



## Full wwPDB EM Validation Report ⓘ

Feb 26, 2024 – 03:56 pm GMT

PDB ID : 8RWZ  
EMDB ID : EMD-19569  
Title : Open non-crosslinked structure Brd4BD2-MZ1-(NEDD8)-CRL2VHL  
Authors : Ciulli, A.; Crowe, C.; Nakacone, M.A.  
Deposited on : 2024-02-05  
Resolution : 4.00 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](mailto: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:

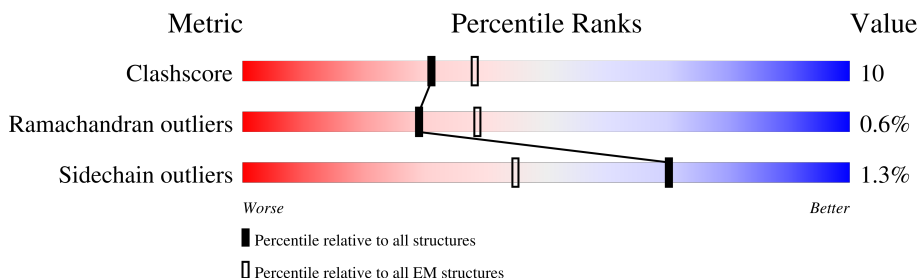
EMDB validation analysis : 0.0.1.dev70  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

# 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 4.00 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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  $\geq 3$ , 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	128	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: center;">28%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="text-align: center;">84%</div> <div style="text-align: center;">5%</div> <div style="text-align: center;">11%</div> </div>
2	B	160	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: center;">23%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="text-align: center;">90%</div> <div style="text-align: center;">10%</div> </div>
3	C	104	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: center;">25%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="text-align: center;">84%</div> <div style="text-align: center;">14%</div> <div style="text-align: center;">..</div> </div>
4	D	97	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: center;">6%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="text-align: center;">59%</div> <div style="text-align: center;">29%</div> <div style="text-align: center;">10%</div> <div style="text-align: center;">.</div> </div>
5	E	745	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: center;">13%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="text-align: center;">81%</div> <div style="text-align: center;">5%</div> <div style="text-align: center;">..</div> <div style="text-align: center;">12%</div> </div>
6	R	199	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: center;">20%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="text-align: center;">39%</div> <div style="text-align: center;">.</div> <div style="text-align: center;">.</div> <div style="text-align: center;">55%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	759	A	501	-	-	X	-
8	ZN	R	301	-	-	X	-

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 19875 atoms, of which 9851 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 Bromodomain-containing protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
1	A	114	1835	591	908	155	170	11	0	0

- Molecule 2 is a protein called von Hippel-Lindau disease tumor suppressor.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
2	B	160	2615	824	1307	245	235	4	0	0

- Molecule 3 is a protein called Elongin-B.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
3	C	104	1647	520	824	138	160	5	0	0

- Molecule 4 is a protein called Elongin-C.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
4	D	97	1522	490	757	123	146	6	0	0

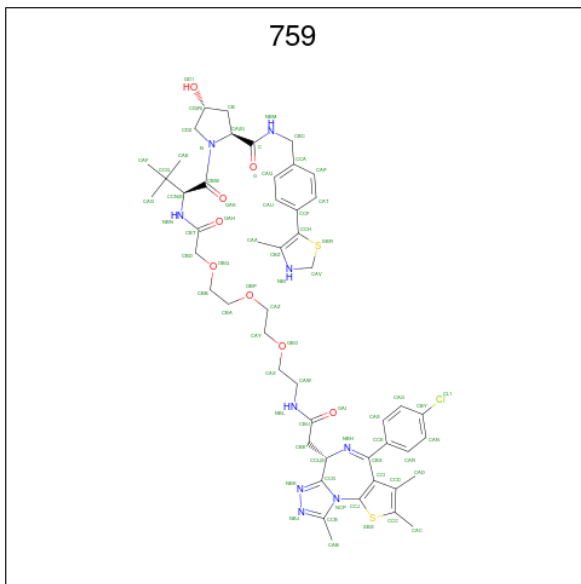
- Molecule 5 is a protein called Cullin-2.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
5	E	658	10756	3436	5363	904	1012	41	0	0

- Molecule 6 is a protein called Rbx1.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
6	R	89	1428	466	692	135	126	9	0	0

- Molecule 7 is (2 {S},4 {R})-1-[(2 {S})-2-[2-[2-[2-[2-[(9 {S})-7-(4-chlorophenyl)-4,5,13-trimethyl-3-thia-1,8,11,12-tetrazatricyclo[8.3.0.0<sup>2,6</sup>]trideca-2(6),4,7,10,12-pentaen-9-yl]ethanoylamino]ethoxy]ethoxy]ethoxy]ethanoylamino]-3,3-dimethyl-butanoyl]- {N}-[[4-(4-methyl-2,3-dihydro-1,3-thiazol-5-yl)phenyl]methyl]-4-oxidanyl-pyrrolidine-2-carboxamide (three-letter code: 759) (formula: C<sub>49</sub>H<sub>62</sub>ClN<sub>9</sub>O<sub>8</sub>S<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf	
			Total	C	Cl	N	O		S
7	A	1	69	49	1	9	8	2	0

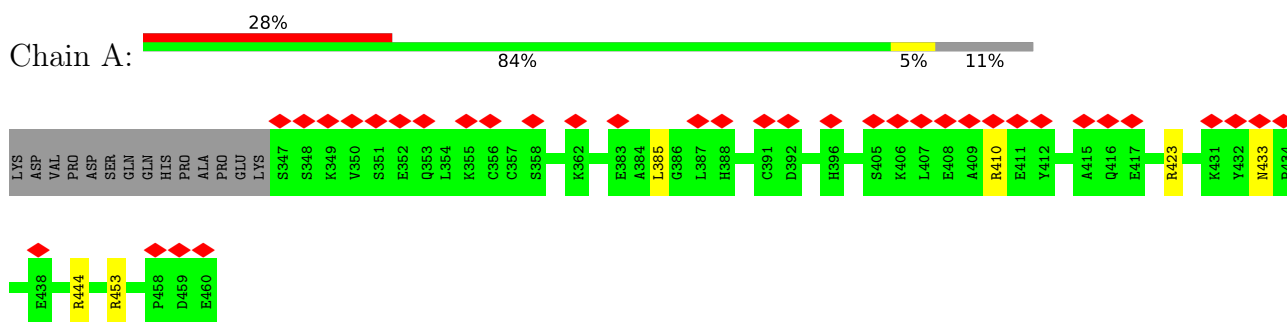
- Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
8	R	3	3	3	0

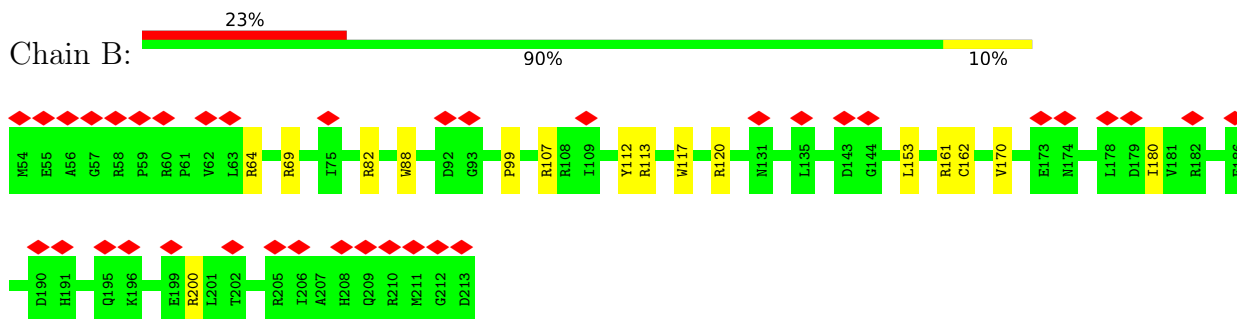
### 3 Residue-property plots [i](#)

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.

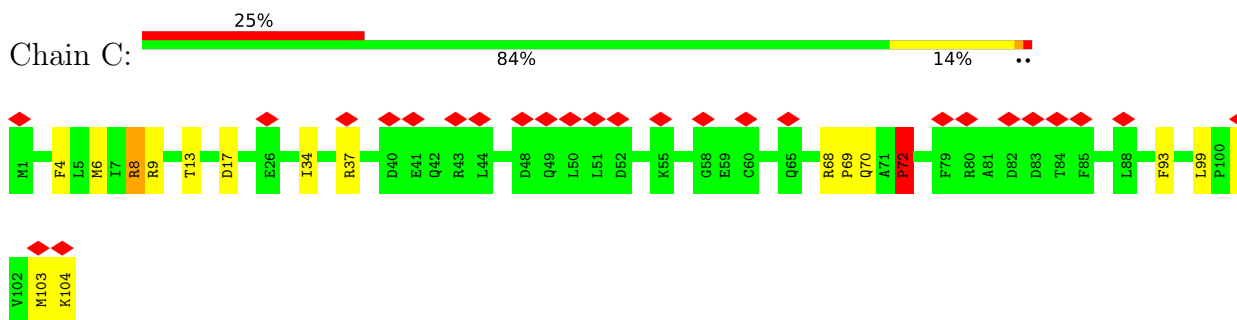
- Molecule 1: Bromodomain-containing protein 4



- Molecule 2: von Hippel-Lindau disease tumor suppressor

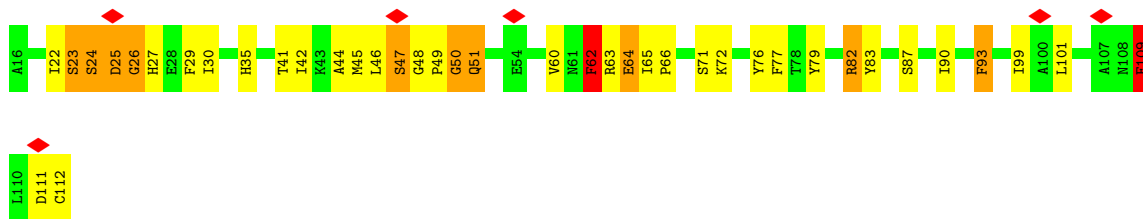


- Molecule 3: Elongin-B

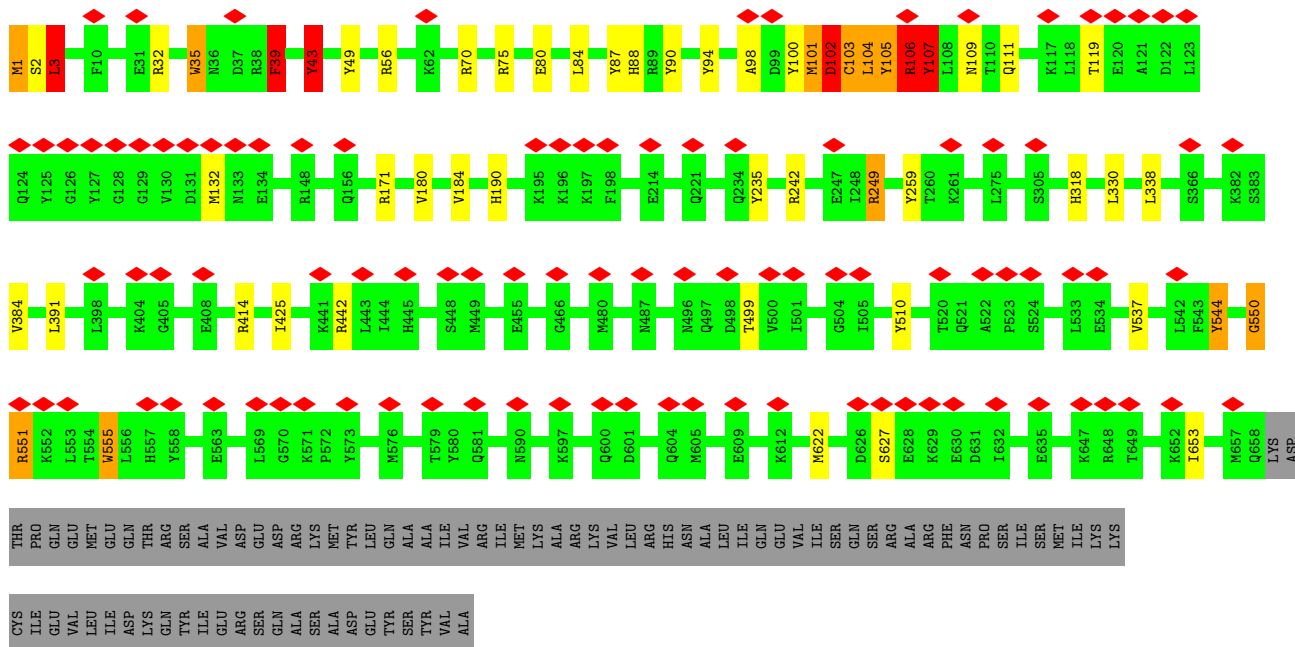
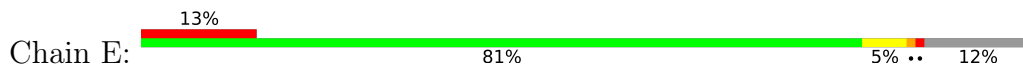


- Molecule 4: Elongin-C

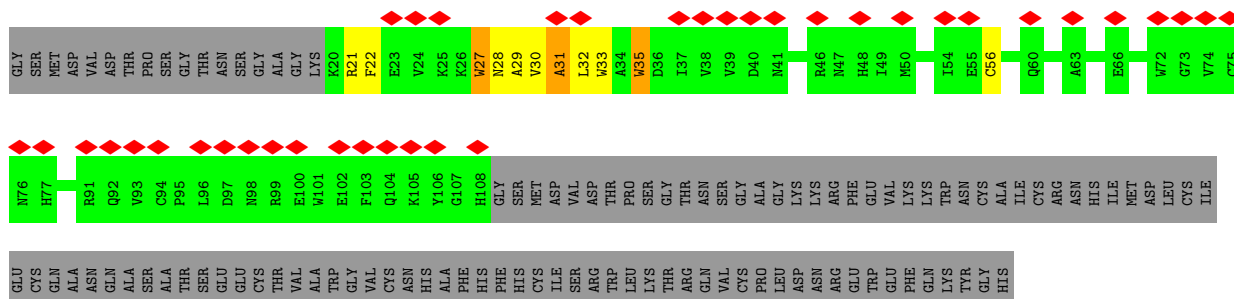
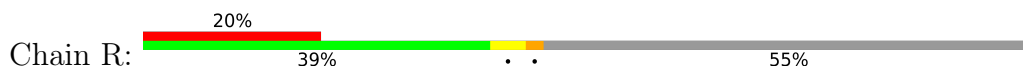




• Molecule 5: Cullin-2



• Molecule 6: Rbx1



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	132697	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	26	Depositor
Minimum defocus (nm)	1700	Depositor
Maximum defocus (nm)	3200	Depositor
Magnification	Not provided	
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	0.789	Depositor
Minimum map value	-0.567	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.04	Depositor
Map size ( $\text{\AA}$ )	378.88, 378.88, 378.88	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.74, 0.74, 0.74	Depositor



## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 759

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	0.70	0/950	0.97	4/1274 (0.3%)
2	B	0.72	0/1341	1.13	8/1824 (0.4%)
3	C	0.66	0/839	1.08	7/1132 (0.6%)
4	D	2.60	4/782 (0.5%)	1.64	21/1057 (2.0%)
5	E	1.20	13/5503 (0.2%)	1.12	34/7416 (0.5%)
6	R	3.71	7/758 (0.9%)	1.51	12/1029 (1.2%)
All	All	1.57	24/10173 (0.2%)	1.19	86/13732 (0.6%)

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
2	B	0	2
4	D	0	2
5	E	0	16
All	All	0	20

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	51	GLN	CA-CB	67.27	3.02	1.53
6	R	31	ALA	CA-C	56.12	2.98	1.52
6	R	35	TRP	CD2-CE2	43.30	1.93	1.41
6	R	35	TRP	CD2-CE3	34.16	1.91	1.40
6	R	35	TRP	CZ3-CH2	33.53	1.93	1.40
6	R	35	TRP	CE3-CZ3	31.27	1.91	1.38
6	R	35	TRP	CE2-CZ2	29.90	1.90	1.39
6	R	35	TRP	CZ2-CH2	28.54	1.91	1.37
5	E	35	TRP	CD2-CE2	26.27	1.72	1.41

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	555	TRP	CD2-CE2	25.53	1.72	1.41
5	E	555	TRP	CD2-CE3	22.23	1.73	1.40
5	E	35	TRP	CD2-CE3	22.22	1.73	1.40
5	E	555	TRP	CZ3-CH2	21.36	1.74	1.40
5	E	35	TRP	CZ3-CH2	20.79	1.73	1.40
5	E	35	TRP	CE3-CZ3	20.54	1.73	1.38
5	E	555	TRP	CE3-CZ3	20.05	1.72	1.38
5	E	555	TRP	CE2-CZ2	18.92	1.72	1.39
5	E	555	TRP	CZ2-CH2	18.39	1.72	1.37
5	E	35	TRP	CE2-CZ2	17.74	1.70	1.39
5	E	35	TRP	CZ2-CH2	17.59	1.70	1.37
5	E	550	GLY	CA-C	7.80	1.64	1.51
4	D	51	GLN	N-CA	6.87	1.60	1.46
4	D	23	SER	CB-OG	-5.20	1.35	1.42
4	D	26	GLY	CA-C	5.19	1.60	1.51

All (86) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	550	GLY	CA-C-O	-16.68	90.58	120.60
6	R	31	ALA	O-C-N	-13.55	101.01	122.70
6	R	31	ALA	CB-CA-C	12.82	129.34	110.10
6	R	31	ALA	N-CA-CB	-11.64	93.81	110.10
6	R	35	TRP	NE1-CE2-CZ2	10.04	141.44	130.40
3	C	8	ARG	NE-CZ-NH2	9.57	125.08	120.30
5	E	249	ARG	NE-CZ-NH2	9.28	124.94	120.30
5	E	35	TRP	CE2-CD2-CG	-8.96	100.13	107.30
6	R	35	TRP	NE1-CE2-CD2	-8.95	98.35	107.30
5	E	104	LEU	N-CA-C	8.79	134.72	111.00
5	E	171	ARG	NE-CZ-NH2	8.68	124.64	120.30
6	R	35	TRP	CG-CD1-NE1	8.61	118.71	110.10
6	R	35	TRP	CE2-CD2-CG	-8.55	100.46	107.30
4	D	26	GLY	N-CA-C	8.06	133.25	113.10
4	D	51	GLN	CB-CA-C	7.89	126.19	110.40
4	D	51	GLN	N-CA-CB	7.85	124.74	110.60
4	D	82	ARG	NE-CZ-NH2	7.73	124.16	120.30
5	E	103	CYS	O-C-N	-7.65	110.45	122.70
5	E	90	TYR	CB-CG-CD2	-7.53	116.48	121.00
4	D	51	GLN	CA-CB-CG	7.52	129.94	113.40
5	E	35	TRP	CB-CG-CD1	-7.52	117.23	127.00
2	B	200	ARG	NE-CZ-NH2	7.41	124.01	120.30
4	D	24	SER	N-CA-C	7.31	130.73	111.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	555	TRP	NE1-CE2-CD2	-7.30	100.00	107.30
5	E	555	TRP	NE1-CE2-CZ2	7.28	138.40	130.40
5	E	442	ARG	NE-CZ-NH2	7.11	123.85	120.30
5	E	103	CYS	CA-C-N	7.07	132.75	117.20
5	E	414	ARG	NE-CZ-NH2	7.01	123.81	120.30
5	E	75	ARG	NE-CZ-NH2	6.94	123.77	120.30
5	E	107	TYR	CB-CG-CD1	-6.80	116.92	121.00
5	E	43	TYR	CB-CG-CD2	-6.78	116.93	121.00
5	E	106	ARG	NE-CZ-NH2	6.74	123.67	120.30
4	D	76	TYR	CB-CG-CD1	-6.73	116.96	121.00
5	E	106	ARG	CB-CA-C	6.70	123.80	110.40
1	A	444	ARG	NE-CZ-NH2	6.67	123.64	120.30
4	D	64	GLU	N-CA-C	6.64	128.93	111.00
5	E	1	MET	C-N-CA	6.61	138.22	121.70
2	B	82	ARG	NE-CZ-NH2	6.47	123.54	120.30
6	R	35	TRP	CG-CD2-CE3	6.38	139.64	133.90
4	D	42	ILE	CA-CB-CG1	-6.36	98.91	111.00
2	B	120	ARG	NE-CZ-NH2	6.35	123.47	120.30
2	B	113	ARG	NE-CZ-NH2	6.34	123.47	120.30
5	E	101	MET	N-CA-CB	6.34	122.01	110.60
5	E	35	TRP	CB-CG-CD2	6.31	134.80	126.60
4	D	50	GLY	N-CA-C	6.27	128.78	113.10
1	A	410	ARG	NE-CZ-NH2	6.19	123.40	120.30
4	D	77	PHE	CB-CG-CD2	-6.18	116.47	120.80
6	R	21	ARG	NE-CZ-NH2	6.16	123.38	120.30
5	E	242	ARG	NE-CZ-NH2	6.14	123.37	120.30
2	B	64	ARG	NE-CZ-NH2	6.04	123.32	120.30
6	R	31	ALA	CA-C-N	5.95	130.30	117.20
5	E	56	ARG	NE-CZ-NH2	5.94	123.27	120.30
3	C	37	ARG	NE-CZ-NH2	5.90	123.25	120.30
2	B	162	CYS	CA-CB-SG	-5.81	103.54	114.00
2	B	107	ARG	NE-CZ-NH2	5.78	123.19	120.30
5	E	249	ARG	NE-CZ-NH1	-5.76	117.42	120.30
4	D	25	ASP	C-N-CA	5.75	134.37	122.30
1	A	423	ARG	NE-CZ-NH2	5.73	123.17	120.30
4	D	93	PHE	CB-CG-CD2	-5.71	116.80	120.80
5	E	70	ARG	NE-CZ-NH2	5.69	123.15	120.30
6	R	27	TRP	CB-CG-CD2	5.69	134.00	126.60
6	R	31	ALA	N-CA-C	5.66	126.27	111.00
5	E	39	PHE	CA-CB-CG	5.65	127.47	113.90
4	D	62	PHE	CB-CG-CD1	5.63	124.74	120.80
4	D	23	SER	CB-CA-C	5.58	120.70	110.10

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	3	LEU	N-CA-C	5.58	126.06	111.00
4	D	51	GLN	N-CA-C	-5.48	96.22	111.00
1	A	453	ARG	NE-CZ-NH2	5.43	123.01	120.30
4	D	77	PHE	CB-CG-CD1	5.38	124.57	120.80
2	B	161	ARG	NE-CZ-NH2	5.38	122.99	120.30
5	E	551	ARG	NE-CZ-NH2	5.36	122.98	120.30
3	C	70	GLN	CB-CA-C	5.27	120.94	110.40
4	D	47	SER	N-CA-C	5.27	125.22	111.00
4	D	49	PRO	C-N-CA	5.22	133.26	122.30
4	D	112	CYS	CA-CB-SG	5.22	123.39	114.00
5	E	555	TRP	CE2-CD2-CG	-5.22	103.13	107.30
5	E	35	TRP	CA-CB-CG	5.20	123.58	113.70
5	E	35	TRP	CG-CD1-NE1	5.20	115.30	110.10
4	D	23	SER	CA-C-N	5.20	128.63	117.20
3	C	8	ARG	NH1-CZ-NH2	-5.18	113.71	119.40
5	E	259	TYR	CB-CG-CD2	-5.15	117.91	121.00
3	C	37	ARG	NE-CZ-NH1	-5.12	117.74	120.30
3	C	9	ARG	CD-NE-CZ	5.06	130.69	123.60
5	E	544	TYR	CB-CG-CD1	-5.02	117.99	121.00
5	E	104	LEU	O-C-N	-5.02	114.67	122.70
3	C	68	ARG	NE-CZ-NH2	5.01	122.81	120.30

There are no chirality outliers.

All (20) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	112	TYR	Sidechain
2	B	69	ARG	Sidechain
4	D	109	PHE	Sidechain
4	D	29	PHE	Sidechain
5	E	100	TYR	Sidechain
5	E	102	ASP	Mainchain
5	E	105	TYR	Sidechain
5	E	106	ARG	Sidechain
5	E	107	TYR	Sidechain
5	E	190	HIS	Sidechain
5	E	235	TYR	Sidechain
5	E	249	ARG	Sidechain
5	E	318	HIS	Sidechain
5	E	32	ARG	Sidechain
5	E	39	PHE	Sidechain
5	E	43	TYR	Sidechain

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type	Group
5	E	49	TYR	Sidechain
5	E	510	TYR	Sidechain
5	E	88	HIS	Sidechain
5	E	94	TYR	Sidechain

## 5.2 Too-close contacts [i](#)

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	927	908	907	3	0
2	B	1308	1307	1301	26	0
3	C	823	824	824	7	0
4	D	765	757	754	93	0
5	E	5393	5363	5362	143	0
6	R	736	692	690	56	0
7	A	69	0	0	27	0
8	R	3	0	0	2	0
All	All	10024	9851	9838	192	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 10.

All (192) 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)
7:A:501:759:SBR	2:B:99:PRO:HB2	1.24	1.76
6:R:35:TRP:CH2	6:R:35:TRP:CZ2	1.91	1.58
6:R:35:TRP:CD2	6:R:35:TRP:CE3	1.91	1.57
6:R:35:TRP:CZ2	6:R:35:TRP:CE2	1.90	1.56
6:R:35:TRP:CH2	6:R:35:TRP:CZ3	1.93	1.56
6:R:35:TRP:CE3	6:R:35:TRP:CZ3	1.91	1.53
5:E:555:TRP:CD2	6:R:31:ALA:HA	1.48	1.46
6:R:35:TRP:CD2	6:R:35:TRP:CE2	1.93	1.42
7:A:501:759:SBR	2:B:99:PRO:CB	2.14	1.36
7:A:501:759:CCF	2:B:99:PRO:HG2	1.55	1.35
4:D:51:GLN:HA	5:E:35:TRP:CD2	1.63	1.33

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:555:TRP:CE3	6:R:31:ALA:HA	1.61	1.33
4:D:51:GLN:HA	5:E:35:TRP:CE3	1.65	1.32
7:A:501:759:CCH	2:B:99:PRO:HG2	1.62	1.29
1:A:433:ASN:HD21	7:A:501:759:CAB	1.50	1.22
4:D:51:GLN:CA	5:E:35:TRP:CE3	2.26	1.19
5:E:555:TRP:CH2	6:R:31:ALA:CA	2.26	1.18
7:A:501:759:CAV	2:B:99:PRO:HB2	1.74	1.18
4:D:51:GLN:CA	5:E:35:TRP:CZ3	2.26	1.18
4:D:51:GLN:CA	5:E:35:TRP:CH2	2.27	1.18
5:E:555:TRP:CE3	6:R:31:ALA:CA	2.26	1.18
4:D:51:GLN:CA	5:E:35:TRP:CZ2	2.28	1.17
5:E:555:TRP:CD2	6:R:31:ALA:CA	2.27	1.17
5:E:555:TRP:CZ3	6:R:31:ALA:CA	2.29	1.16
4:D:51:GLN:CB	5:E:35:TRP:CD2	2.29	1.16
4:D:51:GLN:CA	5:E:35:TRP:CE2	2.28	1.16
5:E:555:TRP:CZ2	6:R:31:ALA:CA	2.29	1.16
4:D:51:GLN:CB	5:E:35:TRP:CE3	2.30	1.15
4:D:51:GLN:CB	5:E:35:TRP:CZ3	2.28	1.15
7:A:501:759:CAF	2:B:88:TRP:HZ3	1.59	1.15
5:E:555:TRP:CE2	6:R:31:ALA:CA	2.30	1.15
4:D:51:GLN:CB	5:E:35:TRP:CH2	2.29	1.14
4:D:51:GLN:CB	5:E:35:TRP:CZ2	2.31	1.14
4:D:51:GLN:CB	5:E:35:TRP:CE2	2.30	1.12
4:D:51:GLN:CA	5:E:35:TRP:CD2	2.31	1.12
5:E:550:GLY:C	6:R:35:TRP:CE3	2.24	1.11
5:E:550:GLY:C	6:R:35:TRP:CZ2	2.25	1.10
5:E:550:GLY:C	6:R:35:TRP:CH2	2.25	1.10
5:E:555:TRP:CZ3	6:R:31:ALA:C	2.25	1.09
5:E:555:TRP:CE2	6:R:31:ALA:C	2.26	1.09
5:E:550:GLY:C	6:R:35:TRP:CZ3	2.26	1.09
5:E:550:GLY:C	6:R:35:TRP:CD2	2.26	1.08
5:E:550:GLY:C	6:R:35:TRP:CE2	2.26	1.08
5:E:551:ARG:N	6:R:35:TRP:CZ3	2.22	1.08
5:E:551:ARG:N	6:R:35:TRP:CH2	2.22	1.07
5:E:555:TRP:CZ2	6:R:31:ALA:C	2.28	1.07
5:E:551:ARG:N	6:R:35:TRP:CE2	2.23	1.07
7:A:501:759:CAT	2:B:99:PRO:HG2	1.85	1.06
5:E:551:ARG:N	6:R:35:TRP:CZ2	2.24	1.06
5:E:555:TRP:CH2	6:R:31:ALA:C	2.29	1.05
5:E:555:TRP:CE3	6:R:31:ALA:C	2.29	1.05
5:E:551:ARG:N	6:R:35:TRP:CD2	2.24	1.05

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:501:759:CCH	2:B:99:PRO:CG	2.34	1.05
5:E:551:ARG:N	6:R:35:TRP:CE3	2.24	1.05
5:E:555:TRP:CD2	6:R:31:ALA:C	2.30	1.04
7:A:501:759:CAF	2:B:88:TRP:CZ3	2.43	1.01
4:D:51:GLN:HB3	5:E:35:TRP:CE2	1.96	1.00
1:A:433:ASN:ND2	7:A:501:759:CAB	2.26	0.98
4:D:51:GLN:HB2	5:E:35:TRP:CH2	1.97	0.96
4:D:26:GLY:H	5:E:1:MET:HA	1.28	0.94
5:E:550:GLY:HA3	6:R:35:TRP:CZ3	2.06	0.91
7:A:501:759:CCF	2:B:99:PRO:CG	2.48	0.90
5:E:550:GLY:CA	6:R:35:TRP:CZ3	2.56	0.88
7:A:501:759:CCH	2:B:99:PRO:CB	2.53	0.86
5:E:550:GLY:CA	6:R:35:TRP:CH2	2.61	0.83
7:A:501:759:CG	2:B:117:TRP:HH2	1.92	0.82
4:D:65:ILE:H	5:E:3:LEU:HD22	1.42	0.82
5:E:550:GLY:C	5:E:551:ARG:N	2.33	0.81
4:D:51:GLN:CG	5:E:35:TRP:CE3	2.63	0.81
4:D:51:GLN:N	5:E:35:TRP:CZ3	2.49	0.80
7:A:501:759:CG	2:B:117:TRP:CH2	2.65	0.80
4:D:51:GLN:HB3	5:E:35:TRP:CD2	2.16	0.80
7:A:501:759:CCH	2:B:99:PRO:HB2	2.11	0.78
5:E:555:TRP:CE2	6:R:31:ALA:CB	2.66	0.78
7:A:501:759:SBR	2:B:99:PRO:CG	2.72	0.78
4:D:51:GLN:C	5:E:35:TRP:CE2	2.58	0.77
5:E:555:TRP:CZ3	6:R:31:ALA:N	2.52	0.77
7:A:501:759:CAV	2:B:99:PRO:CB	2.56	0.76
5:E:551:ARG:CA	6:R:35:TRP:CE2	2.67	0.76
5:E:555:TRP:CZ2	6:R:31:ALA:CB	2.68	0.76
5:E:555:TRP:CE2	6:R:31:ALA:HB1	2.21	0.76
5:E:550:GLY:O	6:R:35:TRP:CE2	2.39	0.75
5:E:555:TRP:CD2	6:R:32:LEU:N	2.54	0.75
4:D:26:GLY:N	5:E:1:MET:HA	2.01	0.74
4:D:51:GLN:HB2	5:E:35:TRP:CZ2	2.14	0.74
4:D:45:MET:HB3	5:E:39:PHE:CD2	2.24	0.73
4:D:51:GLN:CD	5:E:35:TRP:CZ3	2.62	0.73
4:D:47:SER:HA	5:E:102:ASP:C	2.09	0.72
4:D:51:GLN:C	5:E:35:TRP:CZ2	2.61	0.72
5:E:391:LEU:HD13	5:E:425:ILE:HD11	1.72	0.71
4:D:62:PHE:HB2	5:E:3:LEU:HD21	1.72	0.71
5:E:551:ARG:HA	6:R:35:TRP:CE2	2.25	0.70
4:D:65:ILE:N	5:E:3:LEU:HD22	2.07	0.70

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:501:759:OAH	2:B:88:TRP:CH2	2.45	0.70
5:E:550:GLY:O	6:R:35:TRP:CD2	2.45	0.70
4:D:24:SER:H	5:E:3:LEU:N	1.90	0.69
7:A:501:759:OD1	2:B:117:TRP:CZ2	2.47	0.68
5:E:555:TRP:CH2	6:R:31:ALA:O	2.46	0.68
6:R:56:CYS:HG	8:R:301:ZN:ZN	1.04	0.68
4:D:66:PRO:HA	5:E:3:LEU:CB	2.24	0.68
6:R:56:CYS:SG	8:R:301:ZN:ZN	1.83	0.65
4:D:23:SER:CB	5:E:3:LEU:HD12	2.27	0.65
4:D:51:GLN:N	5:E:35:TRP:CH2	2.65	0.64
5:E:555:TRP:CH2	6:R:31:ALA:N	2.66	0.64
4:D:109:PHE:CD1	5:E:107:TYR:CZ	2.86	0.64
4:D:25:ASP:N	5:E:2:SER:H	1.97	0.63
4:D:66:PRO:HA	5:E:3:LEU:HB2	1.79	0.63
4:D:51:GLN:CG	5:E:35:TRP:CZ3	2.80	0.63
5:E:550:GLY:HA3	6:R:35:TRP:CH2	2.32	0.62
7:A:501:759:CAT	2:B:99:PRO:CG	2.70	0.60
7:A:501:759:OD1	2:B:117:TRP:HZ2	1.84	0.60
4:D:65:ILE:C	5:E:3:LEU:HB3	2.20	0.60
4:D:23:SER:HA	5:E:3:LEU:HG	1.82	0.60
1:A:385:LEU:HD11	7:A:501:759:CAC	2.31	0.60
5:E:537:VAL:HG22	6:R:31:ALA:HB3	1.84	0.59
4:D:64:GLU:N	5:E:3:LEU:HD23	2.16	0.59
5:E:555:TRP:CE3	6:R:32:LEU:N	2.69	0.59
4:D:51:GLN:HG3	5:E:35:TRP:CE3	2.37	0.58
5:E:180:VAL:O	5:E:184:VAL:HG23	2.03	0.58
4:D:79:TYR:CE2	4:D:93:PHE:HB2	2.39	0.58
5:E:551:ARG:CA	6:R:35:TRP:CD2	2.85	0.58
5:E:555:TRP:CZ2	6:R:31:ALA:O	2.56	0.58
4:D:24:SER:HA	5:E:1:MET:HB3	1.85	0.57
4:D:51:GLN:HE22	5:E:104:LEU:CA	2.18	0.57
4:D:23:SER:HB3	5:E:3:LEU:HD12	1.88	0.56
4:D:45:MET:CB	5:E:39:PHE:CD2	2.89	0.56
4:D:65:ILE:O	5:E:3:LEU:HD13	2.06	0.56
5:E:43:TYR:HA	5:E:107:TYR:CE2	2.41	0.55
4:D:24:SER:HB3	4:D:63:ARG:HA	1.90	0.54
4:D:51:GLN:HE22	5:E:104:LEU:HB2	1.73	0.53
4:D:23:SER:HB2	5:E:3:LEU:H	1.73	0.53
4:D:45:MET:SD	5:E:39:PHE:HA	2.48	0.53
4:D:24:SER:OG	5:E:3:LEU:HA	2.09	0.52
4:D:50:GLY:C	5:E:35:TRP:CZ3	2.84	0.51

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:109:PHE:CD1	5:E:111:GLN:HG3	2.46	0.51
4:D:45:MET:SD	5:E:39:PHE:CA	3.00	0.50
4:D:109:PHE:CD1	5:E:107:TYR:CE2	3.00	0.49
5:E:551:ARG:C	6:R:35:TRP:CD2	2.85	0.49
3:C:4:PHE:CG	3:C:69:PRO:HA	2.47	0.49
4:D:51:GLN:HE22	5:E:104:LEU:CB	2.26	0.49
5:E:98:ALA:C	5:E:101:MET:H	2.16	0.49
4:D:24:SER:H	5:E:3:LEU:CA	2.26	0.49
5:E:35:TRP:CH2	5:E:103:CYS:HB3	2.48	0.49
4:D:82:ARG:HG3	4:D:83:TYR:CE1	2.47	0.49
4:D:60:VAL:HG22	5:E:39:PHE:CE2	2.48	0.48
4:D:48:GLY:HA3	5:E:105:TYR:H	1.77	0.48
2:B:180:ILE:HG21	4:D:101:LEU:HD11	1.95	0.48
4:D:60:VAL:HG22	5:E:39:PHE:CZ	2.48	0.48
3:C:8:ARG:HG2	3:C:13:THR:HG23	1.96	0.48
4:D:44:ALA:HB1	5:E:106:ARG:HB3	1.96	0.47
4:D:111:ASP:HB2	5:E:111:GLN:HE22	1.78	0.47
4:D:62:PHE:CB	5:E:3:LEU:HD21	2.42	0.47
7:A:501:759:CBZ	2:B:99:PRO:CB	2.93	0.47
4:D:51:GLN:CD	5:E:104:LEU:HD13	2.34	0.47
4:D:51:GLN:OE1	5:E:104:LEU:HD13	2.14	0.47
4:D:51:GLN:NE2	5:E:35:TRP:CZ3	2.83	0.46
4:D:48:GLY:H	5:E:103:CYS:C	2.18	0.46
4:D:44:ALA:HB1	5:E:106:ARG:CA	2.45	0.46
7:A:501:759:OAH	2:B:88:TRP:CZ2	2.69	0.46
4:D:23:SER:OG	5:E:2:SER:HA	2.15	0.46
4:D:25:ASP:H	5:E:2:SER:C	2.19	0.46
5:E:544:TYR:CD2	6:R:33:TRP:HA	2.50	0.46
4:D:25:ASP:N	5:E:2:SER:N	2.62	0.45
4:D:26:GLY:CA	5:E:1:MET:HA	2.46	0.45
5:E:622:MET:SD	5:E:653:ILE:HD11	2.55	0.45
4:D:72:LYS:HE2	4:D:99:ILE:HD11	1.99	0.45
4:D:44:ALA:HB1	5:E:106:ARG:CB	2.47	0.45
4:D:44:ALA:HB1	5:E:106:ARG:C	2.37	0.44
7:A:501:759:OD1	2:B:117:TRP:CH2	2.70	0.44
3:C:34:ILE:HG23	4:D:30:ILE:HG21	2.00	0.43
4:D:23:SER:HB2	5:E:3:LEU:HD12	1.99	0.43
4:D:22:ILE:HG22	5:E:1:MET:HB2	1.99	0.43
5:E:84:LEU:HD22	5:E:184:VAL:HG21	2.01	0.43
5:E:106:ARG:HA	5:E:109:ASN:HB2	2.01	0.43
3:C:93:PHE:CE2	4:D:71:SER:HB2	2.53	0.43

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:87:TYR:C	5:E:87:TYR:CD1	2.92	0.43
4:D:45:MET:HG2	5:E:104:LEU:O	2.19	0.43
7:A:501:759:CCE	7:A:501:759:CAD	2.96	0.42
2:B:153:LEU:O	4:D:90:ILE:HD12	2.18	0.42
4:D:47:SER:HA	5:E:103:CYS:N	2.33	0.42
4:D:27:HIS:H	5:E:1:MET:C	2.22	0.42
4:D:45:MET:C	5:E:103:CYS:O	2.57	0.42
4:D:41:THR:HA	4:D:44:ALA:HB3	2.01	0.42
5:E:330:LEU:HD22	5:E:338:LEU:HB3	2.01	0.42
2:B:170:VAL:CG2	3:C:103:MET:HG2	2.50	0.42
3:C:99:LEU:O	3:C:104:LYS:HE3	2.20	0.42
4:D:50:GLY:HA2	5:E:103:CYS:CB	2.48	0.42
4:D:46:LEU:C	5:E:103:CYS:HA	2.40	0.41
4:D:23:SER:O	5:E:1:MET:CB	2.68	0.41
3:C:6:MET:SD	3:C:72:PRO:HG2	2.61	0.41
5:E:537:VAL:HG22	6:R:31:ALA:CB	2.49	0.40
4:D:23:SER:CA	5:E:3:LEU:HG	2.49	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	112/128 (88%)	112 (100%)	0	0	100	100
2	B	158/160 (99%)	155 (98%)	3 (2%)	0	100	100
3	C	102/104 (98%)	96 (94%)	4 (4%)	2 (2%)	7	40
4	D	95/97 (98%)	90 (95%)	5 (5%)	0	100	100
5	E	654/745 (88%)	637 (97%)	13 (2%)	4 (1%)	25	63
6	R	87/199 (44%)	70 (80%)	16 (18%)	1 (1%)	14	51
All	All	1208/1433 (84%)	1160 (96%)	41 (3%)	7 (1%)	29	63

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	E	3	LEU
5	E	80	GLU
5	E	132	MET
3	C	101	ASP
5	E	102	ASP
6	R	29	ALA
3	C	72	PRO

### 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	A	100/113 (88%)	100 (100%)	0	100	100
2	B	147/147 (100%)	147 (100%)	0	100	100
3	C	92/92 (100%)	90 (98%)	2 (2%)	52	71
4	D	85/85 (100%)	81 (95%)	4 (5%)	26	53
5	E	603/681 (88%)	599 (99%)	4 (1%)	84	90
6	R	78/170 (46%)	74 (95%)	4 (5%)	24	52
All	All	1105/1288 (86%)	1091 (99%)	14 (1%)	70	82

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	17	ASP
3	C	72	PRO
4	D	35	HIS
4	D	62	PHE
4	D	87	SER
4	D	109	PHE
5	E	119	THR
5	E	384	VAL
5	E	499	THR
5	E	627	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
6	R	22	PHE
6	R	27	TRP
6	R	28	ASN
6	R	30	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
4	D	51	GLN

### 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 monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 3 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
7	759	A	501	2,1	69,75,75	2.54	13 (18%)	83,107,107	2.27	15 (18%)

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	759	A	501	2,1	-	7/53/91/91	0/6/7/7

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	501	759	CCI-CBX	-9.62	1.35	1.49
7	A	501	759	CAV-NBI	-7.58	1.34	1.44
7	A	501	759	CCE-CBX	-6.63	1.39	1.49
7	A	501	759	CCH-SBR	-5.80	1.70	1.76
7	A	501	759	NBJ-NBK	-5.68	1.26	1.37
7	A	501	759	CCF-CCH	-5.58	1.35	1.48
7	A	501	759	CBC-CCA	-5.37	1.39	1.51
7	A	501	759	CA-C	-4.16	1.43	1.52
7	A	501	759	CBX-NBH	4.16	1.33	1.28
7	A	501	759	CCI-CCJ	-3.63	1.34	1.40
7	A	501	759	CA-N	3.19	1.53	1.47
7	A	501	759	CCB-NCP	-2.95	1.32	1.37
7	A	501	759	CAA-CBZ	2.48	1.54	1.49

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	501	759	CCL-NBH-CBX	9.77	127.09	117.62
7	A	501	759	CCF-CCH-SBR	8.57	126.29	115.67
7	A	501	759	OBQ-CBD-CBT	-6.39	98.66	112.38
7	A	501	759	CCH-CBZ-NBI	6.01	114.72	105.71
7	A	501	759	CAA-CBZ-CCH	-5.45	124.46	131.01
7	A	501	759	CBW-CCN-NBN	-4.71	102.20	107.34
7	A	501	759	CCI-CBX-CCE	3.65	122.34	118.11
7	A	501	759	CBD-OBQ-CBB	3.28	121.68	113.13
7	A	501	759	SBR-CAV-NBI	3.02	107.11	105.41
7	A	501	759	CBD-CBT-NBN	-2.84	111.43	116.37
7	A	501	759	CCE-CBX-NBH	-2.52	114.39	117.27
7	A	501	759	CCQ-CCN-NBN	-2.42	108.81	111.84
7	A	501	759	CBZ-CCH-SBR	-2.31	105.70	111.58
7	A	501	759	CAV-NBI-CBZ	-2.31	115.93	118.32
7	A	501	759	CAT-CCF-CCH	2.07	124.30	120.83

There are no chirality outliers.

All (7) torsion outliers are listed below:

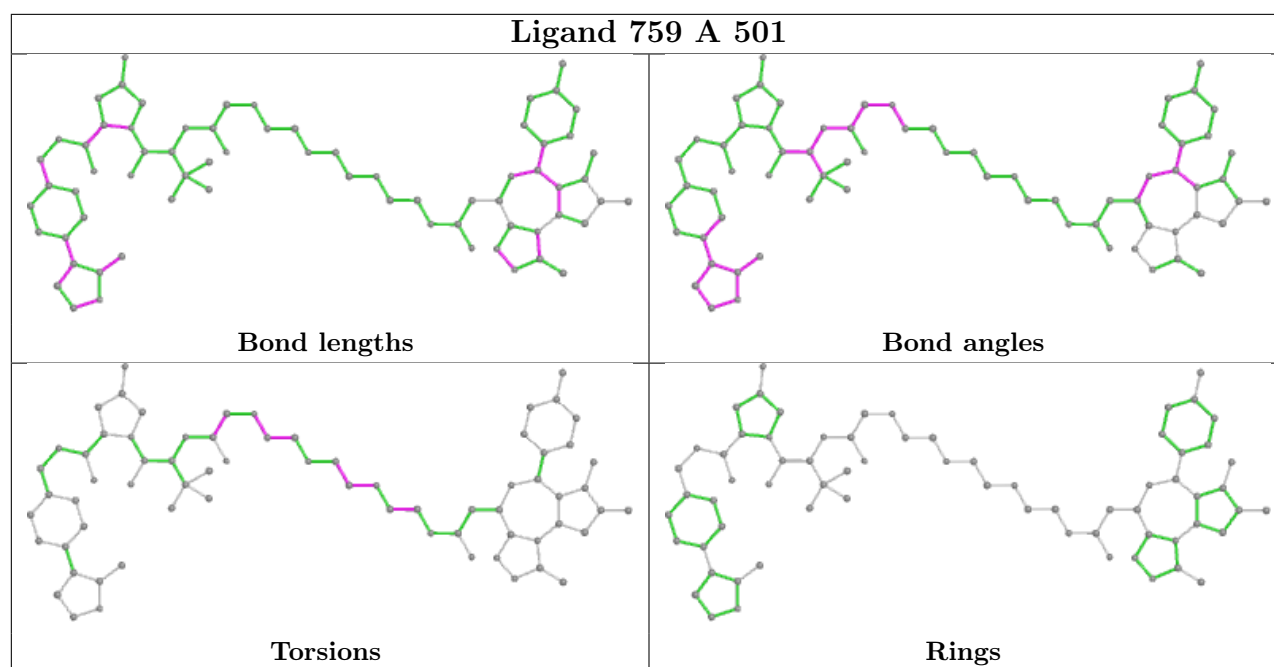
Mol	Chain	Res	Type	Atoms
7	A	501	759	OBP-CBA-CBB-OBQ
7	A	501	759	NBL-CAW-CAX-OBO
7	A	501	759	OBQ-CBD-CBT-NBN
7	A	501	759	OBQ-CBD-CBT-OAH
7	A	501	759	CAZ-CAY-OBO-CAX
7	A	501	759	CBA-CBB-OBQ-CBD
7	A	501	759	OBO-CAY-CAZ-OBP

There are no ring outliers.

1 monomer is involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	501	759	27	0

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



## 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [\(i\)](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
5	E	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	550:GLY	C	551:ARG	N	2.33

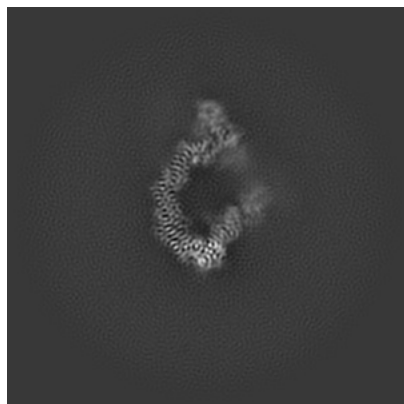
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-19569. These allow visual inspection of the internal detail of the map and identification of artifacts.

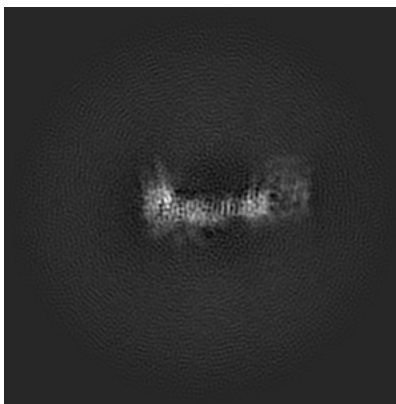
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

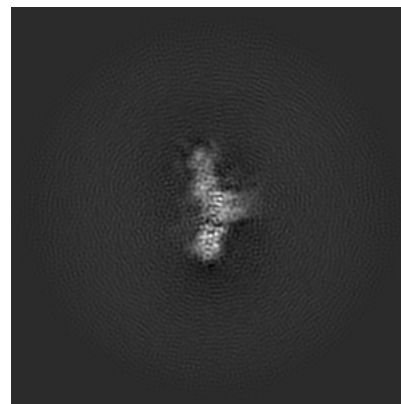
#### 6.1.1 Primary map



X

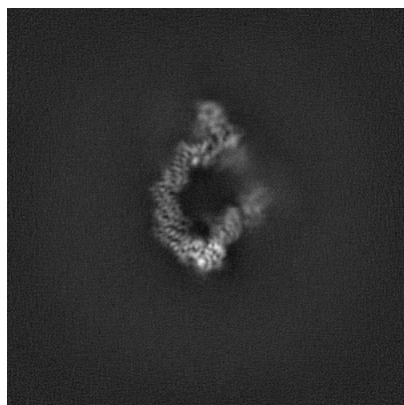


Y

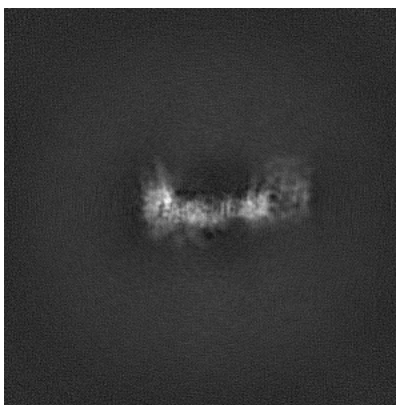


Z

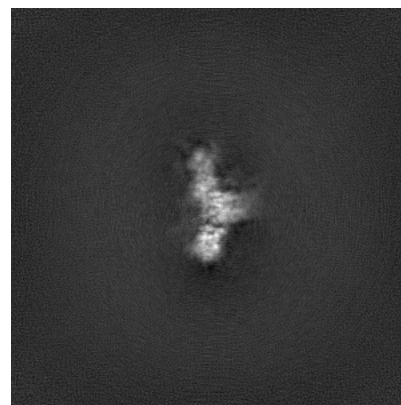
#### 6.1.2 Raw map



X



Y



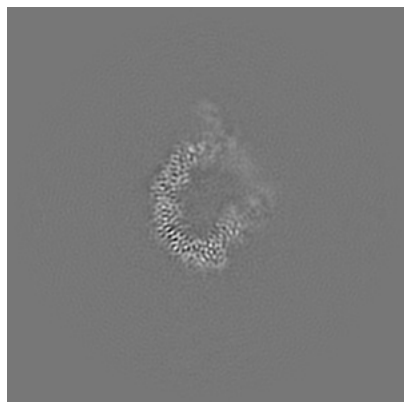
Z

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

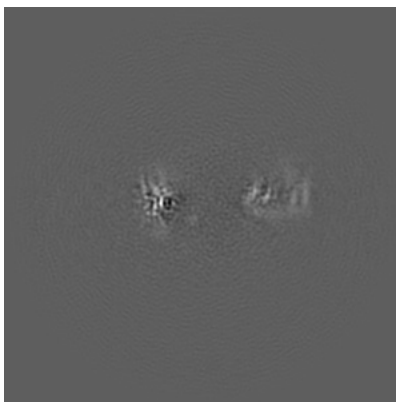


## 6.2 Central slices [i](#)

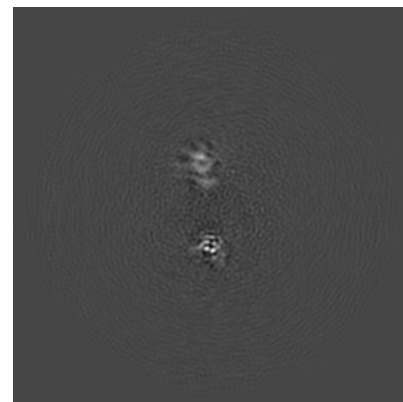
### 6.2.1 Primary map



X Index: 256

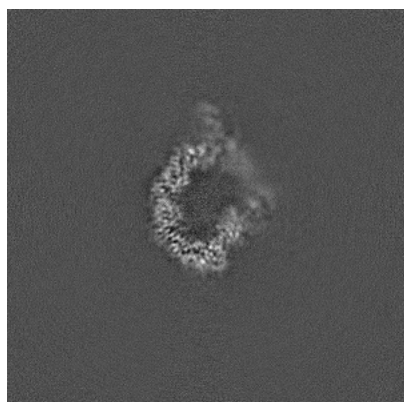


Y Index: 256

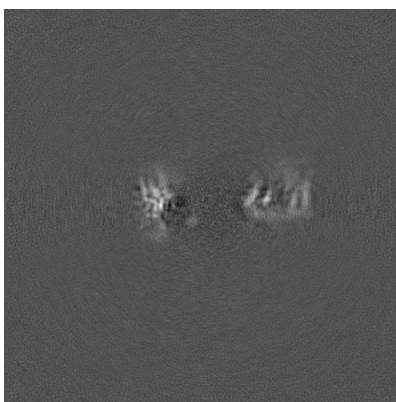


Z Index: 256

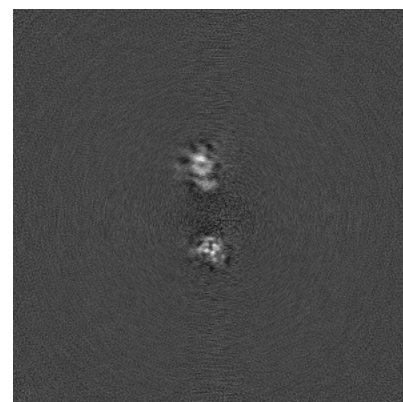
### 6.2.2 Raw map



X Index: 256



Y Index: 256

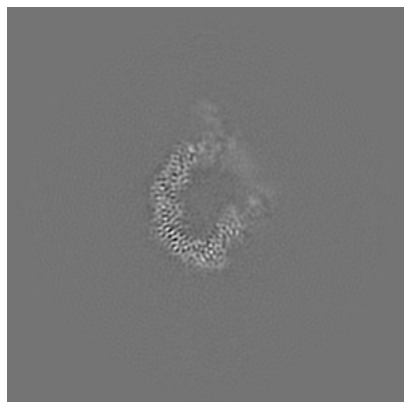


Z Index: 256

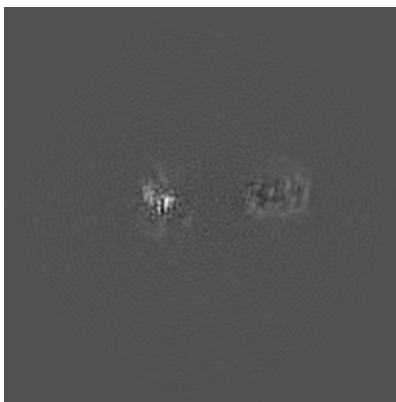
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

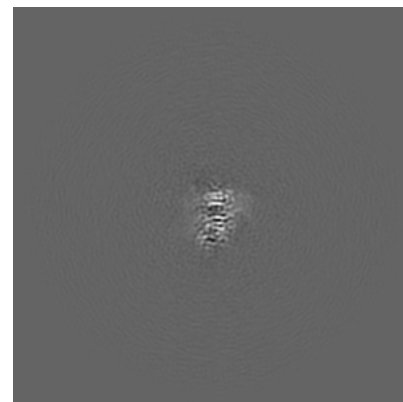
### 6.3.1 Primary map



X Index: 255

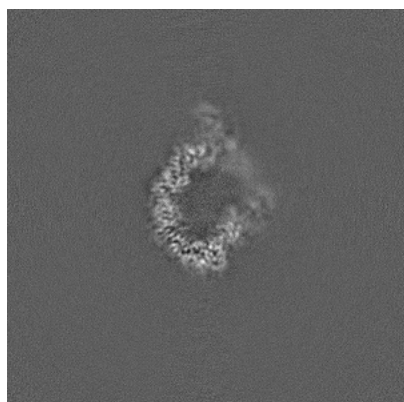


Y Index: 260

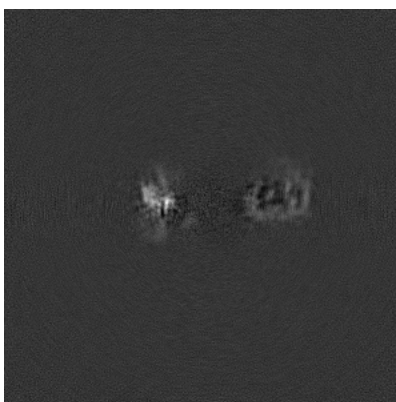


Z Index: 206

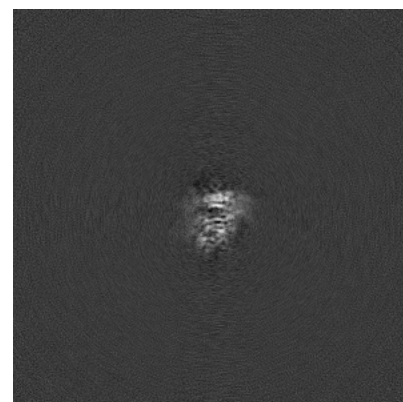
### 6.3.2 Raw map



X Index: 257



Y Index: 259

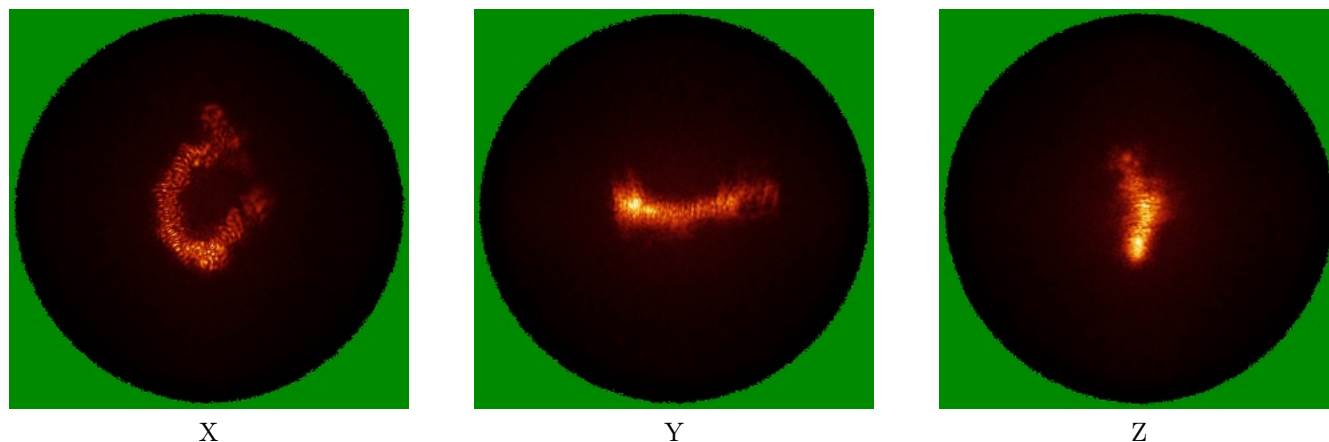


Z Index: 206

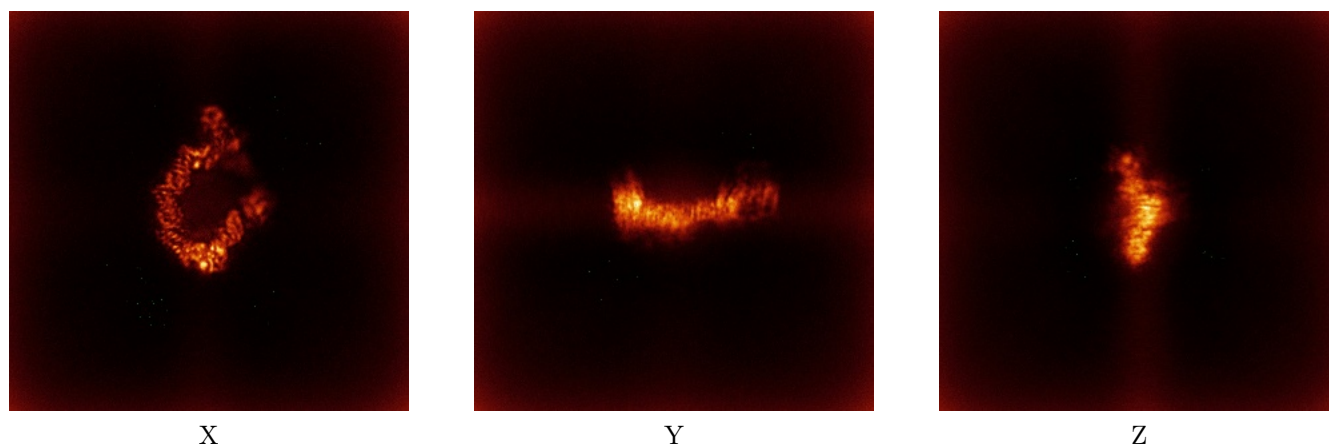
The images above show the largest variance slices of the map in three orthogonal directions.

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

### 6.4.1 Primary map



### 6.4.2 Raw map



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.

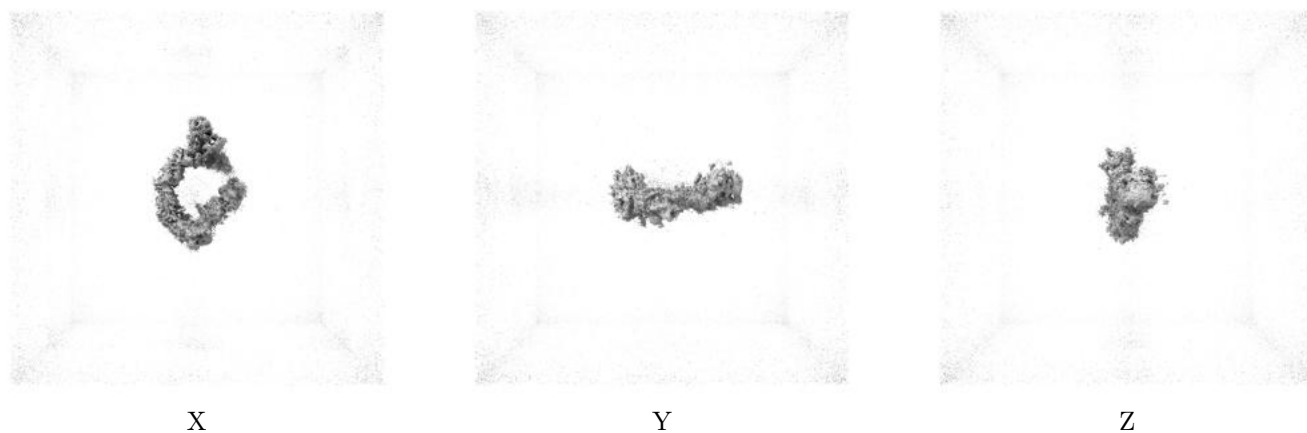
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.04. 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.

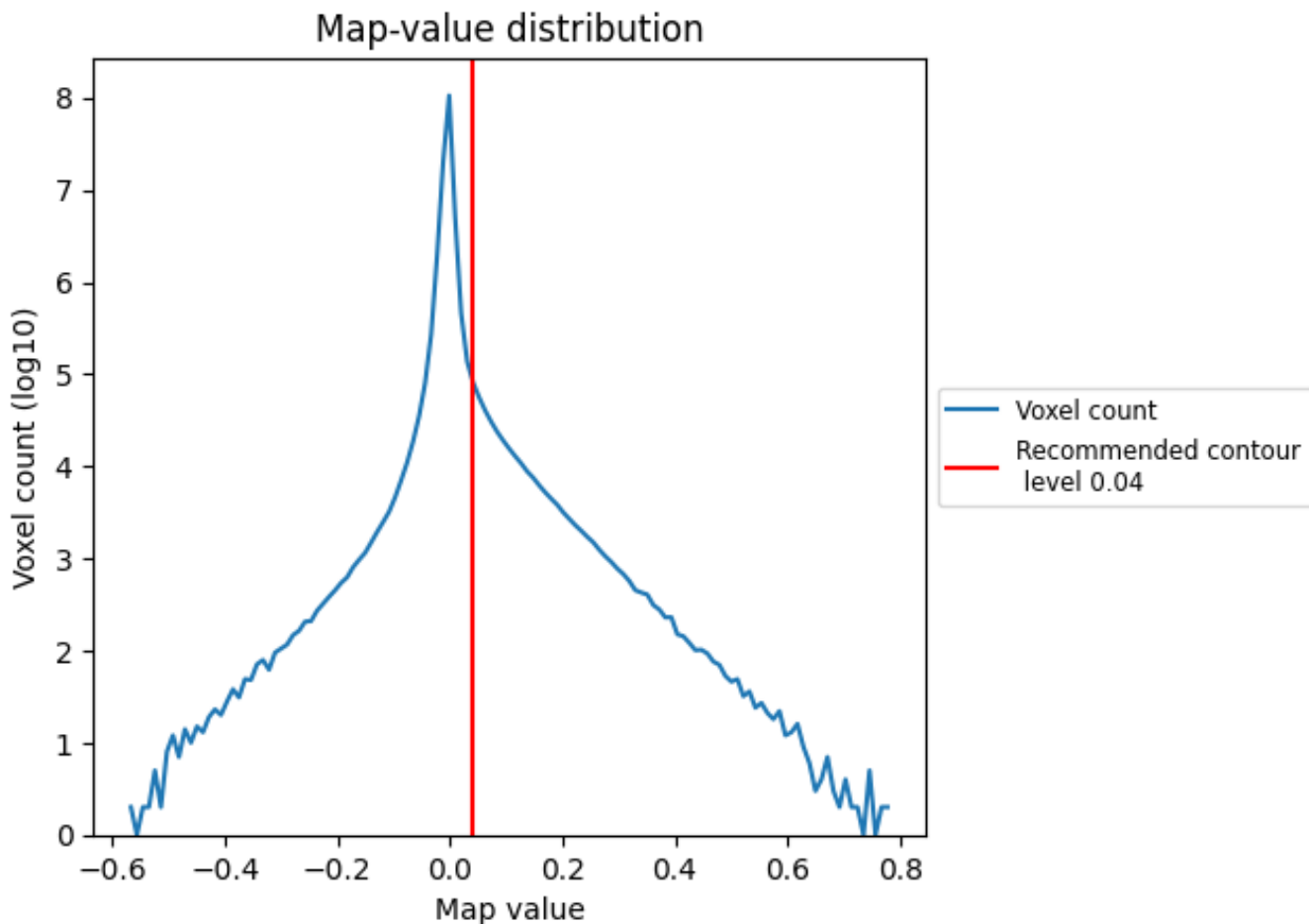
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

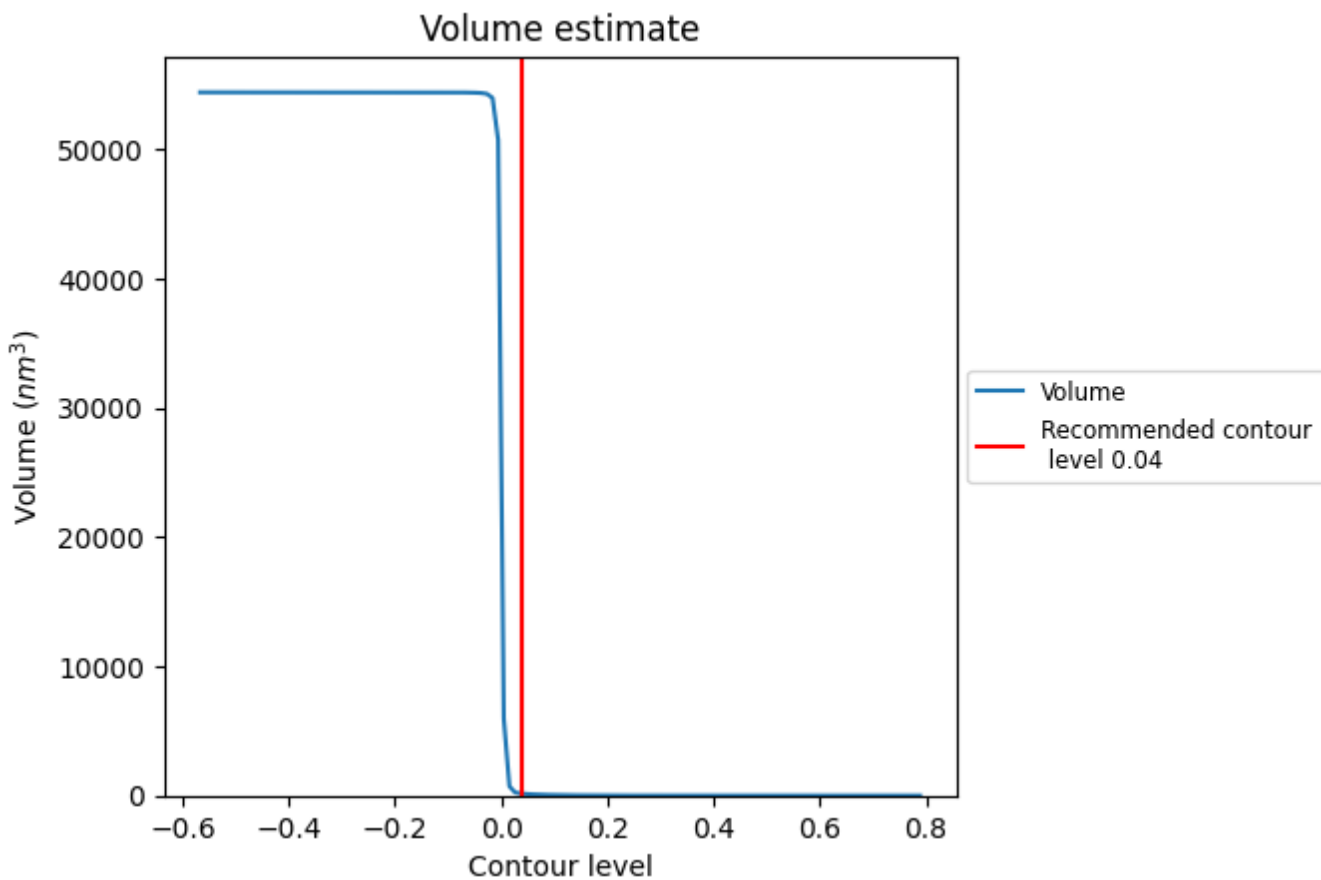
This section contains the results of statistical analysis of the map.

### 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.

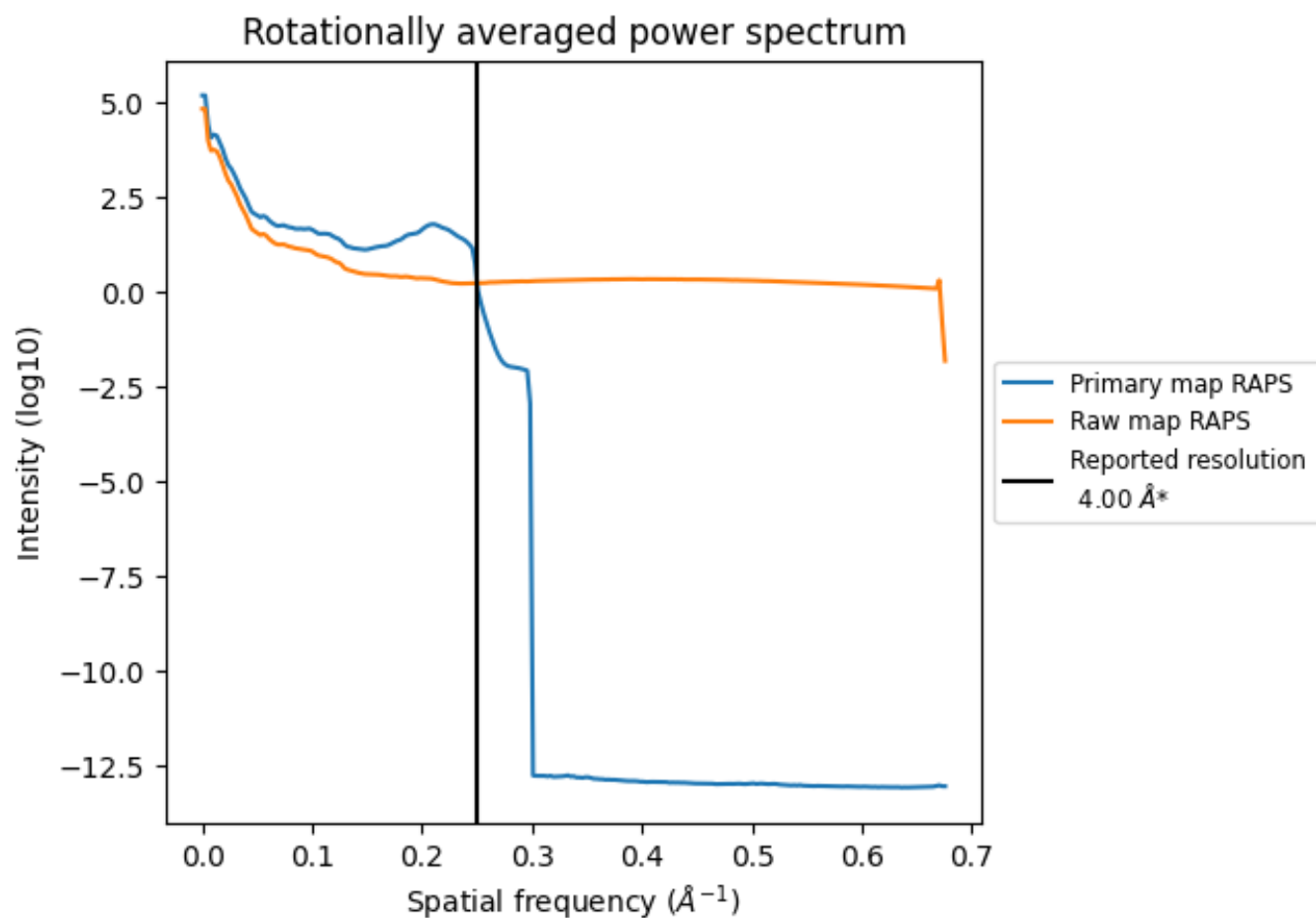
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is  $148 \text{ nm}^3$ ; this corresponds to an approximate mass of 134 kDa.

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

### 7.3 Rotationally averaged power spectrum [i](#)

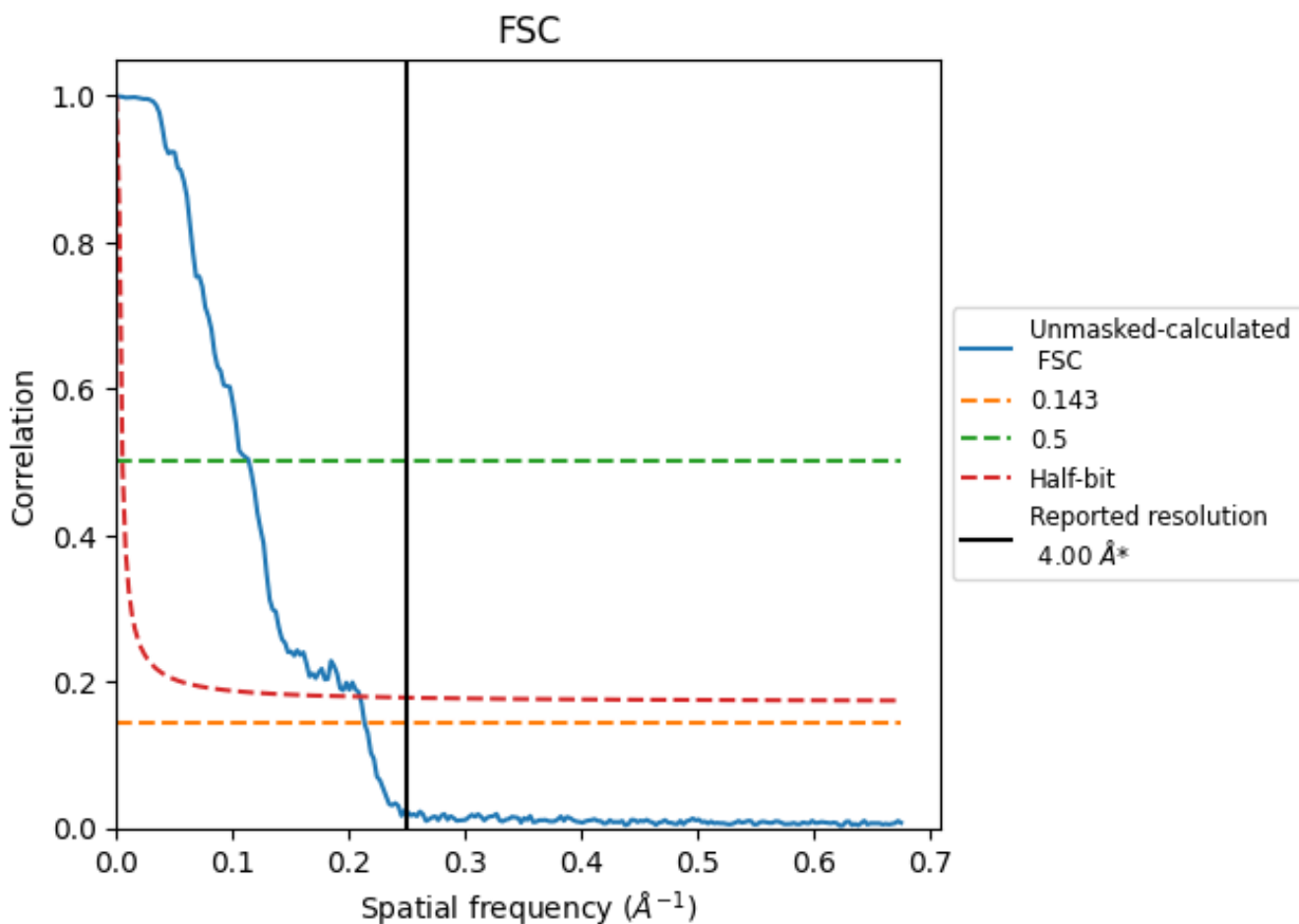


\*Reported resolution corresponds to spatial frequency of 0.250 Å<sup>-1</sup>

## 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 0.250 Å<sup>-1</sup>



## 8.2 Resolution estimates [i](#)

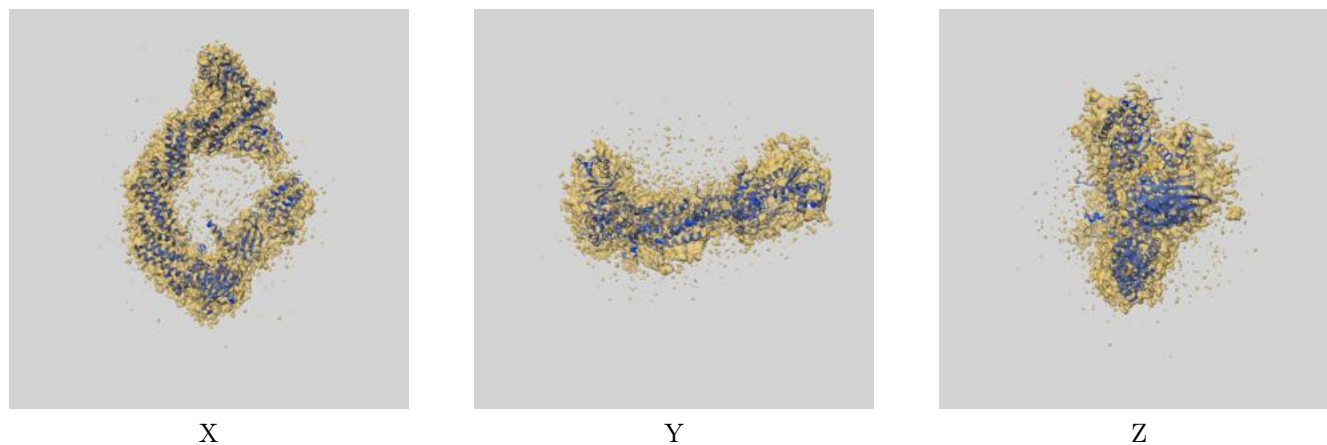
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.00	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.68	8.76	4.77

\*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 4.68 differs from the reported value 4.0 by more than 10 %

## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-19569 and PDB model 8RWZ. Per-residue inclusion information can be found in section [3](#) on page [6](#).

### 9.1 Map-model overlay [i](#)



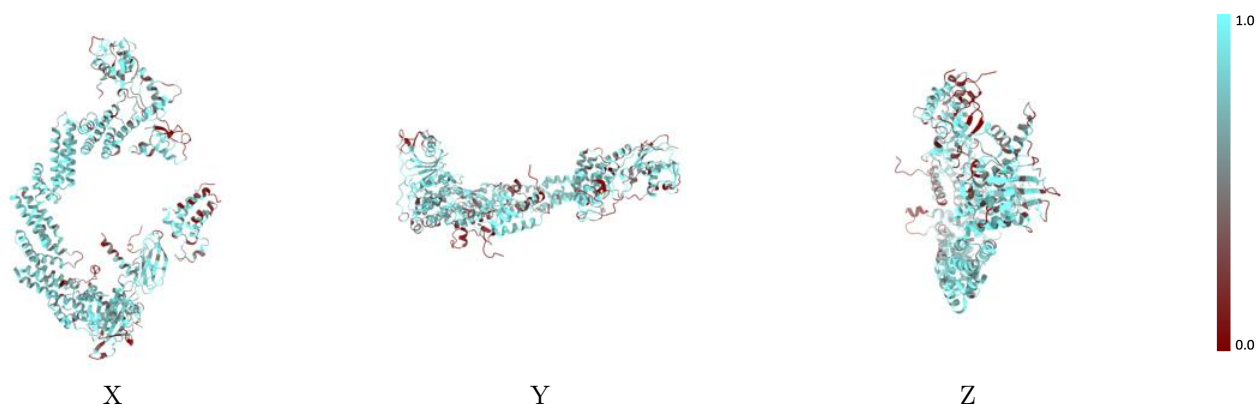
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



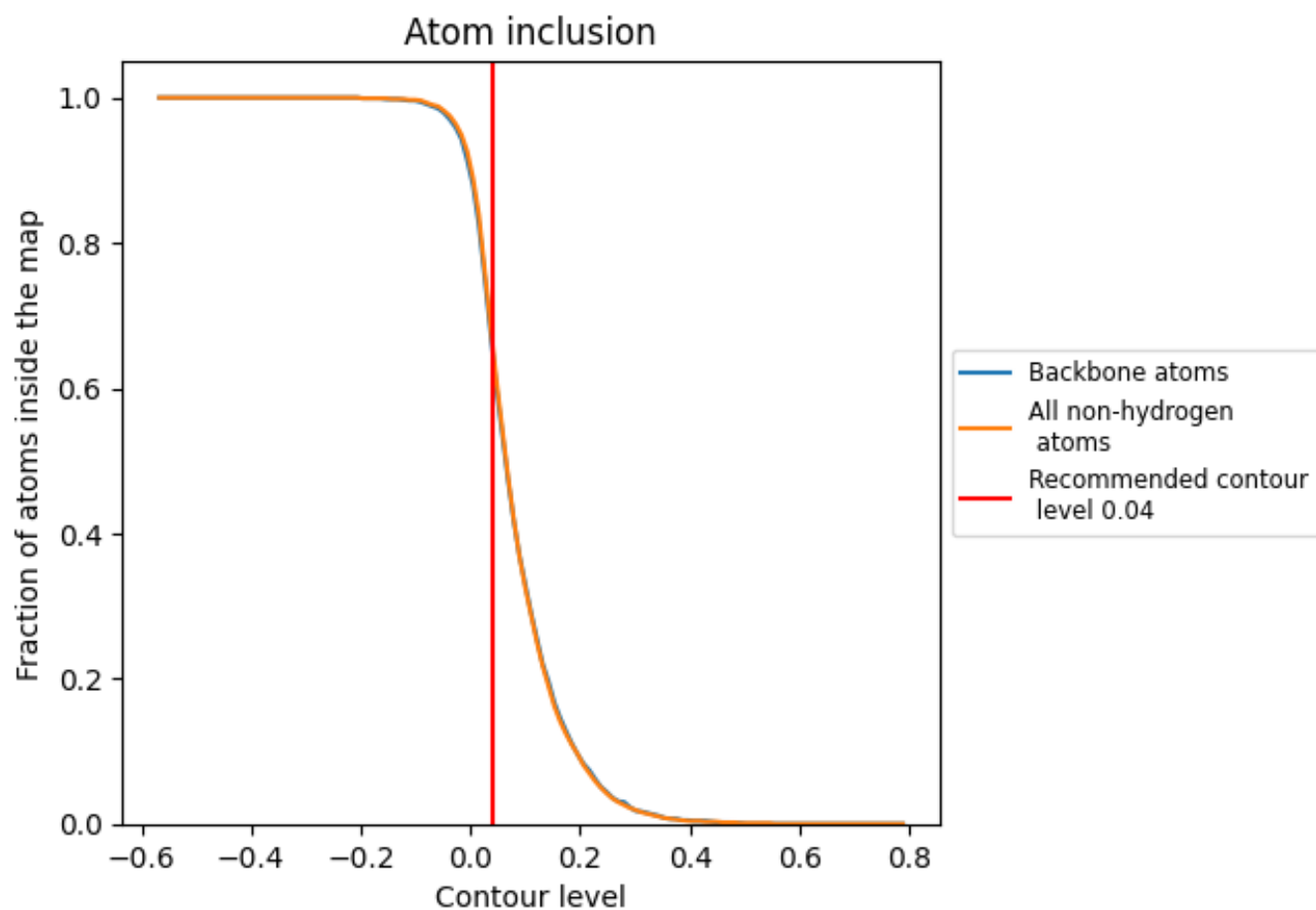
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.04).















## 9.4 Atom inclusion [i](#)



At the recommended contour level, 65% of all backbone atoms, 66% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6630	 0.1470
A	 0.5880	 0.0750
B	 0.6510	 0.1240
C	 0.6300	 0.0640
D	 0.7750	 0.1970
E	 0.7060	 0.1850
R	 0.4900	 0.0430

