



Full wwPDB EM Validation Report ⓘ

Mar 27, 2026 – 01:52 AM UTC

PDB ID : 5OAM / pdb_00005oam
EMDB ID : EMD-3778
Title : Molecular basis of human kinesin-8 function and inhibition
Authors : Locke, J.; Joseph, A.P.; Topf, M.; Moores, C.A.
Deposited on : 2017-06-23
Resolution : 5.50 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

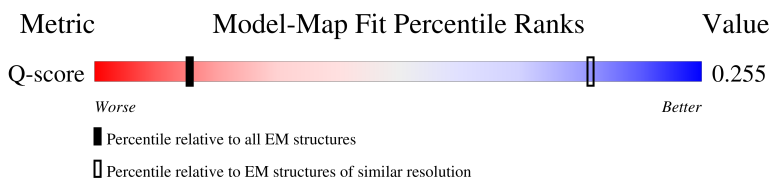
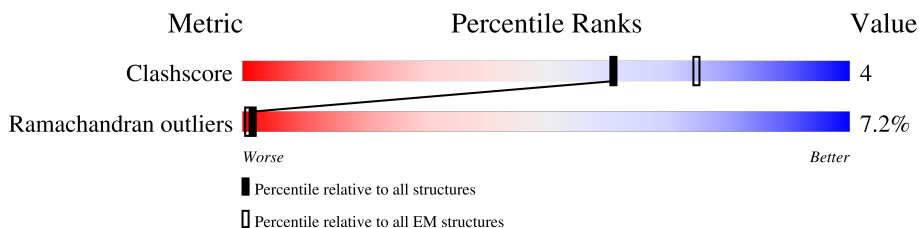
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 5.50 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	520 (5.00 - 6.00)

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	K	377	8% 78% 7% • 13%
2	A	451	78% 12% • 9%
3	B	445	84% 11% • •

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 4788 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 Kinesin-like protein KIF18A.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	K	328	Total	C	N	O	0	0
			1312	656	328	328		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	-2	GLY	-	expression tag	UNP Q8NI77
K	-1	SER	-	expression tag	UNP Q8NI77
K	0	HIS	-	expression tag	UNP Q8NI77

- Molecule 2 is a protein called Tubulin alpha chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	A	412	Total	C	N	O	0	0
			1648	824	412	412		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	136	SER	LEU	conflict	UNP F2Z4C1
A	265	GLY	ILE	conflict	UNP F2Z4C1
A	358	GLU	GLN	conflict	UNP F2Z4C1

- Molecule 3 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	B	426	Total	C	N	O	0	0
			1704	852	426	426		

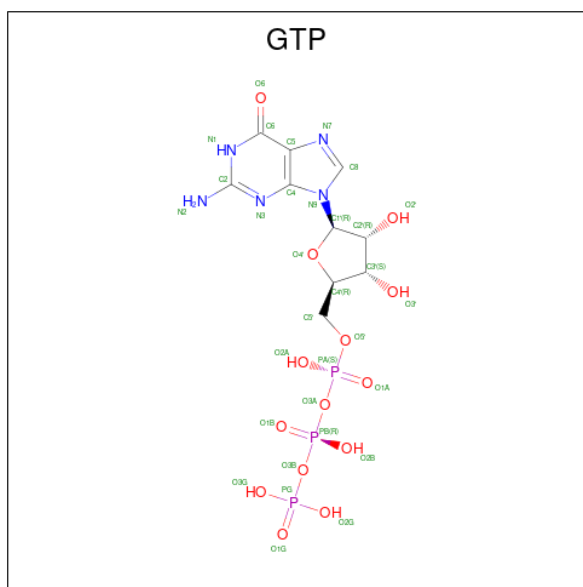
- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	Zn	0
			1	1	

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

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

- Molecule 6 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



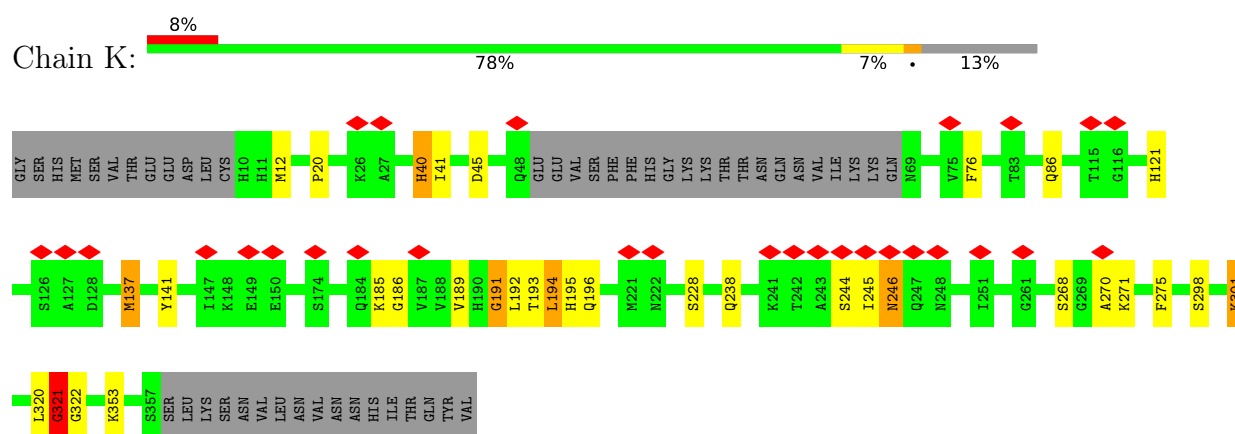
Mol	Chain	Residues	Atoms					AltConf
6	A	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 7 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).

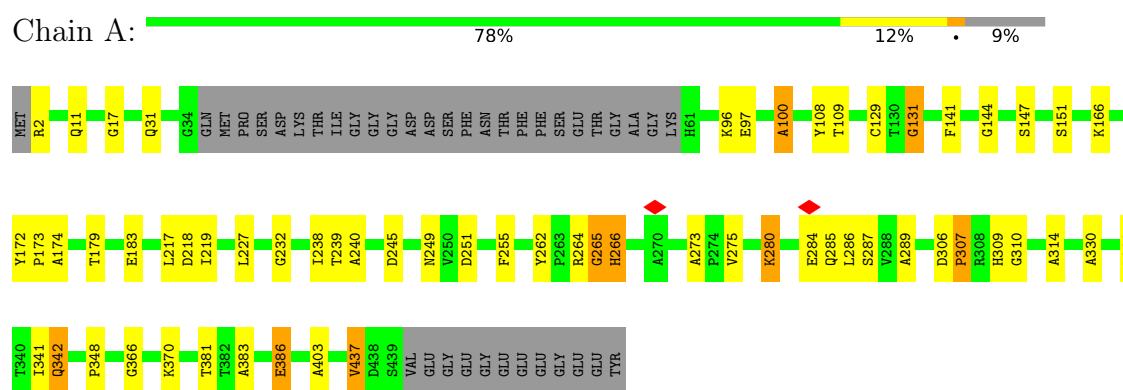
3 Residue-property plots

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

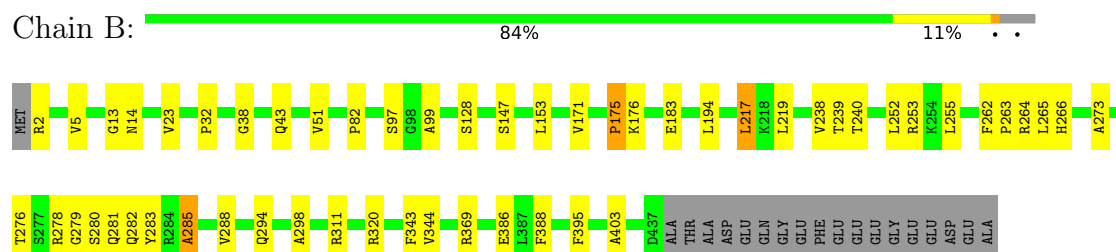
• Molecule 1: Kinesin-like protein KIF18A



• Molecule 2: Tubulin alpha chain



• Molecule 3: Tubulin beta chain



4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=0°, rise=81 Å, axial sym=C1	Depositor
Number of segments used	70395	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	5	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.178	Depositor
Minimum map value	0.000	Depositor
Average map value	0.020	Depositor
Map value standard deviation	0.034	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	107.03, 79.229996, 104.25	wwPDB
Map dimensions	77, 57, 75	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.39, 1.3899999, 1.39	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: ZN, GTP, GDP, MG, TA1

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	K	0.98	2/1310 (0.2%)	1.64	16/1634 (1.0%)
2	A	0.79	0/1646	1.62	12/2054 (0.6%)
3	B	0.83	0/1703	1.63	11/2127 (0.5%)
All	All	0.86	2/4659 (0.0%)	1.63	39/5815 (0.7%)

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	K	0	12
2	A	0	11
3	B	0	10
All	All	0	33

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	41	ILE	CA-C	-8.85	1.41	1.52
1	K	41	ILE	N-CA	-5.14	1.39	1.46

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	41	ILE	N-CA-C	19.42	136.10	107.75
1	K	301	LYS	N-CA-C	15.45	130.46	110.53
1	K	194	LEU	N-CA-C	-7.91	100.47	111.39
2	A	262	TYR	CA-C-N	7.85	128.58	119.47
2	A	262	TYR	C-N-CA	7.85	128.58	119.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	262	PHE	CA-C-N	7.69	129.45	119.84
3	B	262	PHE	C-N-CA	7.69	129.45	119.84
2	A	265	GLY	CA-C-N	7.38	135.64	121.54
2	A	265	GLY	C-N-CA	7.38	135.64	121.54
1	K	228	SER	CA-C-N	7.21	135.48	121.63
1	K	228	SER	C-N-CA	7.21	135.48	121.63
2	A	172	TYR	CA-C-N	7.10	128.72	119.84
2	A	172	TYR	C-N-CA	7.10	128.72	119.84
2	A	174	ALA	CA-C-N	6.97	126.94	119.28
2	A	174	ALA	C-N-CA	6.97	126.94	119.28
1	K	40	HIS	CA-C-N	6.67	131.97	123.10
1	K	40	HIS	C-N-CA	6.67	131.97	123.10
1	K	321	GLY	CA-C-O	-6.53	109.21	120.57
1	K	191	GLY	N-CA-C	-6.41	104.65	115.80
2	A	307	PRO	CA-C-N	6.32	130.70	120.60
2	A	307	PRO	C-N-CA	6.32	130.70	120.60
1	K	196	GLN	CA-C-N	6.22	126.19	120.21
1	K	196	GLN	C-N-CA	6.22	126.19	120.21
1	K	12	MET	N-CA-C	-5.91	100.86	110.20
3	B	217	LEU	N-CA-C	-5.89	98.47	108.26
1	K	353	LYS	CA-C-N	5.78	128.30	120.44
1	K	353	LYS	C-N-CA	5.78	128.30	120.44
3	B	147	SER	CA-C-O	-5.78	114.29	120.42
1	K	137	MET	CA-C-O	-5.75	114.45	120.55
1	K	192	LEU	N-CA-C	-5.72	101.57	110.10
3	B	264	ARG	CA-C-N	5.57	132.17	121.54
3	B	264	ARG	C-N-CA	5.57	132.17	121.54
3	B	14	ASN	N-CA-C	5.46	117.04	111.14
3	B	264	ARG	O-C-N	5.23	129.55	122.59
3	B	194	LEU	CA-C-O	-5.20	115.34	120.70
2	A	306	ASP	CA-C-N	5.05	126.16	119.84
2	A	306	ASP	C-N-CA	5.05	126.16	119.84
3	B	264	ARG	CA-C-O	-5.02	113.33	120.51
3	B	253	ARG	CA-C-O	-5.01	115.74	121.00

There are no chirality outliers.

All (33) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	147	SER	Mainchain
2	A	151	SER	Mainchain
2	A	166	LYS	Mainchain

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Mol	Chain	Res	Type	Group
2	A	17	GLY	Mainchain
2	A	179	THR	Mainchain
2	A	227	LEU	Mainchain
2	A	232	GLY	Mainchain
2	A	280	LYS	Mainchain
2	A	286	LEU	Mainchain
2	A	386	GLU	Mainchain
2	A	437	VAL	Mainchain
3	B	13	GLY	Mainchain
3	B	153	LEU	Mainchain
3	B	171	VAL	Mainchain
3	B	175	PRO	Mainchain
3	B	2	ARG	Mainchain
3	B	255	LEU	Mainchain
3	B	285	ALA	Mainchain
3	B	320	ARG	Mainchain
3	B	388	PHE	Mainchain
3	B	5	VAL	Mainchain
1	K	121	HIS	Mainchain
1	K	137	MET	Mainchain
1	K	141	TYR	Mainchain
1	K	185	LYS	Mainchain
1	K	186	GLY	Mainchain
1	K	238	GLN	Mainchain
1	K	244	SER	Peptide
1	K	246	ASN	Mainchain
1	K	320	LEU	Peptide
1	K	321	GLY	Peptide,Mainchain
1	K	86	GLN	Mainchain

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	K	1312	0	353	12	0
2	A	1648	0	451	10	0
3	B	1704	0	471	3	0
4	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	1	0	0	0	0
6	A	32	0	12	3	0
7	B	28	0	12	0	0
8	B	62	0	51	3	0
All	All	4788	0	1350	27	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 4.

All (27) 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:K:298:SER:C	1:K:301:LYS:H	1.83	0.87
1:K:298:SER:CA	1:K:301:LYS:CA	2.74	0.66
8:B:601:TA1:H261	8:B:601:TA1:H463	1.80	0.62
1:K:40:HIS:O	1:K:76:PHE:N	2.33	0.62
1:K:298:SER:CA	1:K:301:LYS:N	2.64	0.61
1:K:298:SER:CA	1:K:301:LYS:H	2.13	0.61
1:K:298:SER:O	1:K:301:LYS:N	2.35	0.58
2:A:264:ARG:C	2:A:266:HIS:H	2.20	0.49
1:K:193:THR:O	1:K:194:LEU:C	2.52	0.48
2:A:144:GLY:H	6:A:503:GTP:PG	2.37	0.48
2:A:310:GLY:HA3	2:A:383:ALA:N	2.29	0.48
2:A:144:GLY:N	6:A:503:GTP:O3G	2.44	0.47
2:A:11:GLN:N	6:A:503:GTP:O2B	2.49	0.46
3:B:217:LEU:C	3:B:219:LEU:H	2.25	0.45
1:K:268:SER:C	1:K:270:ALA:H	2.25	0.44
2:A:100:ALA:O	2:A:144:GLY:HA3	2.17	0.43
8:B:601:TA1:H463	8:B:601:TA1:C26	2.46	0.43
1:K:321:GLY:O	1:K:322:GLY:C	2.62	0.43
3:B:281:GLN:O	3:B:283:TYR:N	2.52	0.42
2:A:381:THR:C	2:A:383:ALA:H	2.28	0.42
3:B:276:THR:O	8:B:601:TA1:H192	2.19	0.42
1:K:271:LYS:C	1:K:275:PHE:H	2.29	0.41
2:A:310:GLY:HA3	2:A:383:ALA:CA	2.51	0.41
1:K:40:HIS:O	1:K:76:PHE:CA	2.69	0.41
1:K:189:VAL:C	1:K:191:GLY:H	2.28	0.41
2:A:341:ILE:O	2:A:342:GLN:C	2.63	0.40
2:A:2:ARG:N	2:A:131:GLY:O	2.54	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	K	324/377 (86%)	297 (92%)	21 (6%)	6 (2%)	6	31
2	A	408/451 (90%)	297 (73%)	69 (17%)	42 (10%)	0	6
3	B	424/445 (95%)	312 (74%)	77 (18%)	35 (8%)	0	9
All	All	1156/1273 (91%)	906 (78%)	167 (14%)	83 (7%)	2	10

All (83) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	97	GLU
2	A	108	TYR
2	A	109	THR
2	A	141	PHE
2	A	183	GLU
2	A	245	ASP
2	A	266	HIS
2	A	280	LYS
2	A	284	GLU
2	A	285	GLN
2	A	287	SER
2	A	437	VAL
3	B	82	PRO
3	B	97	SER
3	B	175	PRO
3	B	176	LYS
3	B	183	GLU
3	B	239	THR
3	B	252	LEU
3	B	278	ARG
3	B	282	GLN
3	B	288	VAL
3	B	344	VAL
3	B	369	ARG

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Mol	Chain	Res	Type
3	B	403	ALA
1	K	195	HIS
1	K	246	ASN
2	A	96	LYS
2	A	217	LEU
2	A	240	ALA
2	A	251	ASP
2	A	255	PHE
2	A	309	HIS
2	A	342	GLN
2	A	370	LYS
2	A	403	ALA
3	B	32	PRO
3	B	38	GLY
3	B	128	SER
3	B	238	VAL
3	B	265	LEU
3	B	266	HIS
3	B	273	ALA
3	B	279	GLY
3	B	294	GLN
3	B	298	ALA
3	B	311	ARG
3	B	343	PHE
2	A	100	ALA
2	A	173	PRO
2	A	218	ASP
2	A	238	ILE
2	A	249	ASN
2	A	314	ALA
2	A	330	ALA
2	A	339	ARG
2	A	386	GLU
3	B	386	GLU
1	K	20	PRO
1	K	321	GLY
2	A	129	CYS
3	B	240	THR
3	B	280	SER
1	K	245	ILE
2	A	219	ILE
2	A	239	THR

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Mol	Chain	Res	Type
2	A	289	ALA
2	A	366	GLY
3	B	43	GLN
3	B	99	ALA
3	B	263	PRO
3	B	285	ALA
3	B	395	PHE
1	K	45	ASP
2	A	265	GLY
3	B	23	VAL
2	A	273	ALA
2	A	307	PRO
2	A	348	PRO
3	B	51	VAL
2	A	275	VAL
2	A	131	GLY
2	A	31	GLN

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 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 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	$\# Z > 2$
7	GDP	B	600	-	29,30,30	2.85	12 (41%)	45,47,47	3.47	16 (35%)
6	GTP	A	503	5	33,34,34	1.92	3 (9%)	50,54,54	0.94	4 (8%)
8	TA1	B	601	-	68,68,68	2.20	26 (38%)	105,105,105	1.50	13 (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
7	GDP	B	600	-	-	4/16/32/32	0/3/3/3
6	GTP	A	503	5	-	3/22/38/38	0/3/3/3
8	TA1	B	601	-	-	9/41/127/127	0/7/7/7

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	600	GDP	PA-O3A	7.52	1.67	1.59
8	B	601	TA1	C06-C05	6.51	1.50	1.38
6	A	503	GTP	PA-O3A	-5.98	1.53	1.59
7	B	600	GDP	O6-C6	5.95	1.34	1.23
7	B	600	GDP	C8-N9	5.85	1.50	1.37
6	A	503	GTP	PB-O3A	-5.76	1.53	1.59
8	B	601	TA1	C08-C07	-5.68	1.25	1.38
6	A	503	GTP	PB-O3B	5.45	1.65	1.59
8	B	601	TA1	C18-C10	5.35	1.69	1.57
8	B	601	TA1	C05-C04	4.81	1.46	1.39
7	B	600	GDP	C2-N1	4.77	1.49	1.37
8	B	601	TA1	C45-C24	4.23	1.61	1.54
7	B	600	GDP	PB-O2B	-3.91	1.40	1.54
8	B	601	TA1	C36-C31	3.76	1.45	1.39
8	B	601	TA1	O02-C03	3.51	1.41	1.34
7	B	600	GDP	O4'-C1'	3.39	1.49	1.42
8	B	601	TA1	C25-C24	3.37	1.39	1.34
8	B	601	TA1	C46-C45	3.25	1.60	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	601	TA1	C43-C01	3.21	1.60	1.54
8	B	601	TA1	C11-C10	3.08	1.61	1.54
7	B	600	GDP	C8-N7	3.03	1.41	1.32
7	B	600	GDP	C5-N7	-2.87	1.33	1.39
8	B	601	TA1	C43-C26	2.83	1.58	1.52
7	B	600	GDP	C5-C4	2.63	1.45	1.38
8	B	601	TA1	C26-C25	2.62	1.56	1.51
8	B	601	TA1	C01-C45	2.52	1.66	1.56
8	B	601	TA1	C18-C20	2.52	1.62	1.55
7	B	600	GDP	C2-N3	-2.46	1.27	1.33
7	B	600	GDP	PB-O3B	2.44	1.63	1.54
8	B	601	TA1	C04-C03	-2.42	1.44	1.50
8	B	601	TA1	C16-C15	2.35	1.57	1.52
8	B	601	TA1	C41-C42	2.29	1.42	1.38
8	B	601	TA1	C37-C29	2.22	1.54	1.52
8	B	601	TA1	O09-C21	2.18	1.49	1.44
8	B	601	TA1	C33-C32	2.17	1.42	1.38
8	B	601	TA1	C10-C02	2.11	1.62	1.57
8	B	601	TA1	C08-C09	2.10	1.42	1.38
8	B	601	TA1	C39-C38	2.09	1.42	1.38
8	B	601	TA1	C07-C06	2.08	1.42	1.38
8	B	601	TA1	C34-C33	2.02	1.42	1.38
7	B	600	GDP	O3'-C3'	2.00	1.47	1.43

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	600	GDP	N9-C8-N7	-10.74	93.49	113.40
7	B	600	GDP	C8-N7-C5	9.21	120.67	104.26
7	B	600	GDP	C6-C5-N7	8.57	145.88	130.29
7	B	600	GDP	N2-C2-N3	6.30	131.97	119.67
7	B	600	GDP	C6-C5-C4	-6.18	109.53	118.83
7	B	600	GDP	C8-N9-C4	5.84	116.97	106.03
8	B	601	TA1	C06-C05-C04	-5.83	114.63	120.36
8	B	601	TA1	C07-C08-C09	5.79	127.39	120.24
7	B	600	GDP	C5-C6-N1	4.50	124.71	113.25
7	B	600	GDP	N2-C2-N1	-4.26	107.77	116.76
7	B	600	GDP	C2-N3-C4	4.11	119.38	112.30
8	B	601	TA1	C05-C04-C03	-4.05	111.46	120.40
7	B	600	GDP	O6-C6-C5	-3.94	116.12	126.53
7	B	600	GDP	C4-C5-N7	-3.84	104.59	110.67
7	B	600	GDP	C2-N1-C6	-3.82	118.19	125.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	601	TA1	C09-C04-C03	3.62	128.38	120.40
7	B	600	GDP	C2'-C3'-C4'	3.43	109.24	102.61
8	B	601	TA1	C17-C18-C20	3.21	109.79	102.58
8	B	601	TA1	O04-C11-C14	-3.01	101.75	108.13
8	B	601	TA1	C45-C01-C02	2.99	115.22	111.93
7	B	600	GDP	C1'-N9-C8	-2.65	119.20	126.73
8	B	601	TA1	O01-C01-C43	2.48	113.37	107.04
6	A	503	GTP	O3A-PB-O1B	-2.44	103.36	110.70
8	B	601	TA1	C08-C09-C04	-2.35	118.06	120.36
7	B	600	GDP	O2'-C2'-C3'	2.29	119.15	111.82
8	B	601	TA1	C14-C11-C15	-2.27	83.03	85.38
8	B	601	TA1	O06-C15-C11	2.22	93.01	90.58
8	B	601	TA1	C10-C18-C17	-2.21	102.35	106.55
6	A	503	GTP	O2B-PB-O3A	2.19	113.20	107.27
6	A	503	GTP	O5'-C5'-C4'	2.10	116.13	108.99
7	B	600	GDP	C4'-O4'-C1'	2.06	114.01	109.47
6	A	503	GTP	O3G-PG-O3B	2.02	111.39	104.64
8	B	601	TA1	C21-O09-C22	2.01	120.11	115.95

There are no chirality outliers.

All (16) torsion outliers are listed below:

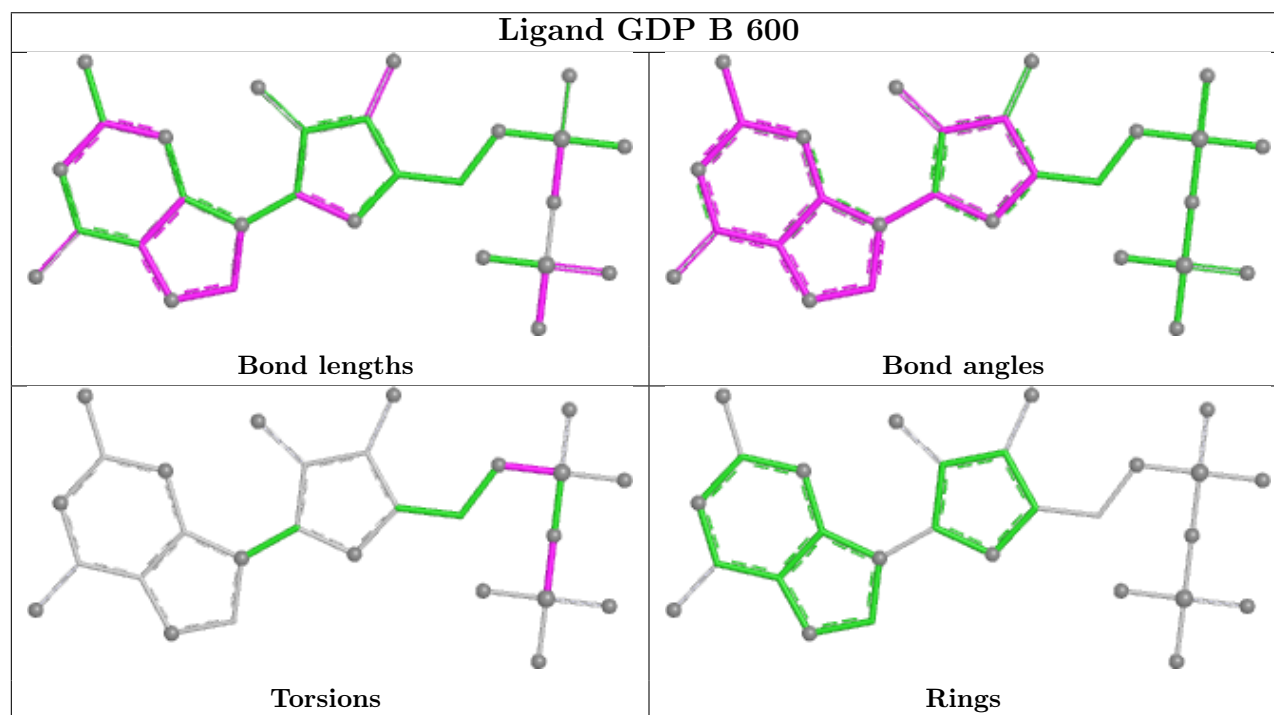
Mol	Chain	Res	Type	Atoms
7	B	600	GDP	PA-O3A-PB-O2B
7	B	600	GDP	C5'-O5'-PA-O3A
7	B	600	GDP	C5'-O5'-PA-O1A
8	B	601	TA1	O02-C03-C04-C05
8	B	601	TA1	O02-C03-C04-C09
8	B	601	TA1	O03-C03-C04-C09
8	B	601	TA1	O03-C03-C04-C05
8	B	601	TA1	N01-C30-C31-C36
8	B	601	TA1	O14-C30-C31-C36
8	B	601	TA1	N01-C30-C31-C32
8	B	601	TA1	O14-C30-C31-C32
6	A	503	GTP	C3'-C4'-C5'-O5'
6	A	503	GTP	O4'-C4'-C5'-O5'
7	B	600	GDP	PA-O3A-PB-O3B
6	A	503	GTP	PG-O3B-PB-O1B
8	B	601	TA1	C15-C11-O04-C12

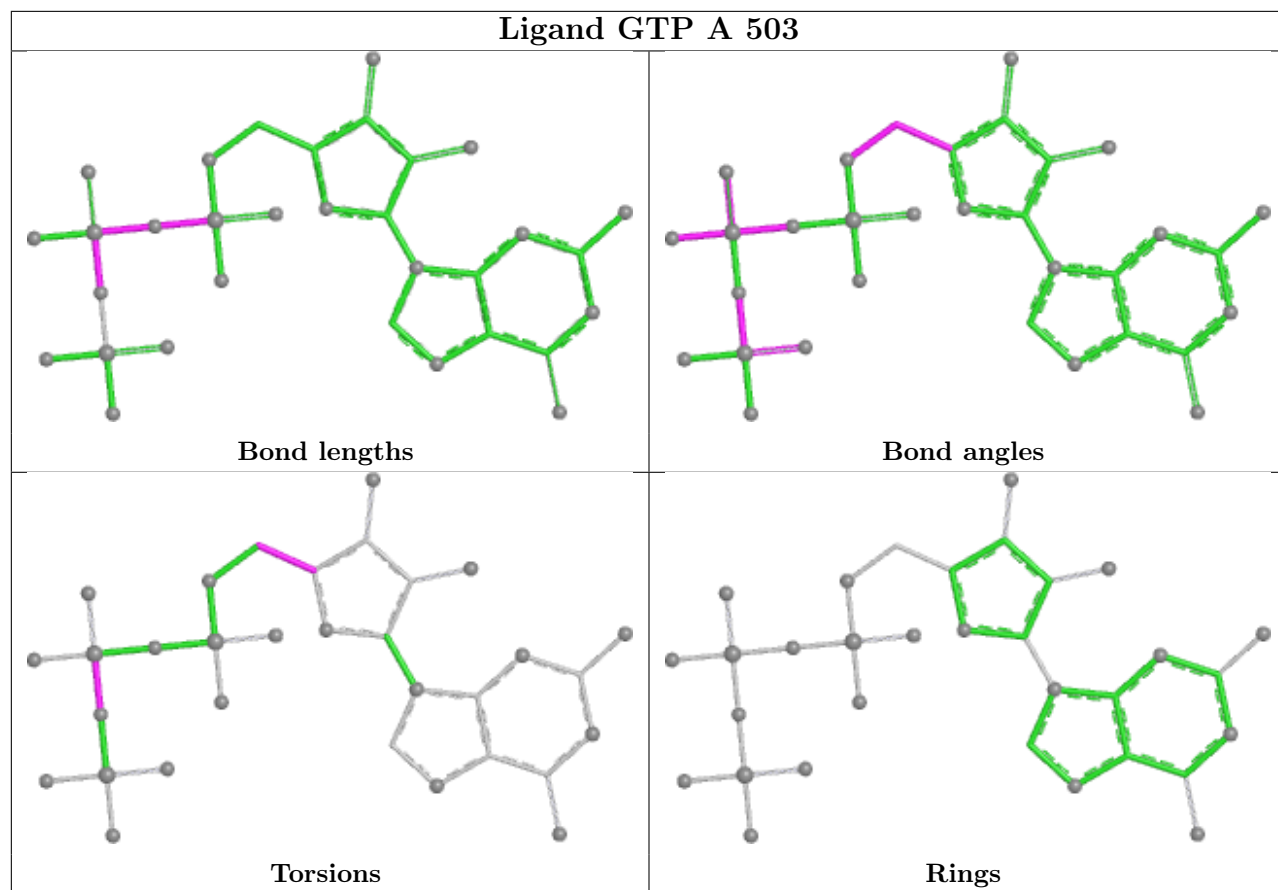
There are no ring outliers.

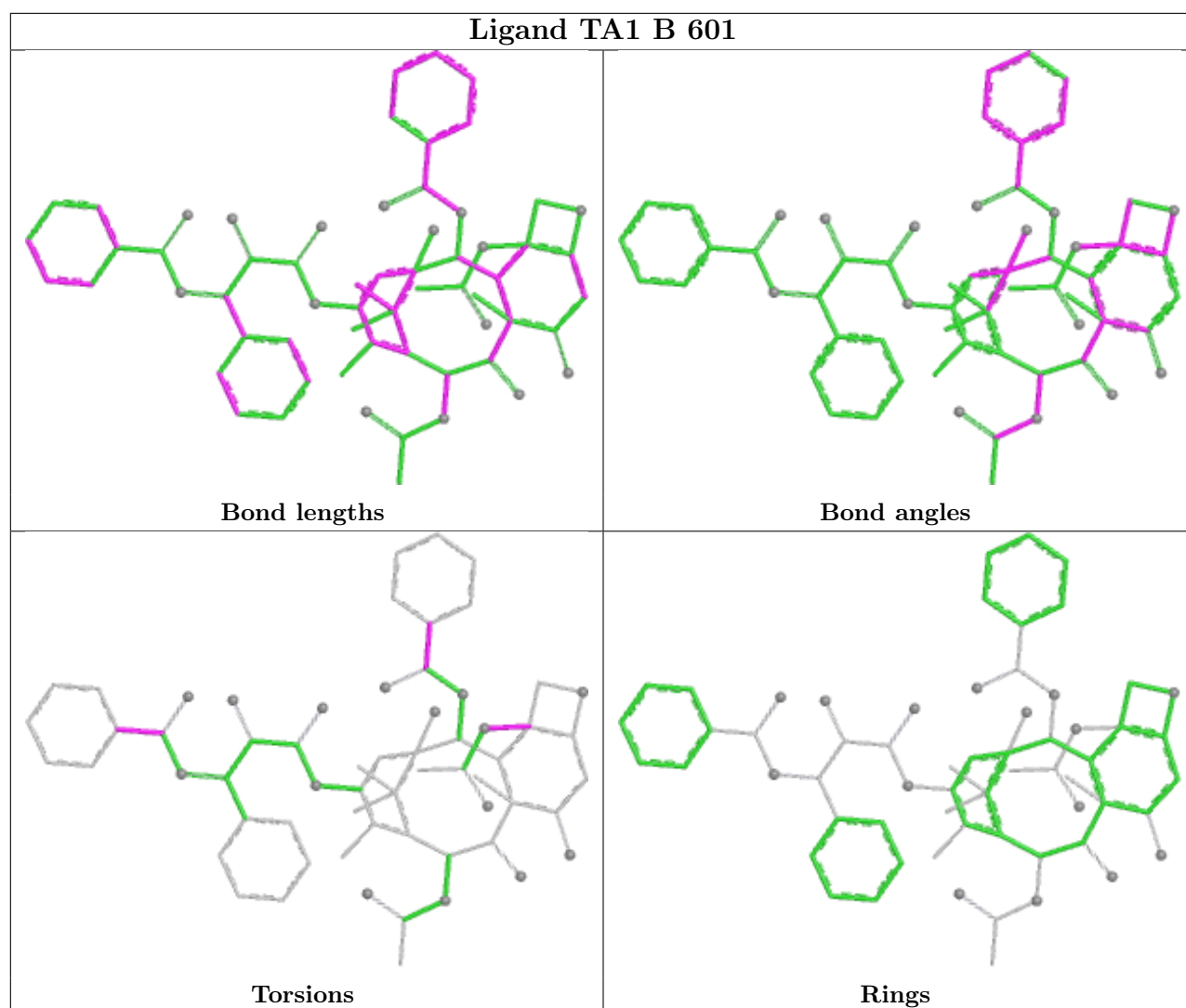
2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	503	GTP	3	0
8	B	601	TA1	3	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-3778. These allow visual inspection of the internal detail of the map and identification of artifacts.

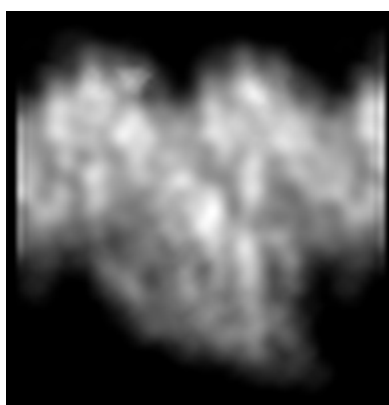
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

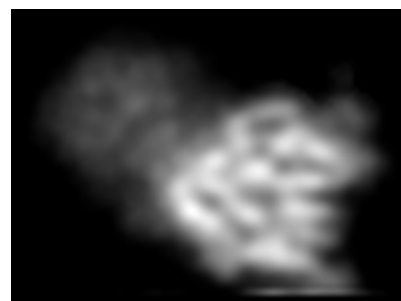
6.1.1 Primary map



X



Y



Z

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

6.2 Central slices [i](#)

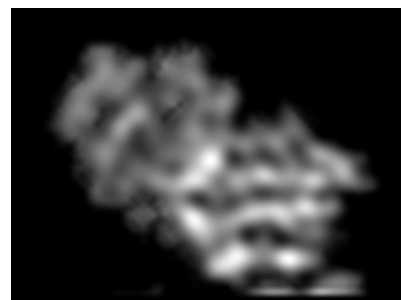
6.2.1 Primary map



X Index: 38



Y Index: 28



Z Index: 37

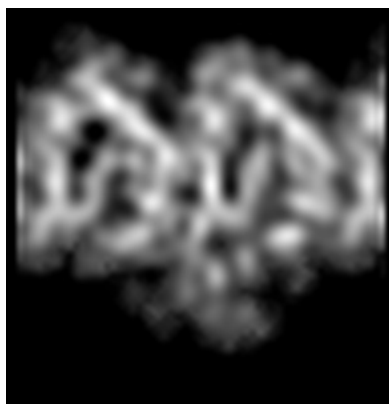
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 53



Y Index: 24



Z Index: 47

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

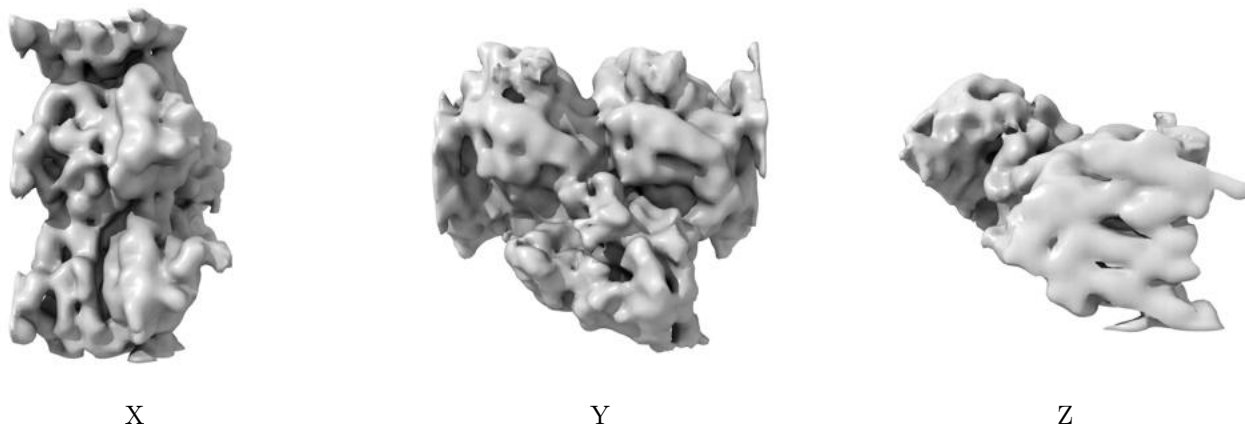


Z

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

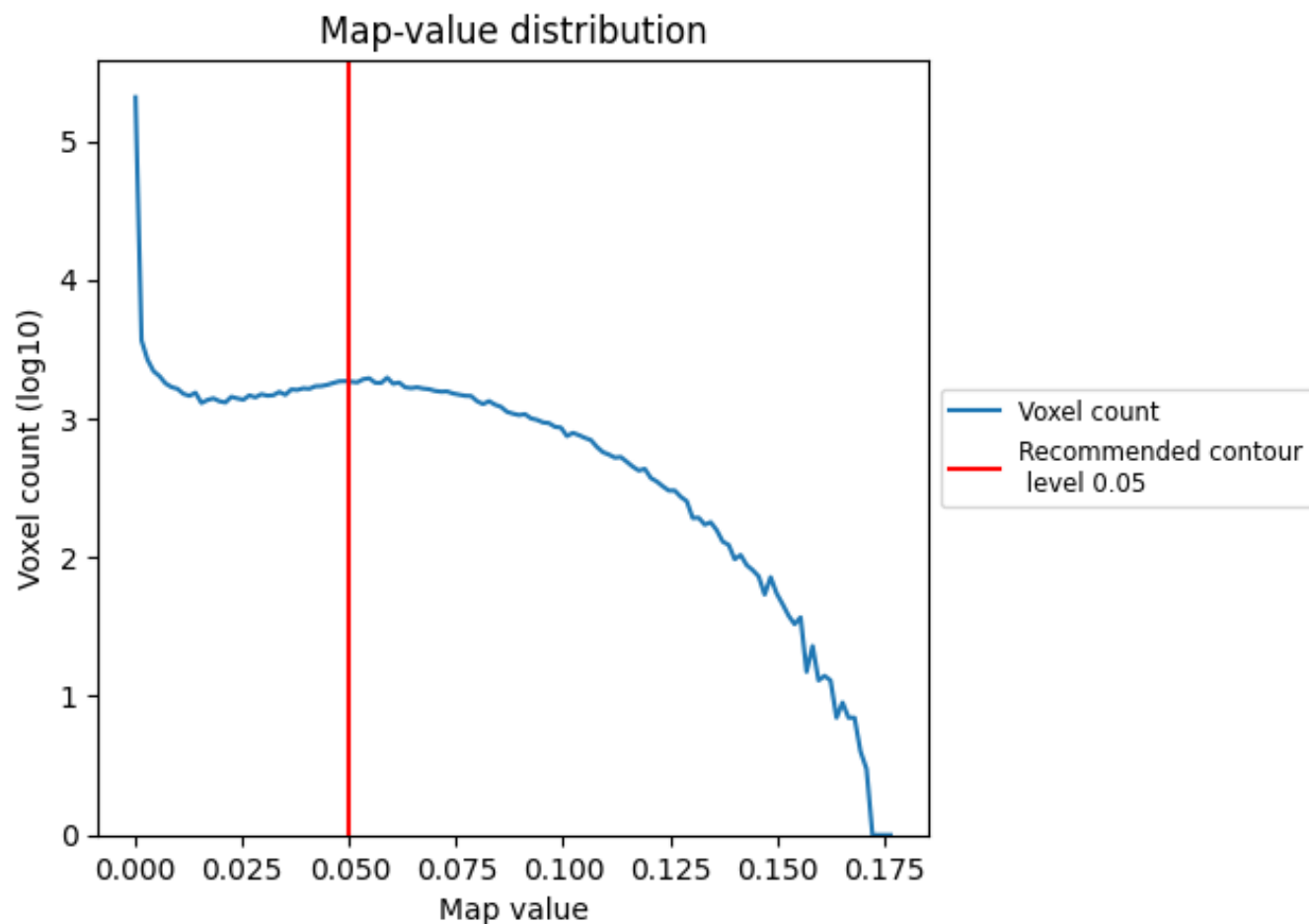
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

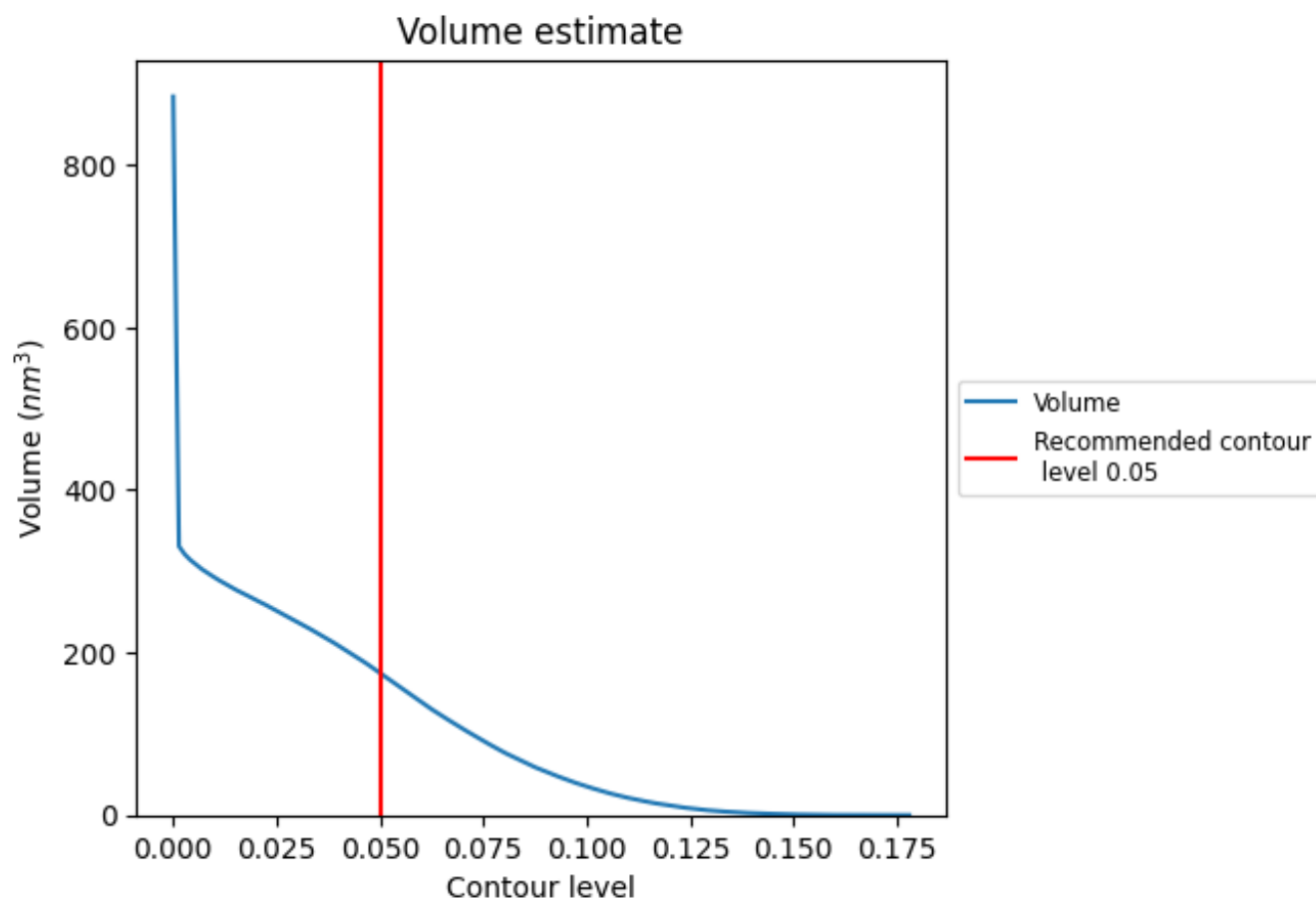
This section contains the results of statistical analysis of the map.

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 175 nm^3 ; this corresponds to an approximate mass of 158 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.

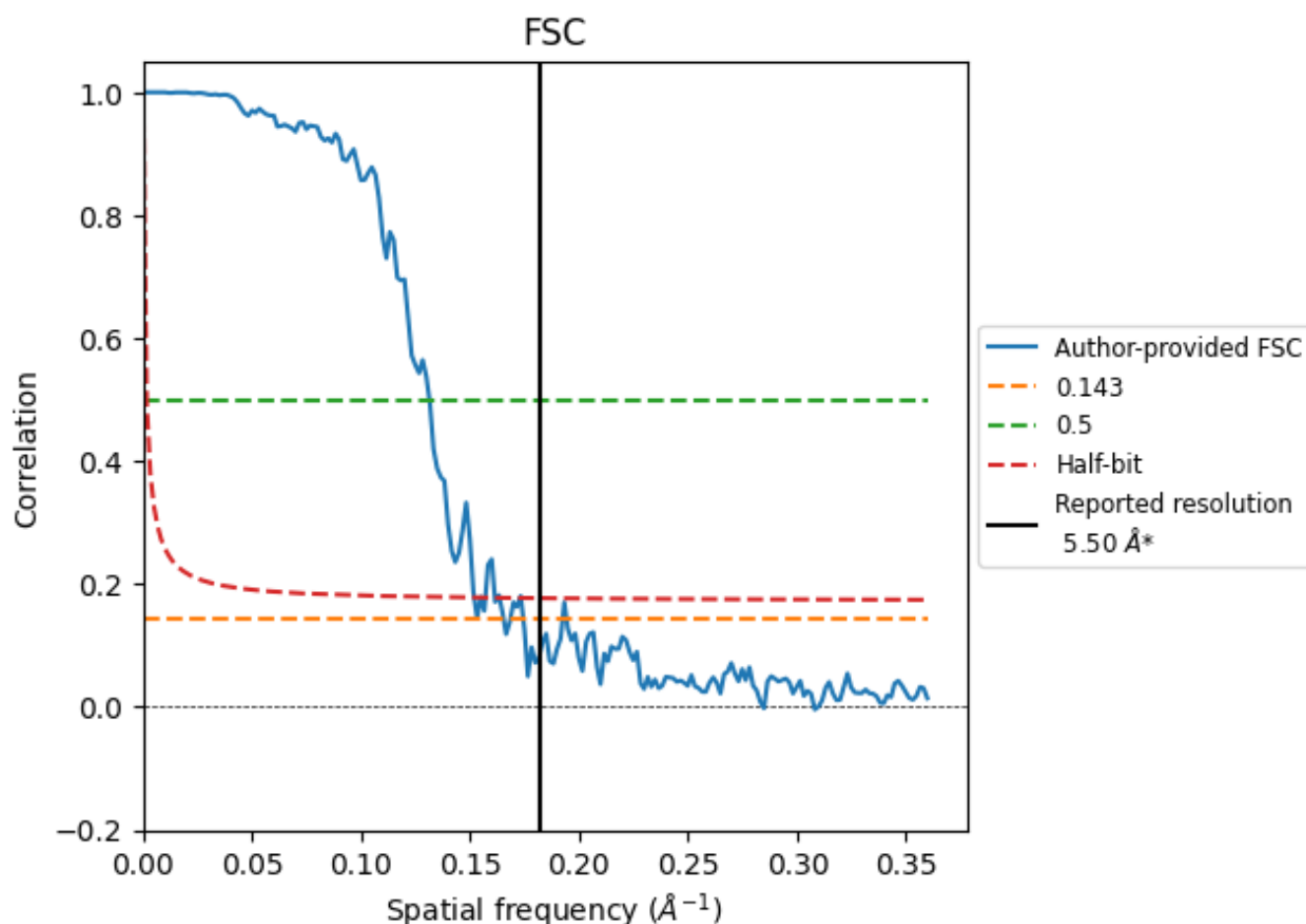
7.3 Rotationally averaged power spectrum [i](#)

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 0.182 Å⁻¹

8.2 Resolution estimates [i](#)

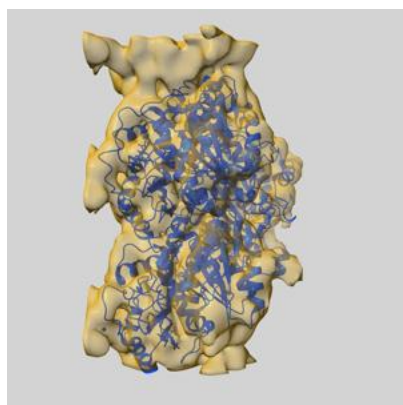
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.50	-	-
Author-provided FSC curve	6.05	7.62	6.58
Unmasked-calculated*	-	-	-

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

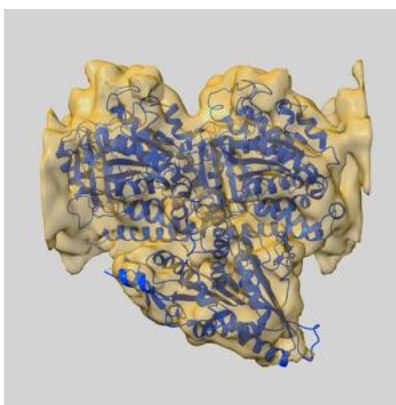
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-3778 and PDB model 5OAM. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

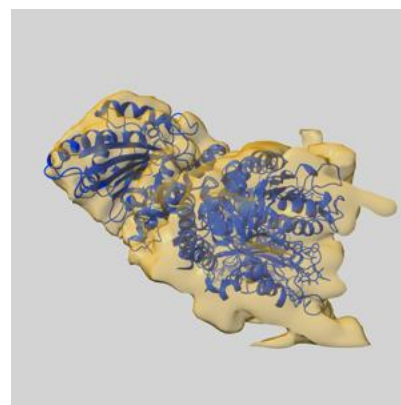
9.1 Map-model overlay [i](#)



X



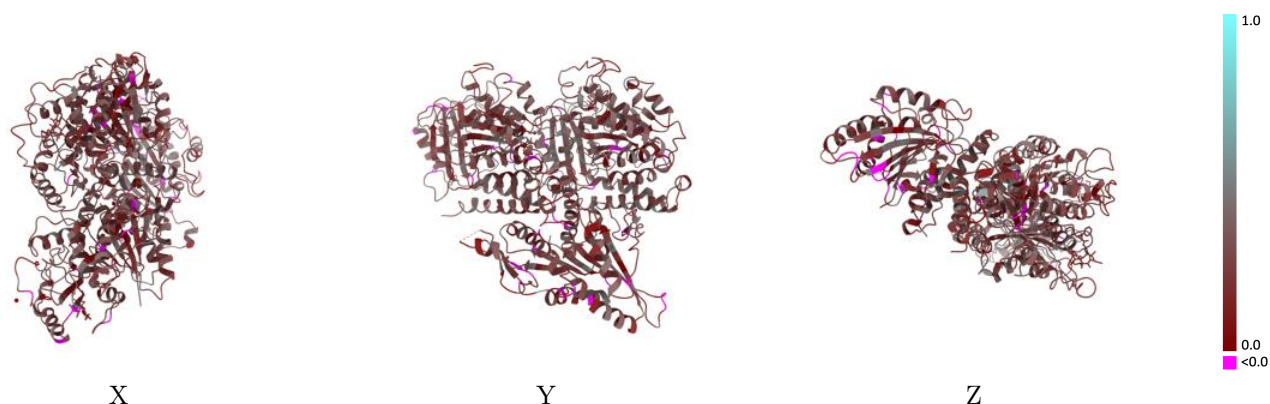
Y



Z

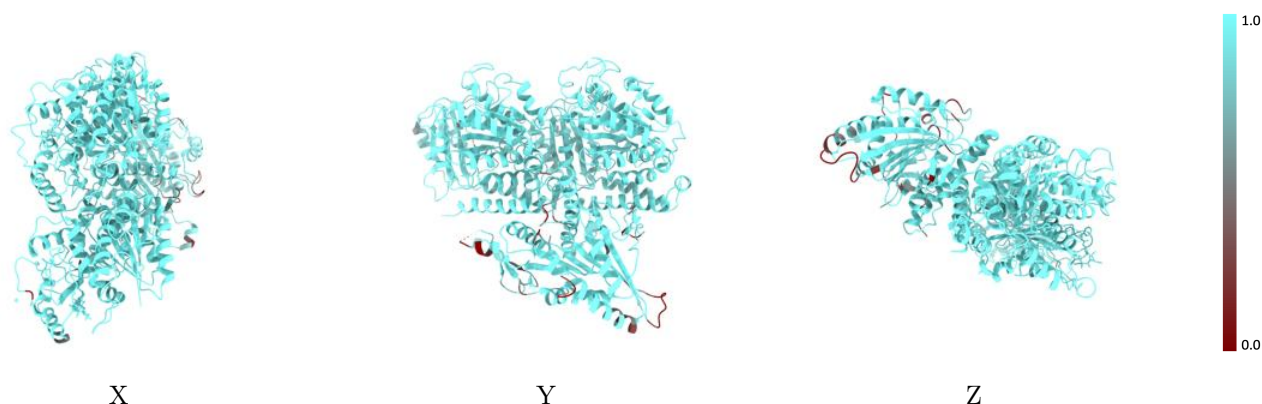
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



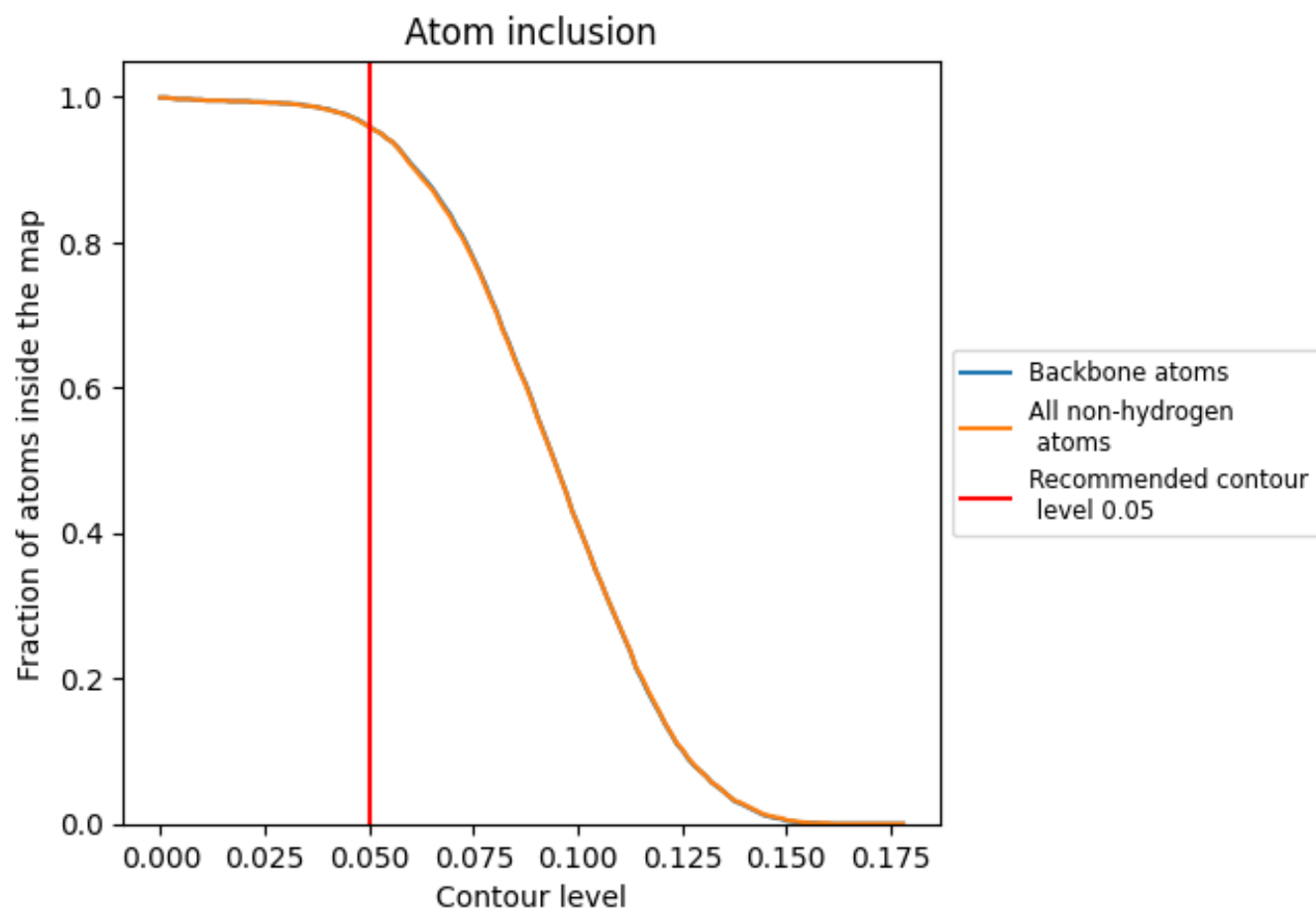
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.05).

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 96% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9590	0.2550
A	0.9880	0.2610
B	0.9960	0.2730
K	0.8720	0.2250

