



Full wwPDB EM Validation Report ⓘ

May 26, 2026 – 10:26 AM JST

PDB ID : 20ZL / pdb_000020zl
EMDB ID : EMD-67434
Title : Cryo-EM structure of the human neurotensin receptor 1 (hNTSR1)-Gi1 complex in the GTP-bound, AHD-open NC state 4, plunge-frozen 0-5 seconds after GTP addition
Authors : Kobayashi, K.; Matsui, T.E.; Fukuda, M.; Kawakami, K.; Yamashita, K.; Kato, H.E.
Deposited on : 2025-12-03
Resolution : 3.10 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:

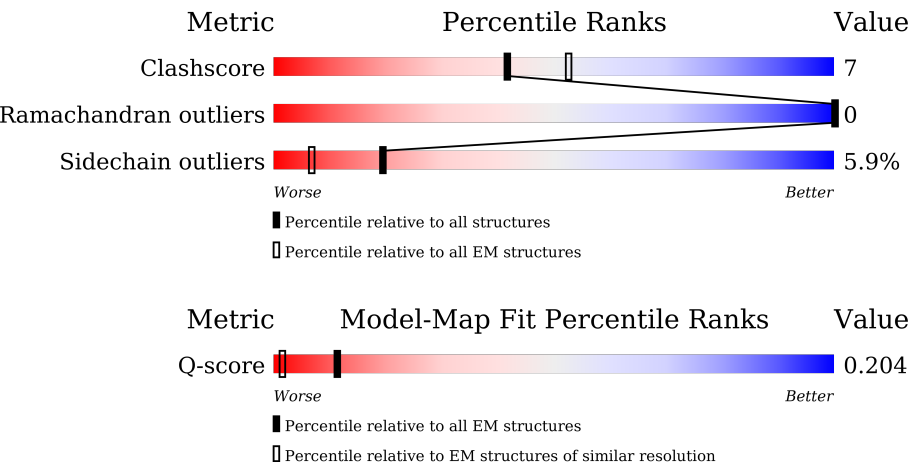
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using 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) : 2.49

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 3.10 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	14724 (2.60 - 3.60)

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	R	436	
2	L	6	
3	A	354	
4	B	358	

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Mol	Chain	Length	Quality of chain
5	C	71	<div><div></div><div>73%</div><div></div><div>25%</div></div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6904 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 Neurotensin receptor type 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	280	Total	C	N	O	S	0	0
			2171	1429	356	373	13		

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	-11	MET	-	initiating methionine	UNP P30989
R	-10	GLY	-	expression tag	UNP P30989
R	-9	GLN	-	expression tag	UNP P30989
R	-8	PRO	-	expression tag	UNP P30989
R	-7	GLY	-	expression tag	UNP P30989
R	-6	ASN	-	expression tag	UNP P30989
R	-5	GLY	-	expression tag	UNP P30989
R	-4	SER	-	expression tag	UNP P30989
R	-3	ALA	-	expression tag	UNP P30989
R	-2	PHE	-	expression tag	UNP P30989
R	-1	LEU	-	expression tag	UNP P30989
R	0	LEU	-	expression tag	UNP P30989
R	1	ALA	-	expression tag	UNP P30989
R	2	PRO	-	expression tag	UNP P30989
R	3	ASN	-	expression tag	UNP P30989
R	4	ARG	-	expression tag	UNP P30989
R	5	SER	-	expression tag	UNP P30989
R	6	HIS	-	expression tag	UNP P30989
R	7	ALA	-	expression tag	UNP P30989
R	8	PRO	-	expression tag	UNP P30989
R	9	ASP	-	expression tag	UNP P30989
R	10	HIS	-	expression tag	UNP P30989
R	11	ASP	-	expression tag	UNP P30989
R	12	VAL	-	expression tag	UNP P30989
R	13	GLU	-	expression tag	UNP P30989
R	14	ASN	-	expression tag	UNP P30989
R	15	LEU	-	expression tag	UNP P30989
R	16	TYR	-	expression tag	UNP P30989

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Chain	Residue	Modelled	Actual	Comment	Reference
R	17	PHE	-	expression tag	UNP P30989
R	18	GLN	-	expression tag	UNP P30989
R	19	GLY	-	expression tag	UNP P30989
R	85	LEU	ALA	engineered mutation	UNP P30989
R	419	LEU	-	expression tag	UNP P30989
R	420	GLU	-	expression tag	UNP P30989
R	421	VAL	-	expression tag	UNP P30989
R	422	LEU	-	expression tag	UNP P30989
R	423	PHE	-	expression tag	UNP P30989
R	424	GLN	-	expression tag	UNP P30989

- Molecule 2 is a protein called LYS-LYS-PRO-TYR-ILE-LEU.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	L	6	Total	C	N	O	0	0
			53	38	8	7		

- Molecule 3 is a protein called Guanine nucleotide-binding protein G(i) subunit alpha-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	218	Total	C	N	O	S	0	0
			1710	1086	286	327	11		

- Molecule 4 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B	338	Total	C	N	O	S	0	0
			2534	1566	453	497	18		

There are 19 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-17	MET	-	initiating methionine	UNP P62873
B	-16	HIS	-	expression tag	UNP P62873
B	-15	HIS	-	expression tag	UNP P62873
B	-14	HIS	-	expression tag	UNP P62873
B	-13	HIS	-	expression tag	UNP P62873
B	-12	HIS	-	expression tag	UNP P62873
B	-11	HIS	-	expression tag	UNP P62873
B	-10	LEU	-	expression tag	UNP P62873
B	-9	GLU	-	expression tag	UNP P62873

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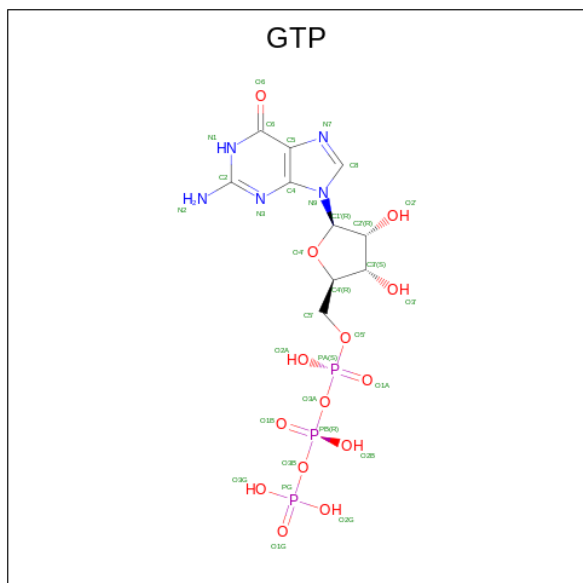
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-8	VAL	-	expression tag	UNP P62873
B	-7	LEU	-	expression tag	UNP P62873
B	-6	PHE	-	expression tag	UNP P62873
B	-5	GLN	-	expression tag	UNP P62873
B	-4	GLY	-	expression tag	UNP P62873
B	-3	PRO	-	expression tag	UNP P62873
B	-2	GLY	-	expression tag	UNP P62873
B	-1	SER	-	expression tag	UNP P62873
B	0	SER	-	expression tag	UNP P62873
B	1	GLY	-	expression tag	UNP P62873

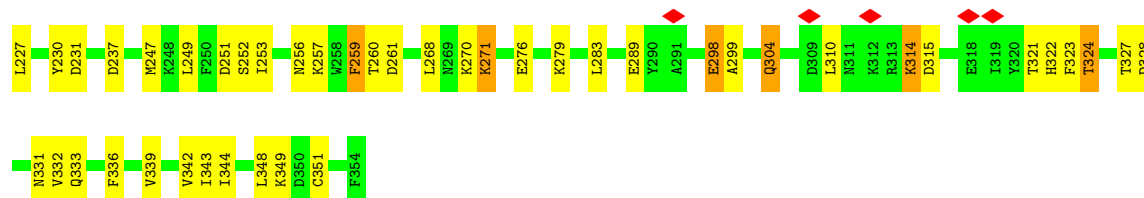
- Molecule 5 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	C	53	Total	C	N	O	S	0	0
			404	256	70	75	3		

- Molecule 6 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$) (labeled as "Ligand of Interest" by depositor).

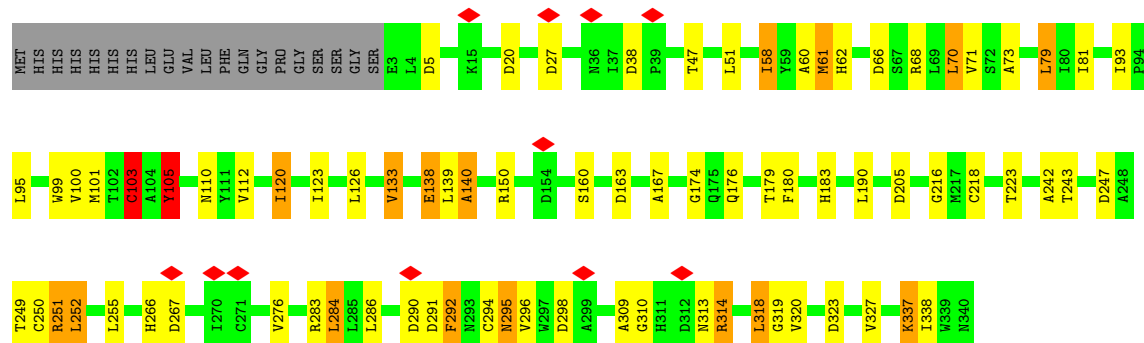


Mol	Chain	Residues	Atoms					AltConf
6	A	1	Total	C	N	O	P	0
			32	10	5	14	3	



• Molecule 4: Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1

Chain B: 72% 17% 6%



• Molecule 5: Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2

Chain C: 73% 25%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	75229	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.230	Depositor
Minimum map value	0.000	Depositor
Average map value	0.012	Depositor
Map value standard deviation	0.045	Depositor
Recommended contour level	0.05	Depositor
Map size (\AA)	163.23329, 163.23329, 163.23329	wwPDB
Map dimensions	118, 118, 118	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.383333, 1.383333, 1.383333	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: GTP

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	R	0.77	3/2226 (0.1%)	1.71	37/3048 (1.2%)
2	L	0.87	0/54	1.25	0/69
3	A	0.76	0/1738	1.77	26/2336 (1.1%)
4	B	0.78	1/2579 (0.0%)	1.60	40/3505 (1.1%)
5	C	0.69	0/410	1.46	0/554
All	All	0.76	4/7007 (0.1%)	1.67	103/9512 (1.1%)

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	R	0	1
4	B	0	3
5	C	0	1
All	All	0	5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	R	330	SER	CA-CB	8.53	1.66	1.53
4	B	183	HIS	CE1-NE2	-6.21	1.26	1.32
1	R	332	GLU	CA-CB	5.36	1.61	1.53
1	R	332	GLU	CA-C	5.13	1.59	1.52

All (103) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	330	SER	CB-CA-C	12.38	130.68	109.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	332	GLU	CB-CA-C	11.29	128.88	110.81
4	B	292	PHE	CA-CB-CG	11.01	124.81	113.80
4	B	163	ASP	CA-CB-CG	10.71	123.31	112.60
1	R	331	ASP	CA-C-N	10.30	134.45	120.54
1	R	331	ASP	C-N-CA	10.30	134.45	120.54
1	R	59	ASP	CA-CB-CG	9.31	121.91	112.60
3	A	276	GLU	CB-CG-CD	9.22	128.27	112.60
4	B	251	ARG	NE-CZ-NH1	-9.04	112.46	121.50
3	A	43	GLU	CB-CA-C	9.04	123.97	111.86
4	B	290	ASP	CA-CB-CG	9.03	121.63	112.60
3	A	271	LYS	CB-CA-C	-8.67	96.12	110.85
4	B	291	ASP	CA-CB-CG	8.21	120.81	112.60
1	R	75	VAL	N-CA-CB	8.10	119.45	110.62
4	B	70	LEU	N-CA-CB	-8.04	97.36	110.71
4	B	27	ASP	CA-CB-CG	7.88	120.48	112.60
4	B	79	LEU	N-CA-CB	-7.67	98.73	110.77
3	A	257	LYS	CB-CA-C	-7.65	98.58	110.81
3	A	315	ASP	CA-CB-CG	7.53	120.13	112.60
4	B	103	CYS	CB-CA-C	-7.51	92.89	109.56
3	A	271	LYS	N-CA-CB	7.22	120.85	110.16
1	R	166	ARG	CA-CB-CG	7.13	128.36	114.10
3	A	188	HIS	CB-CA-C	7.12	123.62	110.10
1	R	79	VAL	N-CA-CB	7.07	118.04	110.62
4	B	110	ASN	CB-CA-C	6.98	120.75	111.82
4	B	66	ASP	CB-CA-C	-6.97	97.73	110.63
4	B	105	TYR	CB-CA-C	6.92	121.23	109.53
1	R	239	VAL	CA-CB-CG1	6.87	122.08	110.40
1	R	348	VAL	N-CA-CB	6.85	119.86	110.54
1	R	330	SER	N-CA-CB	-6.83	99.28	110.41
4	B	251	ARG	NE-CZ-NH2	6.81	125.33	119.20
4	B	140	ALA	N-CA-C	6.79	121.53	112.30
1	R	364	TYR	N-CA-CB	6.62	119.67	110.07
1	R	58	THR	OG1-CB-CG2	-6.55	96.20	109.30
4	B	267	ASP	CA-CB-CG	6.55	119.15	112.60
4	B	323	ASP	CA-CB-CG	6.51	119.11	112.60
4	B	251	ARG	CG-CD-NE	-6.50	97.71	112.00
4	B	68	ARG	NE-CZ-NH2	6.49	125.04	119.20
1	R	372	ARG	N-CA-CB	6.46	119.56	109.94
3	A	188	HIS	CA-CB-CG	6.39	120.19	113.80
4	B	314	ARG	CB-CA-C	-6.34	102.00	109.80
1	R	238	GLN	CB-CA-C	-6.29	100.36	110.79
3	A	260	THR	CA-CB-OG1	-6.26	100.21	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	215	ASP	CA-CB-CG	6.19	118.79	112.60
3	A	259	PHE	N-CA-CB	-6.18	103.24	110.35
3	A	324	THR	CA-CB-OG1	-6.18	100.34	109.60
4	B	205	ASP	CA-CB-CG	6.17	118.77	112.60
3	A	279	LYS	CA-CB-CG	6.16	126.41	114.10
1	R	104	HIS	CB-CG-ND1	6.14	131.91	122.70
4	B	163	ASP	N-CA-CB	-6.07	101.12	110.46
3	A	188	HIS	CB-CG-CD2	-6.01	123.38	131.20
3	A	279	LYS	N-CA-CB	6.01	119.05	110.16
4	B	138	GLU	N-CA-CB	-5.96	100.85	110.69
1	R	58	THR	CA-CB-CG2	5.94	120.60	110.50
4	B	283	ARG	NE-CZ-NH1	-5.91	115.59	121.50
4	B	283	ARG	NE-CZ-NH2	5.91	124.52	119.20
1	R	332	GLU	CB-CG-CD	5.90	122.63	112.60
3	A	261	ASP	CA-CB-CG	5.85	118.45	112.60
4	B	223	THR	CB-CA-C	5.82	120.32	111.76
3	A	279	LYS	CB-CG-CD	5.81	124.66	111.30
3	A	322	HIS	CA-CB-CG	5.80	119.60	113.80
4	B	58	ILE	CA-CB-CG1	5.80	120.26	110.40
4	B	20	ASP	CA-CB-CG	5.77	118.37	112.60
4	B	266	HIS	CA-CB-CG	5.75	119.55	113.80
1	R	104	HIS	CB-CG-CD2	-5.70	123.78	131.20
3	A	298	GLU	CG-CD-OE2	5.69	131.48	118.40
4	B	295	ASN	CB-CA-C	-5.67	99.92	109.72
1	R	51	SER	CA-C-N	5.65	128.17	120.54
1	R	51	SER	C-N-CA	5.65	128.17	120.54
4	B	255	LEU	N-CA-CB	-5.61	101.82	110.13
3	A	257	LYS	N-CA-CB	5.59	118.27	109.94
1	R	372	ARG	CG-CD-NE	-5.56	99.76	112.00
3	A	349	LYS	CB-CA-C	-5.56	101.22	110.68
4	B	223	THR	OG1-CB-CG2	5.56	120.42	109.30
1	R	264	THR	CA-CB-OG1	5.53	117.90	109.60
4	B	38	ASP	CB-CA-C	5.50	117.32	108.91
4	B	66	ASP	CA-CB-CG	5.46	118.06	112.60
1	R	66	VAL	CA-CB-CG1	5.42	119.61	110.40
3	A	193	ASP	CA-CB-CG	5.40	118.00	112.60
3	A	289	GLU	CB-CG-CD	5.40	121.78	112.60
1	R	372	ARG	NE-CZ-NH1	-5.39	116.11	121.50
1	R	368	SER	N-CA-C	5.38	116.82	111.07
4	B	5	ASP	CA-CB-CG	5.34	117.94	112.60
1	R	330	SER	CA-C-N	5.34	128.18	120.38
1	R	330	SER	C-N-CA	5.34	128.18	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	375	PHE	CA-CB-CG	5.33	119.13	113.80
4	B	337	LYS	CB-CG-CD	5.33	123.56	111.30
3	A	251	ASP	CA-CB-CG	5.31	117.91	112.60
3	A	237	ASP	CA-CB-CG	5.29	117.89	112.60
1	R	124	LEU	N-CA-CB	-5.25	101.84	109.82
4	B	318	LEU	N-CA-CB	-5.21	102.76	110.37
1	R	306	ARG	NE-CZ-NH2	5.18	123.86	119.20
3	A	231	ASP	CA-CB-CG	5.17	117.77	112.60
1	R	52	SER	CB-CA-C	-5.16	102.56	110.81
4	B	252	LEU	CB-CA-C	5.13	117.96	110.26
1	R	364	TYR	CA-C-O	-5.09	115.45	120.70
1	R	306	ARG	NE-CZ-NH1	-5.09	116.41	121.50
1	R	200	ALA	CA-C-N	5.05	123.42	120.24
1	R	200	ALA	C-N-CA	5.05	123.42	120.24
4	B	120	ILE	CB-CA-C	5.04	116.98	110.12
4	B	309	ALA	CA-C-N	5.04	125.54	119.94
4	B	309	ALA	C-N-CA	5.04	125.54	119.94
3	A	314	LYS	CB-CG-CD	5.01	122.83	111.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	B	150	ARG	Sidechain
4	B	251	ARG	Sidechain
4	B	310	GLY	Peptide
5	C	27	ARG	Sidechain
1	R	372	ARG	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	R	2171	0	2161	22	0
2	L	53	0	63	0	0
3	A	1710	0	1665	40	0
4	B	2534	0	2403	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	404	0	416	0	0
6	A	32	0	12	0	0
All	All	6904	0	6720	92	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 7.

All (92) 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)
4:B:286:LEU:HD13	4:B:296:VAL:HG22	1.65	0.79
3:A:50:VAL:HG22	3:A:198:MET:HE3	1.67	0.77
3:A:191:PHE:CZ	3:A:333:GLN:HG2	2.20	0.75
3:A:48:THR:HG21	3:A:270:LYS:HE2	1.68	0.75
3:A:304:GLN:CG	3:A:321:THR:HG21	2.20	0.72
1:R:235:VAL:O	1:R:239:VAL:HG12	1.90	0.71
1:R:369:ALA:HA	1:R:372:ARG:HG2	1.74	0.68
3:A:49:ILE:O	3:A:331:ASN:ND2	2.27	0.66
1:R:235:VAL:O	1:R:239:VAL:CG1	2.43	0.66
4:B:120:ILE:HD11	4:B:138:GLU:HB3	1.78	0.65
4:B:51:LEU:HD11	4:B:338:ILE:HD11	1.80	0.64
3:A:214:CYS:SG	4:B:101:MET:SD	2.96	0.64
1:R:52:SER:OG	1:R:53:GLU:N	2.30	0.63
4:B:247:ASP:OD2	4:B:249:THR:OG1	2.16	0.62
3:A:41:ALA:HA	3:A:249:LEU:HD23	1.80	0.62
3:A:52:GLN:HG2	3:A:328:ASP:H	1.65	0.60
3:A:52:GLN:HG2	3:A:328:ASP:N	2.17	0.59
3:A:46:LYS:HA	3:A:49:ILE:HG22	1.83	0.59
3:A:304:GLN:HG3	3:A:321:THR:HG21	1.85	0.58
3:A:52:GLN:HB3	3:A:328:ASP:O	2.04	0.57
3:A:194:LEU:HD13	3:A:336:PHE:CE2	2.40	0.56
3:A:271:LYS:HE2	3:A:323:PHE:HB3	1.86	0.56
4:B:81:ILE:HD11	4:B:126:LEU:HD22	1.87	0.56
3:A:194:LEU:HD13	3:A:336:PHE:HE2	1.70	0.56
1:R:159:VAL:HG12	1:R:252:ILE:HD11	1.87	0.55
3:A:304:GLN:CD	3:A:321:THR:HG21	2.32	0.55
4:B:120:ILE:HD12	4:B:140:ALA:HB2	1.88	0.55
3:A:344:ILE:O	3:A:348:LEU:HD13	2.08	0.54
4:B:320:VAL:HG22	4:B:327:VAL:HG22	1.89	0.54
1:R:325:MET:HG2	1:R:329:ILE:HD12	1.90	0.53
3:A:52:GLN:HG2	3:A:327:THR:HA	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:105:LEU:HD11	1:R:364:TYR:HB3	1.92	0.52
1:R:245:PHE:HB2	1:R:320:HIS:ND1	2.25	0.52
3:A:212:ILE:HG23	3:A:259:PHE:CZ	2.45	0.52
3:A:339:VAL:HA	3:A:342:VAL:HG12	1.92	0.51
4:B:95:LEU:HD13	4:B:100:VAL:HG21	1.93	0.50
1:R:237:ILE:HD12	1:R:327:CYS:HB2	1.94	0.50
1:R:107:SER:OG	1:R:193:TRP:NE1	2.43	0.50
4:B:284:LEU:HD12	4:B:298:ASP:HA	1.95	0.49
4:B:93:ILE:HG23	4:B:133:VAL:HB	1.95	0.49
1:R:156:ALA:HB1	1:R:248:PRO:HG3	1.96	0.48
4:B:60:ALA:HB1	4:B:103:CYS:HB2	1.95	0.48
1:R:77:GLY:CA	1:R:358:THR:HG22	2.45	0.47
3:A:52:GLN:HB3	3:A:331:ASN:HB2	1.96	0.47
4:B:167:ALA:HB1	4:B:176:GLN:HB2	1.96	0.47
4:B:73:ALA:HB2	4:B:79:LEU:HD13	1.97	0.47
4:B:112:VAL:HG22	4:B:126:LEU:HD21	1.97	0.47
3:A:49:ILE:HG12	3:A:331:ASN:HD21	1.80	0.46
3:A:212:ILE:HD12	3:A:259:PHE:CE2	2.50	0.46
4:B:139:LEU:HD22	4:B:174:GLY:HA2	1.98	0.46
4:B:286:LEU:HD12	4:B:295:ASN:O	2.15	0.46
1:R:66:VAL:HG21	1:R:347:MET:HB3	1.96	0.46
3:A:33:GLU:HG3	3:A:195:HIS:HB3	1.98	0.46
4:B:61:MET:HE1	4:B:319:GLY:HA3	1.97	0.46
1:R:99:SER:HA	1:R:102:HIS:CD2	2.51	0.46
4:B:286:LEU:HG	4:B:318:LEU:HD21	1.97	0.46
3:A:210:LYS:O	3:A:213:HIS:CE1	2.69	0.46
3:A:212:ILE:HG21	3:A:256:ASN:ND2	2.31	0.46
1:R:304:VAL:HG21	1:R:366:LEU:HD11	1.97	0.45
1:R:166:ARG:HH11	3:A:351:CYS:HB3	1.81	0.45
1:R:235:VAL:O	1:R:239:VAL:HG13	2.17	0.45
4:B:242:ALA:HB1	4:B:250:CYS:SG	2.57	0.45
1:R:108:LEU:HD21	1:R:360:ASN:HB3	1.98	0.45
3:A:190:THR:HG22	3:A:195:HIS:HA	1.99	0.45
3:A:247:MET:HG3	3:A:310:LEU:HD11	1.98	0.44
3:A:52:GLN:CG	3:A:327:THR:HA	2.48	0.44
3:A:283:LEU:HD21	3:A:299:ALA:HB1	2.00	0.44
1:R:105:LEU:HD11	1:R:364:TYR:CB	2.48	0.44
4:B:71:VAL:HB	4:B:105:TYR:CD1	2.52	0.44
4:B:180:PHE:HE1	4:B:216:GLY:HA2	1.82	0.44
4:B:61:MET:HE2	4:B:62:HIS:HA	2.00	0.44
3:A:208:ARG:HH21	3:A:252:SER:CB	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:156:ALA:HB2	1:R:316:TRP:HZ3	1.83	0.43
3:A:189:PHE:CE1	3:A:332:VAL:HG23	2.53	0.43
4:B:81:ILE:HD11	4:B:126:LEU:CD2	2.49	0.43
4:B:286:LEU:HD11	4:B:294:CYS:HB3	2.01	0.43
4:B:292:PHE:HB3	4:B:314:ARG:HA	2.01	0.43
3:A:212:ILE:HG23	3:A:259:PHE:CE2	2.54	0.43
4:B:112:VAL:HG13	4:B:126:LEU:HD11	1.99	0.43
4:B:120:ILE:CD1	4:B:140:ALA:HB2	2.49	0.42
4:B:47:THR:HG23	4:B:337:LYS:HB3	2.02	0.42
3:A:227:LEU:HD13	3:A:268:LEU:HB3	2.01	0.42
3:A:44:SER:HB2	3:A:225:VAL:HA	2.02	0.42
1:R:249:MET:SD	1:R:313:VAL:HG22	2.60	0.41
3:A:247:MET:CG	3:A:310:LEU:HD11	2.51	0.41
1:R:118:LEU:HD13	1:R:147:LEU:HB3	2.03	0.41
4:B:81:ILE:CD1	4:B:126:LEU:HD22	2.50	0.41
4:B:286:LEU:HD13	4:B:296:VAL:CG2	2.45	0.41
3:A:190:THR:HG22	3:A:195:HIS:CD2	2.57	0.40
3:A:199:PHE:CE2	4:B:99:TRP:HZ2	2.39	0.40
4:B:292:PHE:HB2	4:B:313:ASN:O	2.20	0.40
3:A:38:LEU:HD13	3:A:198:MET:SD	2.62	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	R	272/436 (62%)	263 (97%)	9 (3%)	0	100	100
2	L	4/6 (67%)	4 (100%)	0	0	100	100
3	A	214/354 (60%)	204 (95%)	10 (5%)	0	100	100
4	B	336/358 (94%)	326 (97%)	10 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	C	51/71 (72%)	51 (100%)	0	0	100	100
All	All	877/1225 (72%)	848 (97%)	29 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	R	232/368 (63%)	214 (92%)	18 (8%)	11	38
2	L	6/6 (100%)	6 (100%)	0	100	100
3	A	181/305 (59%)	171 (94%)	10 (6%)	19	50
4	B	265/298 (89%)	250 (94%)	15 (6%)	18	49
5	C	42/58 (72%)	42 (100%)	0	100	100
All	All	726/1035 (70%)	683 (94%)	43 (6%)	19	48

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	R	54	LEU
1	R	66	VAL
1	R	71	LEU
1	R	75	VAL
1	R	88	LEU
1	R	99	SER
1	R	123	GLU
1	R	124	LEU
1	R	230	THR
1	R	239	VAL
1	R	253	SER
1	R	255	LEU
1	R	258	ILE
1	R	261	ASN

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Mol	Chain	Res	Type
1	R	263	LEU
1	R	264	THR
1	R	304	VAL
1	R	365	ASN
3	A	50	VAL
3	A	192	LYS
3	A	201	VAL
3	A	230	TYR
3	A	253	ILE
3	A	298	GLU
3	A	304	GLN
3	A	314	LYS
3	A	324	THR
3	A	343	ILE
4	B	58	ILE
4	B	61	MET
4	B	70	LEU
4	B	103	CYS
4	B	105	TYR
4	B	123	ILE
4	B	133	VAL
4	B	160	SER
4	B	179	THR
4	B	190	LEU
4	B	218	CYS
4	B	243	THR
4	B	252	LEU
4	B	276	VAL
4	B	284	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	R	102	HIS
1	R	172	HIS
1	R	218	HIS
1	R	365	ASN
3	A	204	GLN
3	A	213	HIS
3	A	331	ASN
3	A	333	GLN
4	B	75	GLN

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Mol	Chain	Res	Type
4	B	110	ASN
4	B	132	ASN
4	B	156	GLN
4	B	220	GLN
4	B	239	ASN
4	B	293	ASN
5	C	18	GLN
5	C	59	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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	GTP	A	401	-	30,34,34	0.74	0	46,54,54	0.91	1 (2%)

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	GTP	A	401	-	-	7/22/38/38	0/3/3/3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	401	GTP	O2A-PA-O1A	3.38	128.95	112.24

There are no chirality outliers.

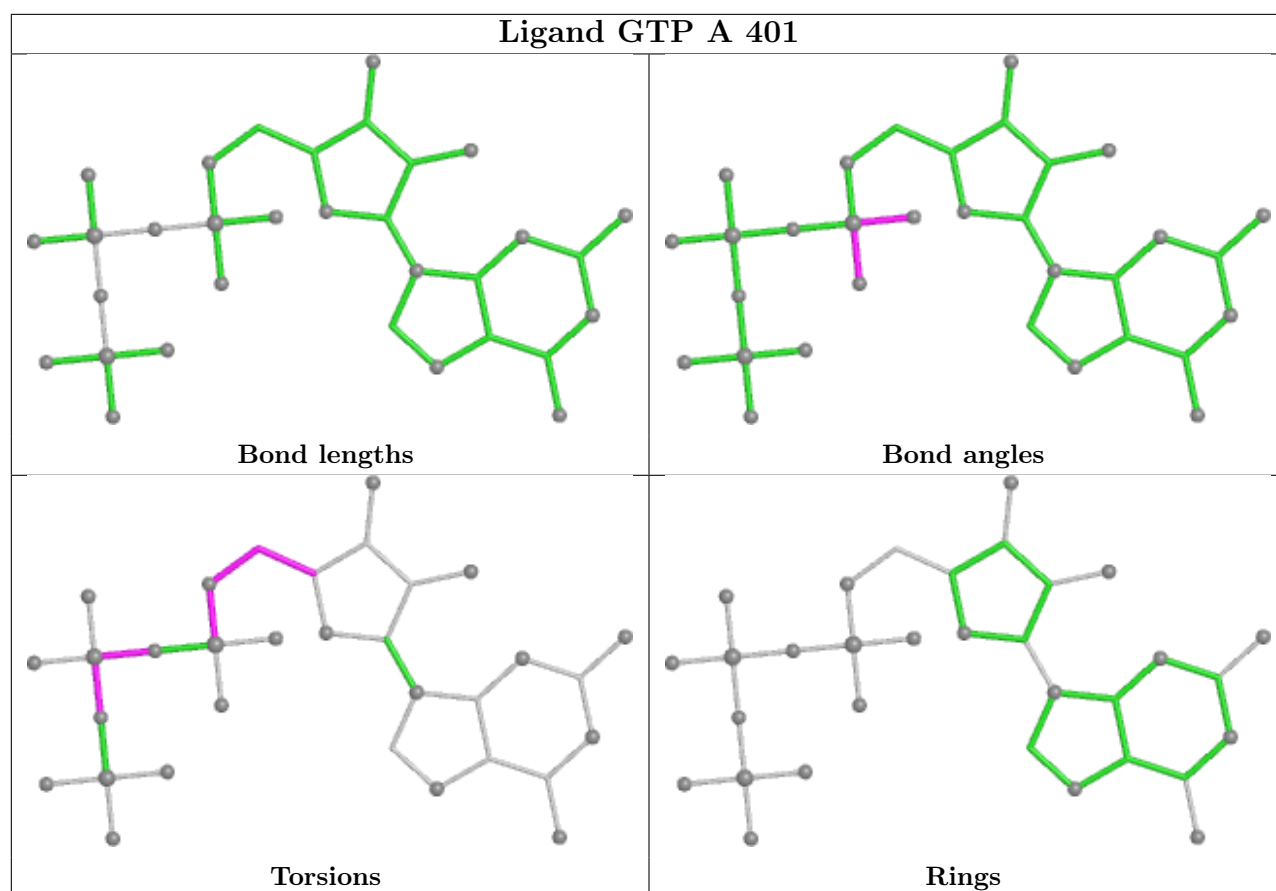
All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	401	GTP	C5'-O5'-PA-O3A
6	A	401	GTP	C5'-O5'-PA-O2A
6	A	401	GTP	O4'-C4'-C5'-O5'
6	A	401	GTP	PG-O3B-PB-O1B
6	A	401	GTP	C4'-C5'-O5'-PA
6	A	401	GTP	PA-O3A-PB-O3B
6	A	401	GTP	C3'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

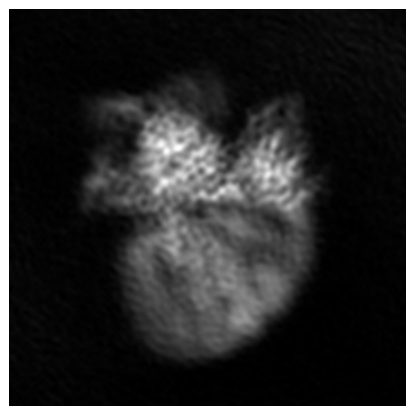
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-67434. These allow visual inspection of the internal detail of the map and identification of artifacts.

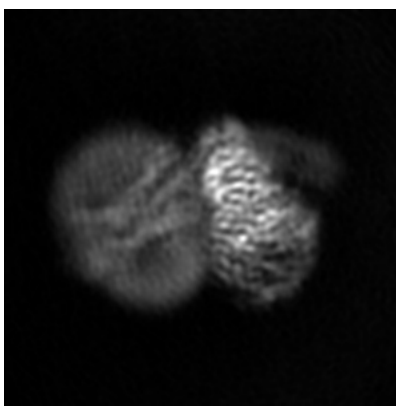
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

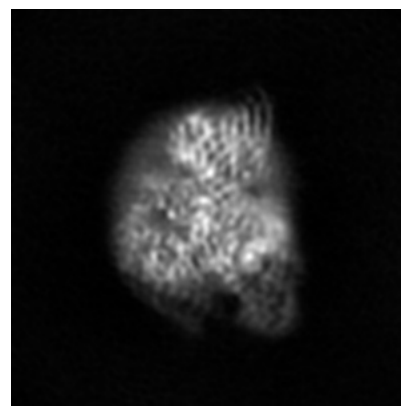
6.1.1 Primary map



X

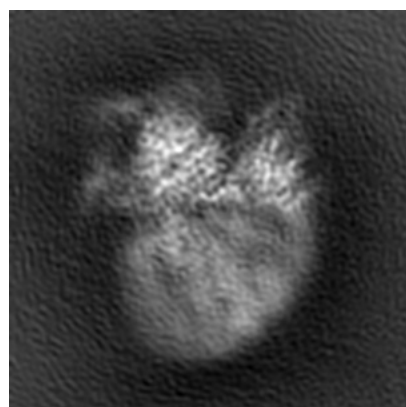


Y

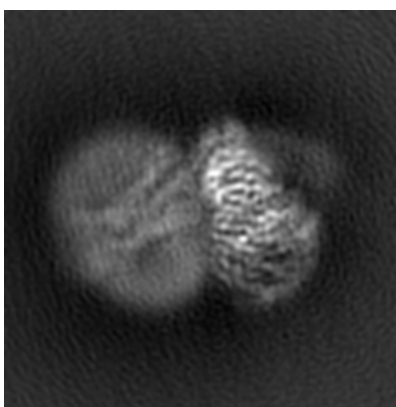


Z

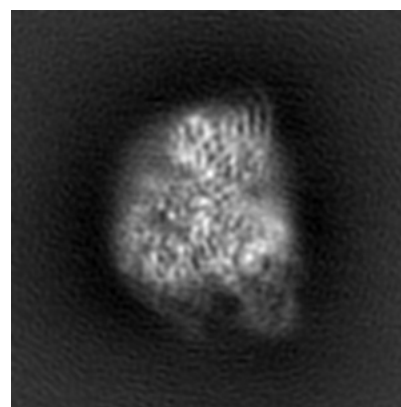
6.1.2 Raw map



X



Y

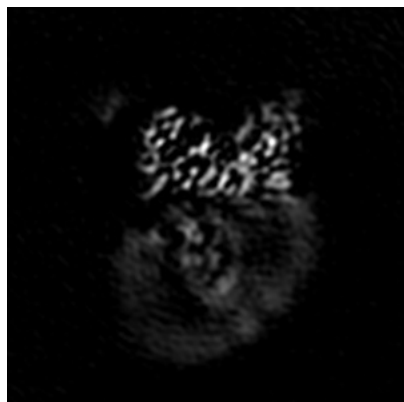


Z

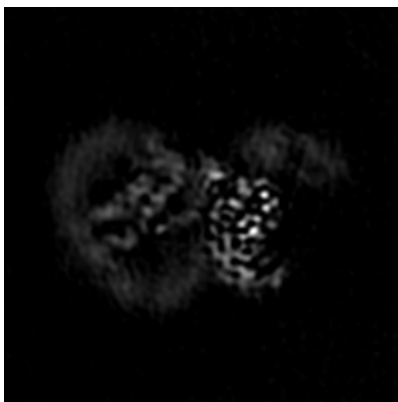
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

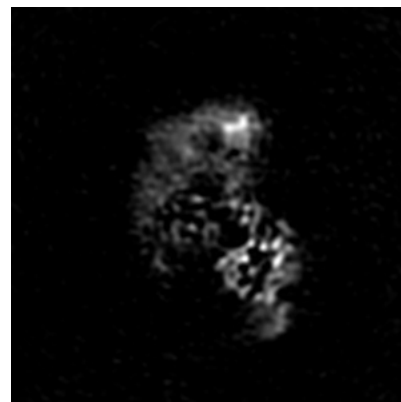
6.2.1 Primary map



X Index: 59

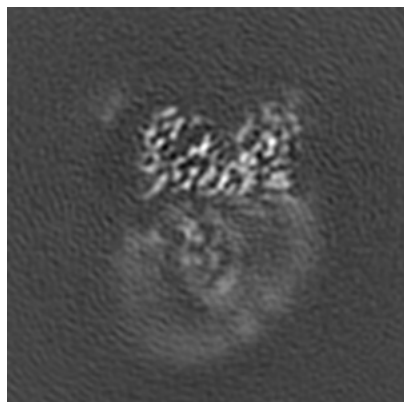


Y Index: 59

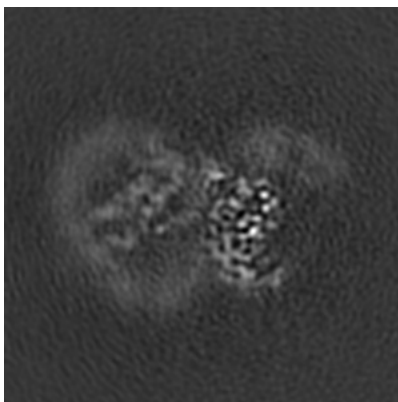


Z Index: 59

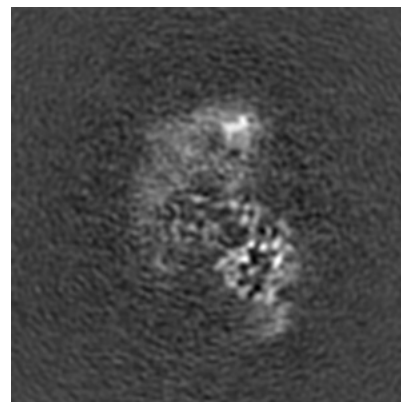
6.2.2 Raw map



X Index: 59



Y Index: 59

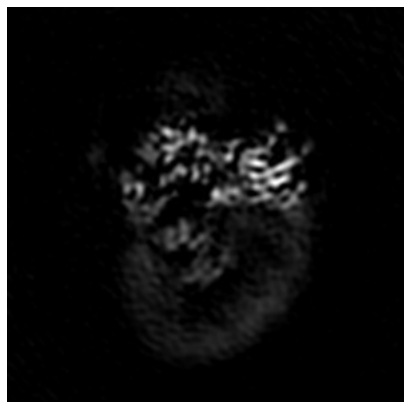


Z Index: 59

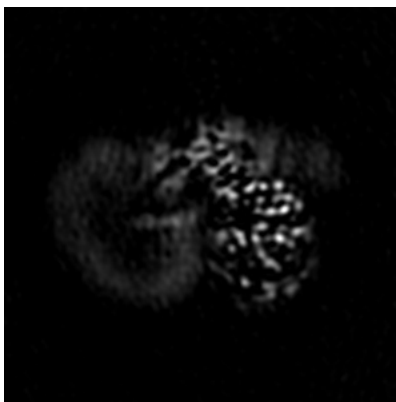
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

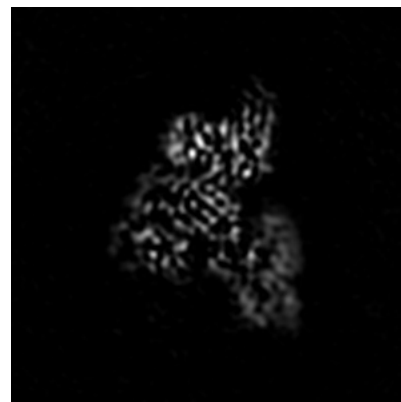
6.3.1 Primary map



X Index: 65

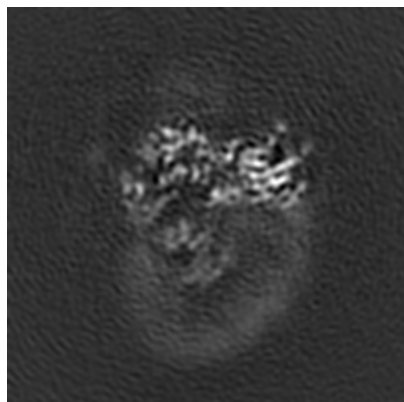


Y Index: 47

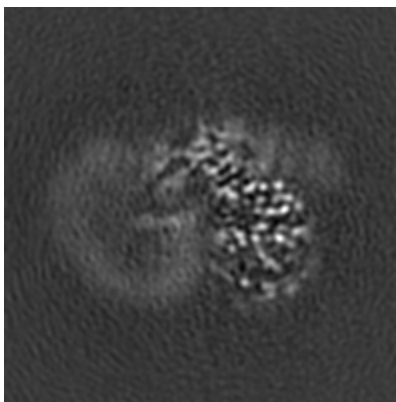


Z Index: 69

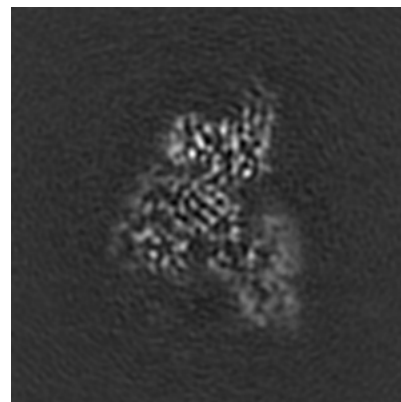
6.3.2 Raw map



X Index: 65



Y Index: 47

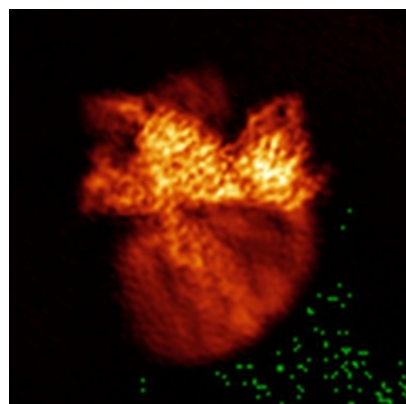


Z Index: 69

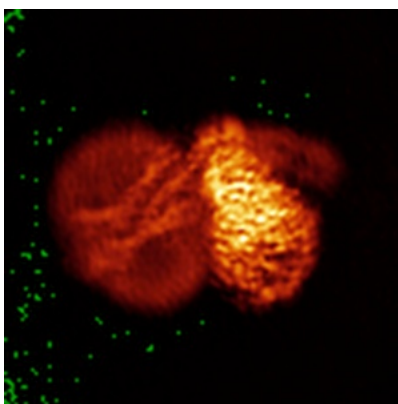
The images above show the largest variance slices of the map in three orthogonal directions.

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

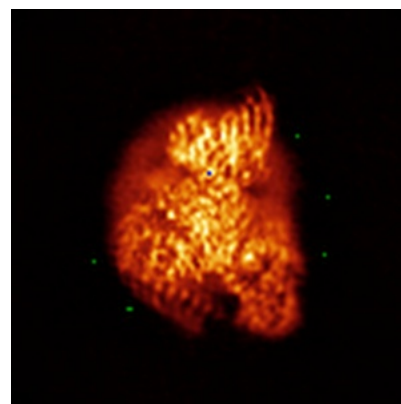
6.4.1 Primary map



X

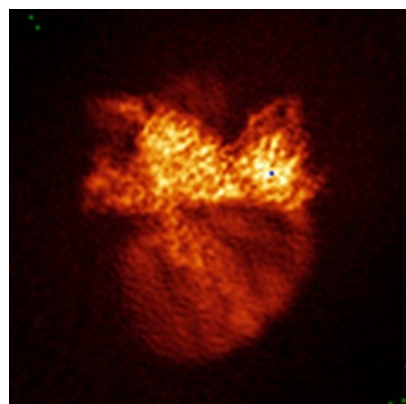


Y

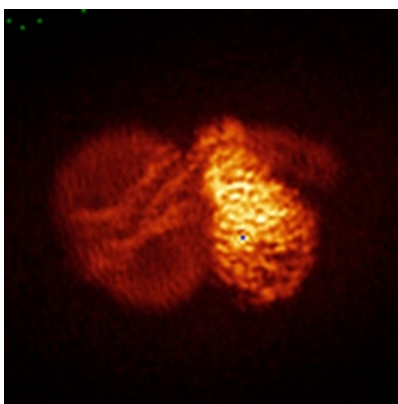


Z

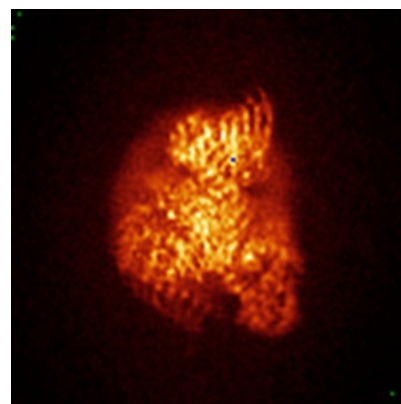
6.4.2 Raw map



X



Y

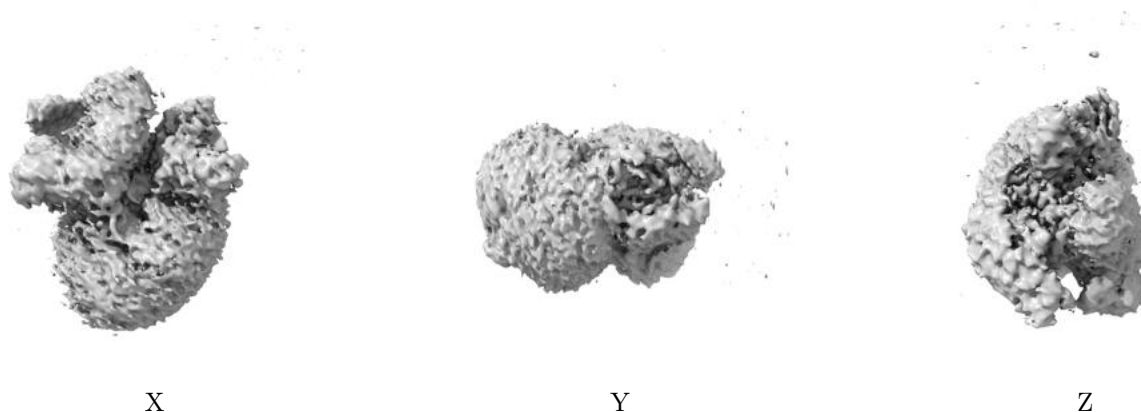


Z

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.

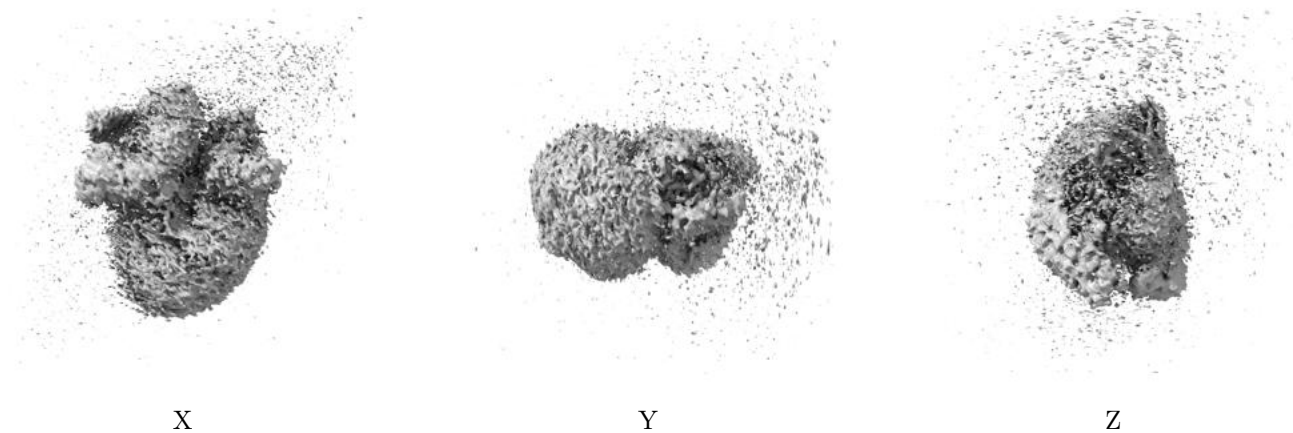
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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.

6.5.2 Raw map



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.

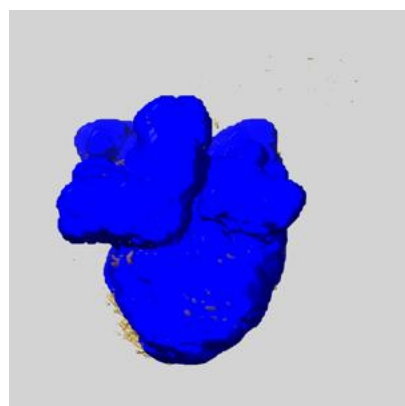
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

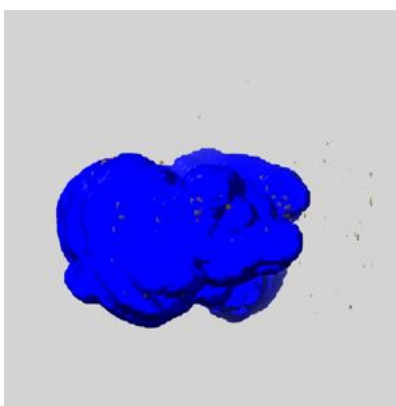
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

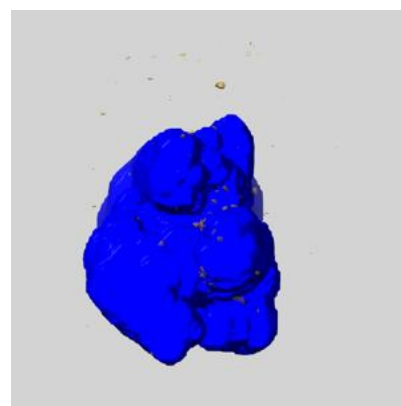
6.6.1 emd_67434_msk_1.map [i](#)



X



Y

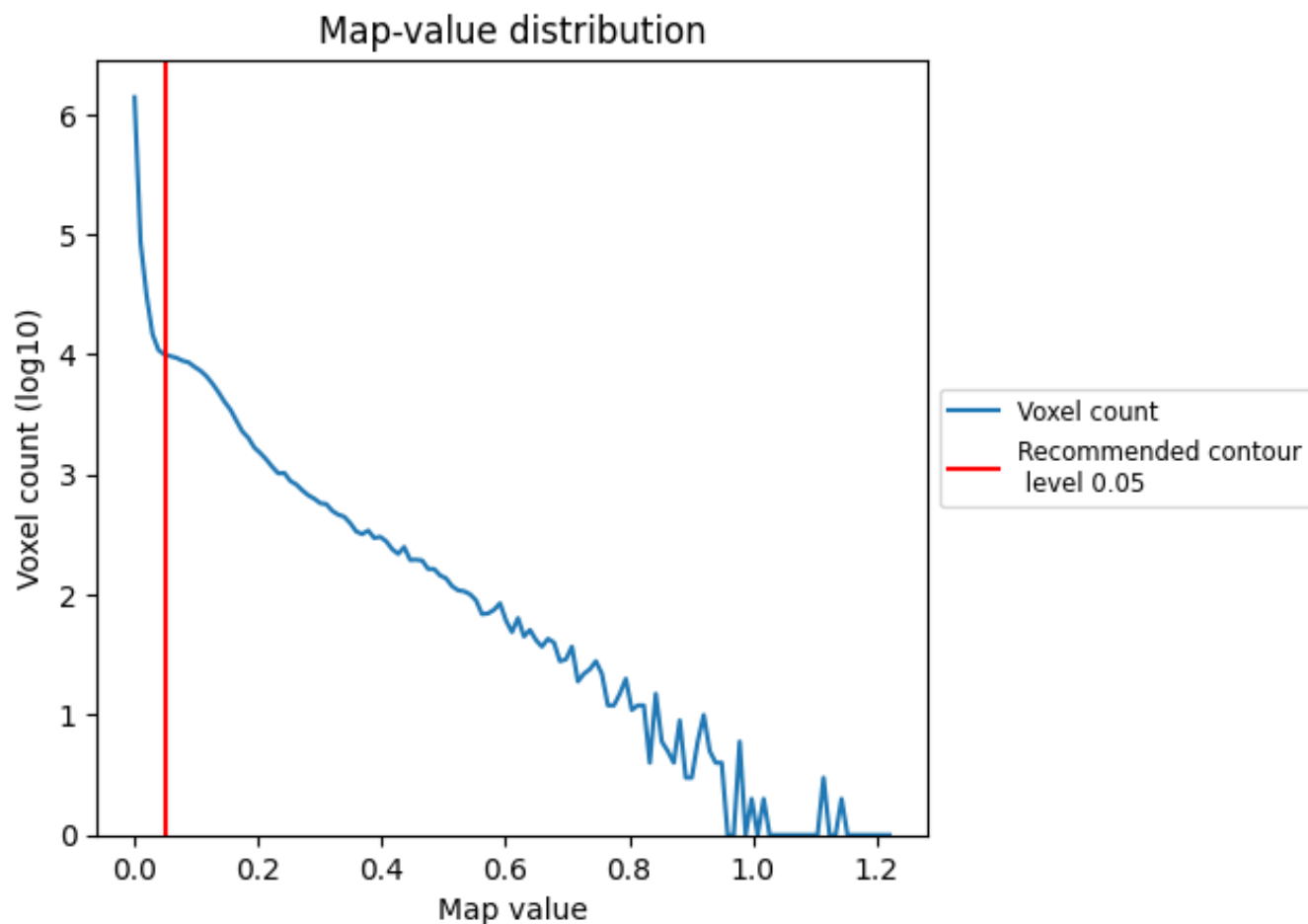


Z

7 Map analysis [i](#)

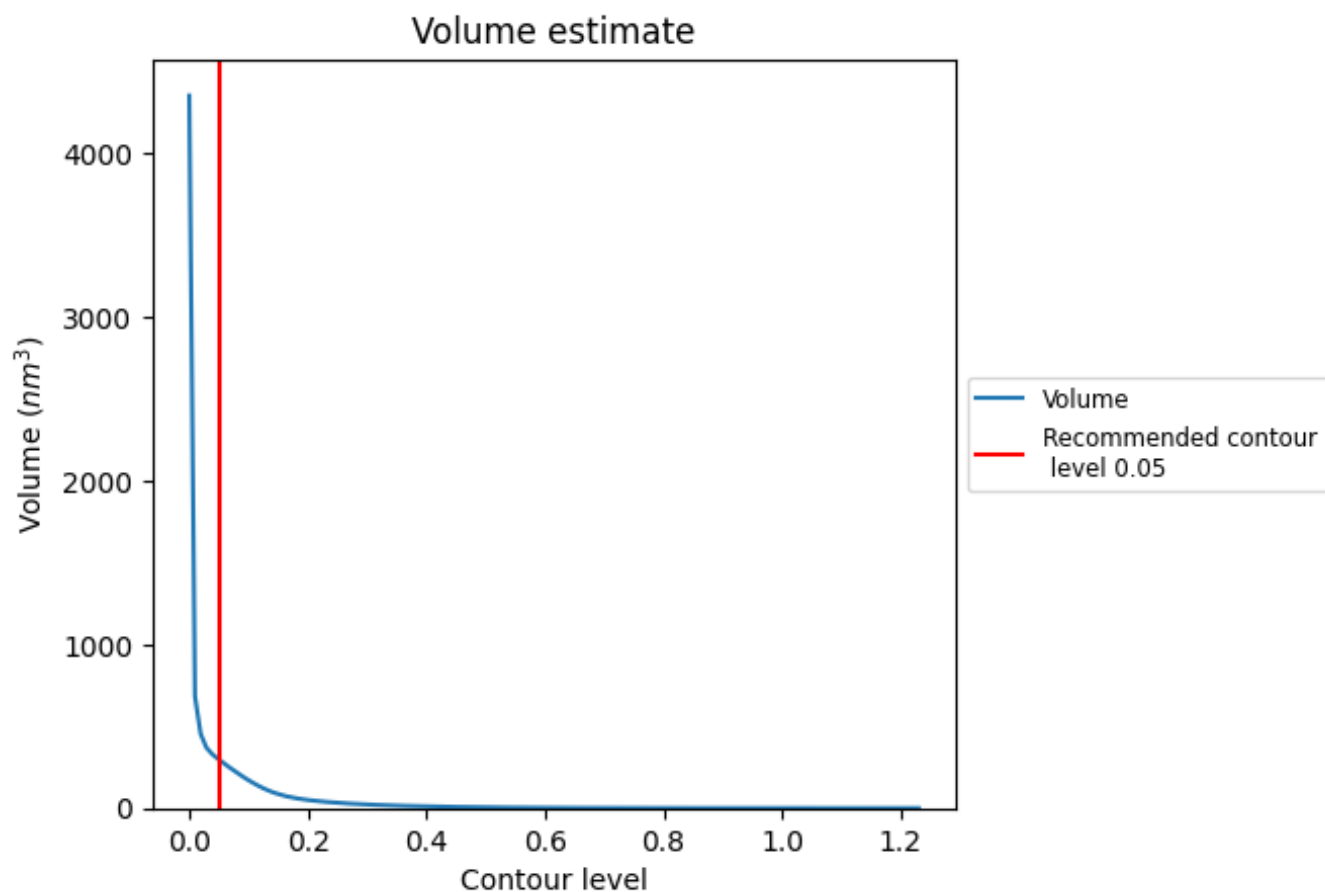
This section contains the results of statistical analysis of the map.

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.

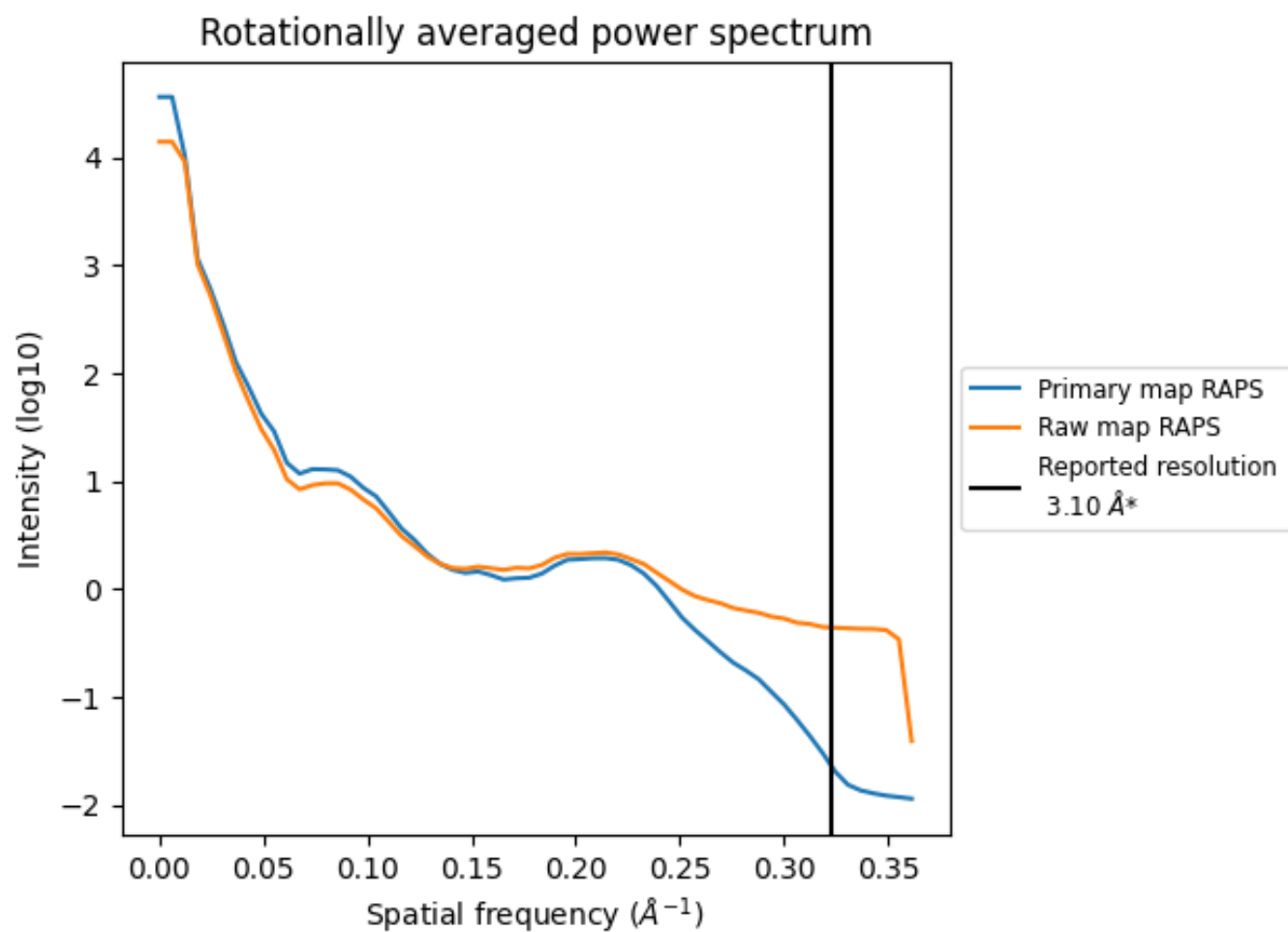
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 297 nm^3 ; this corresponds to an approximate mass of 268 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 0.323 Å⁻¹

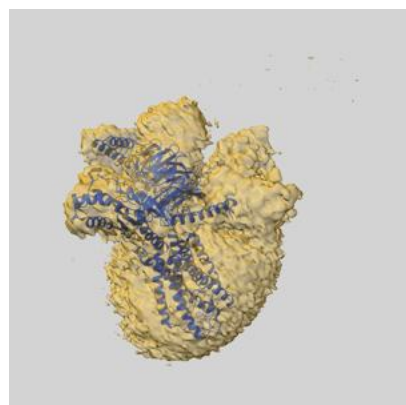
8 Fourier-Shell correlation

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

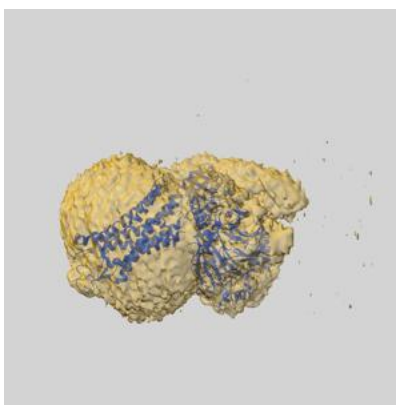
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-67434 and PDB model 20ZL. Per-residue inclusion information can be found in section [3](#) on page [7](#).

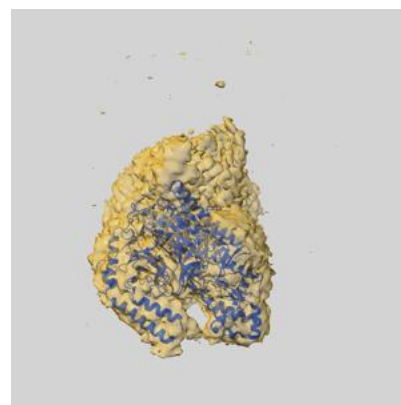
9.1 Map-model overlay [i](#)



X



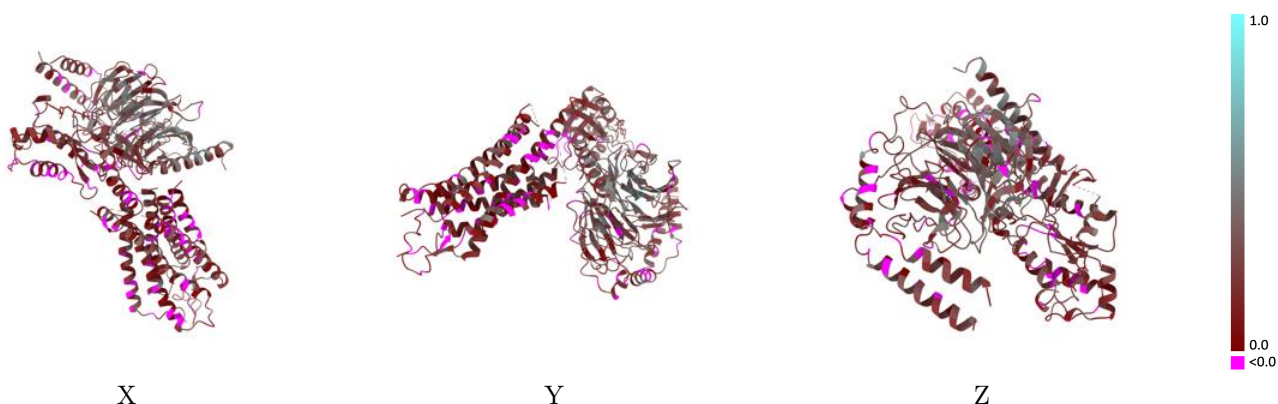
Y



Z

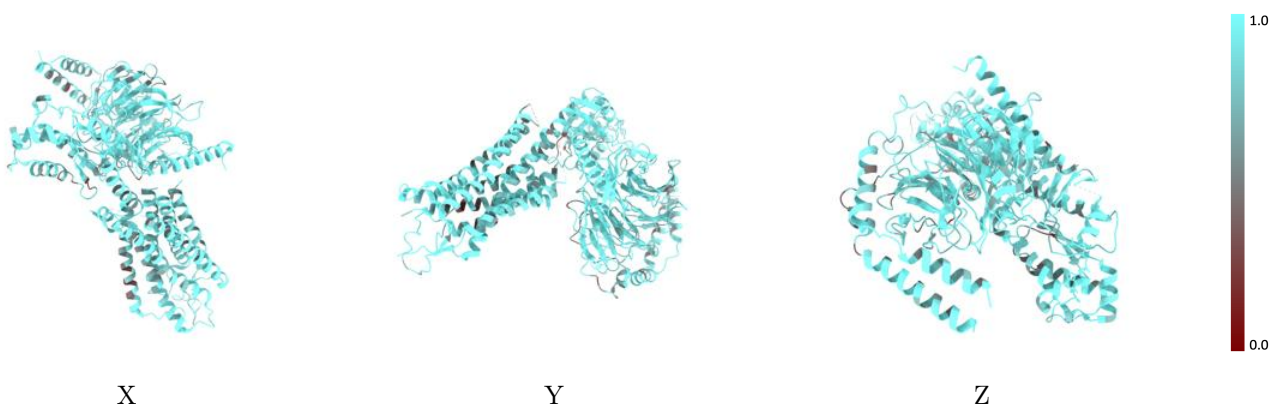
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



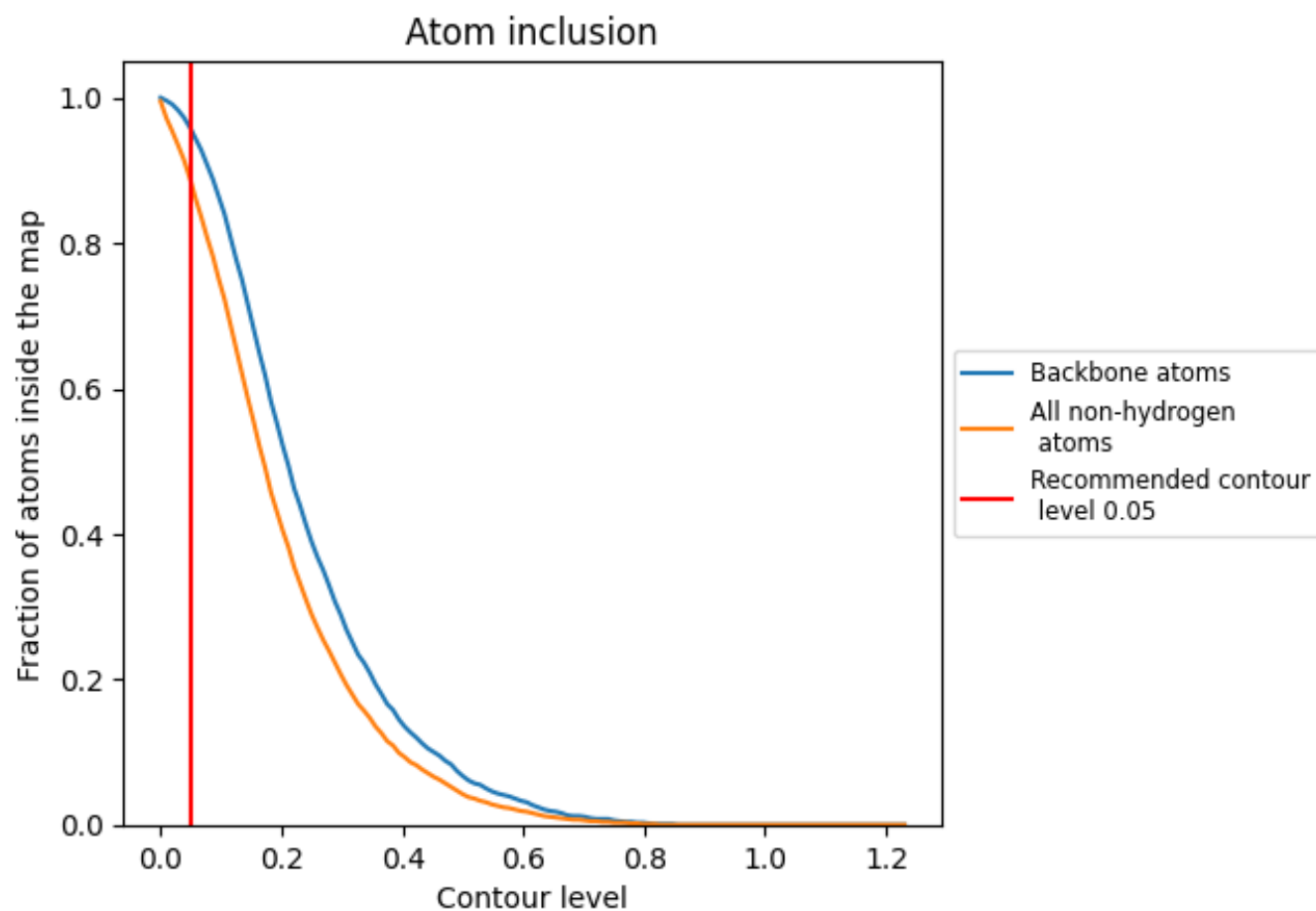
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



At the recommended contour level, 96% of all backbone atoms, 88% 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	<div></div> 0.8850	<div></div> 0.2040
A	<div></div> 0.9010	<div></div> 0.2000
B	<div></div> 0.8820	<div></div> 0.2740
C	<div></div> 0.8870	<div></div> 0.1810
L	<div></div> 0.8080	<div></div> 0.1640
R	<div></div> 0.8780	<div></div> 0.1310

