



Full wwPDB EM Validation Report ⓘ

Jul 9, 2026 – 04:15 pm BST

PDB ID : 9SV3 / pdb_00009sv3
EMDB ID : EMD-55233
Title : Local refinement of EloB/EloC/VHL/CV2a/14-3-3zeta/ERa from pose 1
Authors : Crowe, C.; Nakasone, M.A.; Harzing, T.; Verhoef, C.J.A.; Cossar, P.J.; Ciulli, A.
Deposited on : 2025-09-30
Resolution : 4.30 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

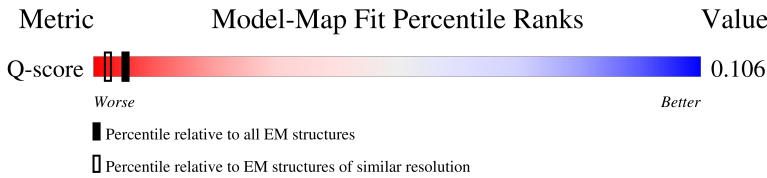
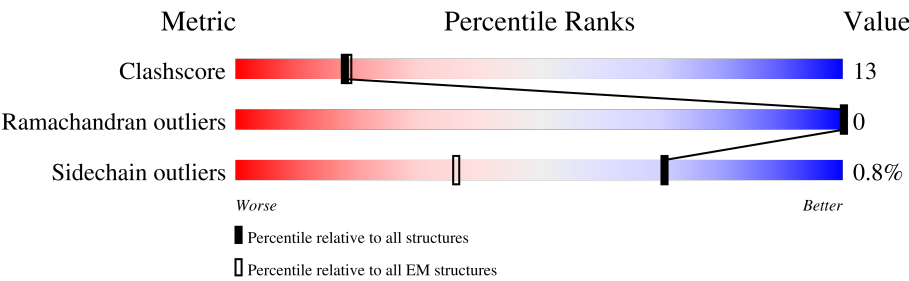
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

1 Overall quality at a glance i

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

The reported resolution of this entry is 4.30 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	4585 (3.80 - 4.80)

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

Mol	Chain	Length	Quality of chain
1	B	97	82% 80% 16% ..
2	C	104	88% 88% 10% ..
3	G	401	99% 99%
3	H	401	99% 99%

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Mol	Chain	Length	Quality of chain
4	D	253	
4	I	253	
5	E	162	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9884 atoms, of which 3182 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 Elongin-C.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	95	Total	C	N	O	S	0	0
			752	482	121	144	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	16	MET	-	initiating methionine	UNP Q15369

- Molecule 2 is a protein called Elongin-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	103	Total	C	N	O	S	0	0
			813	514	136	158	5		

- Molecule 3 is a protein called Estrogen receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	5	Total	C	N	O	P	1	0
			52	29	12	10	1		
3	H	5	Total	C	N	O	P	1	0
			52	29	12	10	1		

There are 220 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	195	MET	-	initiating methionine	UNP P03372
G	196	GLY	-	expression tag	UNP P03372
G	197	HIS	-	expression tag	UNP P03372
G	198	HIS	-	expression tag	UNP P03372
G	199	HIS	-	expression tag	UNP P03372
G	200	HIS	-	expression tag	UNP P03372
G	201	HIS	-	expression tag	UNP P03372
G	202	HIS	-	expression tag	UNP P03372

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Chain	Residue	Modelled	Actual	Comment	Reference
G	203	GLY	-	expression tag	UNP P03372
G	204	GLY	-	expression tag	UNP P03372
G	205	SER	-	expression tag	UNP P03372
G	206	ASP	-	expression tag	UNP P03372
G	207	SER	-	expression tag	UNP P03372
G	208	GLU	-	expression tag	UNP P03372
G	209	VAL	-	expression tag	UNP P03372
G	210	ASN	-	expression tag	UNP P03372
G	211	GLN	-	expression tag	UNP P03372
G	212	GLU	-	expression tag	UNP P03372
G	213	ALA	-	expression tag	UNP P03372
G	214	LYS	-	expression tag	UNP P03372
G	215	PRO	-	expression tag	UNP P03372
G	216	GLU	-	expression tag	UNP P03372
G	217	VAL	-	expression tag	UNP P03372
G	218	LYS	-	expression tag	UNP P03372
G	219	PRO	-	expression tag	UNP P03372
G	220	GLU	-	expression tag	UNP P03372
G	221	VAL	-	expression tag	UNP P03372
G	222	LYS	-	expression tag	UNP P03372
G	223	PRO	-	expression tag	UNP P03372
G	224	GLU	-	expression tag	UNP P03372
G	225	THR	-	expression tag	UNP P03372
G	226	HIS	-	expression tag	UNP P03372
G	227	ILE	-	expression tag	UNP P03372
G	228	ASN	-	expression tag	UNP P03372
G	229	LEU	-	expression tag	UNP P03372
G	230	LYS	-	expression tag	UNP P03372
G	231	VAL	-	expression tag	UNP P03372
G	232	SER	-	expression tag	UNP P03372
G	233	ASP	-	expression tag	UNP P03372
G	234	GLY	-	expression tag	UNP P03372
G	235	SER	-	expression tag	UNP P03372
G	236	SER	-	expression tag	UNP P03372
G	237	GLU	-	expression tag	UNP P03372
G	238	ILE	-	expression tag	UNP P03372
G	239	PHE	-	expression tag	UNP P03372
G	240	PHE	-	expression tag	UNP P03372
G	241	LYS	-	expression tag	UNP P03372
G	242	ILE	-	expression tag	UNP P03372
G	243	LYS	-	expression tag	UNP P03372
G	244	LYS	-	expression tag	UNP P03372

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Chain	Residue	Modelled	Actual	Comment	Reference
G	245	THR	-	expression tag	UNP P03372
G	246	THR	-	expression tag	UNP P03372
G	247	PRO	-	expression tag	UNP P03372
G	248	LEU	-	expression tag	UNP P03372
G	249	ARG	-	expression tag	UNP P03372
G	250	ARG	-	expression tag	UNP P03372
G	251	LEU	-	expression tag	UNP P03372
G	252	MET	-	expression tag	UNP P03372
G	253	GLU	-	expression tag	UNP P03372
G	254	ALA	-	expression tag	UNP P03372
G	255	PHE	-	expression tag	UNP P03372
G	256	ALA	-	expression tag	UNP P03372
G	257	LYS	-	expression tag	UNP P03372
G	258	ARG	-	expression tag	UNP P03372
G	259	GLN	-	expression tag	UNP P03372
G	260	GLY	-	expression tag	UNP P03372
G	261	LYS	-	expression tag	UNP P03372
G	262	GLU	-	expression tag	UNP P03372
G	263	MET	-	expression tag	UNP P03372
G	264	ASP	-	expression tag	UNP P03372
G	265	SER	-	expression tag	UNP P03372
G	266	LEU	-	expression tag	UNP P03372
G	267	ARG	-	expression tag	UNP P03372
G	268	PHE	-	expression tag	UNP P03372
G	269	LEU	-	expression tag	UNP P03372
G	270	TYR	-	expression tag	UNP P03372
G	271	ASP	-	expression tag	UNP P03372
G	272	GLY	-	expression tag	UNP P03372
G	273	ILE	-	expression tag	UNP P03372
G	274	ARG	-	expression tag	UNP P03372
G	275	ILE	-	expression tag	UNP P03372
G	276	GLN	-	expression tag	UNP P03372
G	277	ALA	-	expression tag	UNP P03372
G	278	ASP	-	expression tag	UNP P03372
G	279	GLN	-	expression tag	UNP P03372
G	280	THR	-	expression tag	UNP P03372
G	281	PRO	-	expression tag	UNP P03372
G	282	GLU	-	expression tag	UNP P03372
G	283	ASP	-	expression tag	UNP P03372
G	284	LEU	-	expression tag	UNP P03372
G	285	ASP	-	expression tag	UNP P03372
G	286	MET	-	expression tag	UNP P03372

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Chain	Residue	Modelled	Actual	Comment	Reference
G	287	GLU	-	expression tag	UNP P03372
G	288	ASP	-	expression tag	UNP P03372
G	289	ASN	-	expression tag	UNP P03372
G	290	ASP	-	expression tag	UNP P03372
G	291	ILE	-	expression tag	UNP P03372
G	292	ILE	-	expression tag	UNP P03372
G	293	GLU	-	expression tag	UNP P03372
G	294	ALA	-	expression tag	UNP P03372
G	295	HIS	-	expression tag	UNP P03372
G	296	ARG	-	expression tag	UNP P03372
G	297	GLU	-	expression tag	UNP P03372
G	298	GLN	-	expression tag	UNP P03372
G	299	ILE	-	expression tag	UNP P03372
G	300	GLY	-	expression tag	UNP P03372
G	301	GLY	-	expression tag	UNP P03372
G	305	ALA	SER	engineered mutation	UNP P03372
G	591	ARG	PHE	engineered mutation	UNP P03372
G	592	ARG	PRO	engineered mutation	UNP P03372
H	195	MET	-	initiating methionine	UNP P03372
H	196	GLY	-	expression tag	UNP P03372
H	197	HIS	-	expression tag	UNP P03372
H	198	HIS	-	expression tag	UNP P03372
H	199	HIS	-	expression tag	UNP P03372
H	200	HIS	-	expression tag	UNP P03372
H	201	HIS	-	expression tag	UNP P03372
H	202	HIS	-	expression tag	UNP P03372
H	203	GLY	-	expression tag	UNP P03372
H	204	GLY	-	expression tag	UNP P03372
H	205	SER	-	expression tag	UNP P03372
H	206	ASP	-	expression tag	UNP P03372
H	207	SER	-	expression tag	UNP P03372
H	208	GLU	-	expression tag	UNP P03372
H	209	VAL	-	expression tag	UNP P03372
H	210	ASN	-	expression tag	UNP P03372
H	211	GLN	-	expression tag	UNP P03372
H	212	GLU	-	expression tag	UNP P03372
H	213	ALA	-	expression tag	UNP P03372
H	214	LYS	-	expression tag	UNP P03372
H	215	PRO	-	expression tag	UNP P03372
H	216	GLU	-	expression tag	UNP P03372
H	217	VAL	-	expression tag	UNP P03372
H	218	LYS	-	expression tag	UNP P03372

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Chain	Residue	Modelled	Actual	Comment	Reference
H	219	PRO	-	expression tag	UNP P03372
H	220	GLU	-	expression tag	UNP P03372
H	221	VAL	-	expression tag	UNP P03372
H	222	LYS	-	expression tag	UNP P03372
H	223	PRO	-	expression tag	UNP P03372
H	224	GLU	-	expression tag	UNP P03372
H	225	THR	-	expression tag	UNP P03372
H	226	HIS	-	expression tag	UNP P03372
H	227	ILE	-	expression tag	UNP P03372
H	228	ASN	-	expression tag	UNP P03372
H	229	LEU	-	expression tag	UNP P03372
H	230	LYS	-	expression tag	UNP P03372
H	231	VAL	-	expression tag	UNP P03372
H	232	SER	-	expression tag	UNP P03372
H	233	ASP	-	expression tag	UNP P03372
H	234	GLY	-	expression tag	UNP P03372
H	235	SER	-	expression tag	UNP P03372
H	236	SER	-	expression tag	UNP P03372
H	237	GLU	-	expression tag	UNP P03372
H	238	ILE	-	expression tag	UNP P03372
H	239	PHE	-	expression tag	UNP P03372
H	240	PHE	-	expression tag	UNP P03372
H	241	LYS	-	expression tag	UNP P03372
H	242	ILE	-	expression tag	UNP P03372
H	243	LYS	-	expression tag	UNP P03372
H	244	LYS	-	expression tag	UNP P03372
H	245	THR	-	expression tag	UNP P03372
H	246	THR	-	expression tag	UNP P03372
H	247	PRO	-	expression tag	UNP P03372
H	248	LEU	-	expression tag	UNP P03372
H	249	ARG	-	expression tag	UNP P03372
H	250	ARG	-	expression tag	UNP P03372
H	251	LEU	-	expression tag	UNP P03372
H	252	MET	-	expression tag	UNP P03372
H	253	GLU	-	expression tag	UNP P03372
H	254	ALA	-	expression tag	UNP P03372
H	255	PHE	-	expression tag	UNP P03372
H	256	ALA	-	expression tag	UNP P03372
H	257	LYS	-	expression tag	UNP P03372
H	258	ARG	-	expression tag	UNP P03372
H	259	GLN	-	expression tag	UNP P03372
H	260	GLY	-	expression tag	UNP P03372

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Chain	Residue	Modelled	Actual	Comment	Reference
H	261	LYS	-	expression tag	UNP P03372
H	262	GLU	-	expression tag	UNP P03372
H	263	MET	-	expression tag	UNP P03372
H	264	ASP	-	expression tag	UNP P03372
H	265	SER	-	expression tag	UNP P03372
H	266	LEU	-	expression tag	UNP P03372
H	267	ARG	-	expression tag	UNP P03372
H	268	PHE	-	expression tag	UNP P03372
H	269	LEU	-	expression tag	UNP P03372
H	270	TYR	-	expression tag	UNP P03372
H	271	ASP	-	expression tag	UNP P03372
H	272	GLY	-	expression tag	UNP P03372
H	273	ILE	-	expression tag	UNP P03372
H	274	ARG	-	expression tag	UNP P03372
H	275	ILE	-	expression tag	UNP P03372
H	276	GLN	-	expression tag	UNP P03372
H	277	ALA	-	expression tag	UNP P03372
H	278	ASP	-	expression tag	UNP P03372
H	279	GLN	-	expression tag	UNP P03372
H	280	THR	-	expression tag	UNP P03372
H	281	PRO	-	expression tag	UNP P03372
H	282	GLU	-	expression tag	UNP P03372
H	283	ASP	-	expression tag	UNP P03372
H	284	LEU	-	expression tag	UNP P03372
H	285	ASP	-	expression tag	UNP P03372
H	286	MET	-	expression tag	UNP P03372
H	287	GLU	-	expression tag	UNP P03372
H	288	ASP	-	expression tag	UNP P03372
H	289	ASN	-	expression tag	UNP P03372
H	290	ASP	-	expression tag	UNP P03372
H	291	ILE	-	expression tag	UNP P03372
H	292	ILE	-	expression tag	UNP P03372
H	293	GLU	-	expression tag	UNP P03372
H	294	ALA	-	expression tag	UNP P03372
H	295	HIS	-	expression tag	UNP P03372
H	296	ARG	-	expression tag	UNP P03372
H	297	GLU	-	expression tag	UNP P03372
H	298	GLN	-	expression tag	UNP P03372
H	299	ILE	-	expression tag	UNP P03372
H	300	GLY	-	expression tag	UNP P03372
H	301	GLY	-	expression tag	UNP P03372
H	305	ALA	SER	engineered mutation	UNP P03372

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Chain	Residue	Modelled	Actual	Comment	Reference
H	591	ARG	PHE	engineered mutation	UNP P03372
H	592	ARG	PRO	engineered mutation	UNP P03372

- Molecule 4 is a protein called 14-3-3 protein zeta/delta.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	I	231	Total	C	N	O	S	0	0
			1850	1158	310	372	10		
4	D	231	Total	C	H	N	O	S	0
			3687	1158	1837	310	372	10	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	246	TRP	-	expression tag	UNP P63104
I	247	SER	-	expression tag	UNP P63104
I	248	HIS	-	expression tag	UNP P63104
I	249	PRO	-	expression tag	UNP P63104
I	250	GLN	-	expression tag	UNP P63104
I	251	PHE	-	expression tag	UNP P63104
I	252	GLU	-	expression tag	UNP P63104
I	253	LYS	-	expression tag	UNP P63104
D	246	TRP	-	expression tag	UNP P63104
D	247	SER	-	expression tag	UNP P63104
D	248	HIS	-	expression tag	UNP P63104
D	249	PRO	-	expression tag	UNP P63104
D	250	GLN	-	expression tag	UNP P63104
D	251	PHE	-	expression tag	UNP P63104
D	252	GLU	-	expression tag	UNP P63104
D	253	LYS	-	expression tag	UNP P63104

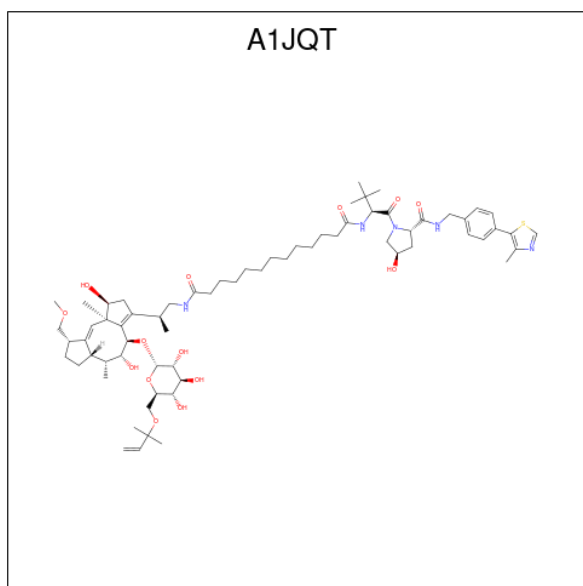
- Molecule 5 is a protein called von Hippel-Lindau disease tumor suppressor.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	152	Total	C	H	N	O	S	0
			2488	787	1242	231	225	3	0

There are 2 discrepancies between the modelled and reference sequences:

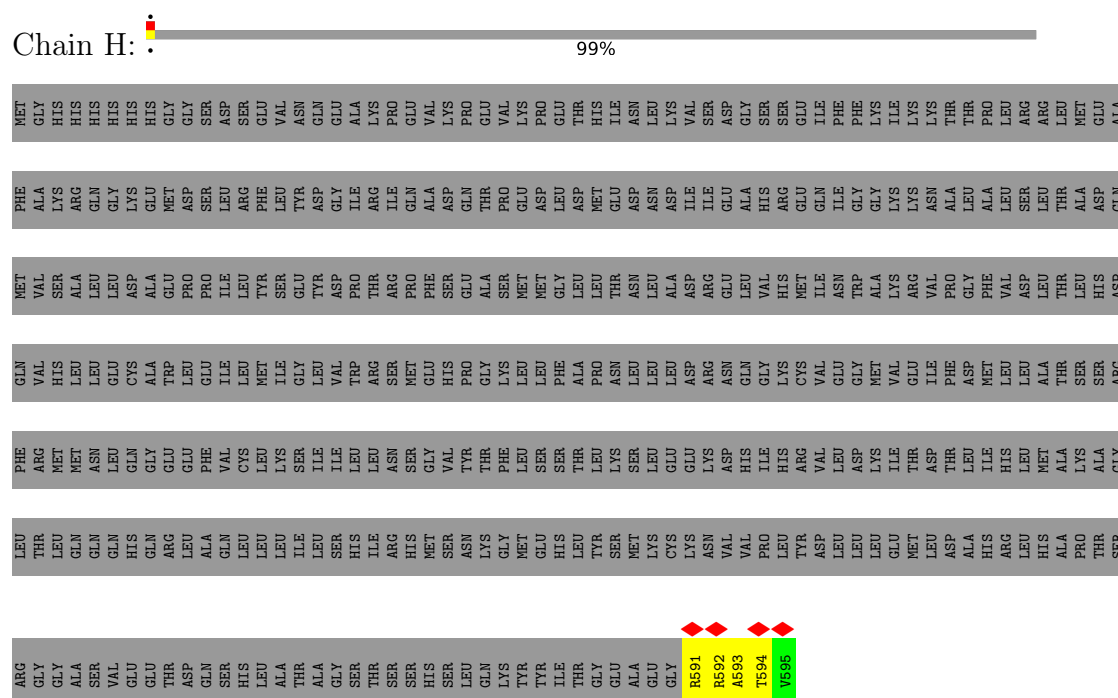
Chain	Residue	Modelled	Actual	Comment	Reference
E	52	GLY	-	expression tag	UNP P40337
E	53	SER	-	expression tag	UNP P40337

- Molecule 6 is {N}'-[(2 {S})-3,3-dimethyl-1-[(2 {S},4 {R})-2-[[4-(4-methyl-1,3-thiazol-5-yl)phenyl]methylcarbamoyl]-4-oxidanyl-pyrrolidin-1-yl]-1-oxidanylidene-butan-2-yl]- {N}-[(2 {S})-2-[(1 {E},3 {R},4 {S},8 {R},9 {R},10 {R},11 {S},14 {S})-14-(methoxymethyl)-3,10-dimethyl-8-[(2 {S},3 {R},4 {S},5 {S},6 {R})-6-(2-methylbut-3-en-2-yloxymethyl)-3,4,5-tris(oxidanyl)oxan-2-yl]oxy-4,9-bis(oxidanyl)-6-tricyclo[9.3.0.0^{3,7}]tetradeca-1,6-dienyl]propyl]tridecanediamide (CCD ID: A1JQT) (formula: C₆₇H₁₀₃N₅O₁₄S) (labeled as "Ligand of Interest" by depositor).

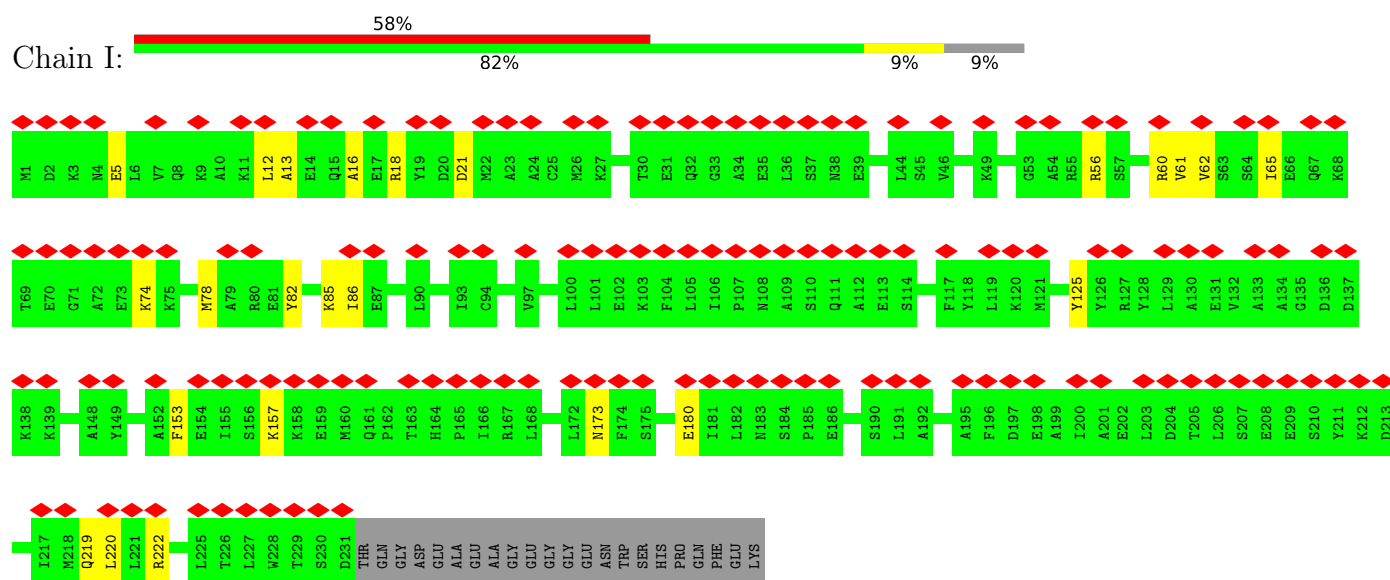


Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	N	O	S	
6	D	1	190	67	103	5	14	1	0

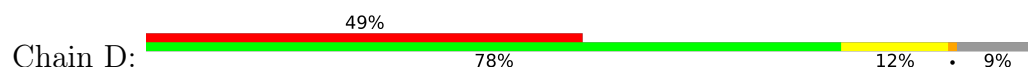
- Molecule 3: Estrogen receptor

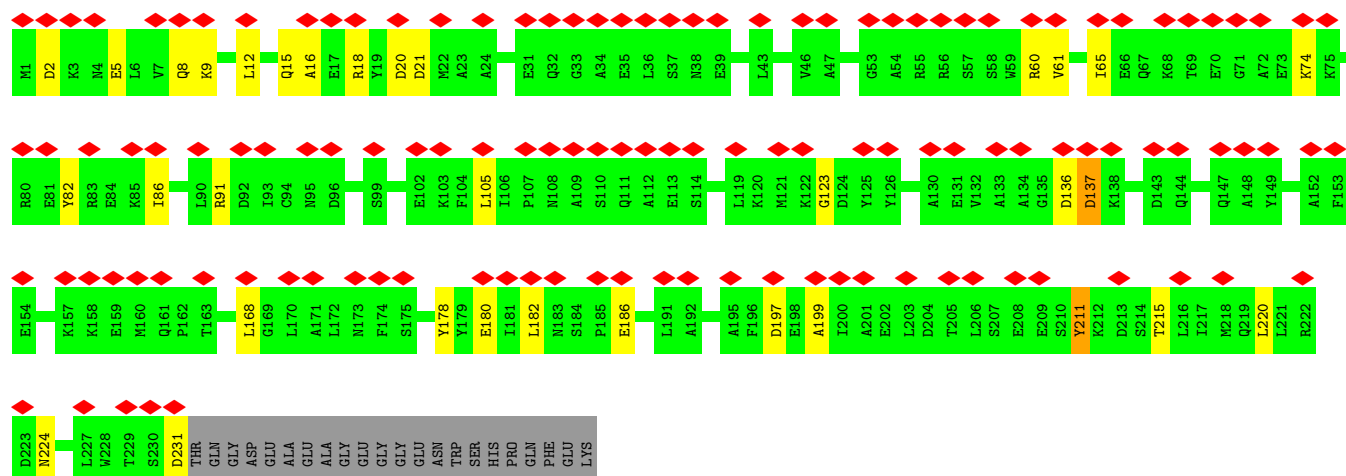


- Molecule 4: 14-3-3 protein zeta/delta

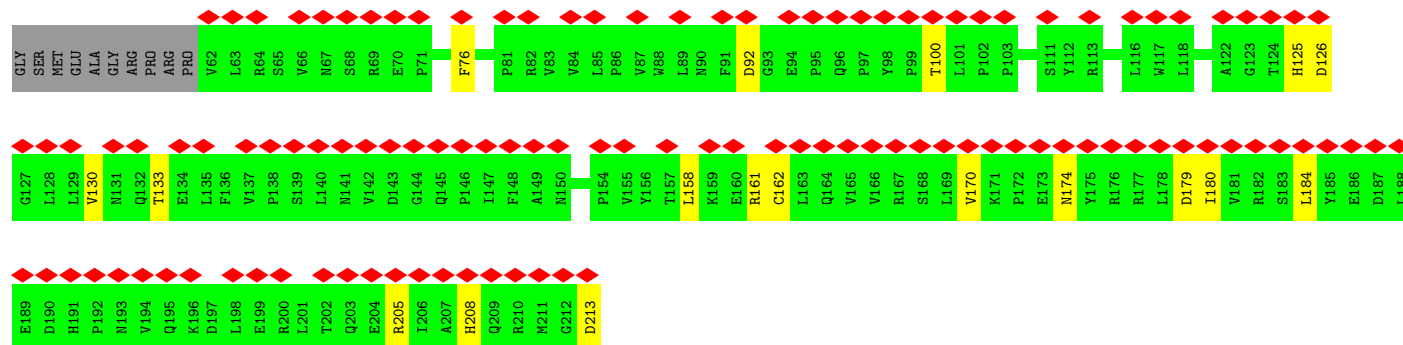
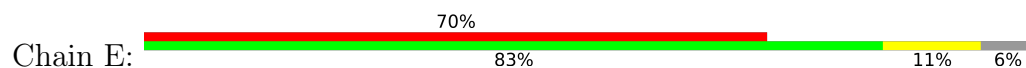


- Molecule 4: 14-3-3 protein zeta/delta





- Molecule 5: von Hippel-Lindau disease tumor suppressor



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	140642	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	33	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2700	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	4.697	Depositor
Minimum map value	-1.358	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.021	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	248.7, 248.7, 248.7	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.829, 0.829, 0.829	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TPO, A1JQT

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	B	0.73	0/769	1.20	3/1040 (0.3%)
2	C	0.73	1/829 (0.1%)	1.13	1/1121 (0.1%)
3	G	0.31	0/38	0.46	0/46
3	H	0.31	0/38	0.46	0/46
4	D	0.95	0/1875	1.70	11/2521 (0.4%)
4	I	0.68	0/1875	1.20	2/2521 (0.1%)
5	E	0.99	0/1277	1.51	10/1738 (0.6%)
All	All	0.83	1/6701 (0.0%)	1.41	27/9033 (0.3%)

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	B	1	1
4	D	0	1
4	I	0	1
5	E	1	1
All	All	2	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	96	PRO	CA-C	5.22	1.54	1.51

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	137	ASP	CA-CB-CG	8.30	120.90	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	197	ASP	CA-CB-CG	7.75	120.34	112.60
4	D	2	ASP	CA-CB-CG	6.98	119.58	112.60
5	E	126	ASP	CA-CB-CG	6.64	119.24	112.60
5	E	125	HIS	CE1-NE2-CD2	-6.56	102.44	109.00
5	E	179	ASP	CA-CB-CG	6.33	118.93	112.60
5	E	92	ASP	CA-CB-CG	6.31	118.91	112.60
1	B	86	SER	CA-C-N	6.18	129.40	120.38
1	B	86	SER	C-N-CA	6.18	129.40	120.38
4	I	173	ASN	OD1-CG-ND2	-5.94	116.66	122.60
5	E	213	ASP	CA-CB-CG	5.94	118.54	112.60
5	E	76	PHE	CA-CB-CG	5.89	119.69	113.80
4	D	21	ASP	CA-CB-CG	5.71	118.31	112.60
5	E	125	HIS	ND1-CE1-NE2	5.66	114.06	108.40
4	I	21	ASP	CA-CB-CG	5.42	118.03	112.60
4	D	91	ARG	CA-C-N	5.31	127.34	120.44
4	D	91	ARG	C-N-CA	5.31	127.34	120.44
4	D	231	ASP	CA-CB-CG	5.29	117.89	112.60
4	D	123	GLY	CA-C-N	5.18	127.18	120.44
4	D	123	GLY	C-N-CA	5.18	127.18	120.44
1	B	87	SER	N-CA-C	5.13	118.32	111.75
5	E	100	THR	N-CA-C	5.12	116.70	110.41
2	C	70	GLN	OE1-CD-NE2	-5.09	117.51	122.60
5	E	208	HIS	CE1-NE2-CD2	-5.06	103.94	109.00
5	E	133	THR	CA-CB-OG1	5.03	117.14	109.60
4	D	105	LEU	CA-C-N	5.01	123.39	120.24
4	D	105	LEU	C-N-CA	5.01	123.39	120.24

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	87	SER	CA
5	E	133	THR	CA

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	33	ARG	Sidechain
4	D	211	TYR	Sidechain
5	E	205	ARG	Sidechain
4	I	125	TYR	Sidechain

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	B	752	0	740	44	0
2	C	813	0	811	23	0
3	G	52	0	53	31	0
3	H	52	0	53	9	0
4	D	1850	1837	1837	112	0
4	I	1850	0	1836	92	0
5	E	1246	1242	1241	33	0
6	D	87	103	0	0	0
All	All	6702	3182	6571	177	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 13.

All (177) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:591:ARG:CZ	4:D:60:ARG:HH22	1.18	1.52
4:I:78:MET:HE3	4:D:9:LYS:CG	1.41	1.51
3:G:591:ARG:NH1	4:D:60:ARG:HH22	1.09	1.46
4:I:78:MET:CE	4:D:9:LYS:HG3	1.43	1.44
4:I:82:TYR:HE1	4:D:16:ALA:CB	1.37	1.38
4:I:12:LEU:CD2	4:D:65:ILE:HG21	1.59	1.32
1:B:112:CYS:O	5:E:158:LEU:HB3	1.26	1.32
3:G:591:ARG:CZ	4:D:60:ARG:NH2	1.94	1.30
3:G:593:ALA:CB	4:D:220:LEU:HD22	1.62	1.27
3:H:592:ARG:NE	4:I:180:GLU:OE1	1.72	1.22
3:G:591:ARG:NH1	4:D:60:ARG:NH2	1.86	1.21
4:I:82:TYR:CE1	4:D:16:ALA:CB	2.30	1.15
4:I:78:MET:HE1	4:D:9:LYS:N	1.62	1.13
3:H:591:ARG:HH22	4:I:60:ARG:NH2	1.46	1.12
4:I:78:MET:HB3	4:D:12:LEU:CD1	1.80	1.11
4:I:65:ILE:HD13	4:D:15:GLN:OE1	1.52	1.08
4:I:86:ILE:CG1	4:D:18:ARG:HH21	1.66	1.08
1:B:112:CYS:SG	5:E:158:LEU:HD22	1.95	1.06
4:I:82:TYR:HE1	4:D:16:ALA:HB3	1.21	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:12:LEU:HD22	4:D:65:ILE:HG21	1.27	1.06
4:I:85:LYS:CE	4:D:18:ARG:NH1	2.21	1.03
4:I:85:LYS:HE2	4:D:18:ARG:NH1	1.73	1.03
4:I:86:ILE:HG13	4:D:18:ARG:NH2	1.74	1.02
1:B:112:CYS:SG	5:E:158:LEU:CD2	2.49	1.01
4:I:78:MET:CE	4:D:9:LYS:N	2.24	0.99
3:G:593:ALA:HB2	4:D:220:LEU:CD2	1.93	0.99
4:I:86:ILE:CG1	4:D:18:ARG:NH2	2.29	0.96
3:H:593:ALA:CB	4:I:220:LEU:HD22	1.97	0.95
3:G:593:ALA:HB2	4:D:220:LEU:HD22	0.97	0.95
3:G:593:ALA:HB1	4:D:220:LEU:HD13	1.49	0.94
3:G:592:ARG:HB2	4:D:224:ASN:OD1	1.68	0.94
3:G:592:ARG:NH2	4:D:180:GLU:OE2	2.01	0.93
3:G:593:ALA:CB	4:D:220:LEU:CD2	2.46	0.92
4:I:85:LYS:CD	4:D:18:ARG:NH1	2.31	0.92
3:H:591:ARG:NH2	4:I:60:ARG:NH2	2.18	0.92
3:G:591:ARG:HH22	4:D:60:ARG:NH1	1.69	0.91
4:I:12:LEU:CD2	4:D:65:ILE:CG2	2.49	0.90
4:I:86:ILE:HG12	4:D:18:ARG:HH21	1.36	0.90
3:G:591:ARG:HH22	4:D:60:ARG:HH12	1.21	0.88
1:B:104:LEU:HB2	5:E:162:CYS:HB3	1.55	0.87
4:I:82:TYR:CE1	4:D:16:ALA:HB3	2.00	0.87
4:I:85:LYS:HD3	4:D:18:ARG:NH1	1.91	0.86
4:I:85:LYS:HE2	4:D:18:ARG:HH12	1.38	0.86
4:I:65:ILE:CD1	4:D:15:GLN:OE1	2.24	0.85
4:I:82:TYR:CE2	4:D:18:ARG:NE	2.45	0.84
4:I:78:MET:CB	4:D:12:LEU:HD11	2.07	0.84
4:I:82:TYR:HE1	4:D:16:ALA:HB2	1.42	0.84
1:B:112:CYS:O	5:E:158:LEU:CB	2.21	0.83
4:I:78:MET:HB3	4:D:12:LEU:HD11	1.61	0.82
1:B:112:CYS:C	5:E:158:LEU:HB3	2.04	0.82
4:I:85:LYS:CD	4:D:18:ARG:HH12	1.90	0.82
4:I:78:MET:CB	4:D:12:LEU:CD1	2.58	0.81
3:G:593:ALA:HB3	4:D:220:LEU:HB3	1.60	0.81
4:I:85:LYS:CE	4:D:18:ARG:HH12	1.90	0.80
4:I:78:MET:HE1	4:D:8:GLN:C	2.07	0.80
3:G:591:ARG:NH2	4:D:60:ARG:NH2	2.29	0.79
4:I:12:LEU:HD21	4:D:65:ILE:HG21	1.64	0.79
1:B:112:CYS:SG	5:E:158:LEU:HD23	2.22	0.78
4:I:16:ALA:HA	4:D:61:VAL:HG11	1.64	0.78
4:I:74:LYS:HE3	4:D:5:GLU:HG2	1.65	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:78:MET:CE	4:D:9:LYS:CG	2.26	0.76
1:B:30:ILE:HB	2:C:14:ILE:HG12	1.67	0.75
4:I:5:GLU:OE1	4:D:74:LYS:HE2	1.87	0.74
4:I:85:LYS:CE	4:D:18:ARG:HH11	1.97	0.74
4:I:74:LYS:CE	4:D:5:GLU:HG2	2.18	0.74
3:H:593:ALA:HB2	4:I:220:LEU:HD22	1.67	0.74
4:I:78:MET:HE1	4:D:9:LYS:H	1.52	0.73
3:G:593:ALA:H	4:D:224:ASN:HD21	1.37	0.73
3:H:591:ARG:NH2	4:I:60:ARG:CZ	2.51	0.73
1:B:107:ALA:HB2	5:E:158:LEU:HG	1.69	0.72
3:G:593:ALA:HB1	4:D:220:LEU:CD1	2.21	0.70
1:B:104:LEU:HD13	5:E:162:CYS:HB2	1.72	0.69
4:I:78:MET:CE	4:D:9:LYS:CA	2.70	0.69
1:B:107:ALA:CB	5:E:158:LEU:HG	2.23	0.69
2:C:102:VAL:CG1	5:E:174:ASN:HB3	2.23	0.69
1:B:68:HIS:HD1	2:C:94:SER:HG	1.40	0.69
1:B:107:ALA:HA	5:E:158:LEU:HD23	1.76	0.68
1:B:29:PHE:HD1	2:C:15:PHE:HE2	1.41	0.68
3:G:591:ARG:NH2	4:D:60:ARG:NH1	2.41	0.67
2:C:102:VAL:O	5:E:170:VAL:HG22	1.95	0.66
4:I:78:MET:HB2	4:D:12:LEU:HD11	1.77	0.66
4:I:65:ILE:HD11	4:D:15:GLN:HB3	1.78	0.65
3:G:591:ARG:NH2	4:D:60:ARG:CZ	2.59	0.64
4:I:78:MET:HE2	4:D:12:LEU:HD12	1.78	0.64
4:I:78:MET:HB3	4:D:12:LEU:HD12	1.75	0.64
4:I:12:LEU:HD21	4:D:65:ILE:CG2	2.24	0.63
4:I:13:ALA:HA	4:D:82:TYR:OH	1.99	0.63
1:B:30:ILE:HD12	2:C:14:ILE:HG12	1.81	0.62
4:I:86:ILE:HG12	4:D:18:ARG:NH2	2.03	0.62
4:I:65:ILE:CD1	4:D:15:GLN:HB3	2.29	0.62
1:B:107:ALA:CB	5:E:158:LEU:HD23	2.29	0.61
4:I:85:LYS:CG	4:D:18:ARG:HH12	2.14	0.61
3:G:591:ARG:HH12	4:D:60:ARG:NH2	1.96	0.61
4:I:78:MET:HE3	4:D:9:LYS:CB	2.28	0.60
4:I:82:TYR:CE1	4:D:16:ALA:HB2	2.22	0.60
1:B:76:TYR:CE1	5:E:158:LEU:HB2	2.37	0.59
1:B:107:ALA:CB	5:E:158:LEU:CD2	2.80	0.59
1:B:104:LEU:CD1	5:E:162:CYS:HB2	2.32	0.59
1:B:112:CYS:C	5:E:158:LEU:CB	2.74	0.58
1:B:29:PHE:HA	2:C:13:THR:O	2.02	0.58
4:I:82:TYR:CE1	4:D:16:ALA:HB1	2.31	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:85:LYS:HG2	4:D:18:ARG:HH12	1.68	0.58
4:I:5:GLU:OE1	4:D:74:LYS:CE	2.52	0.58
4:I:78:MET:HG2	4:D:9:LYS:CE	2.34	0.58
4:I:16:ALA:CA	4:D:61:VAL:HG11	2.32	0.58
1:B:30:ILE:HD12	2:C:14:ILE:CG1	2.35	0.56
3:G:592:ARG:HH21	4:D:180:GLU:CD	2.09	0.56
4:I:153:PHE:CZ	4:I:157:LYS:HE3	2.40	0.56
1:B:104:LEU:HD13	5:E:162:CYS:CB	2.36	0.56
3:G:591:ARG:NH2	4:D:60:ARG:HH12	1.99	0.56
1:B:30:ILE:HG21	2:C:34:ILE:HG21	1.87	0.56
1:B:92:GLU:OE1	5:E:161:ARG:NH2	2.39	0.56
1:B:107:ALA:HB2	5:E:158:LEU:CD2	2.36	0.56
1:B:107:ALA:CA	5:E:158:LEU:HD23	2.36	0.55
4:I:74:LYS:NZ	4:D:5:GLU:HG3	2.21	0.55
3:G:593:ALA:CB	4:D:220:LEU:CG	2.85	0.55
4:I:85:LYS:NZ	4:D:18:ARG:HH11	2.06	0.53
3:G:593:ALA:CB	4:D:220:LEU:HD13	2.32	0.53
4:I:62:VAL:CG2	4:D:16:ALA:HB2	2.38	0.53
4:I:78:MET:HG2	4:D:9:LYS:HE3	1.89	0.53
4:D:178:TYR:CD1	4:D:182:LEU:HD12	2.44	0.52
1:B:68:HIS:HB3	2:C:94:SER:O	2.09	0.52
2:C:102:VAL:HG11	5:E:174:ASN:HB3	1.90	0.52
1:B:107:ALA:CB	5:E:158:LEU:CG	2.88	0.52
3:H:591:ARG:HH22	4:I:60:ARG:HH22	1.49	0.52
2:C:103:MET:HA	5:E:170:VAL:HG22	1.92	0.52
1:B:107:ALA:HB2	5:E:158:LEU:CG	2.37	0.52
4:D:168:LEU:HD21	4:D:199:ALA:HB2	1.93	0.51
4:I:219:GLN:HE22	4:I:222:ARG:HH21	1.60	0.50
1:B:30:ILE:CB	2:C:14:ILE:HG12	2.41	0.49
1:B:98:GLU:HA	2:C:99:LEU:HD13	1.95	0.49
1:B:29:PHE:CD1	2:C:15:PHE:HE2	2.27	0.49
4:I:153:PHE:CE1	4:I:157:LYS:HE3	2.48	0.48
4:I:82:TYR:CE2	4:D:18:ARG:CZ	2.96	0.48
4:I:78:MET:C	4:D:12:LEU:HD13	2.39	0.48
4:I:12:LEU:HD22	4:D:65:ILE:CG2	2.19	0.48
1:B:31:VAL:HG12	2:C:15:PHE:HB2	1.96	0.47
1:B:30:ILE:HD13	2:C:34:ILE:CG2	2.43	0.47
4:I:56:ARG:NH2	4:I:60:ARG:HH22	2.12	0.47
3:G:593:ALA:HB3	4:D:220:LEU:CB	2.39	0.47
2:C:103:MET:HG2	5:E:170:VAL:CG2	2.44	0.47
4:I:74:LYS:CE	4:D:5:GLU:CG	2.91	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:18:ARG:NH1	4:D:86:ILE:HG12	2.31	0.46
4:I:78:MET:CE	4:D:9:LYS:CB	2.90	0.46
4:I:78:MET:HE2	4:D:9:LYS:CA	2.44	0.46
1:B:102:GLU:OE2	2:C:97:PRO:CD	2.64	0.45
1:B:104:LEU:CB	5:E:162:CYS:HB3	2.36	0.45
4:I:78:MET:HE2	4:D:9:LYS:HA	1.99	0.45
4:I:86:ILE:HG13	4:D:18:ARG:HH21	1.35	0.45
4:I:12:LEU:HD23	4:D:65:ILE:HD13	1.98	0.45
3:H:592:ARG:CZ	4:I:180:GLU:OE1	2.55	0.45
3:G:592:ARG:CZ	4:D:180:GLU:OE2	2.62	0.44
4:D:211:TYR:CE1	4:D:215:THR:HG21	2.53	0.44
3:G:591:ARG:NH1	4:D:60:ARG:CZ	2.74	0.44
3:G:593:ALA:CB	4:D:220:LEU:CD1	2.94	0.44
4:I:61:VAL:HG11	4:D:15:GLN:O	2.17	0.44
4:I:78:MET:CE	4:D:8:GLN:C	2.80	0.44
1:B:76:TYR:CG	5:E:158:LEU:HD13	2.53	0.43
4:I:12:LEU:HD23	4:D:65:ILE:HG21	1.80	0.43
5:E:180:ILE:HD12	5:E:184:LEU:HB2	1.99	0.43
3:H:593:ALA:HB1	4:I:220:LEU:HD22	1.90	0.43
1:B:51:GLN:C	1:B:56:GLU:OE1	2.61	0.43
2:C:102:VAL:HG12	5:E:174:ASN:OD1	2.18	0.43
4:I:74:LYS:HZ2	4:D:5:GLU:HG3	1.83	0.43
3:G:592:ARG:NE	4:D:180:GLU:OE2	2.51	0.43
4:I:74:LYS:NZ	4:D:5:GLU:CG	2.82	0.42
3:G:593:ALA:H	4:D:224:ASN:ND2	2.10	0.42
4:I:12:LEU:CD2	4:D:65:ILE:HD13	2.50	0.42
1:B:30:ILE:CD1	2:C:14:ILE:HG12	2.48	0.42
1:B:99:ILE:HG22	2:C:96:PRO:HB3	2.01	0.41
1:B:107:ALA:HB1	5:E:158:LEU:HG	2.02	0.41
4:I:219:GLN:HE22	4:I:222:ARG:NH2	2.17	0.41
1:B:76:TYR:CD1	5:E:158:LEU:HD13	2.56	0.41
1:B:102:GLU:OE2	2:C:97:PRO:HD2	2.20	0.41
4:I:78:MET:HB3	4:D:12:LEU:HD13	1.86	0.41
3:G:591:ARG:CZ	4:D:60:ARG:CZ	2.85	0.41
4:I:78:MET:HG2	4:D:9:LYS:HE2	2.02	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	B	93/97 (96%)	90 (97%)	3 (3%)	0	100	100
2	C	101/104 (97%)	97 (96%)	4 (4%)	0	100	100
3	G	2/401 (0%)	2 (100%)	0	0	100	100
3	H	2/401 (0%)	2 (100%)	0	0	100	100
4	D	229/253 (90%)	223 (97%)	6 (3%)	0	100	100
4	I	229/253 (90%)	227 (99%)	2 (1%)	0	100	100
5	E	150/162 (93%)	139 (93%)	11 (7%)	0	100	100
All	All	806/1671 (48%)	780 (97%)	26 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	B	84/86 (98%)	83 (99%)	1 (1%)	63	73
2	C	91/92 (99%)	91 (100%)	0	100	100
3	G	4/351 (1%)	4 (100%)	0	100	100
3	H	4/351 (1%)	4 (100%)	0	100	100
4	D	201/217 (93%)	197 (98%)	4 (2%)	48	66
4	I	201/217 (93%)	201 (100%)	0	100	100
5	E	141/148 (95%)	140 (99%)	1 (1%)	76	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	726/1462 (50%)	720 (99%)	6 (1%)	70	77

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	87	SER
4	D	20	ASP
4	D	136	ASP
4	D	137	ASP
4	D	186	GLU
5	E	130	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
4	I	42	ASN
4	D	42	ASN
4	D	95	ASN
4	D	224	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	TPO	H	594	3	8,10,11	1.09	1 (12%)	10,14,16	0.99	0
3	TPO	G	594	3	8,10,11	1.10	1 (12%)	10,14,16	0.99	0

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
3	TPO	H	594	3	-	2/9/11/13	-
3	TPO	G	594	3	-	2/9/11/13	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	594	TPO	P-OG1	2.05	1.63	1.59
3	G	594	TPO	P-OG1	2.03	1.63	1.59

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	G	594	TPO	CB-OG1-P-O2P
3	H	594	TPO	CB-OG1-P-O2P
3	G	594	TPO	O-C-CA-CB
3	H	594	TPO	O-C-CA-CB

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand 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	$\# Z > 2$
6	A1JQT	D	301	-	88,93,93	0.99	4 (4%)	102,135,135	1.02	5 (4%)

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
6	A1JQT	D	301	-	-	3/70/156/156	0/7/7/7

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	301	A1JQT	CAZ-NAR	-3.47	1.33	1.38
6	D	301	A1JQT	C24-C26	2.52	1.55	1.53
6	D	301	A1JQT	C28-C09	2.29	1.54	1.50
6	D	301	A1JQT	CBE-CAX	2.25	1.56	1.53

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	301	A1JQT	CBE-NAT-CAV	2.50	127.08	122.03
6	D	301	A1JQT	C14-C10-C11	-2.44	109.22	112.81
6	D	301	A1JQT	CAB-CAZ-NAR	-2.30	116.12	120.94
6	D	301	A1JQT	CAN-SAU-CBB	-2.24	87.77	88.87
6	D	301	A1JQT	C19-C20-C16	2.10	105.91	101.98

There are no chirality outliers.

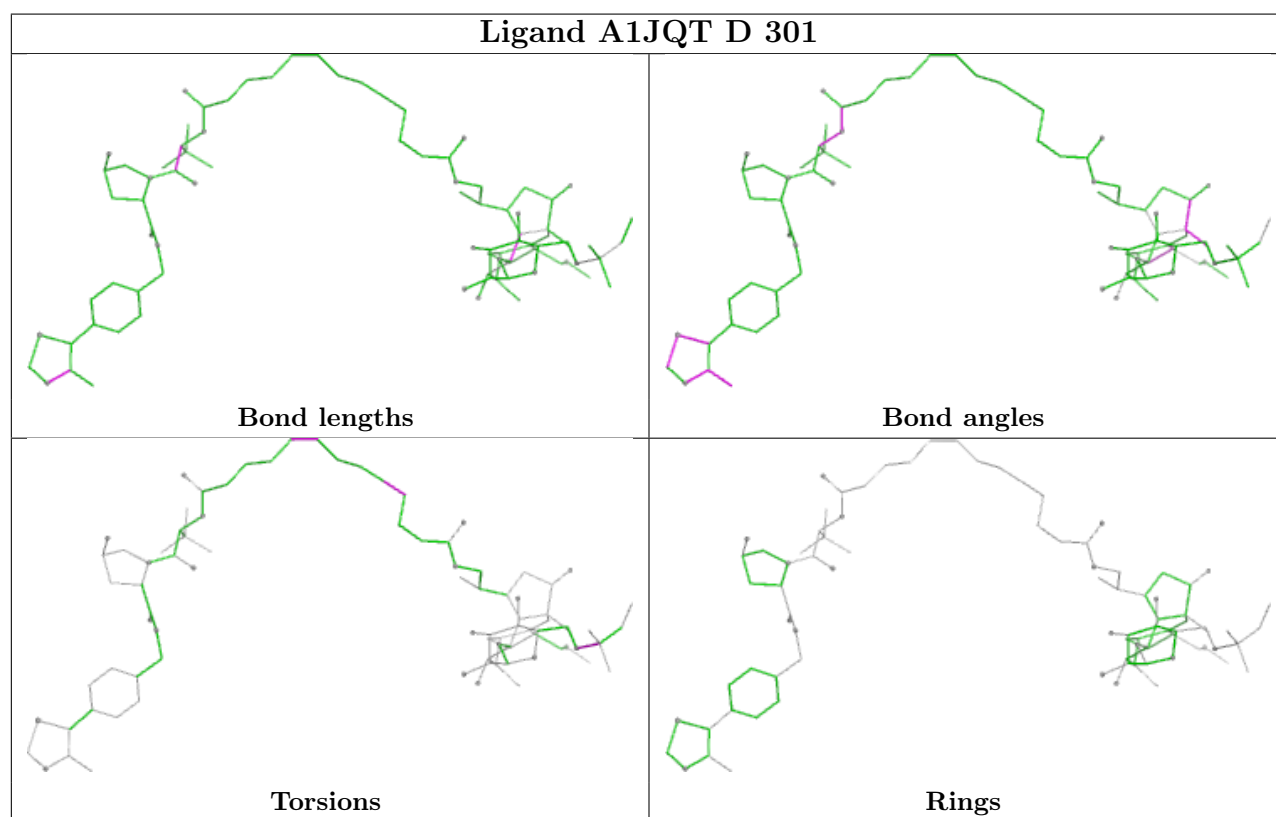
All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	D	301	A1JQT	C62-C63-C64-C65
6	D	301	A1JQT	C2-C3-C4-C5
6	D	301	A1JQT	C41-C40-O39-C38

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

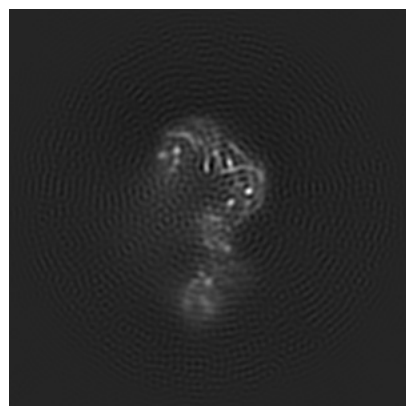
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-55233. These allow visual inspection of the internal detail of the map and identification of artifacts.

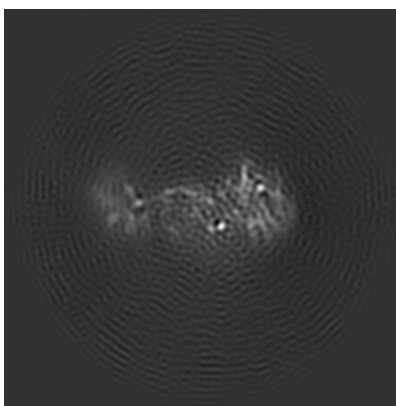
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

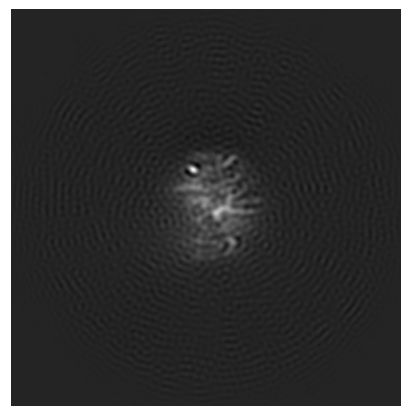
6.1.1 Primary map



X

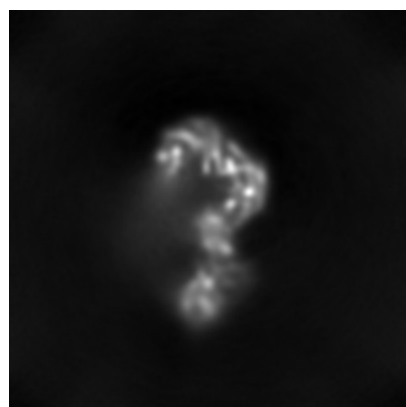


Y

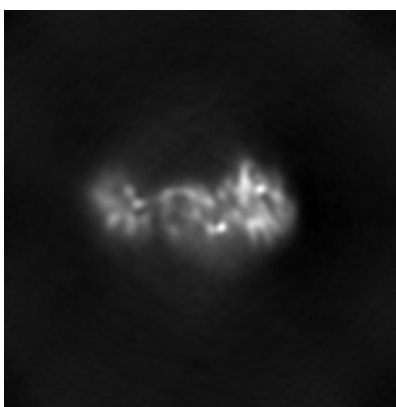


Z

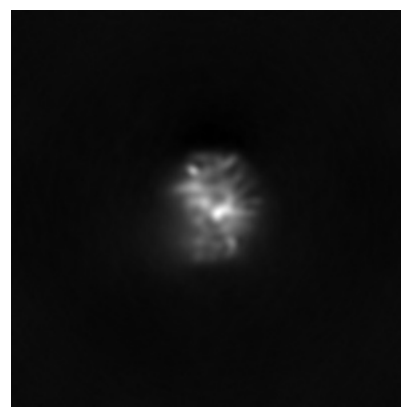
6.1.2 Raw map



X



Y

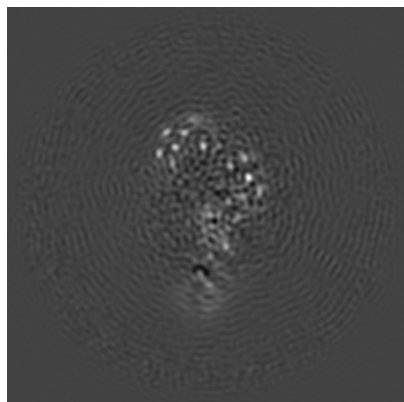


Z

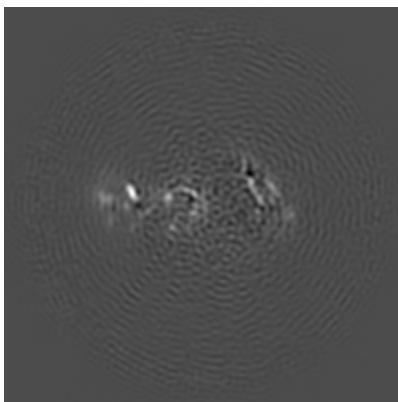
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

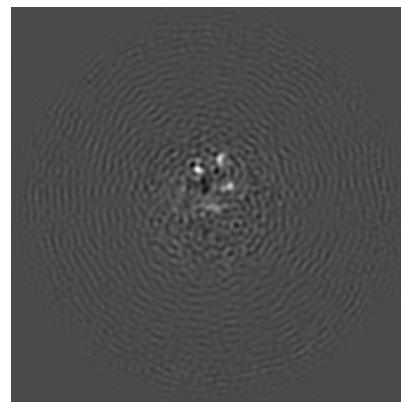
6.2.1 Primary map



X Index: 150

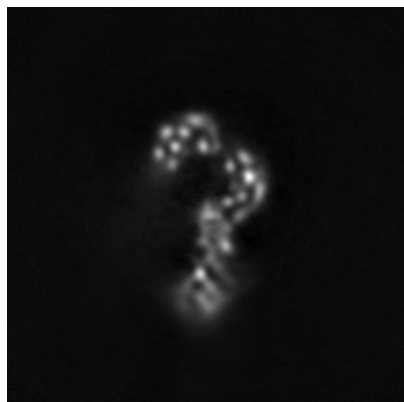


Y Index: 150

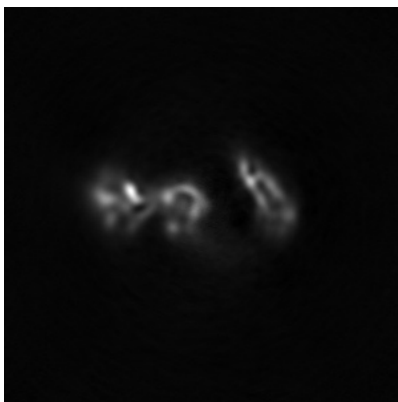


Z Index: 150

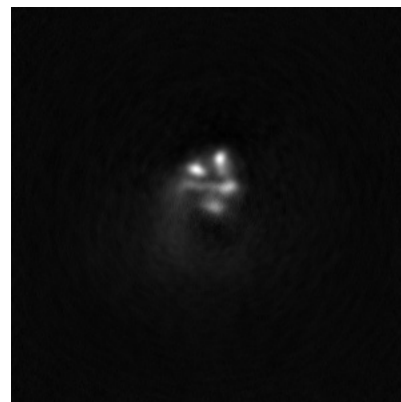
6.2.2 Raw map



X Index: 150



Y Index: 150

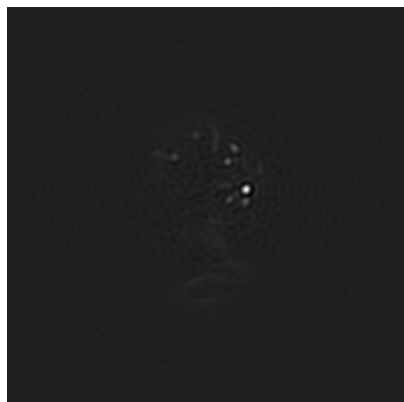


Z Index: 150

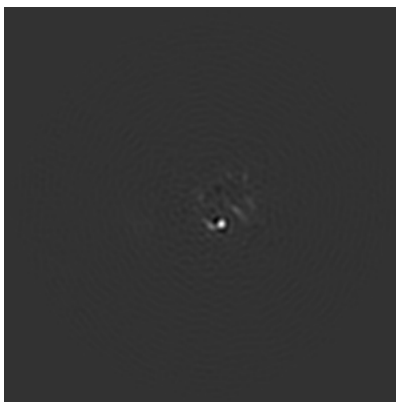
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

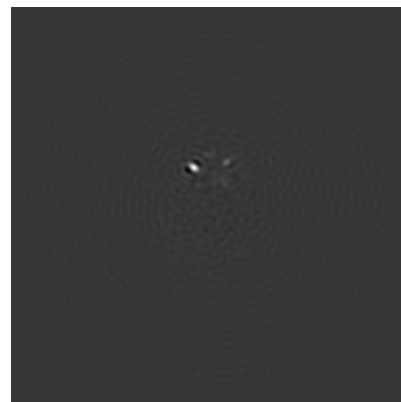
6.3.1 Primary map



X Index: 137



Y Index: 179

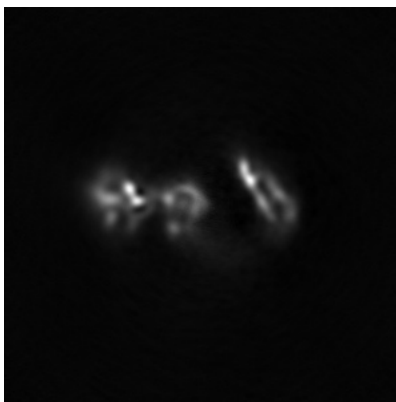


Z Index: 163

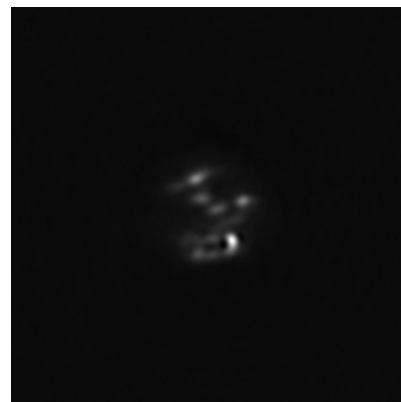
6.3.2 Raw map



X Index: 164



Y Index: 148

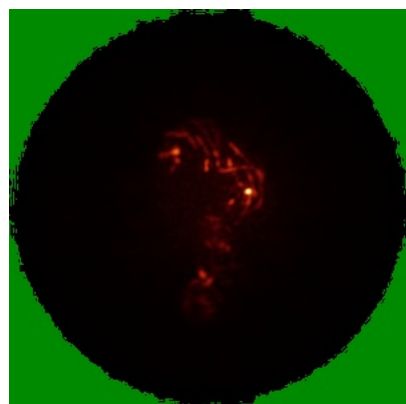


Z Index: 192

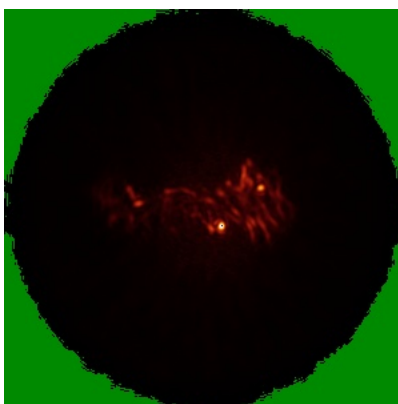
The images above show the largest variance slices of the map in three orthogonal directions.

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

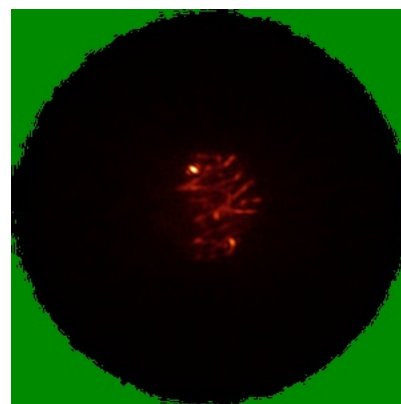
6.4.1 Primary map



X

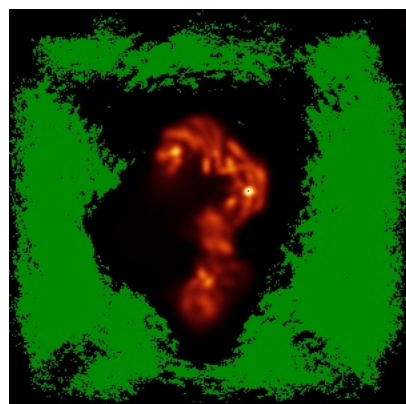


Y

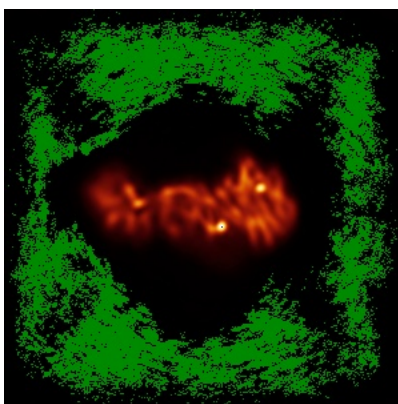


Z

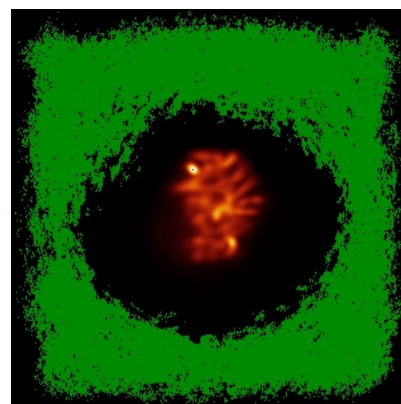
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

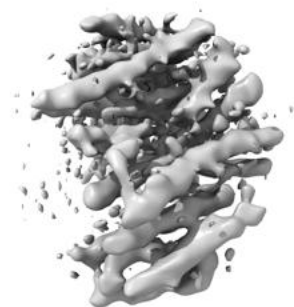
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.15. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

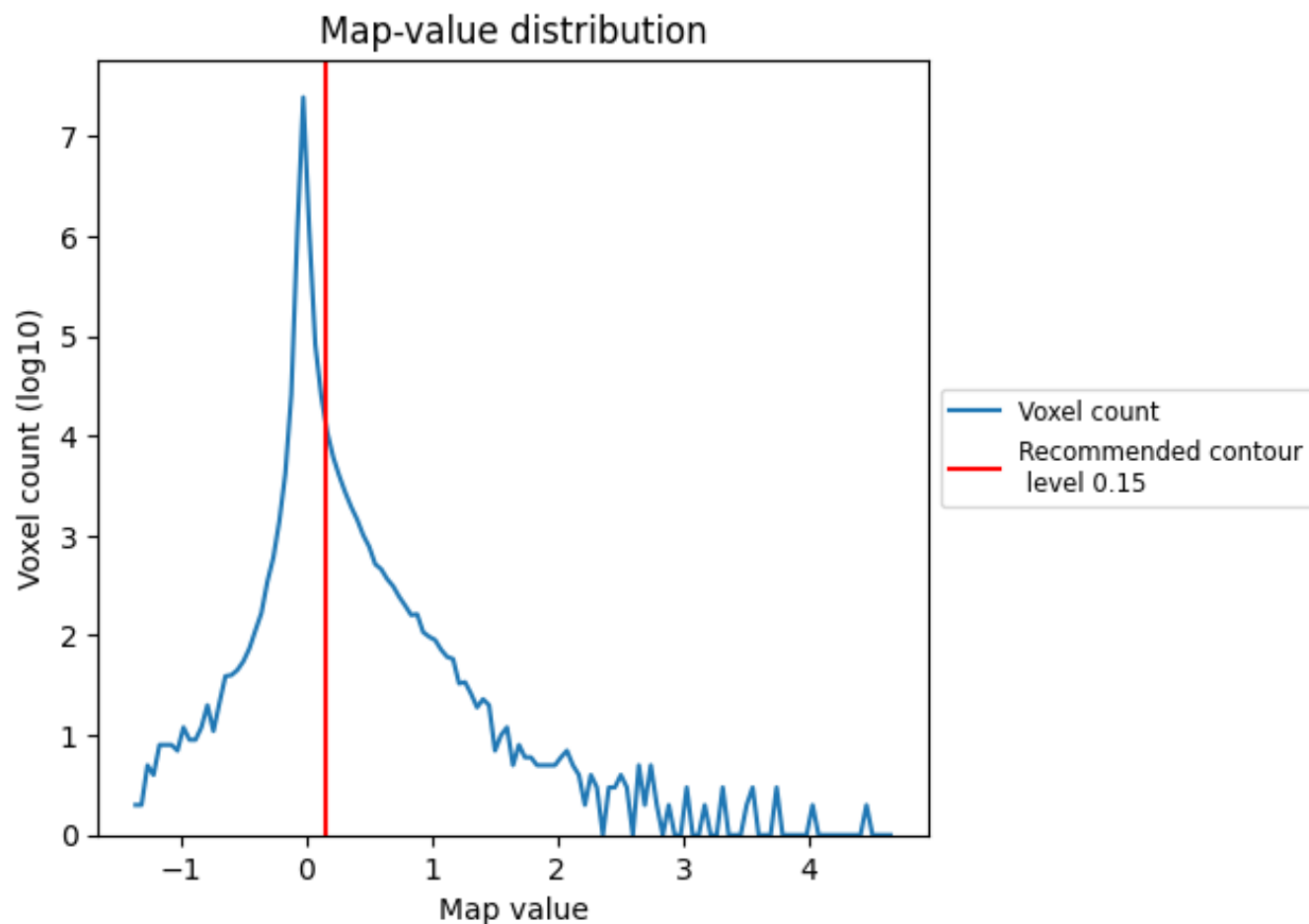
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

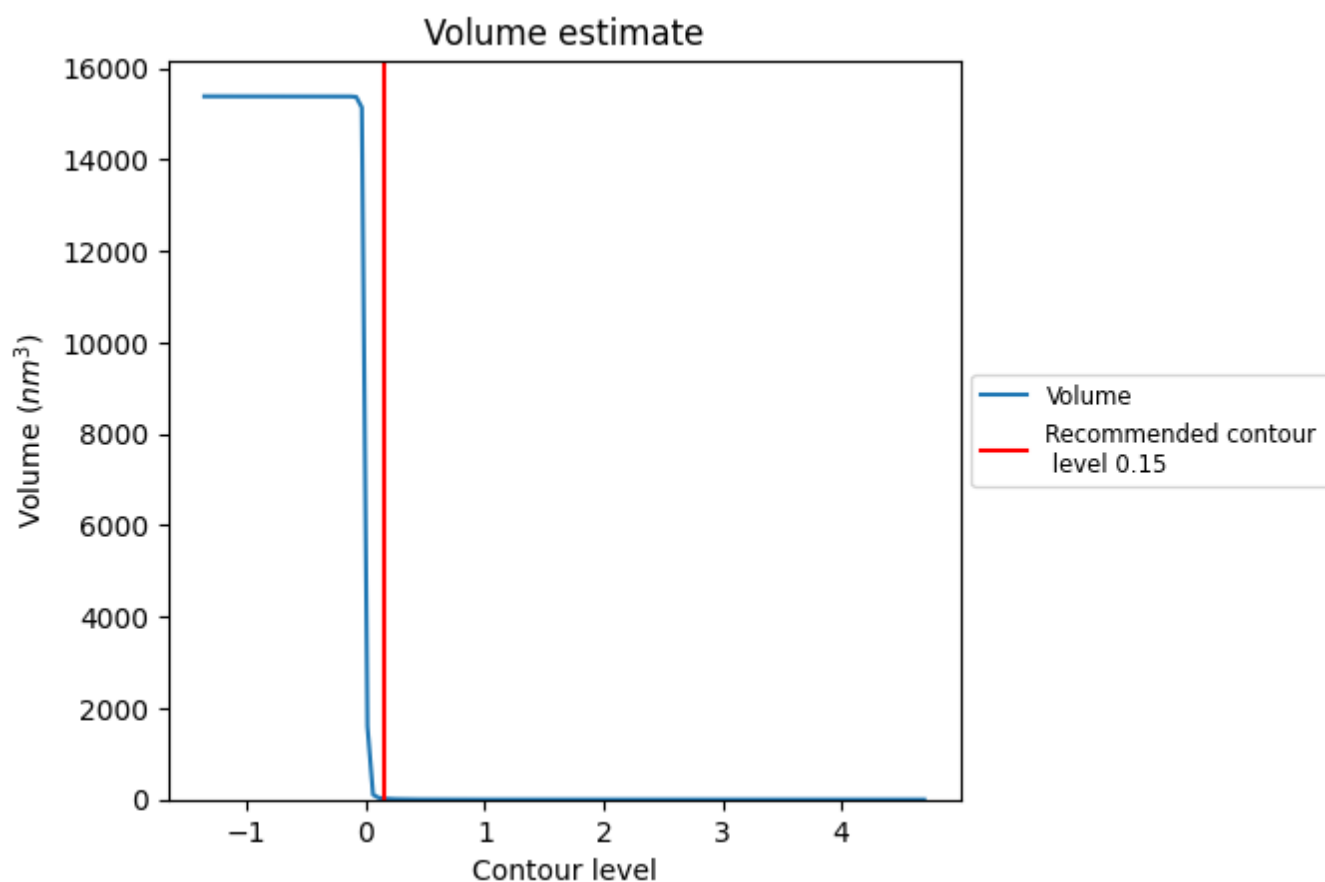
This section contains the results of statistical analysis of the map.

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.

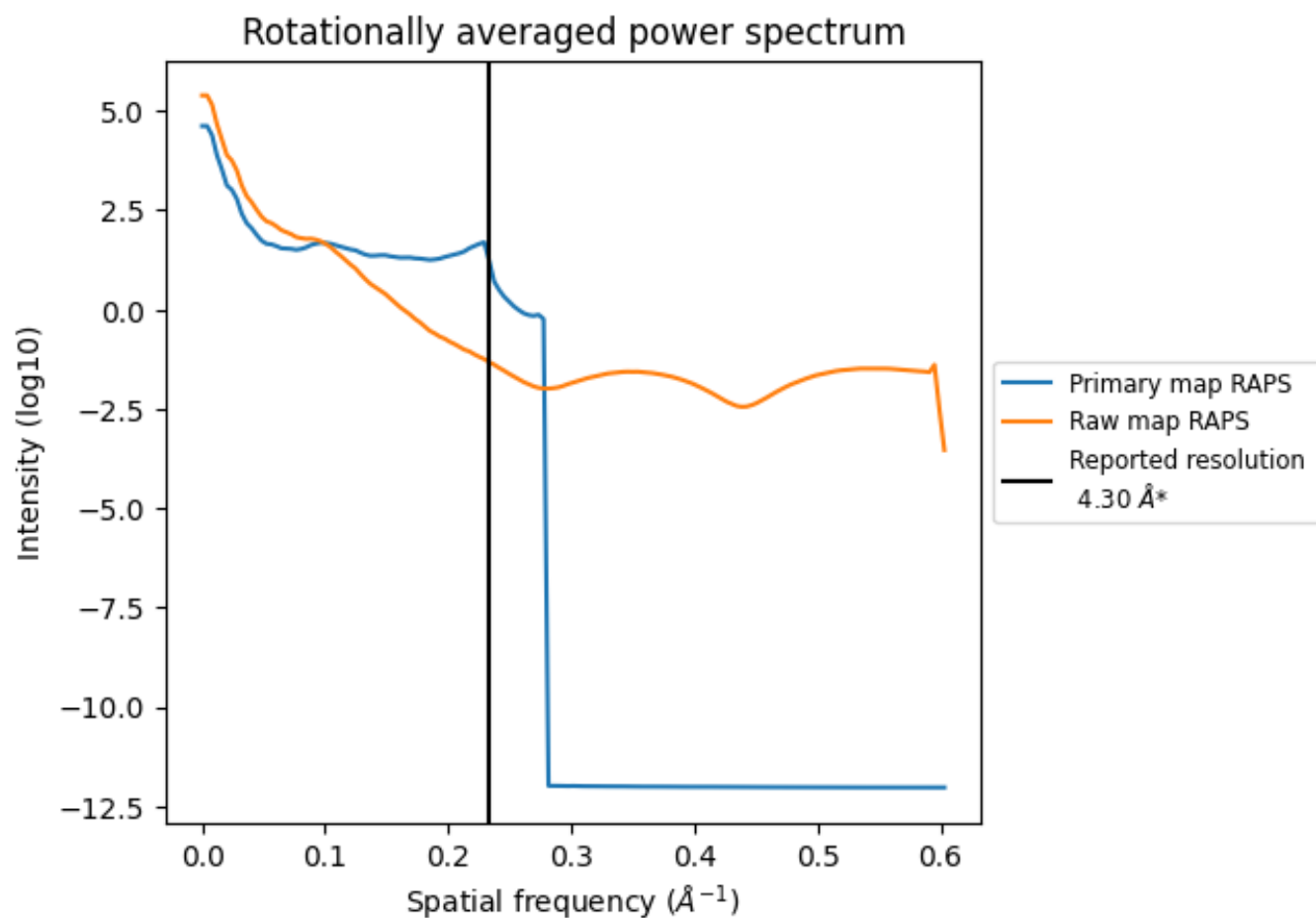
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 23 nm³; this corresponds to an approximate mass of 21 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

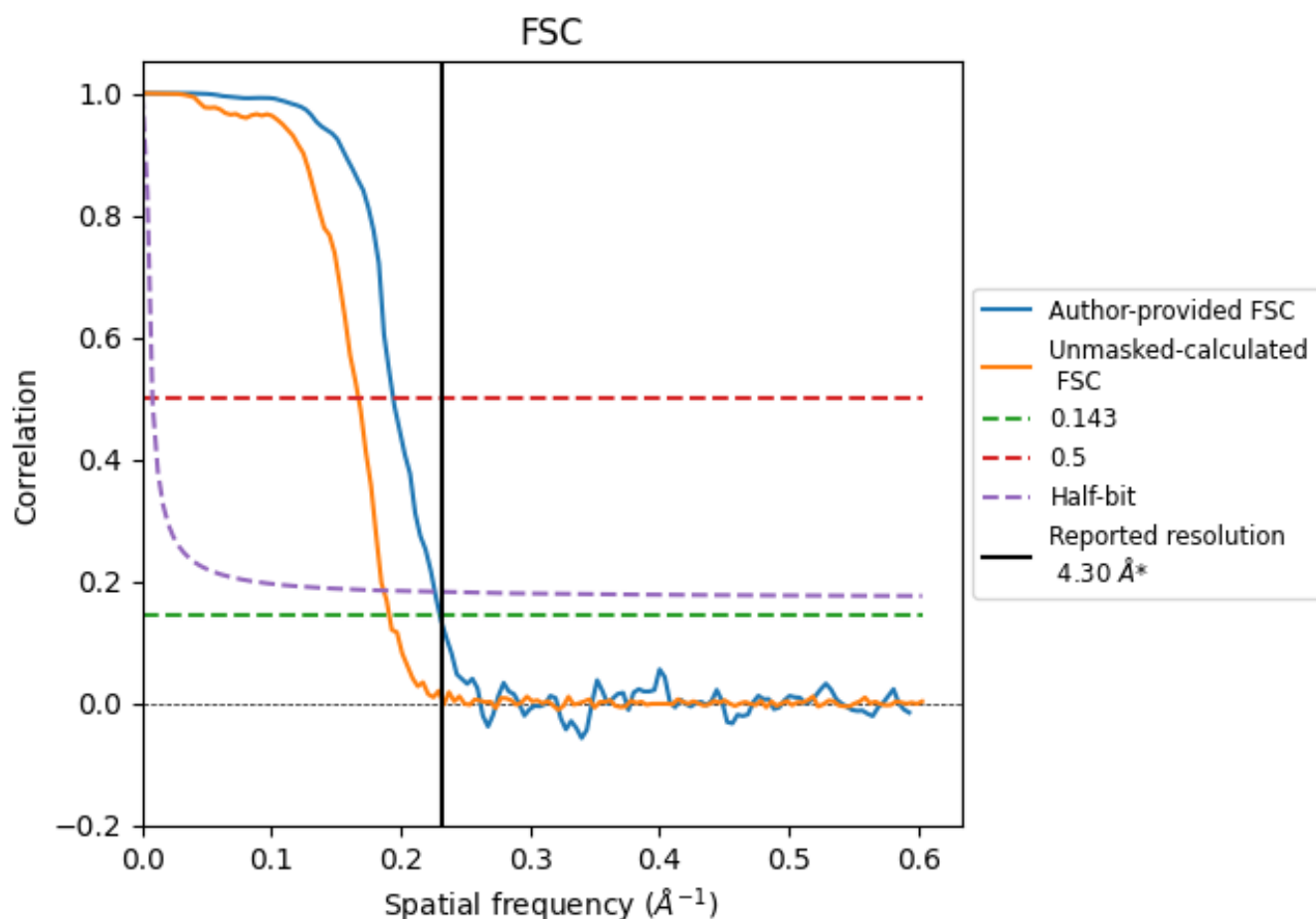


*Reported resolution corresponds to spatial frequency of 0.233 Å⁻¹

8 Fourier-Shell correlation [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 0.233 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

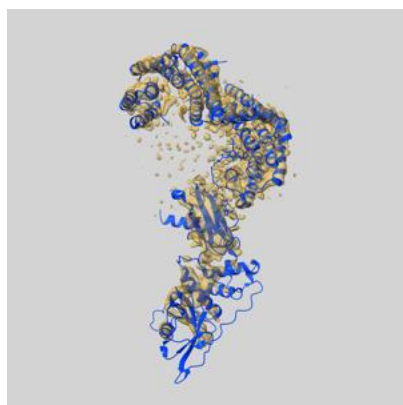
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.30	-	-
Author-provided FSC curve	4.34	5.15	4.42
Unmasked-calculated*	5.23	5.98	5.36

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 5.23 differs from the reported value 4.3 by more than 10 %

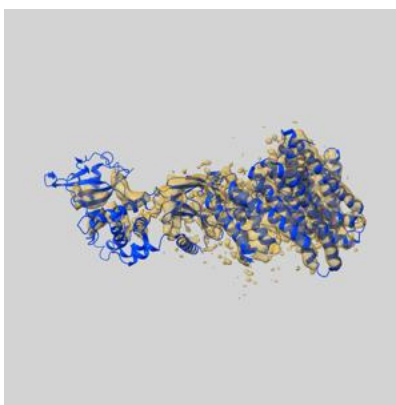
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-55233 and PDB model 9SV3. Per-residue inclusion information can be found in section 3 on page 12.

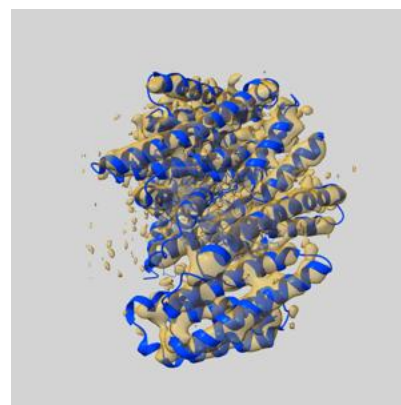
9.1 Map-model overlay [i](#)



X



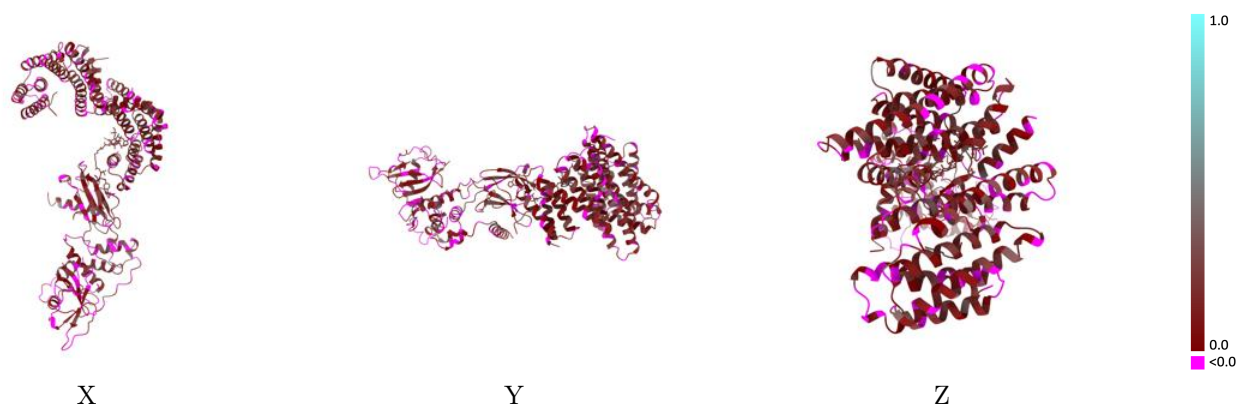
Y



Z

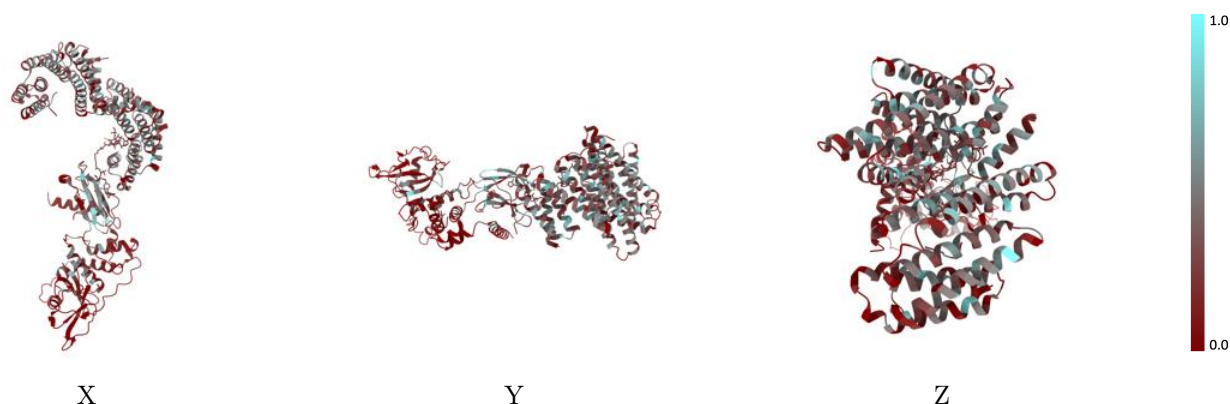
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



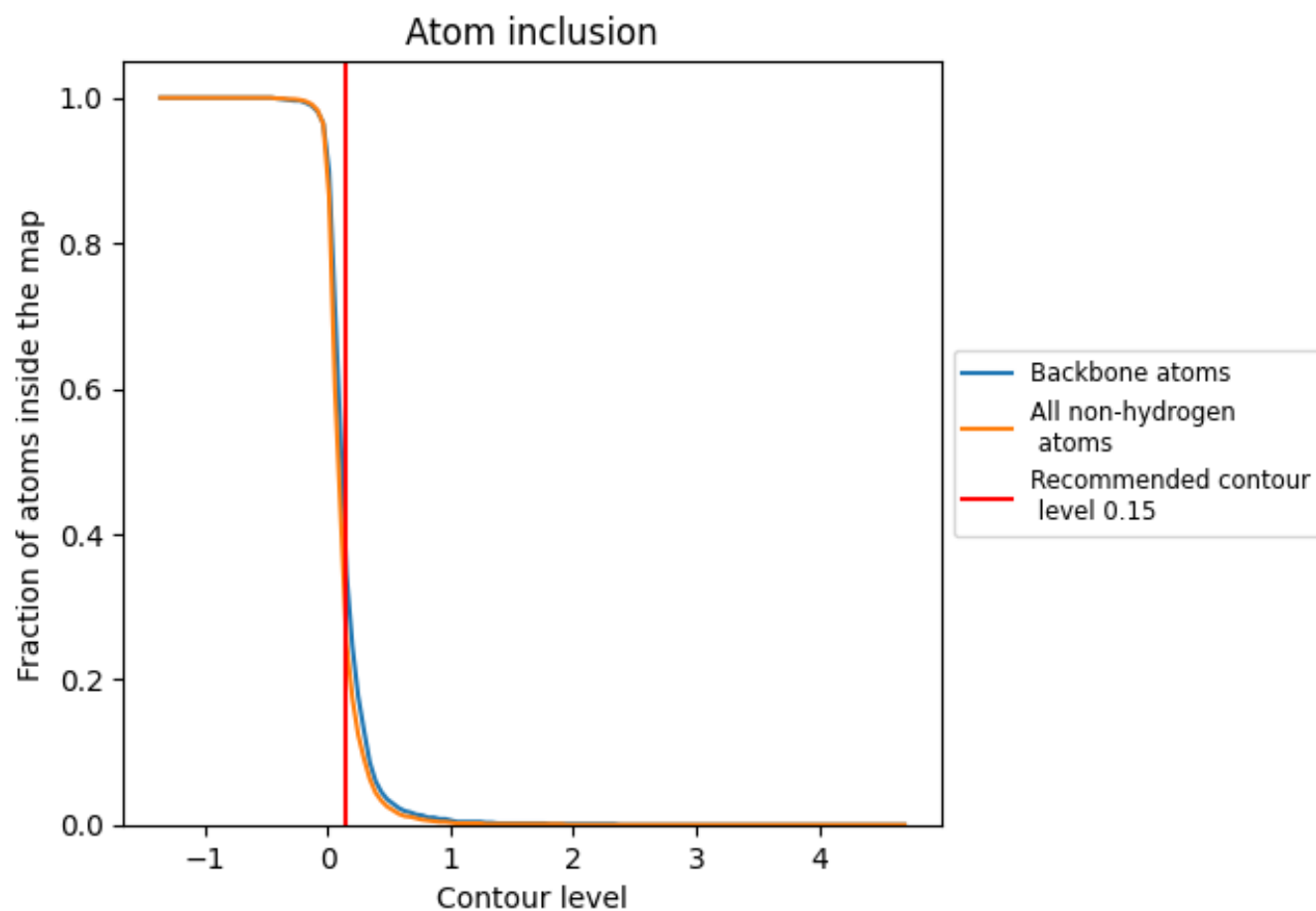
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.15).

9.4 Atom inclusion ⓘ



At the recommended contour level, 36% of all backbone atoms, 26% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.2630	0.1060
B	0.1230	0.0770
C	0.1090	0.0510
D	0.3740	0.1220
E	0.2430	0.1130
G	0.6340	0.3230
H	0.2680	0.2240
I	0.3180	0.1130

1.0

0.0

<0.0