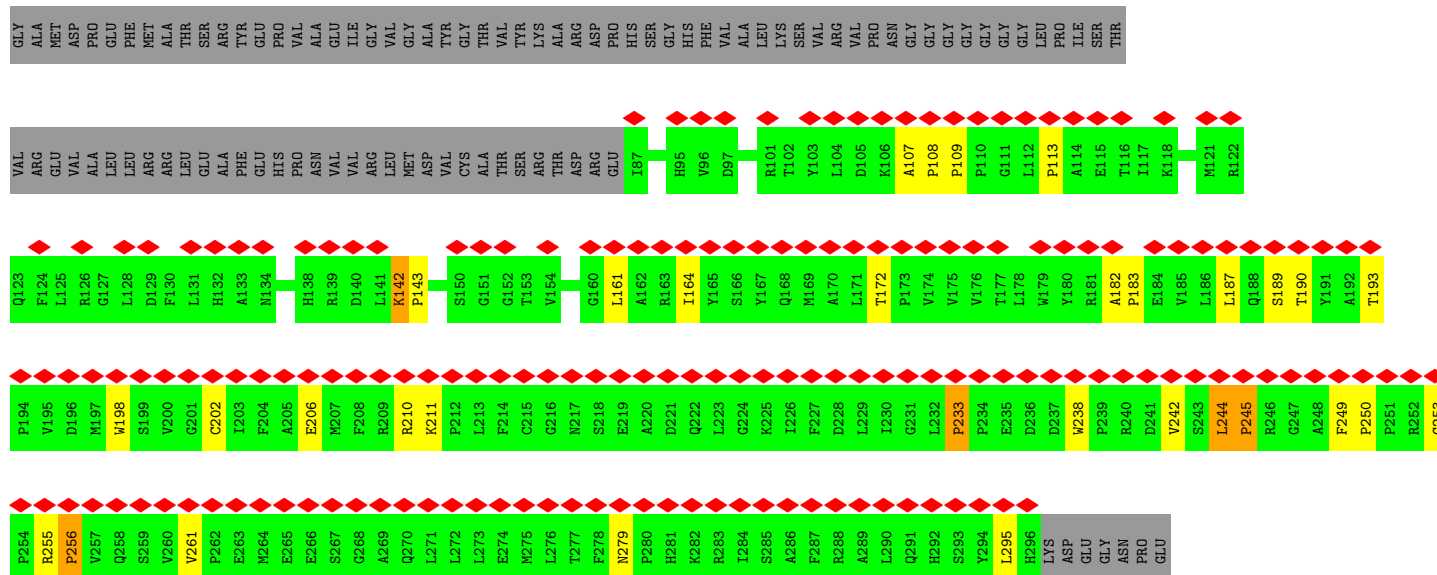
Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total	Mg	0
			1	1	
5	B	1	Total	Mg	0
			1	1	



• Molecule 2: HSP90 CO-CHAPERONE CDC37



• Molecule 3: CYCLIN-DEPENDENT KINASE 4



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	388688	Depositor
Resolution determination method	Not provided	
CTF correction method	Not provided	
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	44	Depositor
Minimum defocus (nm)	1400	Depositor
Maximum defocus (nm)	3800	Depositor
Magnification	22500	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.106	Depositor
Minimum map value	-0.050	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.02	Depositor
Map size ($\text{\AA}$)	336.64, 336.64, 336.64	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.315, 1.315, 1.315	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, MG, SEP

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	0.98	2/5258 (0.0%)	0.92	29/7064 (0.4%)
1	B	1.00	4/5188 (0.1%)	0.92	33/6974 (0.5%)
2	E	0.98	1/1109 (0.1%)	0.83	4/1478 (0.3%)
3	K	0.87	1/1712 (0.1%)	1.21	32/2332 (1.4%)
All	All	0.98	8/13267 (0.1%)	0.96	98/17848 (0.5%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	K	295	LEU	C-N	-7.16	1.23	1.33
1	A	690	ILE	C-N	-7.11	1.23	1.33
2	E	132	LYS	C-N	-7.08	1.23	1.34
1	B	691	ASP	C-N	-6.92	1.23	1.33
1	B	629	ASN	CA-CB	-6.56	1.45	1.53
1	B	632	HIS	CB-CG	-5.54	1.42	1.50
1	A	318	VAL	CA-CB	-5.19	1.47	1.54
1	B	54	ILE	CA-C	-5.07	1.46	1.52

All (98) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	78	ASN	CA-C-N	9.85	129.61	119.56
1	B	78	ASN	C-N-CA	9.85	129.61	119.56
3	K	250	PRO	CA-C-N	9.74	129.82	119.89
3	K	250	PRO	C-N-CA	9.74	129.82	119.89
3	K	108	PRO	CA-C-N	9.61	130.28	120.38
3	K	108	PRO	C-N-CA	9.61	130.28	120.38
3	K	253	GLY	CA-C-N	9.22	129.35	120.31
3	K	253	GLY	C-N-CA	9.22	129.35	120.31
1	B	587	SER	CA-C-N	8.60	128.74	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	587	SER	C-N-CA	8.60	128.74	119.28
3	K	279	ASN	CA-C-N	8.49	128.22	119.56
3	K	279	ASN	C-N-CA	8.49	128.22	119.56
1	A	61	ASP	CA-C-N	8.46	129.29	119.47
1	A	61	ASP	C-N-CA	8.46	129.29	119.47
1	A	78	ASN	CA-C-N	8.46	129.28	119.47
1	A	78	ASN	C-N-CA	8.46	129.28	119.47
1	B	629	ASN	CA-C-N	8.45	130.40	119.84
1	B	629	ASN	C-N-CA	8.45	130.40	119.84
1	A	672	ASP	CA-C-N	8.35	129.16	119.47
1	A	672	ASP	C-N-CA	8.35	129.16	119.47
1	B	61	ASP	CA-C-N	8.35	129.15	119.47
1	B	61	ASP	C-N-CA	8.35	129.15	119.47
1	B	292	ASN	CA-C-N	8.33	128.82	119.32
1	B	292	ASN	C-N-CA	8.33	128.82	119.32
1	B	76	ILE	CA-C-N	8.27	128.30	119.78
1	B	76	ILE	C-N-CA	8.27	128.30	119.78
3	K	261	VAL	CA-C-N	8.20	128.71	119.93
3	K	261	VAL	C-N-CA	8.20	128.71	119.93
1	B	632	HIS	CA-C-N	8.05	128.13	119.28
1	B	632	HIS	C-N-CA	8.05	128.13	119.28
1	B	672	ASP	CA-C-N	8.04	128.80	119.47
1	B	672	ASP	C-N-CA	8.04	128.80	119.47
1	A	335	ILE	CA-C-N	7.85	127.86	119.78
1	A	335	ILE	C-N-CA	7.85	127.86	119.78
3	K	107	ALA	CA-C-N	7.77	128.38	120.38
3	K	107	ALA	C-N-CA	7.77	128.38	120.38
1	A	632	HIS	CA-C-N	7.77	128.17	119.32
1	A	632	HIS	C-N-CA	7.77	128.17	119.32
2	E	20	HIS	CA-C-N	7.66	127.70	119.28
2	E	20	HIS	C-N-CA	7.66	127.70	119.28
1	A	515	GLU	CA-C-N	7.64	127.53	119.05
1	A	515	GLU	C-N-CA	7.64	127.53	119.05
1	A	587	SER	CA-C-N	7.54	127.26	119.64
1	A	587	SER	C-N-CA	7.54	127.26	119.64
1	B	335	ILE	CA-C-N	7.46	127.39	119.85
1	B	335	ILE	C-N-CA	7.46	127.39	119.85
3	K	238	TRP	CA-C-N	7.41	127.42	119.78
3	K	238	TRP	C-N-CA	7.41	127.42	119.78
1	A	629	ASN	CA-C-N	7.38	127.05	119.82
1	A	629	ASN	C-N-CA	7.38	127.05	119.82
3	K	233	PRO	CA-C-N	7.36	129.04	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	233	PRO	C-N-CA	7.36	129.04	119.84
2	E	112	MET	CA-C-N	7.33	127.33	119.78
2	E	112	MET	C-N-CA	7.33	127.33	119.78
1	B	286	LYS	CA-C-N	7.30	127.28	119.76
1	B	286	LYS	C-N-CA	7.30	127.28	119.76
3	K	249	PHE	CA-C-N	7.30	127.90	120.38
3	K	249	PHE	C-N-CA	7.30	127.90	120.38
1	A	339	ALA	CA-C-N	7.23	127.80	120.14
1	A	339	ALA	C-N-CA	7.23	127.80	120.14
1	B	370	ILE	CA-C-N	7.19	127.18	119.78
1	B	370	ILE	C-N-CA	7.19	127.18	119.78
1	A	211	TYR	CA-C-N	7.05	127.30	119.90
1	A	211	TYR	C-N-CA	7.05	127.30	119.90
1	A	292	ASN	CA-C-N	6.83	128.37	119.84
1	A	292	ASN	C-N-CA	6.83	128.37	119.84
3	K	109	PRO	CA-C-N	6.75	128.28	119.84
3	K	109	PRO	C-N-CA	6.75	128.28	119.84
3	K	182	ALA	CA-C-N	6.72	126.98	119.32
3	K	182	ALA	C-N-CA	6.72	126.98	119.32
3	K	211	LYS	CA-C-N	6.67	128.18	119.84
3	K	211	LYS	C-N-CA	6.67	128.18	119.84
1	B	515	GLU	CA-C-N	6.67	126.61	119.28
1	B	515	GLU	C-N-CA	6.67	126.61	119.28
1	A	286	LYS	CA-C-N	6.48	126.83	119.83
1	A	286	LYS	C-N-CA	6.48	126.83	119.83
1	B	339	ALA	CA-C-N	6.29	126.81	120.14
1	B	339	ALA	C-N-CA	6.29	126.81	120.14
1	B	211	TYR	CA-C-N	6.22	126.55	119.83
1	B	211	TYR	C-N-CA	6.22	126.55	119.83
3	K	172	THR	CA-C-N	6.18	125.86	119.56
3	K	172	THR	C-N-CA	6.18	125.86	119.56
3	K	193	THR	CA-C-N	6.15	125.71	119.19
3	K	193	THR	C-N-CA	6.15	125.71	119.19
1	A	370	ILE	CA-C-N	5.84	126.33	120.14
1	A	370	ILE	C-N-CA	5.84	126.33	120.14
3	K	244	LEU	CA-C-N	5.83	127.12	119.84
3	K	244	LEU	C-N-CA	5.83	127.12	119.84
1	B	173	GLU	CA-C-N	5.66	127.64	120.51
1	B	173	GLU	C-N-CA	5.66	127.64	120.51
3	K	142	LYS	CA-C-N	5.56	126.79	119.84
3	K	142	LYS	C-N-CA	5.56	126.79	119.84
1	B	543	LEU	CA-C-N	5.55	126.78	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	543	LEU	C-N-CA	5.55	126.78	119.84
1	B	54	ILE	CB-CA-C	-5.53	104.89	111.97
1	A	76	ILE	CA-C-N	5.18	125.63	120.14
1	A	76	ILE	C-N-CA	5.18	125.63	120.14
1	A	54	ILE	CB-CA-C	-5.12	105.42	111.97

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	A	5174	5226	5224	15	0
1	B	5104	5139	5137	26	0
2	E	1104	1070	1069	3	0
3	K	1666	1678	1677	11	0
4	A	31	0	12	3	0
4	B	31	0	12	2	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
All	All	13112	13113	13131	59	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 2.

All (59) 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:606:MET:CE	1:B:612:ARG:CZ	2.17	1.21
1:B:609:GLN:HB2	1:B:612:ARG:CG	1.78	1.12
1:B:609:GLN:HB2	1:B:612:ARG:HG3	1.31	1.10
1:B:606:MET:HE3	1:B:612:ARG:NE	1.79	0.97
1:B:609:GLN:CB	1:B:612:ARG:HG2	1.99	0.93
1:B:606:MET:HE3	1:B:612:ARG:CZ	2.02	0.89
1:A:128:GLN:O	1:A:128:GLN:HG2	1.73	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:609:GLN:HB2	1:B:612:ARG:HG2	1.56	0.88
1:B:606:MET:HE2	1:B:612:ARG:CZ	2.02	0.86
1:B:609:GLN:CB	1:B:612:ARG:CG	2.51	0.86
4:A:725:ATP:O2G	4:A:725:ATP:O2A	2.00	0.79
1:B:606:MET:HE2	1:B:612:ARG:NH2	1.98	0.79
1:B:606:MET:HE1	1:B:612:ARG:CZ	2.14	0.77
4:B:725:ATP:O2B	4:B:725:ATP:O2G	2.03	0.76
1:B:609:GLN:HB3	1:B:612:ARG:HG2	1.68	0.74
1:B:606:MET:CE	1:B:612:ARG:NE	2.43	0.72
1:B:606:MET:HE1	1:B:612:ARG:NH1	2.12	0.64
1:B:606:MET:CE	1:B:612:ARG:NH1	2.62	0.62
2:E:132:LYS:HG2	2:E:133:PRO:N	2.15	0.61
1:A:279:GLN:O	1:A:279:GLN:HG3	2.02	0.60
1:A:124:SER:OG	1:A:358:ARG:NH1	2.36	0.59
1:A:38:ILE:HD12	1:A:38:ILE:C	2.33	0.53
4:A:725:ATP:N3	4:A:725:ATP:H2'	2.24	0.52
1:B:606:MET:CE	1:B:612:ARG:NH2	2.59	0.51
3:K:255:ARG:O	3:K:256:PRO:C	2.54	0.51
1:A:221:ARG:HB2	1:A:273:LYS:HB2	1.92	0.50
4:A:725:ATP:O3A	4:A:725:ATP:O1G	2.30	0.50
3:K:210:ARG:HG2	3:K:210:ARG:O	2.11	0.50
1:B:220:GLU:HG2	1:B:220:GLU:O	2.12	0.50
3:K:206:GLU:O	3:K:210:ARG:N	2.45	0.49
1:A:597:GLY:HA2	1:A:621:MET:SD	2.53	0.48
3:K:142:LYS:HB2	3:K:143:PRO:CD	2.44	0.47
3:K:244:LEU:HB3	3:K:245:PRO:HD2	1.97	0.47
3:K:142:LYS:HB2	3:K:143:PRO:HD2	1.97	0.47
1:A:594:SER:OG	1:A:596:TYR:O	2.33	0.46
1:B:219:LYS:O	1:B:220:GLU:C	2.59	0.46
2:E:131:THR:O	2:E:132:LYS:CB	2.64	0.45
1:B:299:GLU:OE1	1:B:299:GLU:N	2.39	0.45
3:K:161:LEU:HA	3:K:164:ILE:HG12	1.99	0.45
3:K:187:LEU:HD22	3:K:242:VAL:HG13	1.98	0.45
1:A:389:ASN:OD1	1:A:389:ASN:C	2.58	0.45
3:K:189:SER:OG	3:K:190:THR:N	2.50	0.45
3:K:183:PRO:O	3:K:187:LEU:HG	2.17	0.44
1:A:316:LEU:C	1:A:316:LEU:HD23	2.43	0.44
1:B:83:THR:HG22	1:B:184:HIS:HA	2.00	0.43
1:B:141:GLU:OE1	1:B:186:LYS:NZ	2.52	0.43
1:A:486:ILE:O	1:A:486:ILE:HG23	2.19	0.43
1:B:93:MET:SD	4:B:725:ATP:H1'	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:598:TRP:CD1	1:A:602:MET:SD	3.14	0.41
3:K:198:TRP:CH2	3:K:202:CYS:SG	3.11	0.41
1:B:627:GLU:HA	1:B:627:GLU:OE1	2.20	0.41
1:A:492:GLU:H	1:A:492:GLU:CD	2.29	0.41
1:A:444:ASP:OD1	1:A:444:ASP:C	2.64	0.40
1:B:21:ILE:HA	1:B:24:LEU:HB3	2.03	0.40
1:B:139:VAL:HG12	1:B:185:LEU:HD22	2.03	0.40
1:B:78:ASN:C	1:B:78:ASN:OD1	2.62	0.40
2:E:131:THR:O	2:E:132:LYS:HB2	2.21	0.40
1:A:456:ARG:HB3	1:A:466:MET:HG2	2.01	0.40
1:A:473:VAL:HA	1:A:476:MET:SD	2.61	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	635/727 (87%)	612 (96%)	20 (3%)	3 (0%)	24 59
1	B	627/727 (86%)	607 (97%)	18 (3%)	2 (0%)	36 69
2	E	129/378 (34%)	123 (95%)	5 (4%)	1 (1%)	16 50
3	K	208/310 (67%)	183 (88%)	21 (10%)	4 (2%)	6 33
All	All	1599/2142 (75%)	1525 (95%)	64 (4%)	10 (1%)	23 55

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	132	LYS
3	K	256	PRO
1	A	174	PRO
1	A	281	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	691	ASP
3	K	113	PRO
1	A	128	GLN
3	K	233	PRO
3	K	245	PRO
1	B	127	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	577/653 (88%)	577 (100%)	0	100	100
1	B	569/653 (87%)	569 (100%)	0	100	100
2	E	119/340 (35%)	119 (100%)	0	100	100
3	K	183/262 (70%)	183 (100%)	0	100	100
All	All	1448/1908 (76%)	1448 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	442	HIS
1	A	461	GLN
1	B	189	GLN
1	B	205	HIS
1	B	298	GLN
1	B	458	HIS
1	B	524	GLN
1	B	674	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SEP	E	13	2	8,9,10	1.47	1 (12%)	7,12,14	1.26	1 (14%)

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
2	SEP	E	13	2	-	0/6/8/10	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	13	SEP	P-O1P	3.31	1.60	1.50

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	13	SEP	OG-CB-CA	3.06	111.12	108.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 2 are 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
4	ATP	A	725	5	32,33,33	1.46	6 (18%)	48,52,52	1.73	7 (14%)
4	ATP	B	725	5	32,33,33	1.52	7 (21%)	48,52,52	1.74	6 (12%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ATP	A	725	5	-	9/22/38/38	0/3/3/3
4	ATP	B	725	5	-	8/22/38/38	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	725	ATP	C5-C4	4.75	1.47	1.39
4	B	725	ATP	C5-C4	4.71	1.47	1.39
4	B	725	ATP	PB-O3A	-3.42	1.55	1.59
4	B	725	ATP	C5-N7	-2.78	1.34	1.39
4	A	725	ATP	PB-O3B	-2.68	1.56	1.59
4	A	725	ATP	C5-C6	2.52	1.48	1.41
4	B	725	ATP	C5-C6	2.35	1.47	1.41
4	A	725	ATP	C4-N9	-2.27	1.33	1.37
4	B	725	ATP	PA-O3A	-2.22	1.57	1.59
4	A	725	ATP	C5-N7	-2.20	1.35	1.39
4	A	725	ATP	C8-N7	2.16	1.35	1.31
4	B	725	ATP	C4-N9	-2.16	1.33	1.37
4	B	725	ATP	C8-N7	2.07	1.35	1.31

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	725	ATP	C5-C4-N3	-5.86	118.65	126.72
4	B	725	ATP	C5-C4-N3	-5.75	118.80	126.72
4	A	725	ATP	N3-C4-N9	4.56	134.93	127.17
4	B	725	ATP	N3-C4-N9	4.44	134.73	127.17
4	A	725	ATP	C2-N3-C4	3.71	120.89	111.83
4	B	725	ATP	C2-N3-C4	3.66	120.76	111.83
4	A	725	ATP	N3-C2-N1	-3.37	123.48	128.58
4	B	725	ATP	N3-C2-N1	-3.31	123.57	128.58
4	A	725	ATP	C4-C5-N7	-3.11	107.02	110.58
4	B	725	ATP	C4-C5-N7	-3.02	107.12	110.58
4	B	725	ATP	C3'-C2'-C1'	2.38	105.96	101.46
4	A	725	ATP	C4-N9-C8	2.18	108.02	105.74
4	A	725	ATP	O2B-PB-O1B	2.10	122.23	112.44

There are no chirality outliers.

All (17) torsion outliers are listed below:

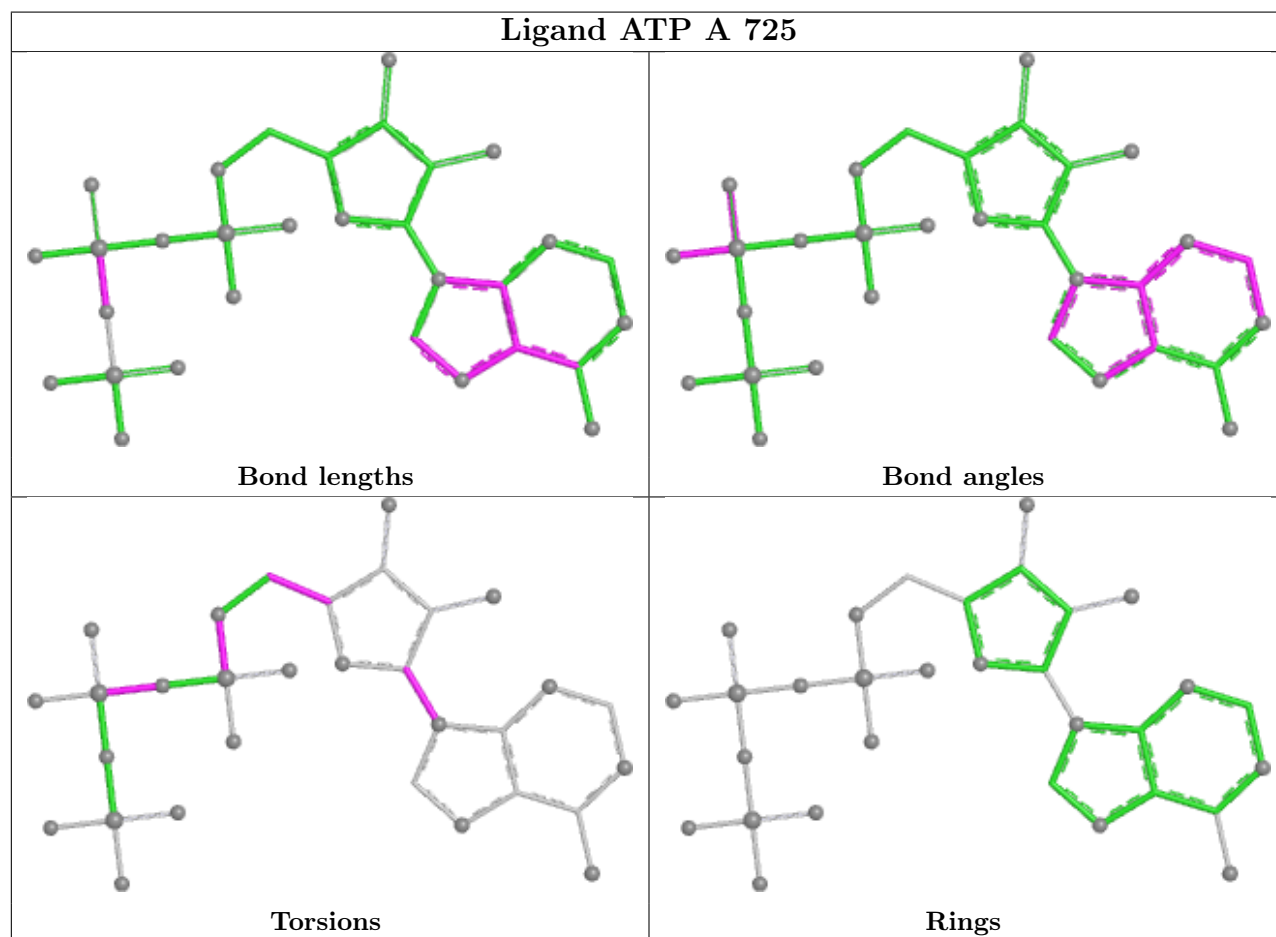
Mol	Chain	Res	Type	Atoms
4	A	725	ATP	O4'-C4'-C5'-O5'
4	B	725	ATP	C5'-O5'-PA-O2A
4	B	725	ATP	C5'-O5'-PA-O3A
4	A	725	ATP	C3'-C4'-C5'-O5'
4	B	725	ATP	O4'-C4'-C5'-O5'
4	B	725	ATP	C3'-C4'-C5'-O5'
4	A	725	ATP	PA-O3A-PB-O2B
4	B	725	ATP	PG-O3B-PB-O2B
4	A	725	ATP	C5'-O5'-PA-O1A
4	A	725	ATP	C5'-O5'-PA-O2A
4	A	725	ATP	C5'-O5'-PA-O3A
4	B	725	ATP	PB-O3A-PA-O2A
4	A	725	ATP	C2'-C1'-N9-C4
4	A	725	ATP	C2'-C1'-N9-C8
4	B	725	ATP	PB-O3A-PA-O1A
4	A	725	ATP	PA-O3A-PB-O1B
4	B	725	ATP	PG-O3B-PB-O1B

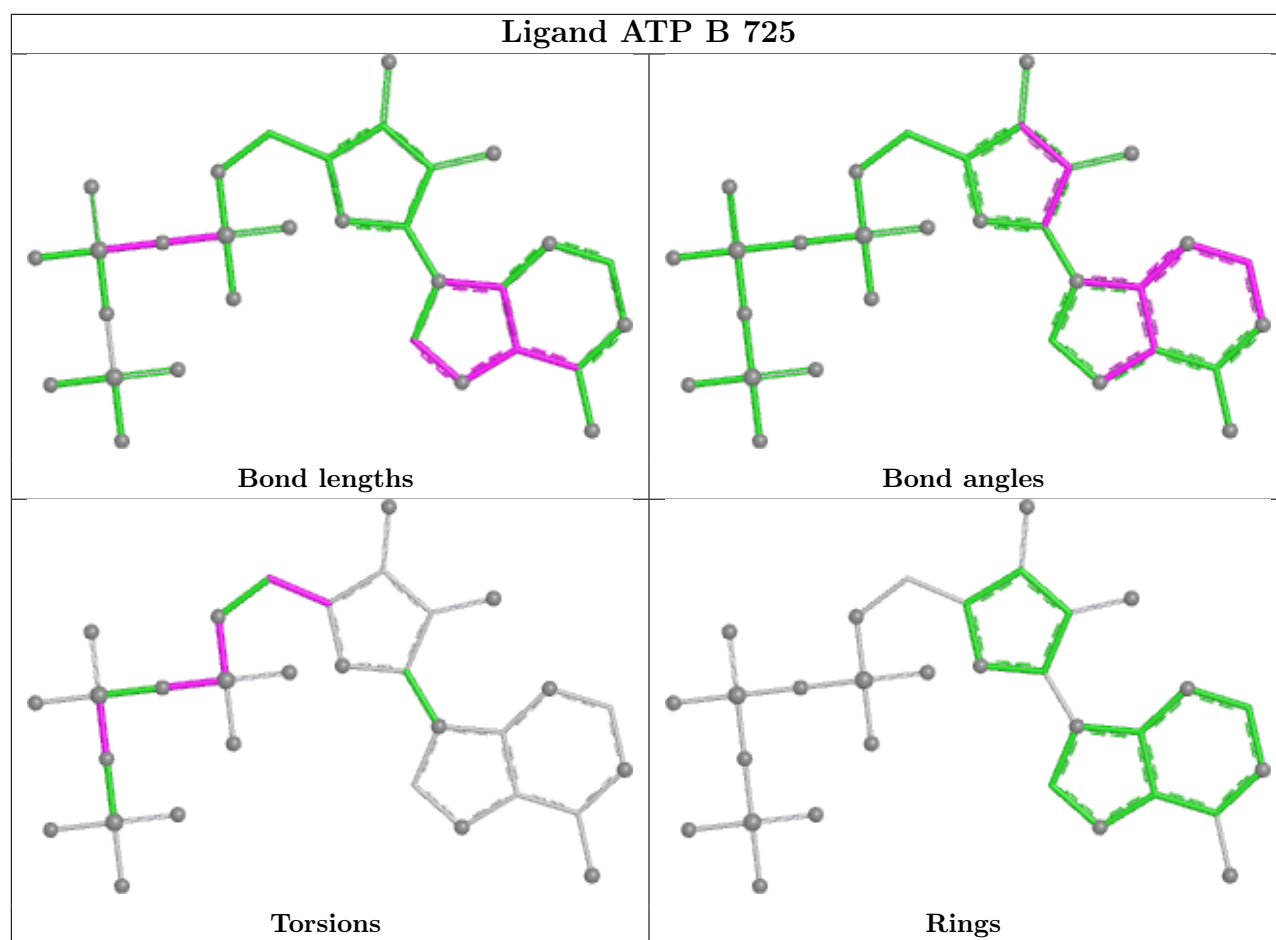
There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	725	ATP	3	0
4	B	725	ATP	2	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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

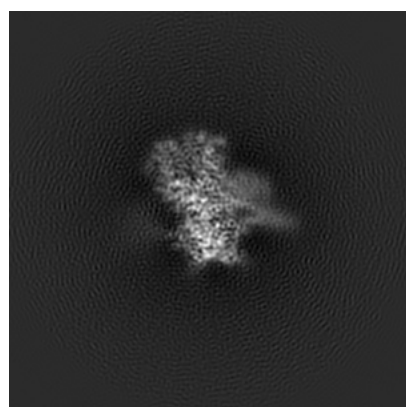
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3337. These allow visual inspection of the internal detail of the map and identification of artifacts.

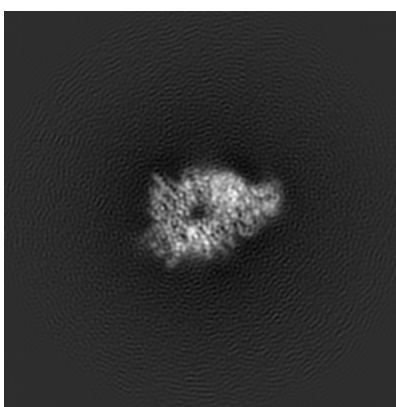
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

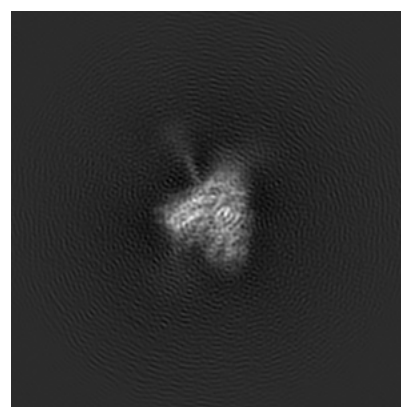
6.1.1 Primary map



X



Y

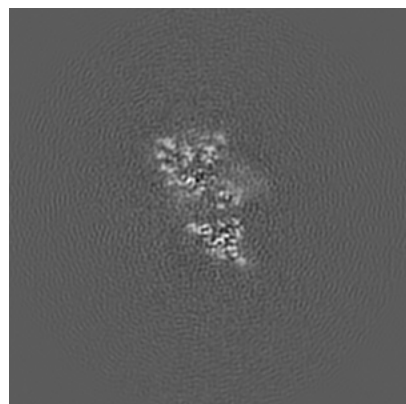


Z

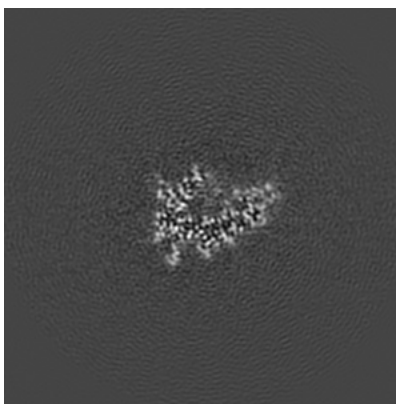
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

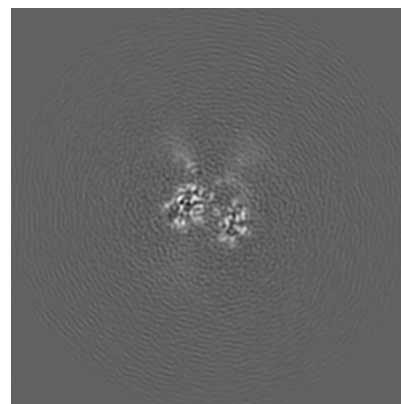
6.2.1 Primary map



X Index: 128



Y Index: 128

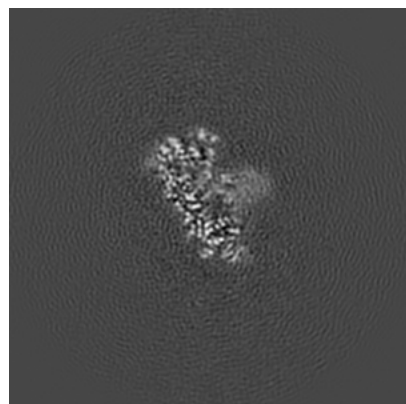


Z Index: 128

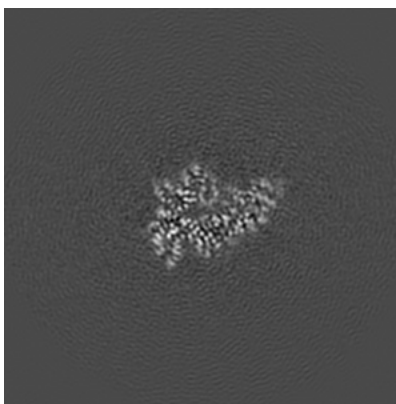
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

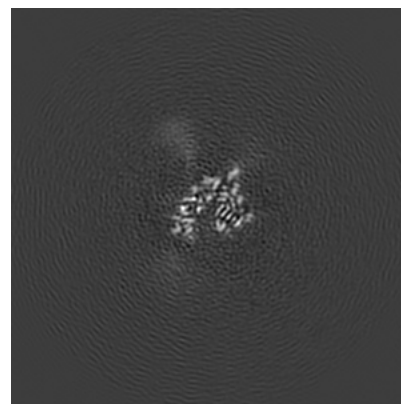
6.3.1 Primary map



X Index: 138



Y Index: 126

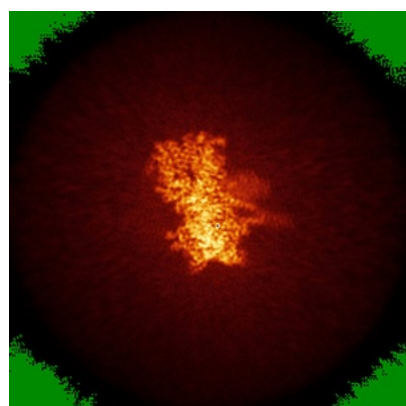


Z Index: 118

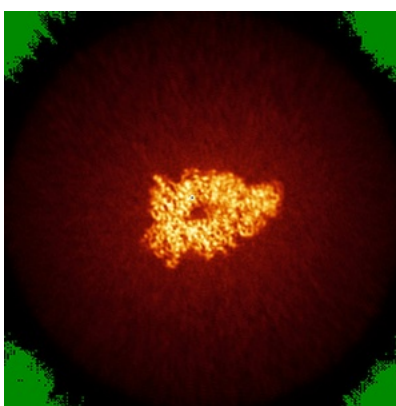
The images above show the largest variance slices of the map in three orthogonal directions.

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

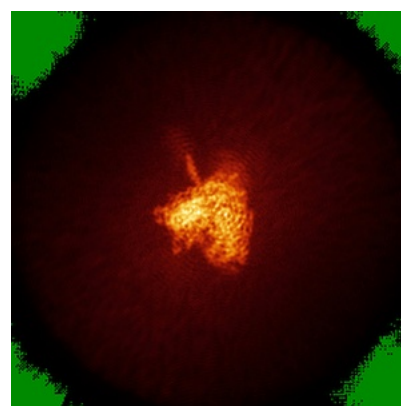
6.4.1 Primary map



X



Y

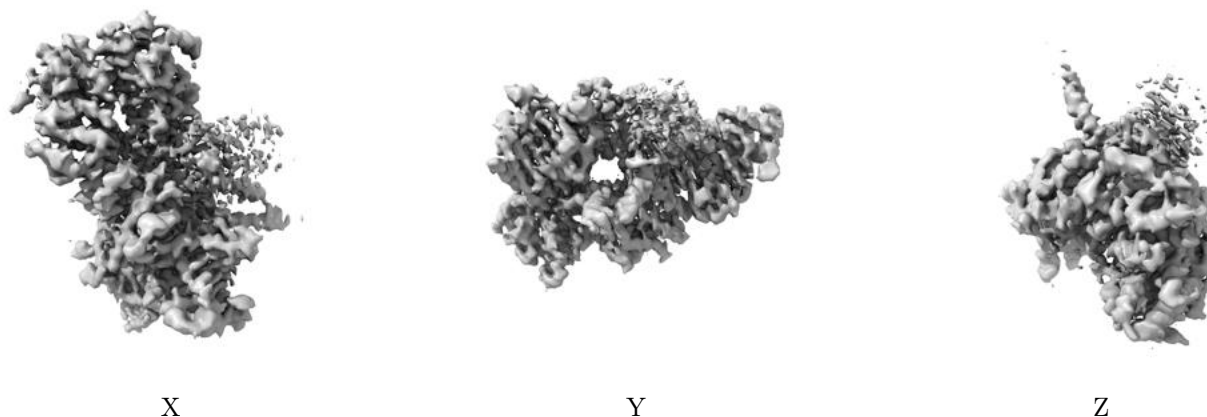


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

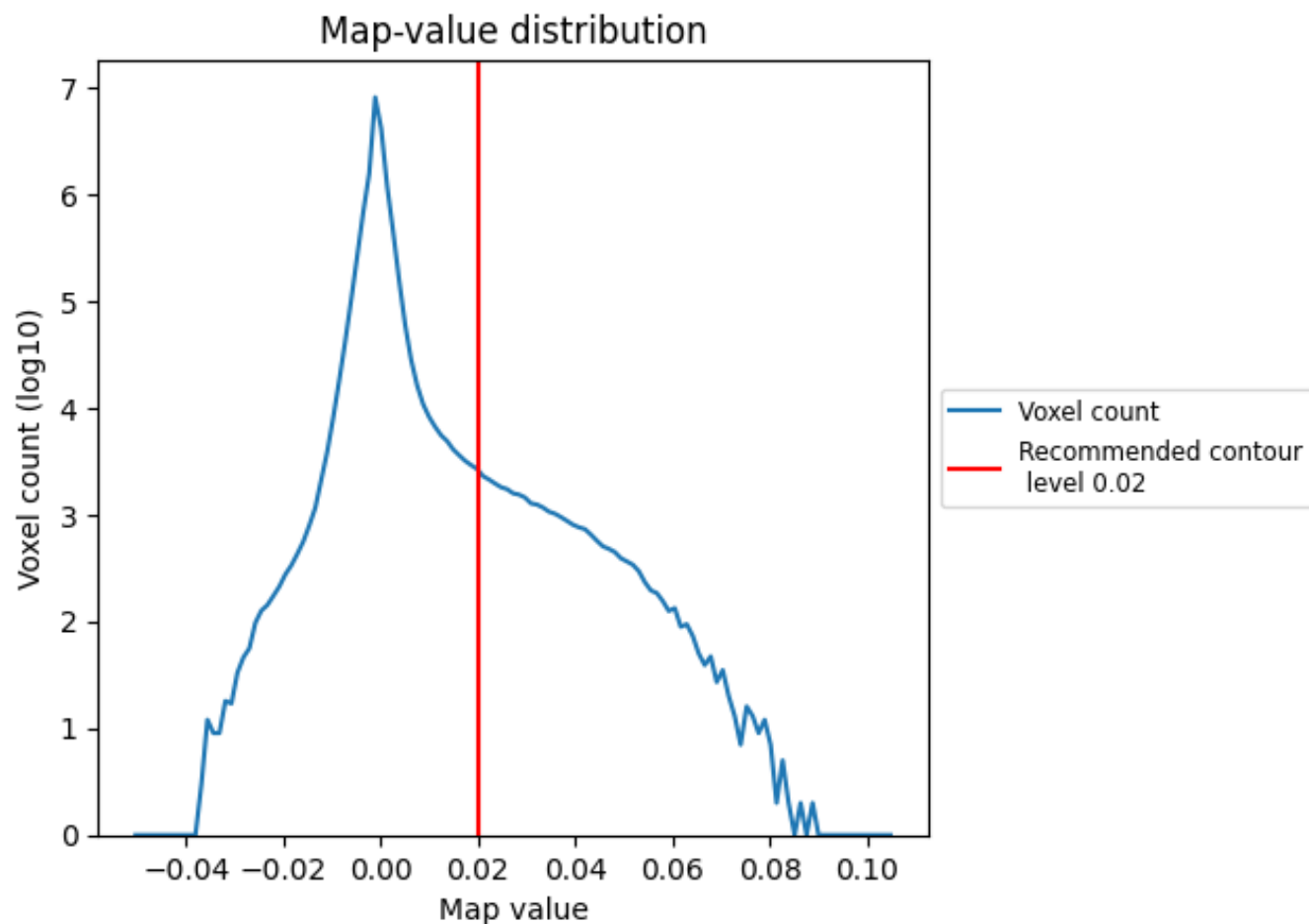
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

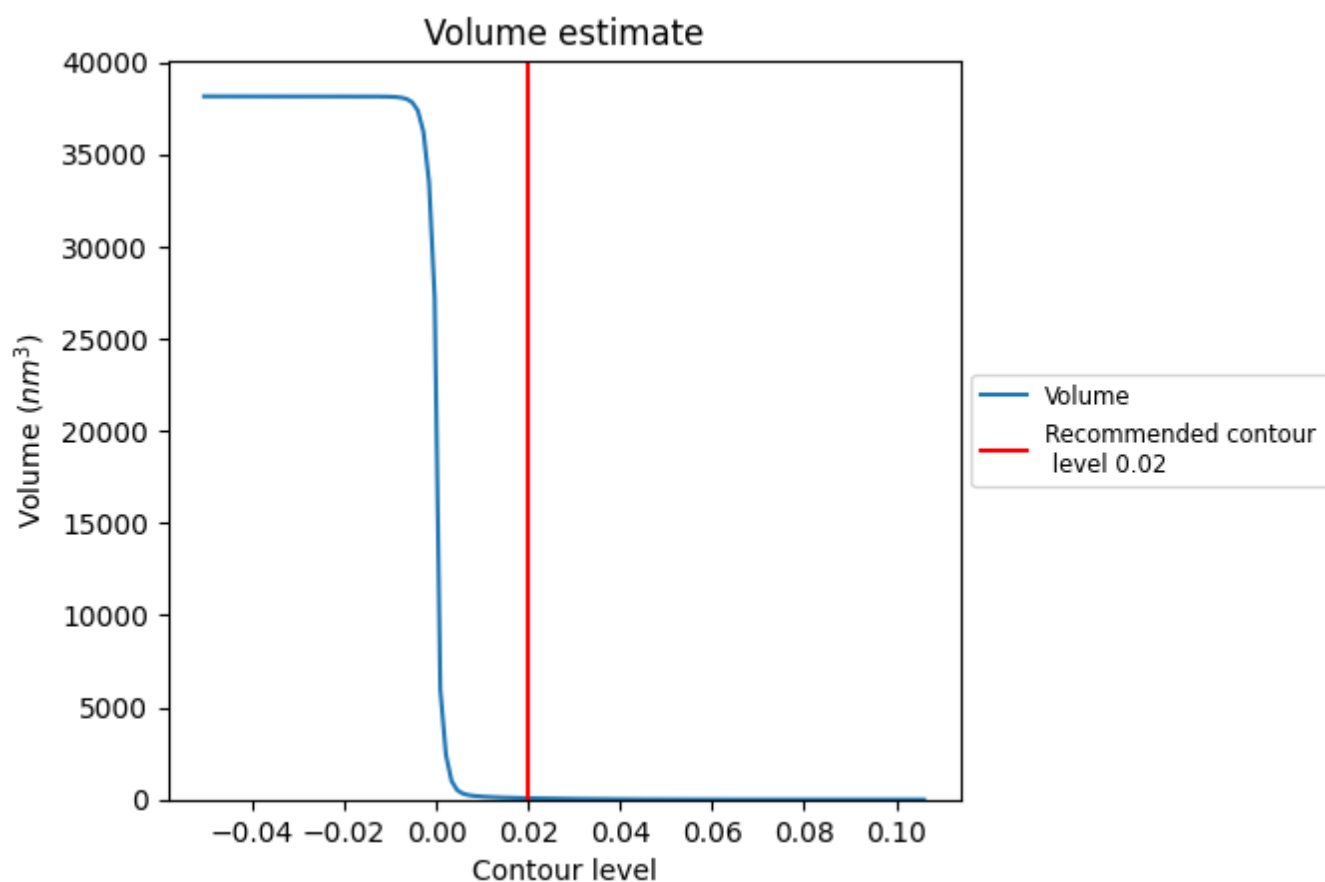
This section contains the results of statistical analysis of the map.

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.

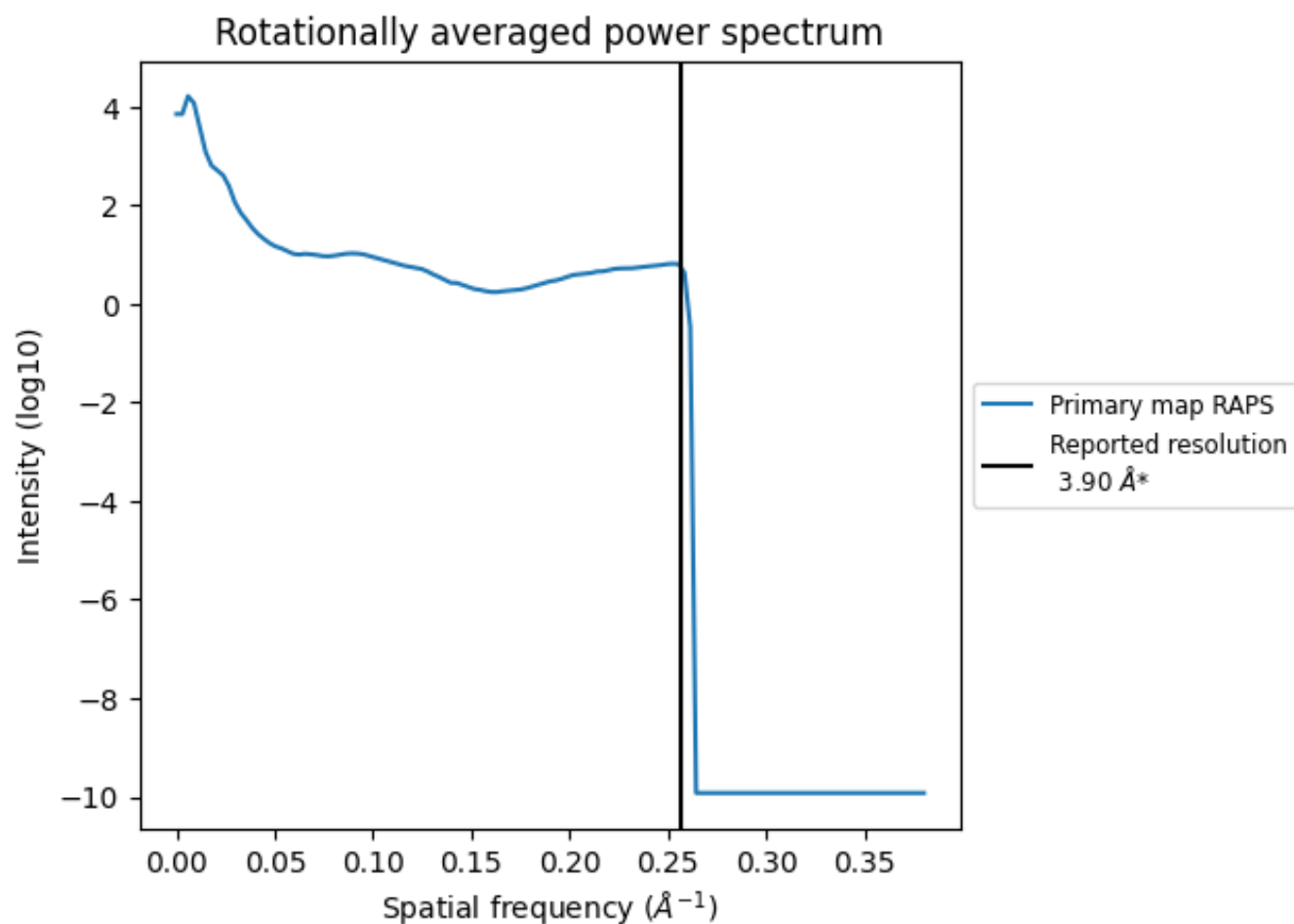
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 73 nm³; this corresponds to an approximate mass of 66 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 ⓘ

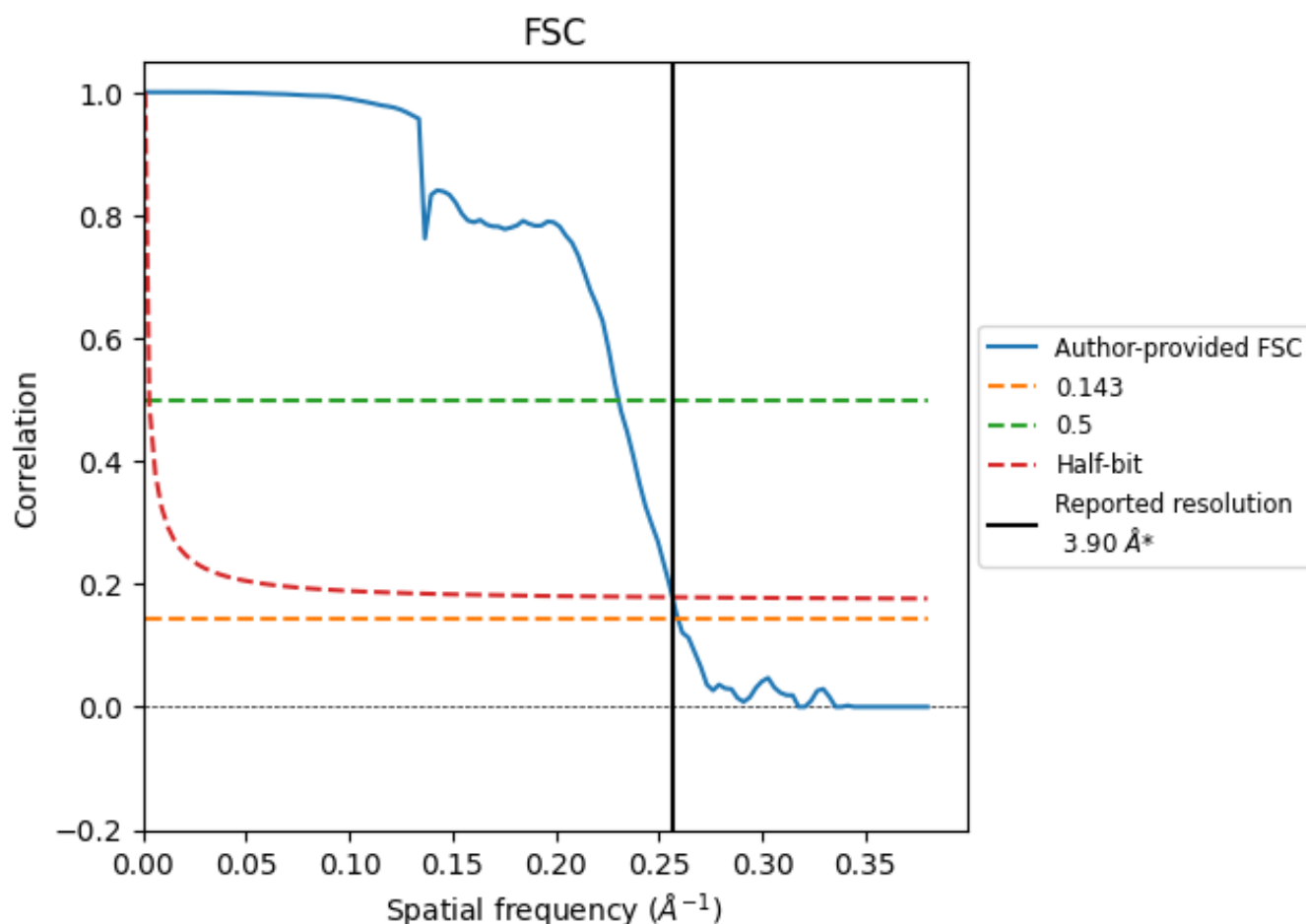


*Reported resolution corresponds to spatial frequency of 0.256 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.256 Å⁻¹

8.2 Resolution estimates [i](#)

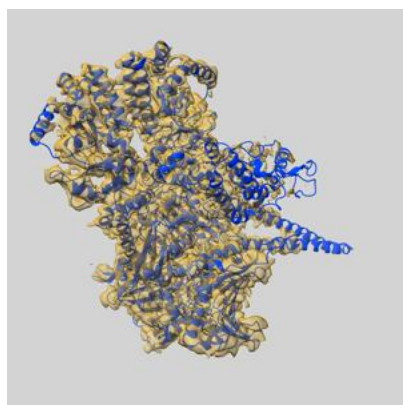
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	-	-	-
Author-provided FSC curve	3.86	4.34	3.90
Unmasked-calculated*	-	-	-

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

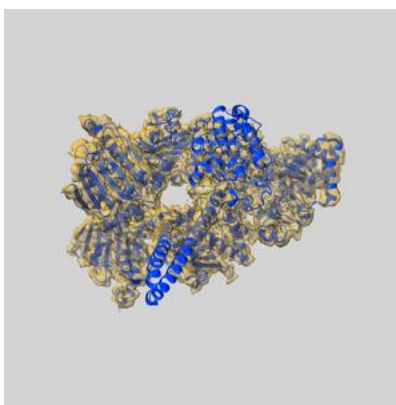
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-3337 and PDB model 5FWK. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

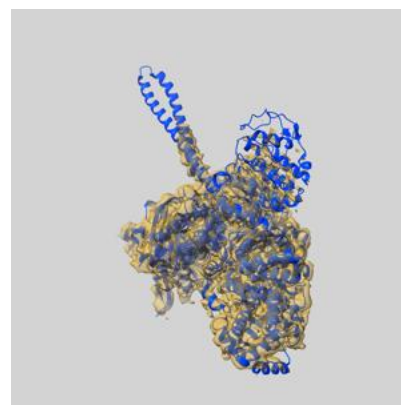
9.1 Map-model overlay [i](#)



X



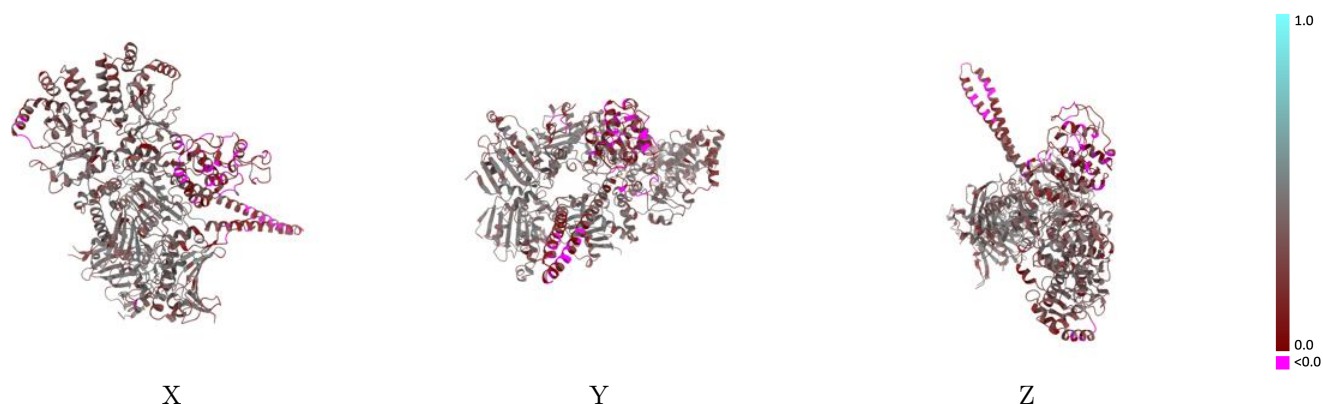
Y



Z

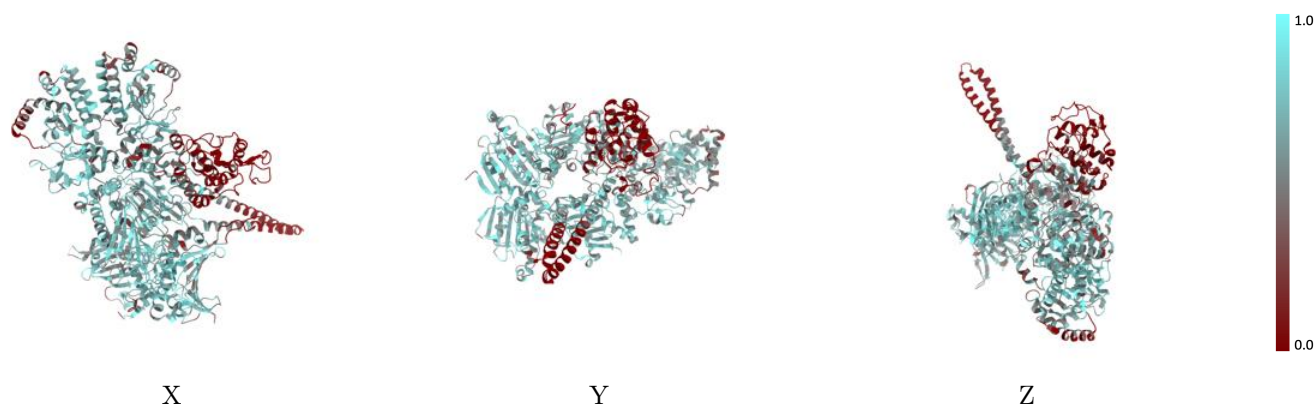
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



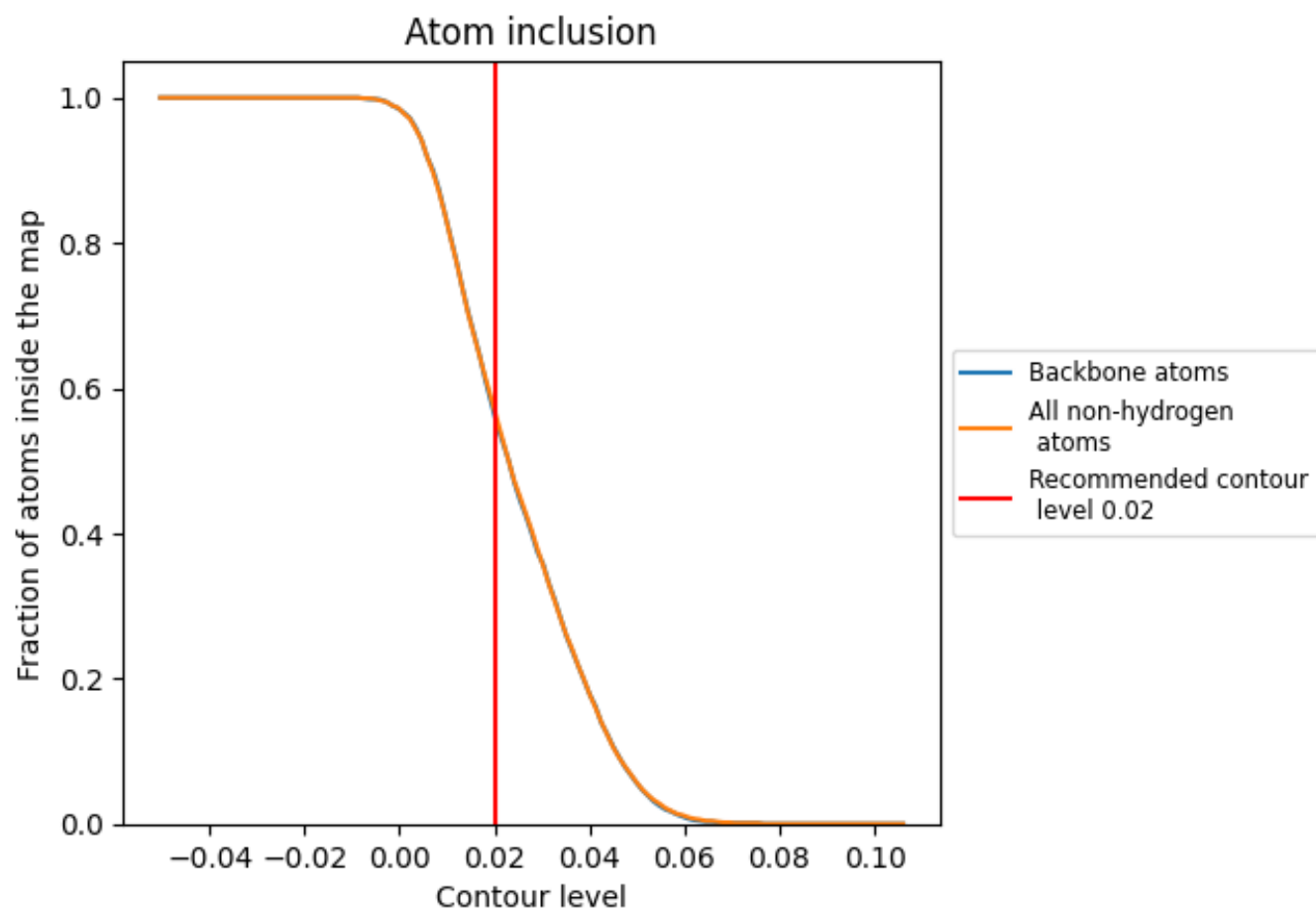
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).

9.4 Atom inclusion [i](#)



At the recommended contour level, 56% of all backbone atoms, 57% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5690	0.3260
A	0.6430	0.3550
B	0.6700	0.3720
E	0.4120	0.2380
K	0.1560	0.1520

