



Full wwPDB EM Validation Report ⓘ

May 26, 2026 – 10:28 AM JST

PDB ID : 20ZI / pdb_000020zi
EMDB ID : EMD-67431
Title : Cryo-EM structure of the human neurotensin receptor 1 (hNTSR1)-Gi1 complex in the GTP-bound, AHD-open NC state 1, 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 : 2.70 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:

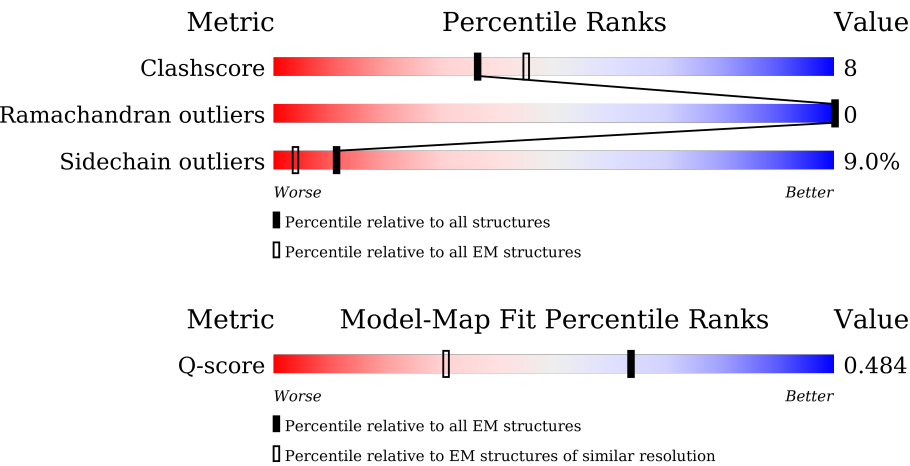
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 2.70 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	10327 (2.20 - 3.20)

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

Mol	Chain	Length	Quality of chain
1	A	354	<div><div>49%</div><div>10%</div><div>38%</div></div>
2	B	358	<div><div>73%</div><div>18%</div><div>6%</div></div>
3	C	71	<div><div>72%</div><div>24%</div></div>
4	D	259	<div><div>75%</div><div>14%</div><div>11%</div></div>

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Mol	Chain	Length	Quality of chain
5	R	436	<div><div></div><div></div><div></div><div></div><div></div></div> <div>39%22%7%30%</div>
6	L	6	<div><div></div><div></div><div></div><div></div><div></div></div> <div>17%33%50%</div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8934 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 Guanine nucleotide-binding protein G(i) subunit alpha-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	218	Total	C	N	O	S	0	0
			1754	1117	292	333	12		

- Molecule 2 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	338	Total	C	N	O	S	0	0
			2585	1596	461	507	21		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	54	Total	C	N	O	S	0	0
			410	259	71	77	3		

- Molecule 4 is a protein called scFv16.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	231	Total	C	N	O	S	0	0
			1758	1118	293	337	10		

- Molecule 5 is a protein called Neurotensin receptor type 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	R	305	Total	C	N	O	S	0	0
			2374	1552	397	409	16		

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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

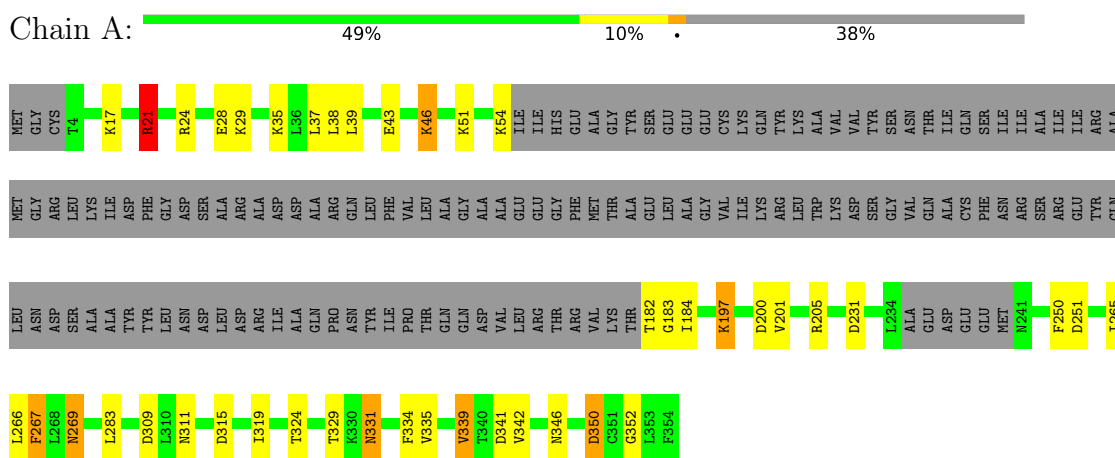
- Molecule 6 is a protein called LYS-LYS-PRO-TYR-ILE-LEU.

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

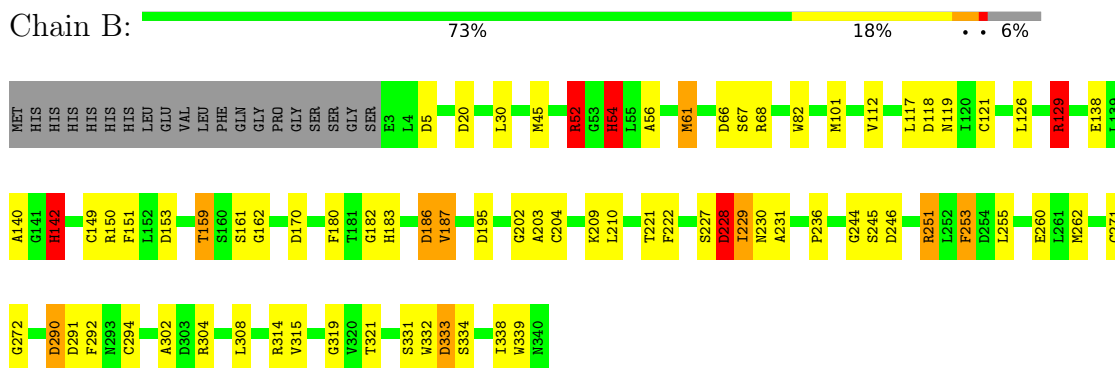
3 Residue-property plots

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.

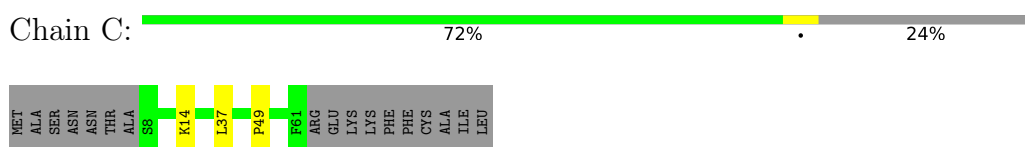
- Molecule 1: Guanine nucleotide-binding protein G(i) subunit alpha-1




- Molecule 2: Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1

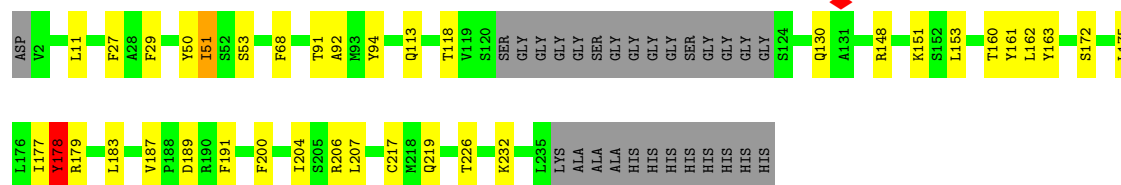


- Molecule 3: Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2



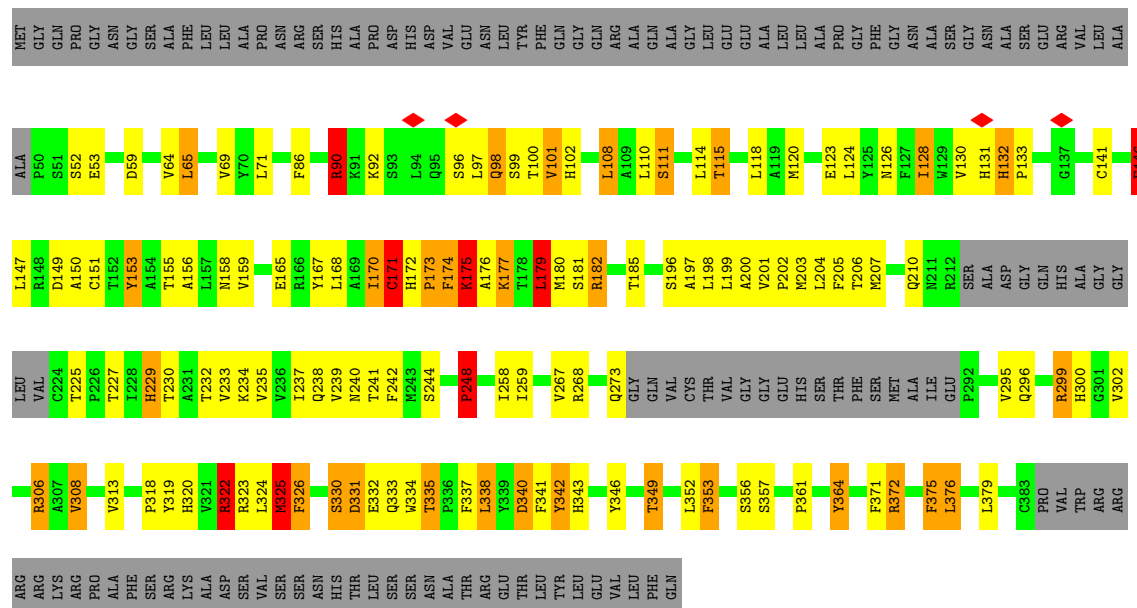
- Molecule 4: scFv16

Chain D:  75% 14% 11%



- Molecule 5: Neurotensin receptor type 1

Chain R:  39% 22% 7% 30%



- Molecule 6: LYS-LYS-PRO-TYR-ILE-LEU

Chain L:  17% 33% 50%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	332320	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	0.510	Depositor
Minimum map value	0.000	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.013	Depositor
Recommended contour level	0.05	Depositor
Map size (\AA)	249.0, 249.0, 249.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.83, 0.83, 0.83	Depositor

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.74	0/1783	1.56	16/2391 (0.7%)
2	B	0.89	2/2632 (0.1%)	1.62	43/3570 (1.2%)
3	C	0.68	0/416	1.52	1/562 (0.2%)
4	D	0.83	2/1802 (0.1%)	1.42	13/2446 (0.5%)
5	R	0.83	2/2429 (0.1%)	1.84	54/3317 (1.6%)
6	L	0.79	0/54	2.02	3/69 (4.3%)
All	All	0.83	6/9116 (0.1%)	1.63	130/12355 (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	A	0	3
2	B	0	5
4	D	0	4
5	R	0	5
All	All	0	17

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	R	330	SER	CA-CB	-7.44	1.41	1.53
2	B	161	SER	CA-CB	-6.02	1.43	1.53
2	B	142	HIS	CE1-NE2	-5.97	1.26	1.32
4	D	51	ILE	CB-CG1	-5.79	1.41	1.53
4	D	53	SER	CA-CB	-5.46	1.44	1.53
5	R	332	GLU	CA-CB	-5.14	1.45	1.53

All (130) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	129	ARG	NE-CZ-NH2	-13.49	107.06	119.20
1	A	21	ARG	NE-CZ-NH2	-12.73	107.75	119.20
5	R	306	ARG	NE-CZ-NH2	-10.05	110.15	119.20
5	R	172	HIS	CB-CA-C	-8.86	98.59	113.04
2	B	333	ASP	CA-CB-CG	8.77	121.37	112.60
5	R	322	ARG	NE-CZ-NH1	-8.66	112.84	121.50
1	A	21	ARG	NE-CZ-NH1	8.46	129.96	121.50
5	R	242	PHE	N-CA-CB	8.43	122.24	110.01
2	B	228	ASP	CB-CA-C	-8.35	97.32	109.84
5	R	322	ARG	CD-NE-CZ	8.11	135.75	124.40
1	A	21	ARG	CB-CA-C	-7.87	97.47	110.85
5	R	179	LEU	N-CA-C	7.86	120.61	111.02
2	B	253	PHE	CA-CB-CG	7.81	121.61	113.80
2	B	292	PHE	CA-CB-CG	7.74	121.54	113.80
1	A	267	PHE	CA-CB-CG	7.55	121.35	113.80
4	D	161	TYR	N-CA-CB	-7.54	101.90	110.35
5	R	375	PHE	CA-CB-CG	7.53	121.33	113.80
2	B	186	ASP	CA-CB-CG	7.48	120.08	112.60
5	R	229	HIS	CA-CB-CG	7.34	121.14	113.80
2	B	54	HIS	CA-CB-CG	7.33	121.13	113.80
2	B	187	VAL	N-CA-CB	7.31	118.69	110.72
5	R	90	ARG	CD-NE-CZ	7.27	134.58	124.40
5	R	322	ARG	N-CA-CB	7.22	120.85	110.16
2	B	52	ARG	CB-CA-C	-7.20	98.68	112.43
5	R	337	PHE	CA-CB-CG	7.11	120.91	113.80
1	A	21	ARG	CG-CD-NE	-7.10	96.38	112.00
2	B	119	ASN	CA-CB-CG	7.07	119.67	112.60
4	D	50	TYR	N-CA-CB	-7.06	98.35	111.13
2	B	56	ALA	CA-C-O	-6.99	113.63	121.25
5	R	248	PRO	N-CA-CB	-6.96	95.56	103.15
5	R	174	PHE	CA-C-N	-6.93	111.51	120.65
5	R	174	PHE	C-N-CA	-6.93	111.51	120.65
5	R	371	PHE	CA-CB-CG	6.92	120.72	113.80
4	D	68	PHE	CA-CB-CG	6.85	120.65	113.80
5	R	171	CYS	CA-C-O	6.83	130.28	120.51
5	R	174	PHE	N-CA-CB	-6.73	100.08	109.91
5	R	175	LYS	CA-C-N	-6.70	111.32	120.44
5	R	175	LYS	C-N-CA	-6.70	111.32	120.44
2	B	68	ARG	CA-CB-CG	6.66	127.42	114.10
5	R	375	PHE	N-CA-C	-6.65	103.13	111.11
4	D	179	ARG	N-CA-C	-6.62	99.32	109.65
2	B	66	ASP	CA-CB-CG	6.58	119.19	112.60
2	B	129	ARG	NE-CZ-NH1	6.58	128.08	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	R	375	PHE	N-CA-CB	6.54	119.69	109.94
4	D	178	TYR	N-CA-CB	-6.51	101.57	110.95
5	R	64	VAL	CG1-CB-CG2	6.50	125.10	110.80
5	R	302	VAL	N-CA-CB	6.47	119.34	110.54
5	R	238	GLN	N-CA-CB	6.42	119.51	109.94
1	A	200	ASP	CA-CB-CG	6.39	118.99	112.60
5	R	146	PHE	CA-CB-CG	6.38	120.18	113.80
6	L	11	TYR	CA-CB-CG	6.37	125.36	113.90
2	B	151	PHE	CA-CB-CG	6.34	120.14	113.80
5	R	238	GLN	CB-CA-C	-6.31	100.72	110.81
4	D	29	PHE	CA-CB-CG	6.23	120.03	113.80
6	L	10	PRO	N-CA-CB	-6.21	96.73	103.25
2	B	118	ASP	CA-CB-CG	6.21	118.81	112.60
5	R	326	PHE	N-CA-CB	6.18	118.93	109.91
2	B	339	TRP	CA-C-O	-6.16	114.61	121.51
5	R	340	ASP	CA-CB-CG	6.03	118.62	112.60
5	R	299	ARG	N-CA-CB	6.01	118.95	110.12
5	R	306	ARG	CG-CD-NE	-5.99	98.81	112.00
5	R	172	HIS	N-CA-C	5.93	120.30	112.35
5	R	173	PRO	CA-C-N	-5.86	112.91	120.65
5	R	173	PRO	C-N-CA	-5.86	112.91	120.65
5	R	177	LYS	CA-C-N	-5.86	112.48	120.44
5	R	177	LYS	C-N-CA	-5.86	112.48	120.44
5	R	364	TYR	N-CA-CB	5.85	118.82	110.16
2	B	195	ASP	CA-CB-CG	5.83	118.43	112.60
5	R	115	THR	N-CA-CB	5.82	118.45	110.01
2	B	304	ARG	N-CA-CB	5.79	119.09	109.60
1	A	231	ASP	CA-CB-CG	5.78	118.38	112.60
1	A	352	GLY	N-CA-C	-5.76	107.73	115.21
2	B	170	ASP	CA-CB-CG	5.76	118.36	112.60
5	R	52	SER	CA-CB-OG	-5.66	99.79	111.10
2	B	222	PHE	CA-CB-CG	5.64	119.44	113.80
5	R	65	LEU	N-CA-CB	5.63	118.18	110.01
1	A	28	GLU	CB-CA-C	5.63	120.13	110.79
5	R	299	ARG	CA-CB-CG	5.59	125.28	114.10
4	D	179	ARG	N-CA-CB	5.59	120.04	110.65
1	A	251	ASP	CA-CB-CG	5.58	118.18	112.60
5	R	308	VAL	N-CA-CB	5.56	118.11	110.54
2	B	54	HIS	CA-C-O	-5.55	114.33	120.38
2	B	290	ASP	CA-CB-CG	5.55	118.15	112.60
2	B	180	PHE	CA-CB-CG	5.53	119.33	113.80
1	A	43	GLU	N-CA-C	-5.53	106.42	112.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	183	LEU	N-CA-CB	-5.52	101.24	111.13
2	B	52	ARG	N-CA-CB	-5.51	100.66	110.14
2	B	236	PRO	N-CA-C	5.50	121.08	113.65
5	R	59	ASP	CA-CB-CG	5.50	118.11	112.60
5	R	64	VAL	CA-CB-CG1	-5.50	101.05	110.40
5	R	185	THR	CA-CB-OG1	-5.49	101.37	109.60
2	B	230	ASN	N-CA-C	-5.48	107.24	114.31
2	B	129	ARG	CB-CA-C	-5.47	99.23	110.38
2	B	20	ASP	CA-CB-CG	5.46	118.06	112.60
2	B	138	GLU	CB-CA-C	5.45	120.39	111.23
5	R	108	LEU	N-CA-C	-5.45	105.24	111.07
1	A	341	ASP	CA-CB-CG	5.44	118.04	112.60
6	L	9	LYS	CB-CA-C	5.44	120.88	110.17
2	B	291	ASP	CA-CB-CG	5.42	118.02	112.60
5	R	342	TYR	CB-CA-C	-5.40	102.65	110.96
5	R	306	ARG	NE-CZ-NH1	5.39	126.89	121.50
2	B	251	ARG	NE-CZ-NH1	-5.39	116.11	121.50
5	R	331	ASP	CA-CB-CG	5.39	117.99	112.60
4	D	130	GLN	CB-CA-C	-5.33	101.36	109.89
2	B	101	MET	CB-CA-C	5.33	119.39	110.44
4	D	27	PHE	CA-CB-CG	5.32	119.12	113.80
4	D	189	ASP	CA-CB-CG	5.31	117.91	112.60
1	A	309	ASP	CA-CB-CG	5.30	117.90	112.60
5	R	341	PHE	CA-CB-CG	5.29	119.09	113.80
5	R	353	PHE	CB-CA-C	5.27	119.81	110.85
2	B	5	ASP	CA-CB-CG	5.27	117.87	112.60
2	B	292	PHE	CB-CA-C	5.26	119.49	111.80
2	B	236	PRO	N-CA-CB	-5.26	97.71	103.39
5	R	322	ARG	CG-CD-NE	-5.26	100.43	112.00
1	A	315	ASP	CA-CB-CG	5.25	117.85	112.60
2	B	182	GLY	CA-C-O	-5.23	114.55	120.30
2	B	183	HIS	CB-CG-CD2	-5.22	124.42	131.20
5	R	325	MET	CG-SD-CE	5.22	112.38	100.90
4	D	163	TYR	CB-CA-C	5.20	119.08	109.71
2	B	140	ALA	CA-C-O	-5.18	115.57	121.68
4	D	191	PHE	CA-CB-CG	5.16	118.96	113.80
2	B	182	GLY	N-CA-C	5.15	120.27	113.37
2	B	251	ARG	CD-NE-CZ	5.15	131.61	124.40
3	C	49	PRO	N-CA-C	5.13	120.57	113.65
2	B	153	ASP	CA-CB-CG	5.09	117.69	112.60
1	A	311	ASN	N-CA-CB	5.03	118.08	109.87
1	A	201	VAL	N-CA-CB	-5.03	104.75	112.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	230	ASN	CB-CA-C	5.02	117.46	109.02
5	R	170	ILE	CA-C-O	-5.01	115.54	120.85
5	R	353	PHE	CA-CB-CG	5.00	118.80	113.80

There are no chirality outliers.

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	21	ARG	Sidechain
1	A	24	ARG	Sidechain
1	A	350	ASP	Mainchain
2	B	129	ARG	Sidechain
2	B	150	ARG	Sidechain
2	B	251	ARG	Sidechain
2	B	338	ILE	Mainchain
2	B	52	ARG	Mainchain
4	D	148	ARG	Sidechain
4	D	178	TYR	Mainchain
4	D	206	ARG	Sidechain
4	D	51	ILE	Mainchain
5	R	171	CYS	Peptide
5	R	182	ARG	Sidechain
5	R	306	ARG	Sidechain
5	R	322	ARG	Sidechain
5	R	90	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	A	1754	0	1744	17	0
2	B	2585	0	2479	33	0
3	C	410	0	421	0	0
4	D	1758	0	1685	10	0
5	R	2374	0	2404	77	0
6	L	53	0	63	5	0
All	All	8934	0	8796	135	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 8.

All (135) 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)
5:R:168:LEU:HD22	5:R:175:LYS:HG3	1.58	0.86
5:R:206:THR:HG23	5:R:207:MET:HE2	1.61	0.83
2:B:187:VAL:HG12	2:B:203:ALA:HB2	1.64	0.79
1:A:350:ASP:O	5:R:101:VAL:HG21	1.82	0.78
4:D:113:GLN:HA	4:D:172:SER:OG	1.90	0.71
4:D:153:LEU:HD21	4:D:219:GLN:HB2	1.72	0.71
5:R:150:ALA:HB2	5:R:200:ALA:HB2	1.74	0.70
5:R:372:ARG:O	5:R:376:LEU:N	2.23	0.70
5:R:115:THR:HG22	5:R:151:CYS:HB3	1.76	0.68
1:A:266:LEU:HD13	1:A:319:ILE:HG23	1.78	0.66
5:R:175:LYS:HD2	5:R:179:LEU:HG	1.77	0.66
5:R:96:SER:HB3	5:R:182:ARG:HB2	1.78	0.66
5:R:325:MET:HE2	5:R:342:TYR:HD2	1.61	0.64
5:R:330:SER:OG	5:R:333:GLN:HG2	1.98	0.64
5:R:101:VAL:HG22	5:R:165:GLU:OE2	1.98	0.64
1:A:269:ASN:HB3	1:A:324:THR:HG23	1.78	0.64
5:R:170:ILE:HD13	5:R:259:ILE:HG23	1.79	0.64
1:A:250:PHE:CE1	1:A:266:LEU:HD11	2.34	0.63
5:R:98:GLN:O	5:R:101:VAL:N	2.31	0.63
5:R:124:LEU:O	5:R:128:ILE:HB	1.99	0.62
5:R:108:LEU:HG	5:R:158:ASN:HB3	1.82	0.62
5:R:326:PHE:HA	5:R:334:TRP:CZ3	2.35	0.62
5:R:173:PRO:O	5:R:174:PHE:C	2.42	0.61
5:R:126:ASN:HD22	5:R:133:PRO:HD2	1.66	0.61
5:R:338:LEU:HD23	5:R:338:LEU:H	1.66	0.60
5:R:322:ARG:HE	5:R:322:ARG:C	2.10	0.60
5:R:325:MET:HE2	5:R:342:TYR:CD2	2.36	0.59
5:R:203:MET:HA	5:R:206:THR:HG22	1.85	0.58
5:R:241:THR:HG21	5:R:324:LEU:CD2	2.34	0.58
5:R:235:VAL:O	5:R:239:VAL:HG23	2.05	0.57
1:A:184:ILE:HD13	2:B:117:LEU:HB3	1.87	0.56
5:R:99:SER:O	5:R:102:HIS:N	2.39	0.56
5:R:319:TYR:HA	5:R:349:THR:HG23	1.86	0.56
2:B:246:ASP:HA	2:B:272:GLY:HA2	1.86	0.56
5:R:241:THR:HG21	5:R:324:LEU:HD21	1.88	0.56
1:A:342:VAL:HG22	1:A:346:ASN:ND2	2.21	0.55
2:B:187:VAL:CG1	2:B:203:ALA:HB2	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:175:LEU:HD21	4:D:178:TYR:HB3	1.90	0.54
5:R:319:TYR:HA	5:R:349:THR:CG2	2.38	0.54
5:R:132:HIS:CE1	6:L:12:ILE:HD11	2.43	0.53
2:B:204:CYS:HA	2:B:228:ASP:HB3	1.90	0.53
1:A:37:LEU:HD22	1:A:39:LEU:HG	1.91	0.52
5:R:96:SER:O	5:R:99:SER:N	2.38	0.52
2:B:61:MET:HE1	2:B:319:GLY:HA3	1.91	0.52
2:B:202:GLY:HA3	2:B:229:ILE:HD11	1.92	0.52
5:R:98:GLN:C	5:R:100:THR:N	2.66	0.52
5:R:326:PHE:HA	5:R:334:TRP:CH2	2.44	0.52
5:R:153:TYR:CE2	5:R:199:LEU:HB3	2.45	0.52
5:R:340:ASP:HA	5:R:343:HIS:NE2	2.26	0.51
5:R:175:LYS:O	5:R:179:LEU:HB2	2.10	0.51
5:R:101:VAL:O	5:R:102:HIS:C	2.52	0.51
5:R:99:SER:O	5:R:100:THR:C	2.54	0.50
5:R:156:ALA:HB1	5:R:248:PRO:HG2	1.93	0.50
5:R:357:SER:O	5:R:361:PRO:HD2	2.12	0.50
5:R:96:SER:CB	5:R:182:ARG:HB2	2.41	0.50
1:A:38:LEU:HD23	1:A:46:LYS:HD2	1.94	0.49
2:B:142:HIS:CE1	2:B:159:THR:CG2	2.96	0.49
5:R:171:CYS:SG	5:R:175:LYS:HG2	2.53	0.49
2:B:262:MET:HE2	2:B:302:ALA:HB2	1.94	0.49
4:D:91:THR:HG23	4:D:118:THR:HA	1.95	0.49
5:R:335:THR:HG23	5:R:338:LEU:HD21	1.95	0.49
5:R:197:ALA:O	5:R:200:ALA:HB3	2.12	0.49
5:R:199:LEU:O	5:R:202:PRO:HD2	2.12	0.49
5:R:174:PHE:O	5:R:175:LYS:C	2.53	0.48
1:A:265:ILE:HD13	1:A:335:VAL:HG23	1.95	0.48
2:B:52:ARG:O	2:B:82:TRP:HH2	1.96	0.48
5:R:99:SER:HA	5:R:102:HIS:CG	2.49	0.47
5:R:175:LYS:O	5:R:176:ALA:C	2.54	0.47
5:R:210:GLN:HE21	5:R:227:THR:HA	1.80	0.47
4:D:162:LEU:HD22	4:D:200:PHE:CG	2.49	0.47
2:B:202:GLY:HA3	2:B:229:ILE:CD1	2.45	0.47
5:R:237:ILE:HD11	6:L:13:LEU:HD11	1.97	0.47
2:B:227:SER:O	2:B:245:SER:OG	2.33	0.47
1:A:331:ASN:O	1:A:334:PHE:N	2.47	0.47
2:B:229:ILE:C	2:B:229:ILE:HD12	2.40	0.46
2:B:253:PHE:HD1	2:B:260:GLU:HA	1.80	0.46
5:R:86:PHE:O	5:R:90:ARG:N	2.44	0.46
6:L:13:LEU:HD12	6:L:13:LEU:HA	1.77	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:187:VAL:HA	2:B:203:ALA:HA	1.97	0.46
2:B:210:LEU:HD22	2:B:255:LEU:HD12	1.97	0.46
1:A:197:LYS:HB3	1:A:197:LYS:HE3	1.58	0.46
5:R:318:PRO:O	5:R:322:ARG:N	2.48	0.46
5:R:196:SER:O	5:R:197:ALA:C	2.59	0.46
4:D:92:ALA:HB3	4:D:94:TYR:HE1	1.81	0.45
4:D:162:LEU:HD11	4:D:217:CYS:HB2	1.98	0.45
4:D:204:ILE:HG21	4:D:207:LEU:HD23	1.97	0.45
2:B:271:CYS:HB2	2:B:290:ASP:HB2	1.98	0.45
5:R:372:ARG:O	5:R:375:PHE:HB3	2.17	0.45
2:B:331:SER:OG	2:B:333:ASP:OD1	2.34	0.45
5:R:146:PHE:CD1	5:R:204:LEU:HD12	2.51	0.45
2:B:52:ARG:O	2:B:82:TRP:CH2	2.69	0.45
2:B:67:SER:HB2	2:B:321:THR:HB	1.99	0.45
2:B:231:ALA:O	2:B:244:GLY:N	2.50	0.45
2:B:228:ASP:OD1	2:B:228:ASP:N	2.40	0.44
4:D:175:LEU:HD21	4:D:178:TYR:CB	2.46	0.44
5:R:71:LEU:HA	5:R:71:LEU:HD13	1.61	0.44
5:R:322:ARG:NH1	6:L:13:LEU:OXT	2.50	0.44
2:B:54:HIS:O	2:B:334:SER:OG	2.28	0.44
2:B:121:CYS:HG	2:B:149:CYS:HG	1.63	0.44
5:R:320:HIS:CE1	5:R:323:ARG:HH22	2.36	0.44
5:R:325:MET:CE	5:R:342:TYR:HD2	2.30	0.44
5:R:120:MET:HE2	5:R:124:LEU:HD23	2.00	0.44
2:B:334:SER:OG	2:B:334:SER:O	2.36	0.44
5:R:111:SER:O	5:R:115:THR:HG23	2.17	0.43
5:R:201:VAL:HG12	5:R:205:PHE:CZ	2.53	0.43
5:R:96:SER:HB3	5:R:182:ARG:HD3	2.01	0.43
1:A:342:VAL:O	1:A:346:ASN:ND2	2.50	0.43
1:A:350:ASP:HA	5:R:98:GLN:HG3	2.00	0.43
5:R:167:TYR:HE2	5:R:258:ILE:HG21	1.83	0.43
5:R:155:THR:O	5:R:159:VAL:HG23	2.18	0.43
2:B:314:ARG:HD2	2:B:332:TRP:CZ3	2.54	0.43
4:D:113:GLN:N	4:D:113:GLN:OE1	2.47	0.43
1:A:250:PHE:CZ	1:A:266:LEU:HD11	2.53	0.43
2:B:209:LYS:HG2	2:B:221:THR:OG1	2.19	0.42
5:R:98:GLN:O	5:R:101:VAL:HG23	2.18	0.42
5:R:181:SER:OG	5:R:182:ARG:N	2.47	0.42
2:B:294:CYS:SG	2:B:315:VAL:HG11	2.59	0.42
2:B:142:HIS:HE1	2:B:159:THR:CG2	2.33	0.42
5:R:203:MET:CA	5:R:206:THR:HG22	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:45:MET:HE3	2:B:308:LEU:HD11	2.03	0.41
5:R:118:LEU:HD21	5:R:151:CYS:SG	2.60	0.41
1:A:182:THR:OG1	1:A:183:GLY:N	2.54	0.41
2:B:30:LEU:HD23	2:B:262:MET:SD	2.60	0.41
2:B:112:VAL:HG13	2:B:126:LEU:HD11	2.02	0.41
2:B:162:GLY:HA2	2:B:186:ASP:HB2	2.01	0.41
5:R:322:ARG:HD3	5:R:346:TYR:HA	2.03	0.41
5:R:131:HIS:HB3	5:R:133:PRO:HD3	2.02	0.41
5:R:170:ILE:CD1	5:R:259:ILE:HG23	2.48	0.41
5:R:331:ASP:HB3	6:L:9:LYS:HD2	2.03	0.41
1:A:342:VAL:HG22	1:A:346:ASN:HD21	1.85	0.41
5:R:335:THR:CB	5:R:338:LEU:HD21	2.50	0.41
1:A:339:VAL:HA	1:A:342:VAL:HG12	2.04	0.40
5:R:98:GLN:O	5:R:99:SER:C	2.65	0.40
5:R:323:ARG:O	5:R:326:PHE:N	2.54	0.40
5:R:128:ILE:HG22	5:R:130:VAL:HB	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	212/354 (60%)	209 (99%)	3 (1%)	0	100	100
2	B	336/358 (94%)	331 (98%)	5 (2%)	0	100	100
3	C	52/71 (73%)	52 (100%)	0	0	100	100
4	D	227/259 (88%)	224 (99%)	3 (1%)	0	100	100
5	R	299/436 (69%)	289 (97%)	10 (3%)	0	100	100
6	L	4/6 (67%)	1 (25%)	3 (75%)	0	100	100
All	All	1130/1484 (76%)	1106 (98%)	24 (2%)	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	A	193/305 (63%)	178 (92%)	15 (8%)	11	29
2	B	278/298 (93%)	271 (98%)	7 (2%)	42	71
3	C	43/58 (74%)	41 (95%)	2 (5%)	23	51
4	D	190/209 (91%)	183 (96%)	7 (4%)	30	59
5	R	257/368 (70%)	203 (79%)	54 (21%)	1	3
6	L	6/6 (100%)	4 (67%)	2 (33%)	0	1
All	All	967/1244 (78%)	880 (91%)	87 (9%)	11	23

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LYS
1	A	21	ARG
1	A	29	LYS
1	A	35	LYS
1	A	46	LYS
1	A	51	LYS
1	A	54	LYS
1	A	197	LYS
1	A	205	ARG
1	A	267	PHE
1	A	269	ASN
1	A	283	LEU
1	A	329	THR
1	A	331	ASN
1	A	339	VAL
2	B	54	HIS
2	B	61	MET
2	B	129	ARG
2	B	142	HIS

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Mol	Chain	Res	Type
2	B	159	THR
2	B	228	ASP
2	B	229	ILE
3	C	14	LYS
3	C	37	LEU
4	D	11	LEU
4	D	151	LYS
4	D	160	THR
4	D	177	ILE
4	D	187	VAL
4	D	226	THR
4	D	232	LYS
5	R	53	GLU
5	R	65	LEU
5	R	69	VAL
5	R	92	LYS
5	R	97	LEU
5	R	98	GLN
5	R	101	VAL
5	R	110	LEU
5	R	111	SER
5	R	114	LEU
5	R	123	GLU
5	R	128	ILE
5	R	132	HIS
5	R	141	CYS
5	R	146	PHE
5	R	147	LEU
5	R	149	ASP
5	R	153	TYR
5	R	171	CYS
5	R	175	LYS
5	R	177	LYS
5	R	179	LEU
5	R	180	MET
5	R	198	LEU
5	R	225	THR
5	R	229	HIS
5	R	230	THR
5	R	232	THR
5	R	233	VAL
5	R	234	LYS

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Mol	Chain	Res	Type
5	R	240	ASN
5	R	244	SER
5	R	248	PRO
5	R	267	VAL
5	R	268	ARG
5	R	273	GLN
5	R	295	VAL
5	R	296	GLN
5	R	299	ARG
5	R	300	HIS
5	R	308	VAL
5	R	313	VAL
5	R	322	ARG
5	R	325	MET
5	R	335	THR
5	R	338	LEU
5	R	349	THR
5	R	352	LEU
5	R	353	PHE
5	R	356	SER
5	R	364	TYR
5	R	372	ARG
5	R	376	LEU
5	R	379	LEU
6	L	10	PRO
6	L	11	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	188	HIS
1	A	204	GLN
1	A	346	ASN
2	B	119	ASN
2	B	125	ASN
2	B	156	GLN
2	B	176	GLN
2	B	259	GLN
3	C	18	GLN
3	C	44	HIS
4	D	39	GLN
4	D	77	ASN

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Mol	Chain	Res	Type
4	D	167	GLN
5	R	102	HIS
5	R	126	ASN
5	R	261	ASN
5	R	269	GLN
5	R	296	GLN
5	R	300	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

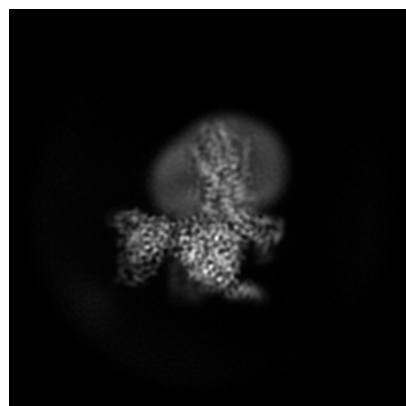
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-67431. These allow visual inspection of the internal detail of the map and identification of artifacts.

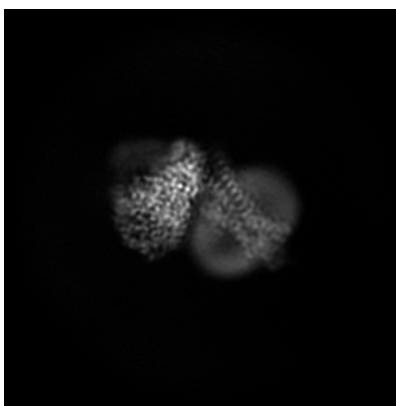
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

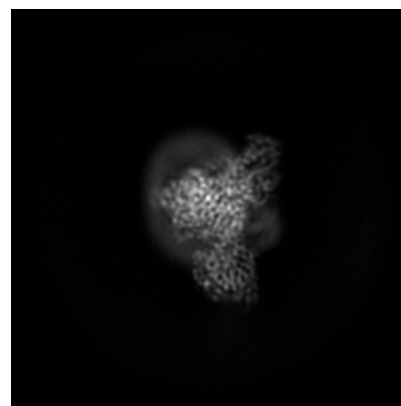
6.1.1 Primary map



X

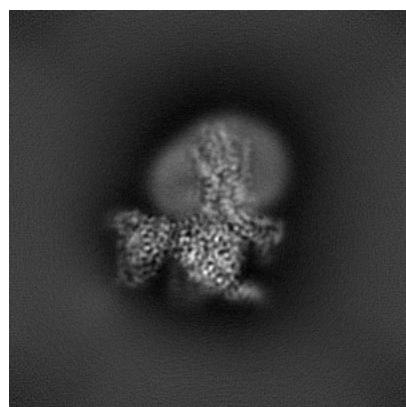


Y

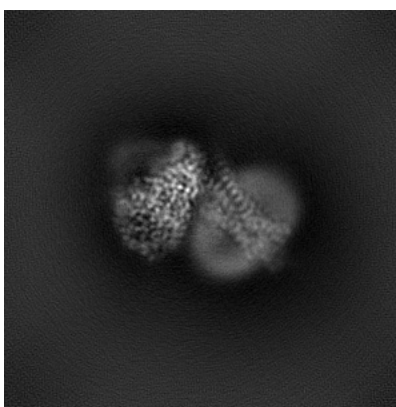


Z

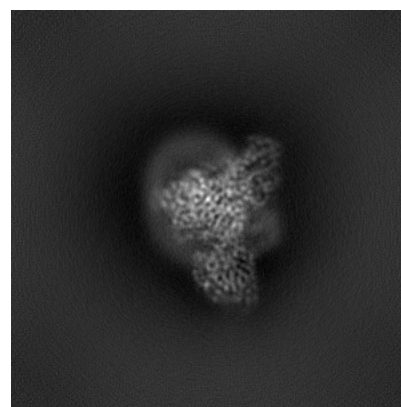
6.1.2 Raw map



X



Y

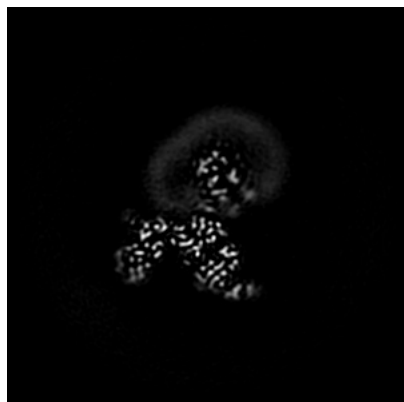


Z

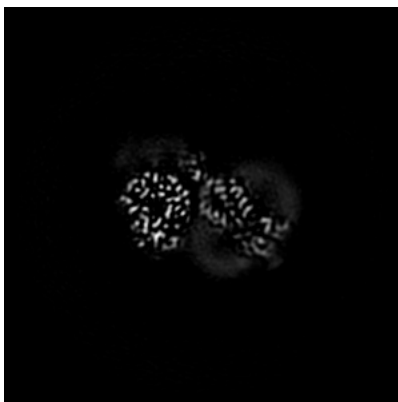
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

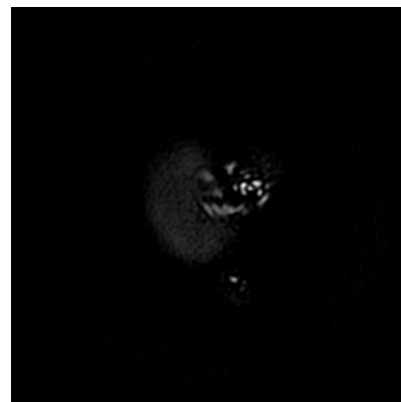
6.2.1 Primary map



X Index: 150

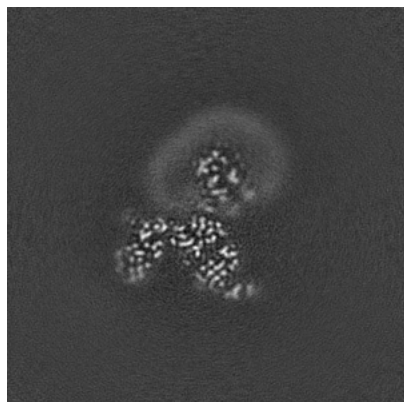


Y Index: 150

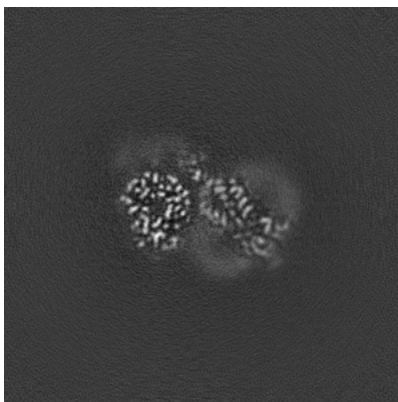


Z Index: 150

6.2.2 Raw map



X Index: 150



Y Index: 150

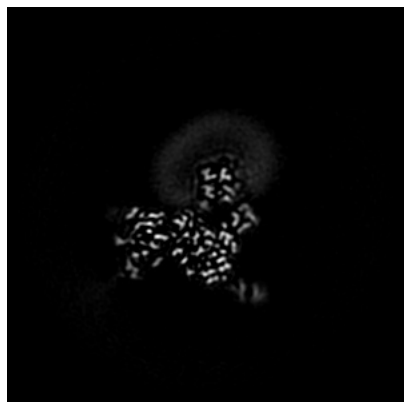


Z Index: 150

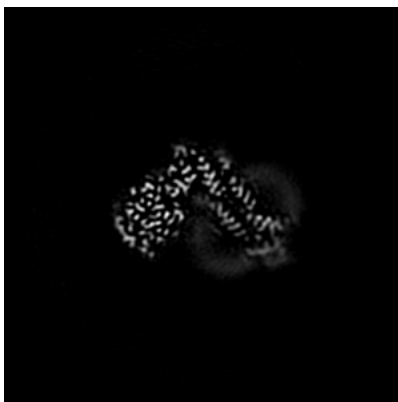
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

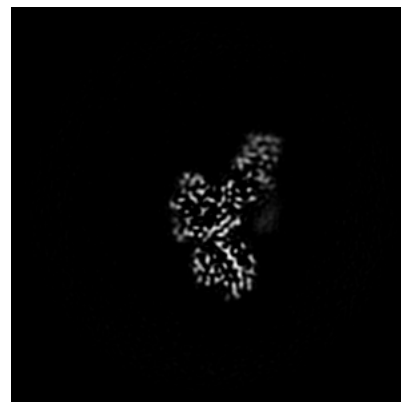
6.3.1 Primary map



X Index: 163

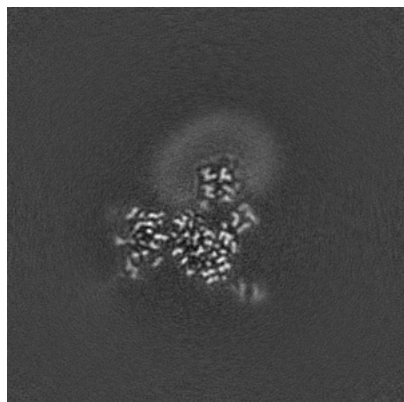


Y Index: 163

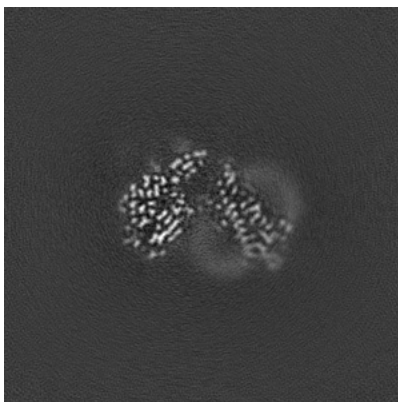


Z Index: 127

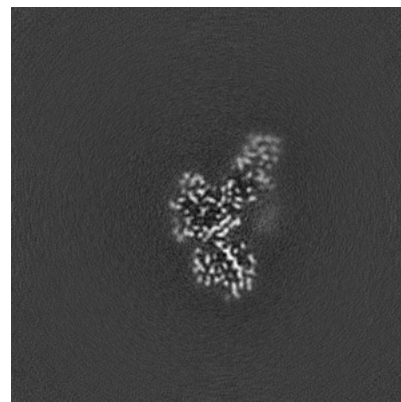
6.3.2 Raw map



X Index: 163



Y Index: 156

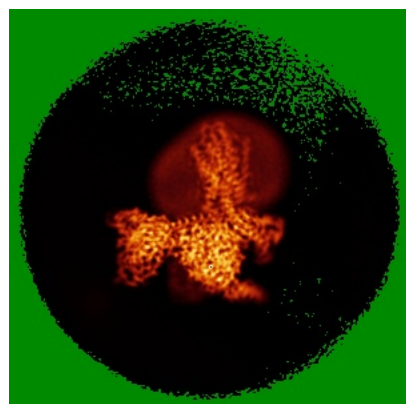


Z Index: 127

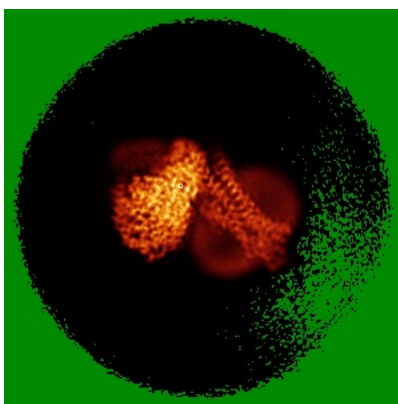
The images above show the largest variance slices of the map in three orthogonal directions.

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

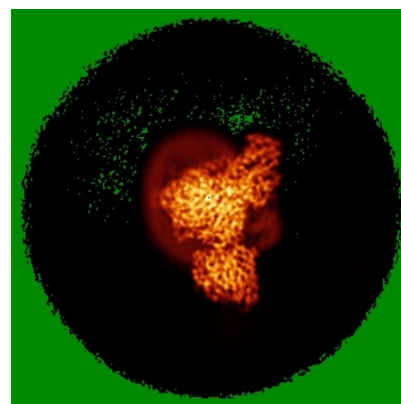
6.4.1 Primary map



X

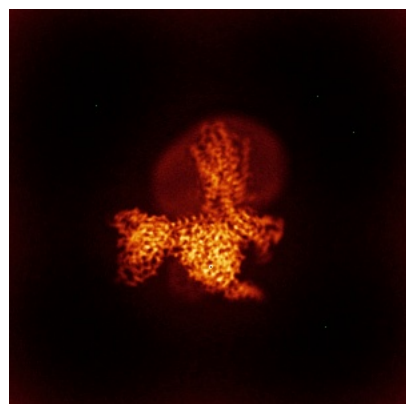


Y

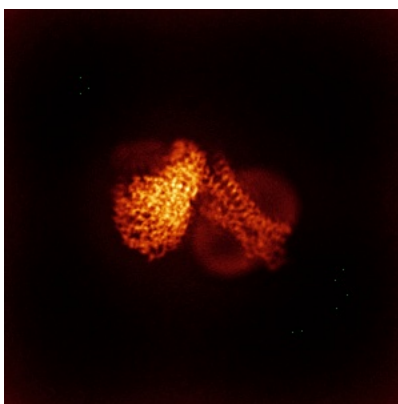


Z

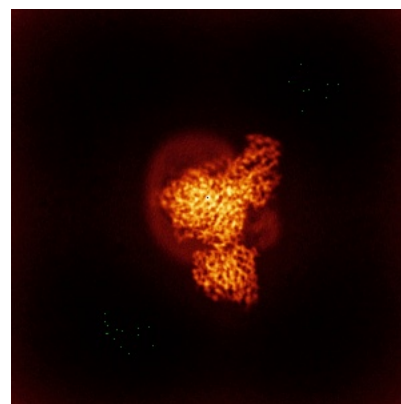
6.4.2 Raw map



X



Y

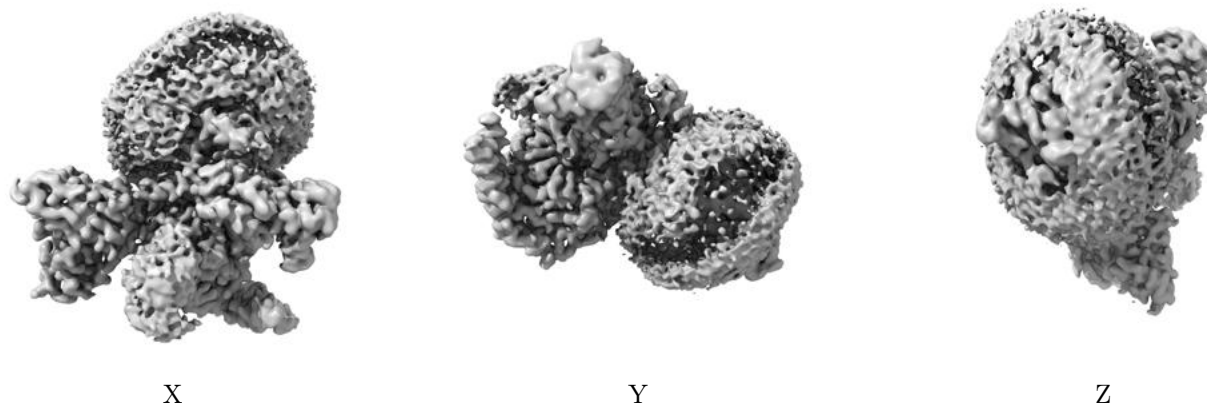


Z

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.

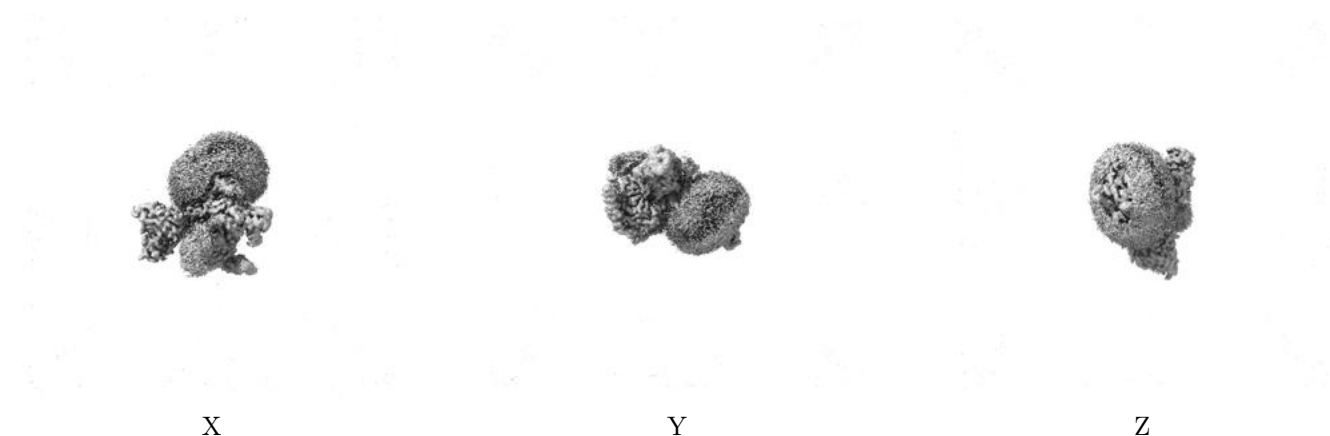
6.5 Orthogonal surface views [i](#)

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.

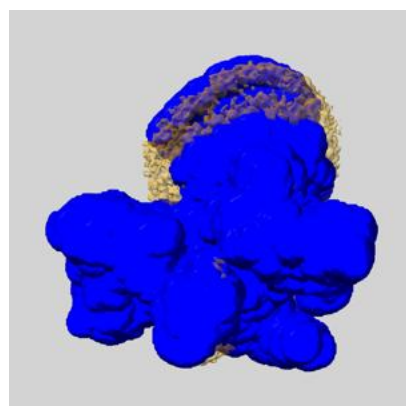
6.6 Mask visualisation [i](#)

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

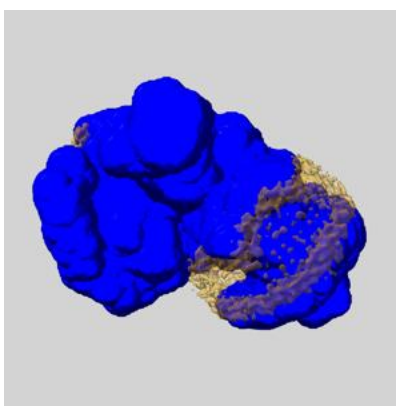
A mask typically either:

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

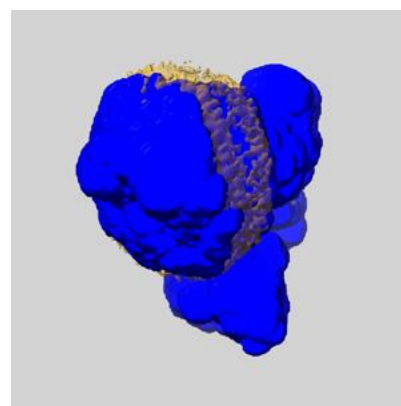
6.6.1 emd_67431_msk_1.map [i](#)



X



Y

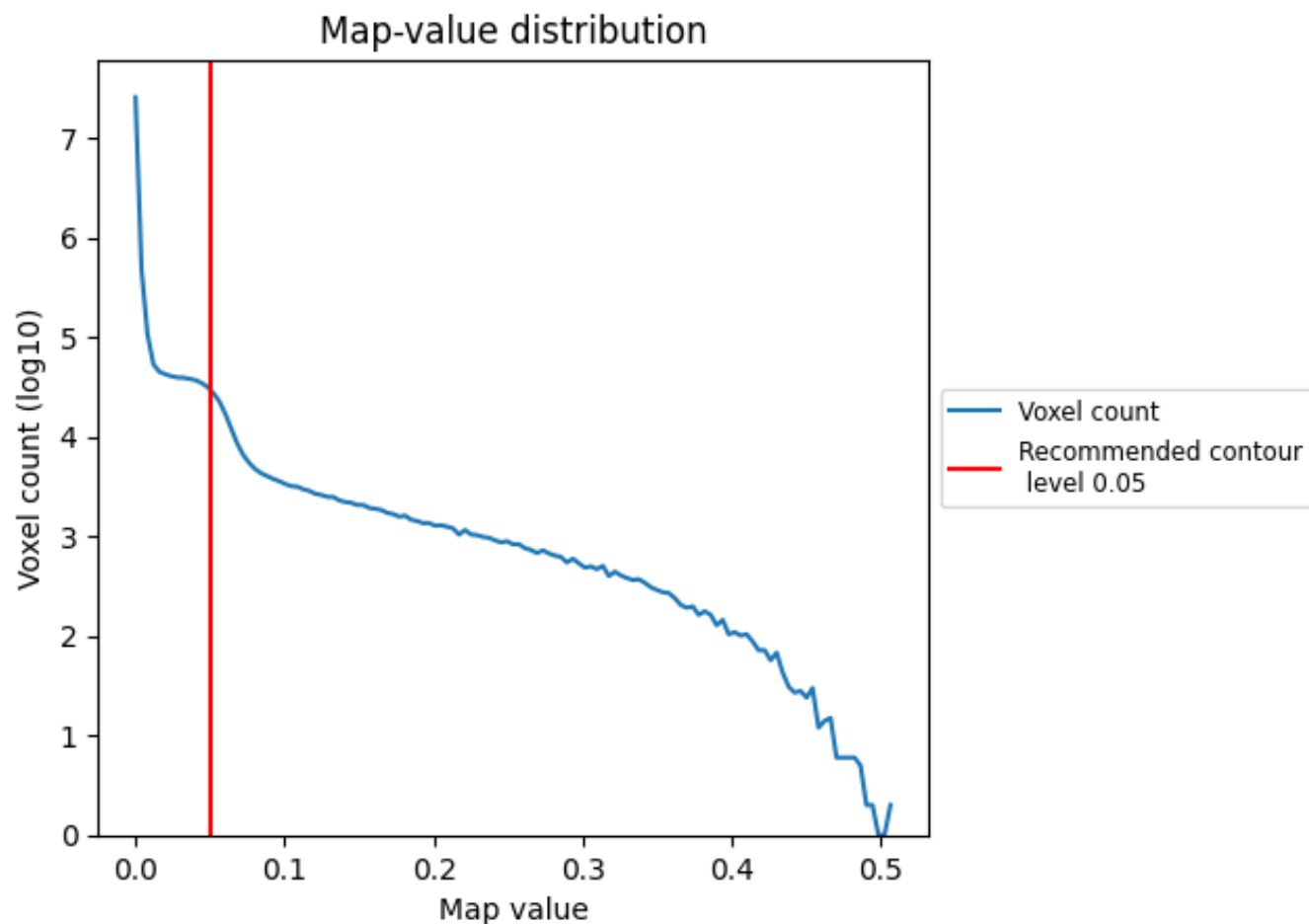


Z

7 Map analysis [i](#)

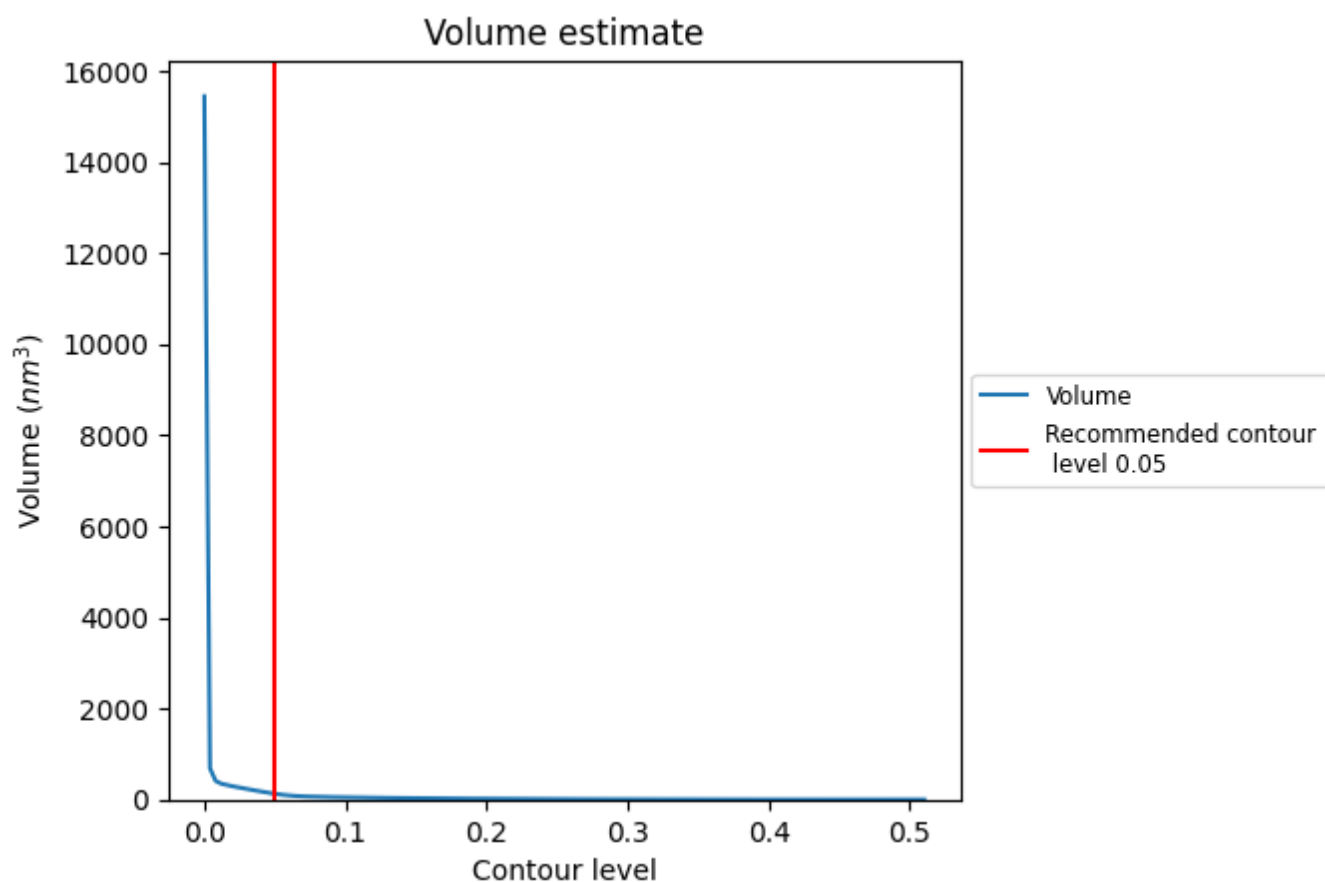
This section contains the results of statistical analysis of the map.

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.

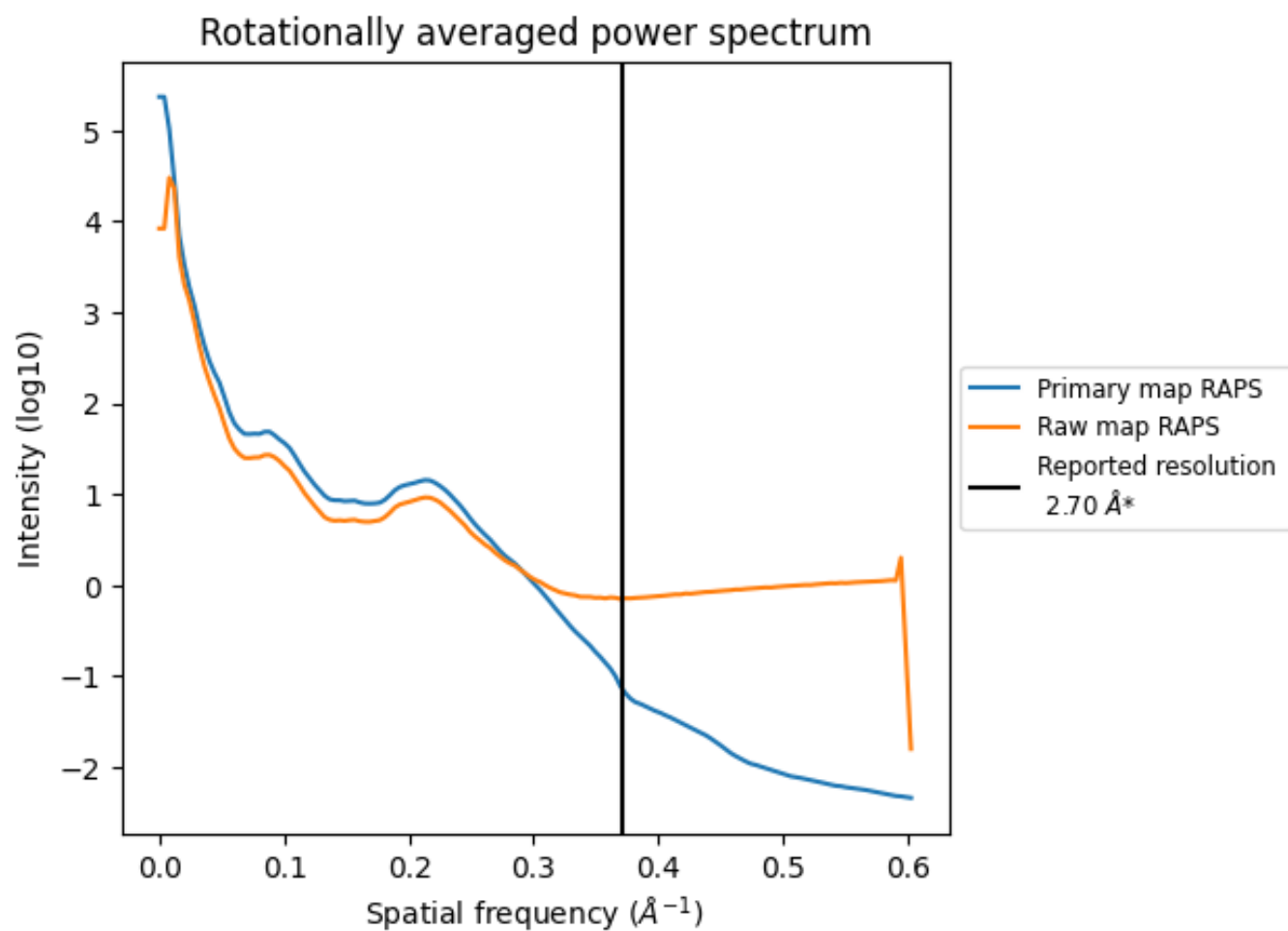
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 127 nm³; this corresponds to an approximate mass of 115 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 ⓘ

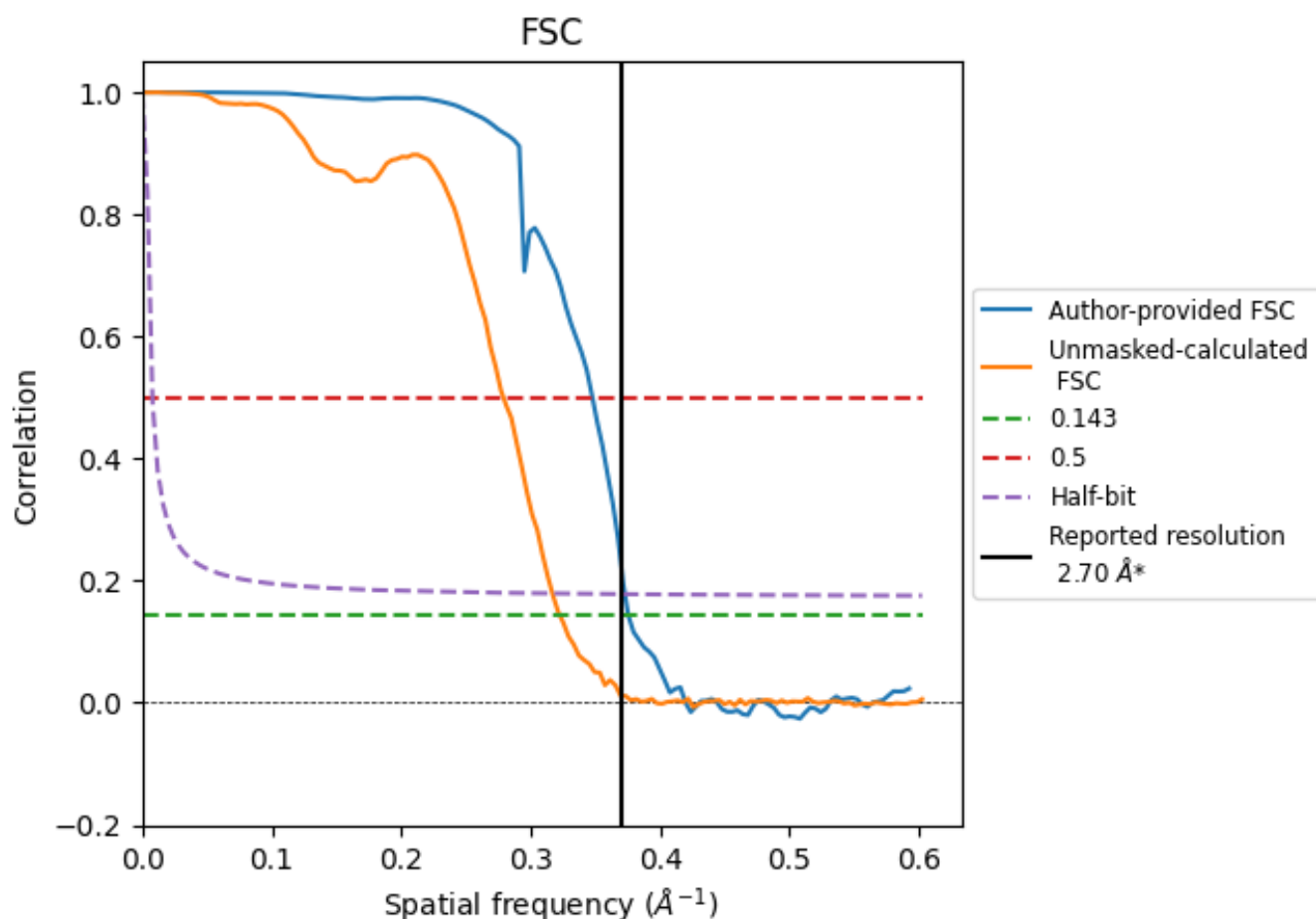


*Reported resolution corresponds to spatial frequency of 0.370 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.370 \AA^{-1}

8.2 Resolution estimates [i](#)

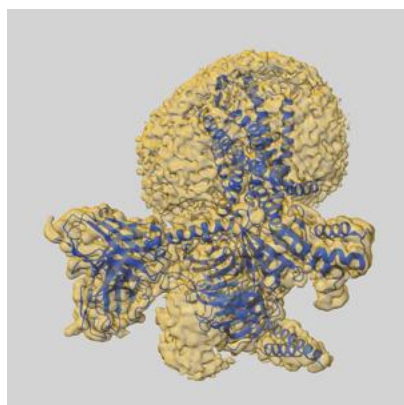
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	2.66	2.88	2.68
Unmasked-calculated*	3.10	3.58	3.16

*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 3.10 differs from the reported value 2.7 by more than 10 %

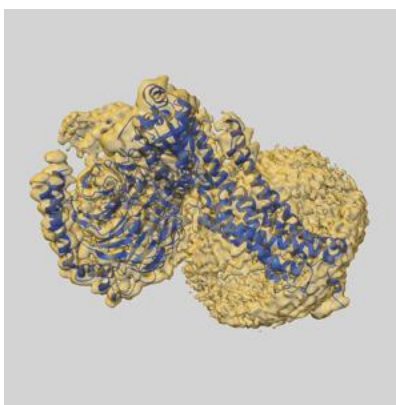
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-67431 and PDB model 20ZI. Per-residue inclusion information can be found in section [3](#) on page [7](#).

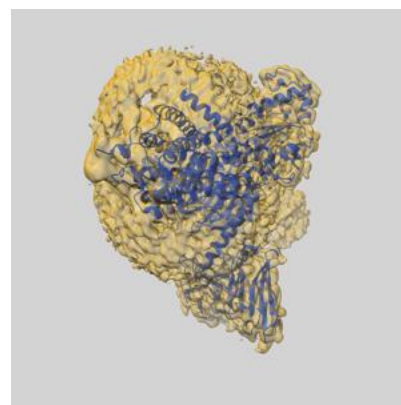
9.1 Map-model overlay [i](#)



X



Y



Z

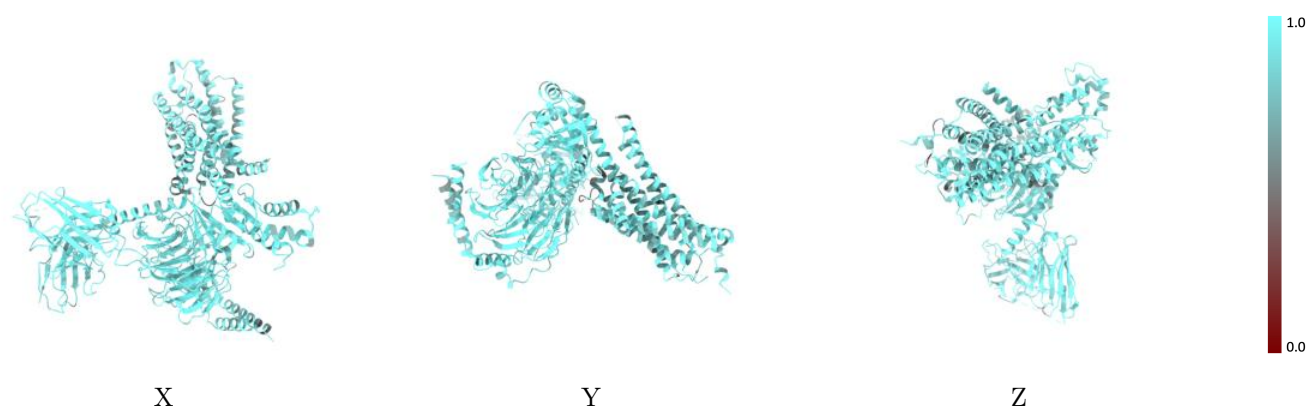
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



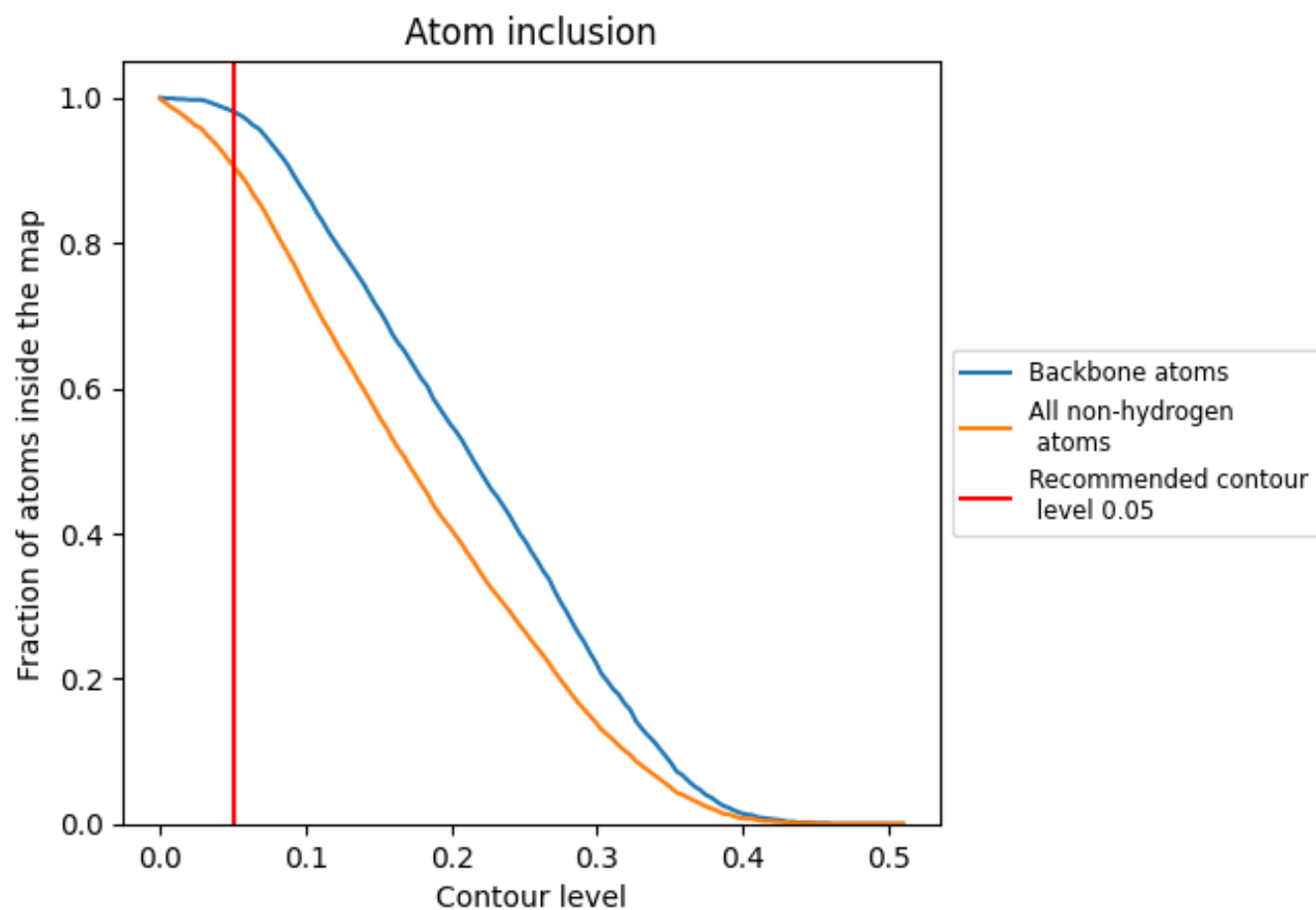
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



At the recommended contour level, 98% of all backbone atoms, 91% 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></div></div> 0.9060	<div><div></div></div> 0.4840
A	<div><div></div></div> 0.9200	<div><div></div></div> 0.5050
B	<div><div></div></div> 0.9460	<div><div></div></div> 0.5430
C	<div><div></div></div> 0.8790	<div><div></div></div> 0.4740
D	<div><div></div></div> 0.9400	<div><div></div></div> 0.5310
L	<div><div></div></div> 0.8270	<div><div></div></div> 0.4390
R	<div><div></div></div> 0.8360	<div><div></div></div> 0.3710

1.0

0.0

<0.0