



## Full wwPDB EM Validation Report ⓘ

Apr 7, 2025 – 05:05 pm BST

PDB ID : 9GM7 / pdb\_00009gm7  
EMDB ID : EMD-51443  
Title : MukBEF in a nucleotide-bound state with open neck gate (monomer)  
Authors : Burmann, F.; Lowe, J.  
Deposited on : 2024-08-28  
Resolution : 4.30 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](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.dev117  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.42

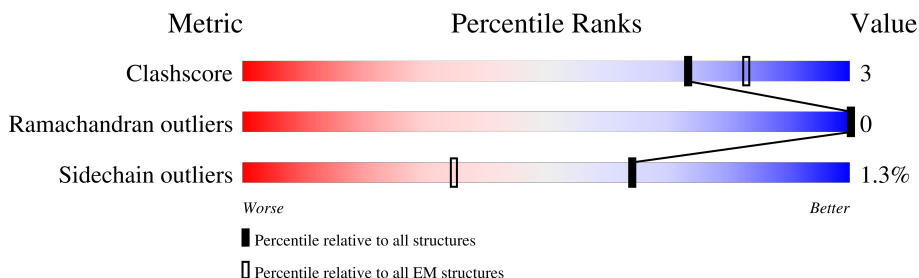
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.30 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	C	440	
1	D	440	
2	E	240	
2	F	240	
3	G	78	
3	I	78	
4	A	1482	
4	B	1482	

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
3	4HH	G	36	-	-	X	-

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 67711 atoms, of which 33622 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 Chromosome partition protein MukF.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	C	440	Total	C	H	N	O	S	0	0
			6982	2218	3451	614	686	13		
1	D	290	Total	C	H	N	O	S	0	0
			4567	1444	2260	402	451	10		

- Molecule 2 is a protein called Chromosome partition protein MukE.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	E	212	Total	C	H	N	O	S	0	0
			3441	1090	1719	301	322	9		
2	F	198	Total	C	H	N	O	S	0	0
			3246	1029	1627	284	298	8		

- Molecule 3 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	G	72	Total	C	H	N	O	P S	0	0
			1147	360	564	87	133	1 2		
3	I	72	Total	C	H	N	O	P S	0	0
			1147	360	564	87	133	1 2		

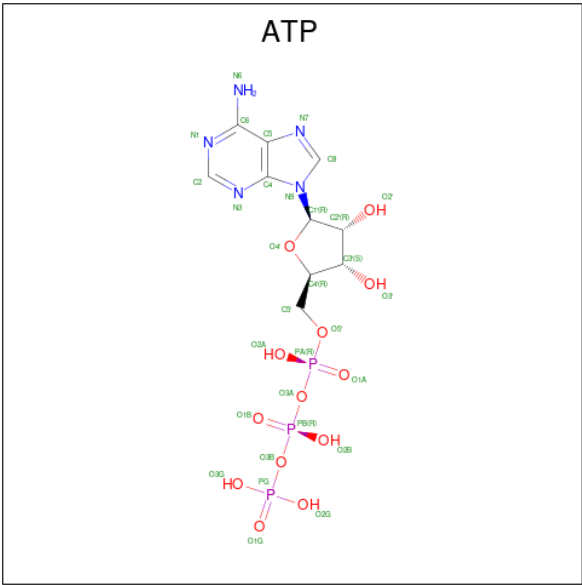
- Molecule 4 is a protein called Chromosome partition protein MukB.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	A	1467	Total	C	H	N	O	S	0	0
			23547	7298	11707	2188	2314	40		
4	B	1467	Total	C	H	N	O	S	0	0
			23546	7298	11706	2188	2314	40		

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 6 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).

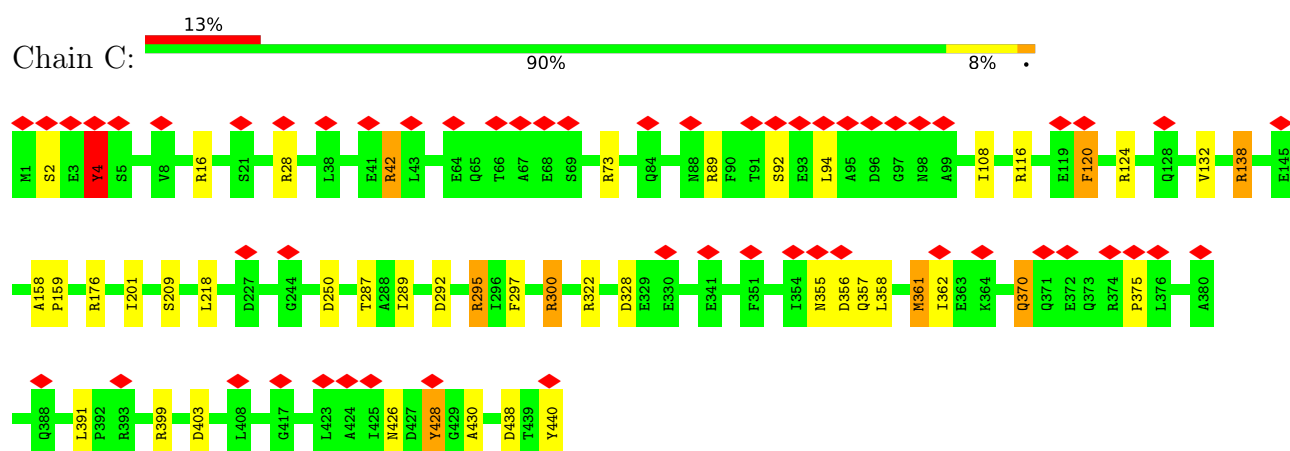


Mol	Chain	Residues	Atoms							AltConf
6	A	1	Total	C	H	N	O	P	0	
			43	10	12	5	13	3		
6	B	1	Total	C	H	N	O	P	0	
			43	10	12	5	13	3		

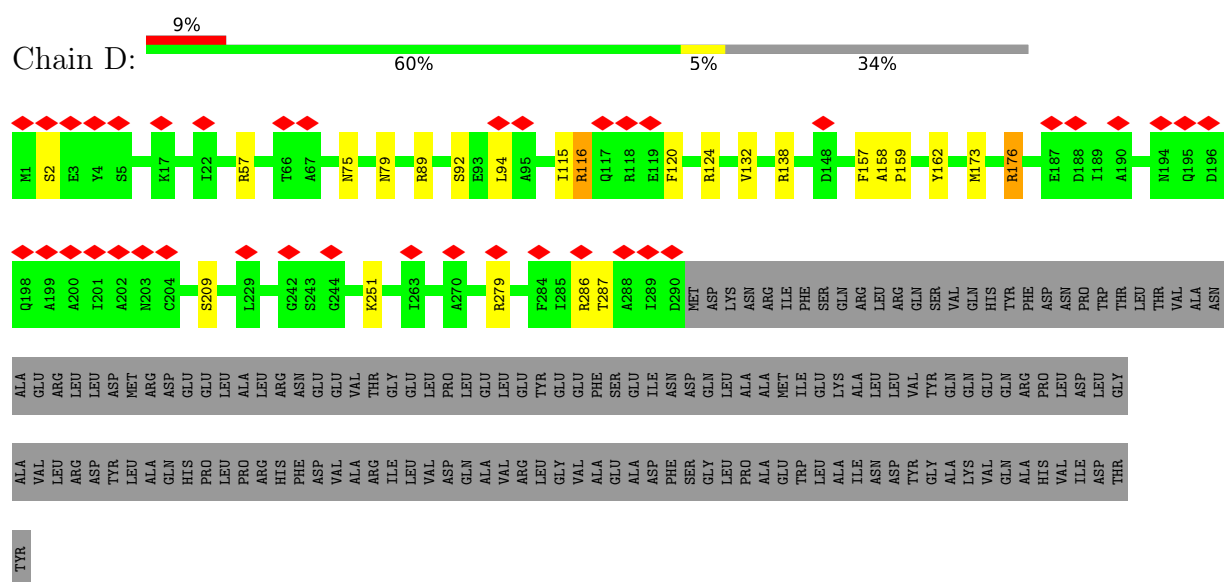
### 3 Residue-property plots

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.

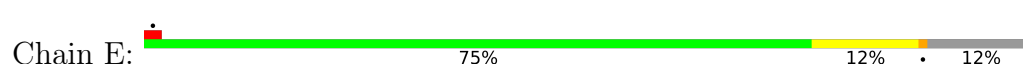
#### • Molecule 1: Chromosome partition protein MukF

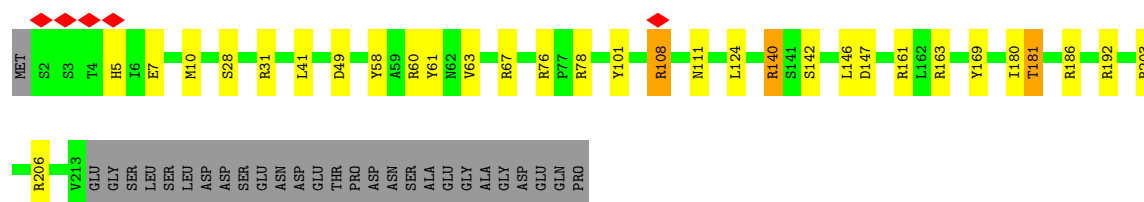


#### • Molecule 1: Chromosome partition protein MukF

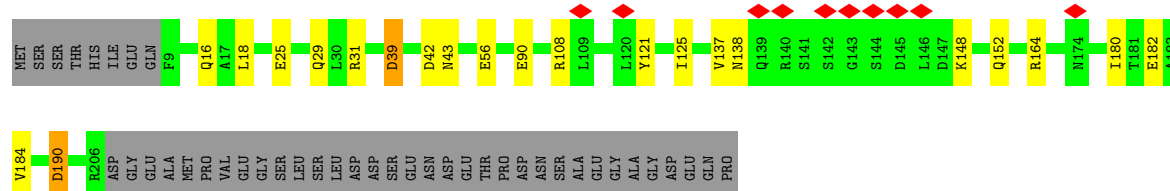


#### • Molecule 2: Chromosome partition protein MukE

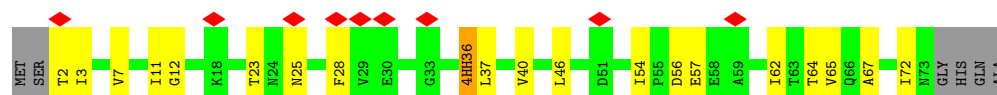




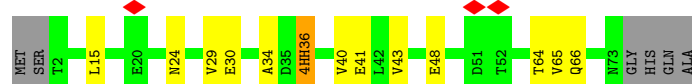
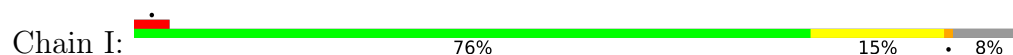
• Molecule 2: Chromosome partition protein MukE



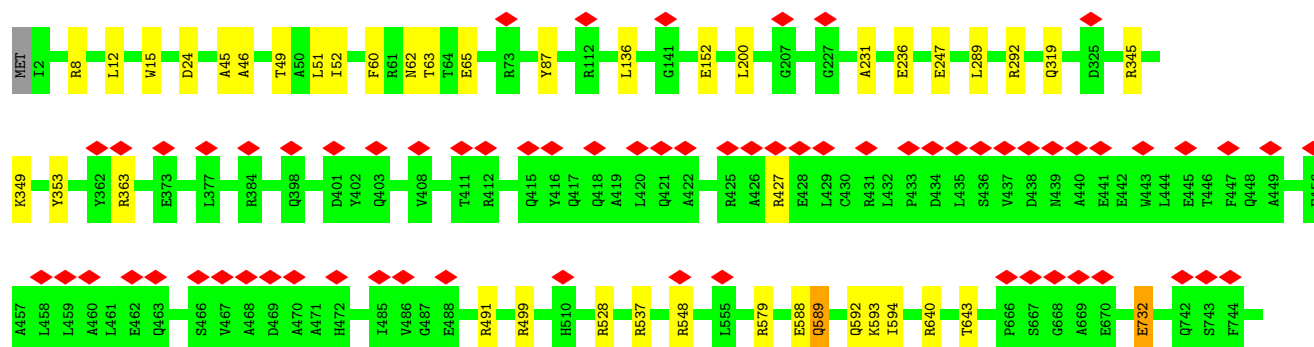
• Molecule 3: Acyl carrier protein

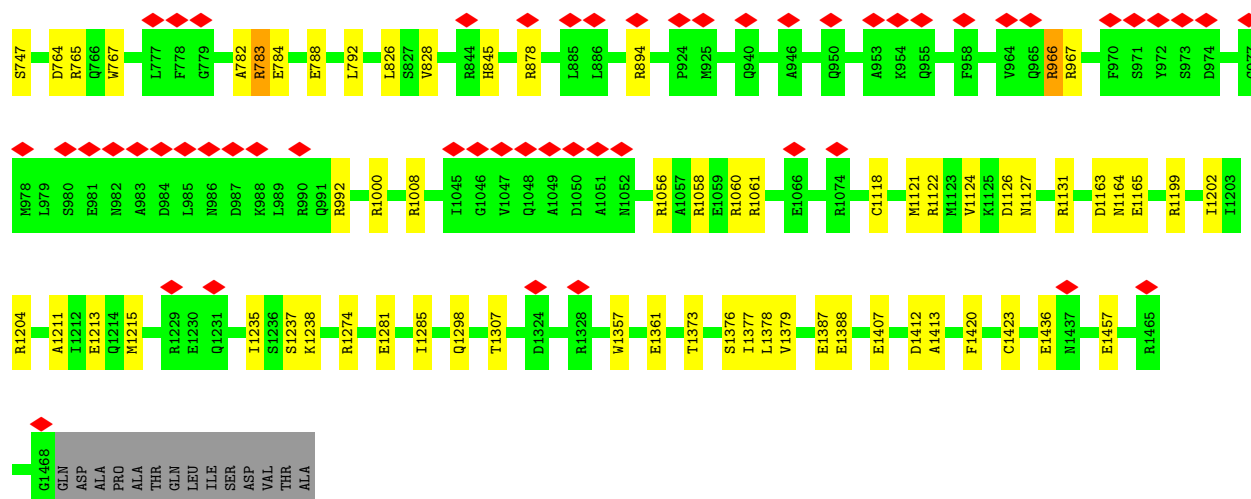


• Molecule 3: Acyl carrier protein

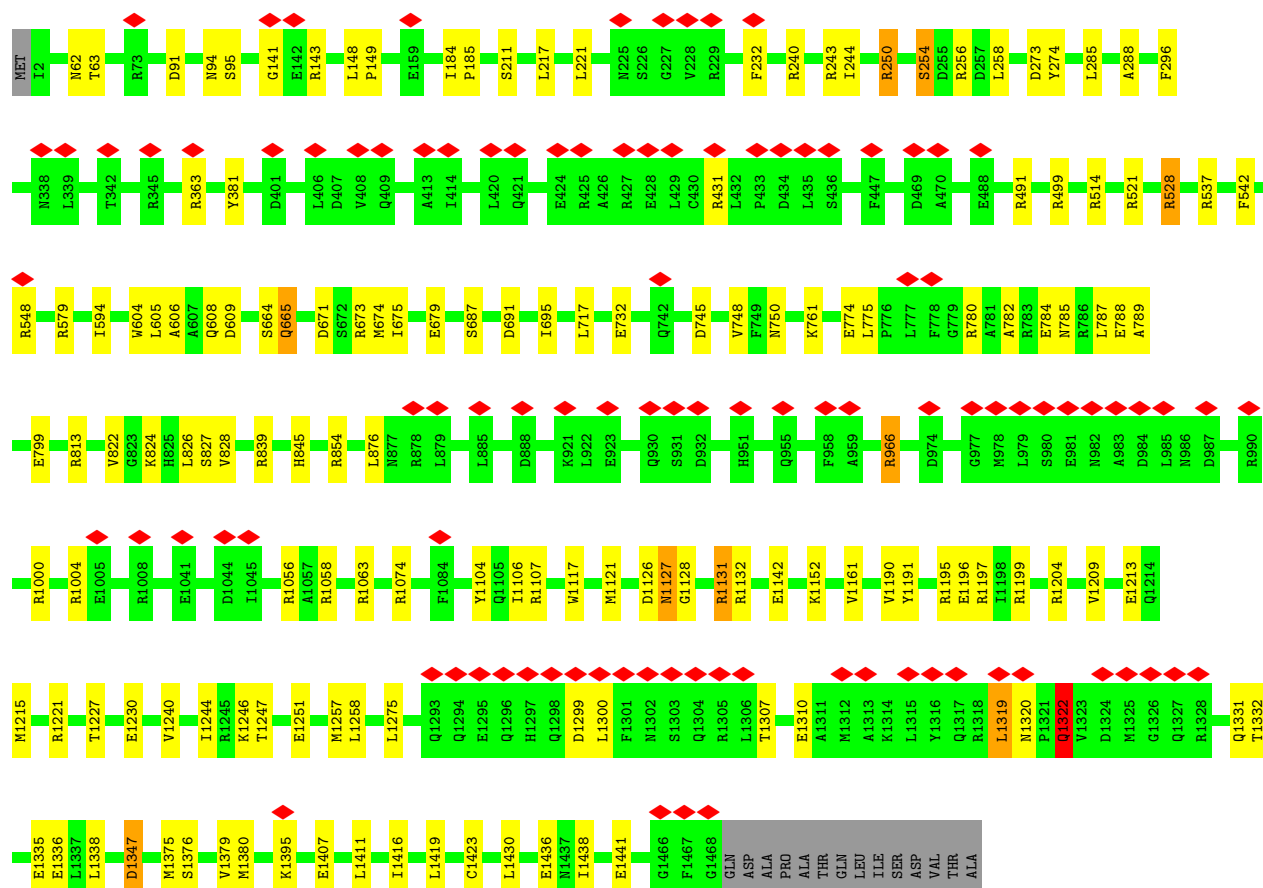
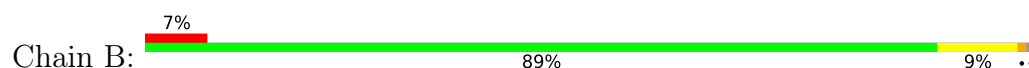


• Molecule 4: Chromosome partition protein MukB





• Molecule 4: Chromosome partition protein MukB





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	34436	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.044	Depositor
Minimum map value	-0.017	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.012	Depositor
Map size (Å)	460.97998, 460.97998, 460.97998	wwPDB
Map dimensions	312, 312, 312	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.4775, 1.4775, 1.4775	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 4HH, ATP, MG

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	C	0.65	3/3592 (0.1%)	0.96	10/4862 (0.2%)
1	D	0.62	0/2343	0.97	7/3165 (0.2%)
2	E	1.32	17/1753 (1.0%)	1.35	15/2361 (0.6%)
2	F	0.69	4/1648 (0.2%)	0.76	2/2218 (0.1%)
3	G	0.25	0/558	0.42	0/754
3	I	0.25	0/558	0.41	0/754
4	A	0.47	1/11999 (0.0%)	0.79	20/16166 (0.1%)
4	B	0.70	24/11999 (0.2%)	0.90	36/16166 (0.2%)
All	All	0.66	49/34450 (0.1%)	0.89	90/46446 (0.2%)

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	C	0	8
1	D	0	5
2	E	0	3
4	A	0	3
4	B	0	2
All	All	0	21

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	295	ARG	C-N	-13.06	1.04	1.34
4	A	589	GLN	C-N	7.61	1.51	1.34
2	F	31	ARG	CZ-NH2	-7.37	1.23	1.33
4	B	1132	ARG	CZ-NH2	-7.37	1.23	1.33
4	B	1131	ARG	CZ-NH2	-7.35	1.23	1.33

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	203	ARG	CZ-NH2	-7.32	1.23	1.33
2	E	31	ARG	CZ-NH2	-7.31	1.23	1.33
4	B	1199	ARG	CZ-NH2	-7.26	1.23	1.33
2	E	206	ARG	CZ-NH2	-7.25	1.23	1.33
1	C	322	ARG	CZ-NH2	-7.24	1.23	1.33
4	B	1221	ARG	CZ-NH2	-7.21	1.23	1.33
4	B	240	ARG	CZ-NH2	-7.20	1.23	1.33
4	B	1197	ARG	CZ-NH2	-7.20	1.23	1.33
4	B	250	ARG	CZ-NH2	-7.18	1.23	1.33
2	F	164	ARG	CZ-NH2	-7.17	1.23	1.33
4	B	243	ARG	CZ-NH2	-7.10	1.23	1.33
2	E	67	ARG	CZ-NH2	-7.10	1.23	1.33
2	E	60	ARG	CZ-NH2	-7.05	1.23	1.33
4	B	250	ARG	CZ-NH1	-6.92	1.24	1.33
2	F	31	ARG	CZ-NH1	-6.83	1.24	1.33
2	E	31	ARG	CZ-NH1	-6.80	1.24	1.33
4	B	240	ARG	CZ-NH1	-6.80	1.24	1.33
1	C	322	ARG	CZ-NH1	-6.80	1.24	1.33
4	B	243	ARG	CZ-NH1	-6.80	1.24	1.33
2	E	206	ARG	CZ-NH1	-6.79	1.24	1.33
2	E	67	ARG	CZ-NH1	-6.77	1.24	1.33
2	E	60	ARG	CZ-NH1	-6.77	1.24	1.33
4	B	1199	ARG	CZ-NH1	-6.75	1.24	1.33
2	F	164	ARG	CZ-NH1	-6.72	1.24	1.33
4	B	1221	ARG	CZ-NH1	-6.69	1.24	1.33
2	E	203	ARG	CZ-NH1	-6.65	1.24	1.33
4	B	1191	TYR	CD2-CE2	-6.64	1.29	1.39
4	B	1131	ARG	CZ-NH1	-6.62	1.24	1.33
4	B	1197	ARG	CZ-NH1	-6.62	1.24	1.33
4	B	1132	ARG	CZ-NH1	-6.60	1.24	1.33
2	E	58	TYR	CD1-CE1	-6.30	1.29	1.39
2	E	61	TYR	CD2-CE2	-6.06	1.30	1.39
2	E	61	TYR	CD1-CE1	-6.01	1.30	1.39
2	E	58	TYR	CD2-CE2	-5.97	1.30	1.39
4	B	1191	TYR	CD1-CE1	-5.89	1.30	1.39
4	B	296	PHE	C-N	-5.69	1.22	1.33
4	B	1128	GLY	N-CA	-5.41	1.38	1.46
4	B	1190	VAL	CB-CG2	-5.35	1.41	1.52
2	E	63	VAL	CB-CG1	-5.34	1.41	1.52
4	B	254	SER	CB-OG	-5.05	1.35	1.42
2	E	63	VAL	CB-CG2	-5.05	1.42	1.52
4	B	1209	VAL	CB-CG2	-5.05	1.42	1.52

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	28	SER	CB-OG	-5.03	1.35	1.42
4	B	1209	VAL	CB-CG1	-5.02	1.42	1.52

All (90) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	295	ARG	C-N-CA	10.48	147.91	121.70
4	B	966	ARG	NE-CZ-NH2	9.24	124.92	120.30
4	B	1056	ARG	NE-CZ-NH2	8.80	124.70	120.30
1	C	42	ARG	NE-CZ-NH1	-8.78	115.91	120.30
1	D	116	ARG	NE-CZ-NH2	8.61	124.61	120.30
2	E	58	TYR	CB-CG-CD2	8.20	125.92	121.00
4	B	528	ARG	NE-CZ-NH2	7.86	124.23	120.30
1	D	176	ARG	CB-CG-CD	7.55	131.23	111.60
4	B	363	ARG	NE-CZ-NH2	7.54	124.07	120.30
4	A	966	ARG	NE-CZ-NH2	7.14	123.87	120.30
1	C	116	ARG	NE-CZ-NH2	6.92	123.76	120.30
4	B	1131	ARG	CD-NE-CZ	6.90	133.26	123.60
4	B	521	ARG	NE-CZ-NH2	6.88	123.74	120.30
4	B	1221	ARG	CD-NE-CZ	6.78	133.10	123.60
4	B	499	ARG	NE-CZ-NH2	6.77	123.68	120.30
2	E	186	ARG	NE-CZ-NH2	6.74	123.67	120.30
4	B	1132	ARG	CD-NE-CZ	6.70	132.98	123.60
4	B	548	ARG	NE-CZ-NH2	6.63	123.61	120.30
4	B	1191	TYR	CB-CG-CD2	6.62	124.97	121.00
4	B	579	ARG	NE-CZ-NH2	6.59	123.59	120.30
4	B	431	ARG	NE-CZ-NH2	6.58	123.59	120.30
4	B	1195	ARG	NE-CZ-NH2	6.56	123.58	120.30
4	B	1063	ARG	NE-CZ-NH2	6.53	123.56	120.30
1	C	16	ARG	NE-CZ-NH2	6.47	123.54	120.30
2	E	60	ARG	CD-NE-CZ	6.43	132.60	123.60
4	B	243	ARG	CG-CD-NE	6.42	125.28	111.80
1	C	176	ARG	NE-CZ-NH1	-6.40	117.10	120.30
2	F	31	ARG	CD-NE-CZ	6.39	132.55	123.60
2	E	31	ARG	CD-NE-CZ	6.39	132.55	123.60
4	A	1056	ARG	NE-CZ-NH2	6.38	123.49	120.30
4	A	537	ARG	NE-CZ-NH2	6.36	123.48	120.30
1	D	138	ARG	NE-CZ-NH2	6.36	123.48	120.30
4	B	491	ARG	NE-CZ-NH2	6.35	123.48	120.30
1	C	4	TYR	CB-CG-CD2	-6.28	117.23	121.00
4	B	1319	LEU	CA-CB-CG	6.23	129.64	115.30
4	B	1074	ARG	NE-CZ-NH2	6.20	123.40	120.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	108	ARG	NE-CZ-NH2	6.18	123.39	120.30
4	A	878	ARG	NE-CZ-NH2	6.17	123.39	120.30
4	B	256	ARG	CD-NE-CZ	6.17	132.24	123.60
4	B	1197	ARG	CD-NE-CZ	6.12	132.16	123.60
4	A	992	ARG	NE-CZ-NH2	6.11	123.36	120.30
4	B	1058	ARG	NE-CZ-NH2	6.08	123.34	120.30
1	C	297	PHE	CB-CG-CD2	-6.07	116.55	120.80
4	A	589	GLN	O-C-N	6.03	132.35	122.70
2	E	67	ARG	CG-CD-NE	6.03	124.46	111.80
4	B	243	ARG	CA-CB-CG	5.92	126.44	113.40
4	A	499	ARG	NE-CZ-NH2	5.90	123.25	120.30
4	A	548	ARG	NE-CZ-NH2	5.90	123.25	120.30
2	E	67	ARG	CD-NE-CZ	5.89	131.85	123.60
4	B	1204	ARG	NE-CZ-NH2	5.86	123.23	120.30
4	B	243	ARG	CD-NE-CZ	5.86	131.80	123.60
1	D	251	LYS	CB-CG-CD	5.81	126.70	111.60
2	E	76	ARG	NE-CZ-NH2	5.80	123.20	120.30
4	A	363	ARG	NE-CZ-NH2	5.75	123.18	120.30
2	E	78	ARG	NE-CZ-NH2	5.57	123.08	120.30
4	A	894	ARG	NE-CZ-NH1	-5.55	117.52	120.30
4	A	1056	ARG	NE-CZ-NH1	-5.54	117.53	120.30
4	B	537	ARG	NE-CZ-NH2	5.51	123.06	120.30
4	A	491	ARG	NE-CZ-NH2	5.49	123.04	120.30
4	B	1000	ARG	NE-CZ-NH2	5.47	123.03	120.30
2	E	192	ARG	NE-CZ-NH2	5.44	123.02	120.30
1	C	73	ARG	NE-CZ-NH2	5.41	123.00	120.30
4	B	1215	MET	CA-CB-CG	5.41	122.49	113.30
4	A	579	ARG	NE-CZ-NH2	5.39	122.99	120.30
2	F	164	ARG	CD-NE-CZ	5.38	131.13	123.60
4	A	345	ARG	NE-CZ-NH2	5.38	122.99	120.30
1	D	57	ARG	NE-CZ-NH2	5.38	122.99	120.30
4	A	1008	ARG	NE-CZ-NH2	5.38	122.99	120.30
4	A	894	ARG	NE-CZ-NH2	5.35	122.97	120.30
2	E	61	TYR	CB-CG-CD2	5.35	124.21	121.00
1	D	176	ARG	CD-NE-CZ	5.33	131.07	123.60
1	C	42	ARG	NE-CZ-NH2	5.29	122.95	120.30
4	B	854	ARG	NE-CZ-NH2	5.29	122.95	120.30
1	C	138	ARG	NE-CZ-NH2	5.29	122.94	120.30
4	A	1061	ARG	NE-CZ-NH2	5.27	122.94	120.30
2	E	58	TYR	CD1-CG-CD2	-5.26	112.12	117.90
4	A	427	ARG	NE-CZ-NH2	5.25	122.93	120.30
4	A	528	ARG	NE-CZ-NH2	5.25	122.93	120.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	381	TYR	CB-CG-CD2	-5.25	117.85	121.00
4	B	514	ARG	NE-CZ-NH2	5.23	122.92	120.30
4	B	1221	ARG	CA-CB-CG	5.22	124.88	113.40
1	D	157	PHE	CB-CG-CD1	-5.19	117.17	120.80
4	B	1004	ARG	NE-CZ-NH2	5.18	122.89	120.30
4	B	1322	GLN	CA-CB-CG	5.17	124.78	113.40
2	E	67	ARG	CA-CB-CG	5.14	124.71	113.40
4	A	1000	ARG	NE-CZ-NH2	5.09	122.85	120.30
4	B	1191	TYR	CD1-CG-CD2	-5.07	112.33	117.90
4	B	1199	ARG	CD-NE-CZ	5.04	130.65	123.60
2	E	61	TYR	CD1-CG-CD2	-5.01	112.38	117.90
2	E	163	ARG	NE-CZ-NH2	5.01	122.81	120.30

There are no chirality outliers.

All (21) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	A	1058	ARG	Sidechain
4	A	966	ARG	Sidechain
4	A	967	ARG	Sidechain
4	B	528	ARG	Sidechain
4	B	966	ARG	Sidechain
1	C	120	PHE	Sidechain
1	C	124	ARG	Sidechain
1	C	138	ARG	Sidechain
1	C	28	ARG	Sidechain
1	C	300	ARG	Sidechain
1	C	4	TYR	Sidechain
1	C	42	ARG	Sidechain
1	C	89	ARG	Sidechain
1	D	116	ARG	Sidechain
1	D	120	PHE	Sidechain
1	D	124	ARG	Sidechain
1	D	162	TYR	Sidechain
1	D	89	ARG	Sidechain
2	E	101	TYR	Sidechain
2	E	140	ARG	Sidechain
2	E	161	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	C	3531	3451	3450	19	0
1	D	2307	2260	2260	5	0
2	E	1722	1719	1718	12	0
2	F	1619	1627	1626	16	0
3	G	583	564	563	24	0
3	I	583	564	563	10	0
4	A	11840	11707	11705	60	0
4	B	11840	11706	11705	86	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	31	12	12	0	0
6	B	31	12	12	0	0
All	All	34089	33622	33614	207	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 3.

All (207) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:36:4HH:CL3	3:G:40:VAL:HG21	1.87	1.04
4:B:1127:ASN:O	4:B:1127:ASN:ND2	1.91	1.02
3:I:48:GLU:OE1	4:B:1107:ARG:NE	2.04	0.90
3:G:36:4HH:SU	4:A:292:ARG:HD3	2.14	0.87
4:B:665:GLN:NE2	4:B:671:ASP:OD2	2.11	0.84
3:G:36:4HH:HT3	3:G:56:ASP:OD1	1.85	0.76
3:G:23:THR:OG1	3:G:25:ASN:OD1	2.04	0.74
4:A:1412:ASP:OD1	4:A:1413:ALA:N	2.20	0.73
4:B:1127:ASN:HD22	4:B:1127:ASN:C	1.88	0.71
3:G:36:4HH:CL3	3:G:40:VAL:CG2	2.68	0.68
3:G:36:4HH:HB2	3:G:36:4HH:HJ2	1.74	0.68
4:A:1298:GLN:N	4:A:1298:GLN:OE1	2.27	0.68
4:B:273:ASP:OD1	4:B:274:TYR:N	2.26	0.68
4:A:784:GLU:OE1	4:A:784:GLU:N	2.28	0.67
4:A:826:LEU:HD21	4:B:827:SER:HA	1.75	0.67

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1436:GLU:O	4:A:1436:GLU:OE1	2.12	0.67
3:G:36:4HH:HJ2	3:G:36:4HH:CB	2.25	0.66
3:G:46:LEU:HD21	3:G:72:ILE:HD11	1.78	0.66
4:B:1332:THR:O	4:B:1336:GLU:N	2.30	0.64
4:A:1457:GLU:OE1	4:A:1457:GLU:N	2.28	0.62
3:G:36:4HH:ON	3:G:40:VAL:CG2	2.48	0.62
4:A:231:ALA:HB2	4:B:665:GLN:CB	2.30	0.62
4:B:254:SER:O	4:B:258:LEU:HD22	2.01	0.60
3:G:36:4HH:HS3	4:A:289:LEU:HD22	1.83	0.60
3:I:24:ASN:O	3:I:66:GLN:N	2.35	0.59
4:B:788:GLU:OE1	4:B:789:ALA:N	2.35	0.59
2:E:10:MET:SD	2:F:18:LEU:HD11	2.43	0.59
4:B:1142:GLU:OE1	4:B:1142:GLU:N	2.36	0.59
2:F:148:LYS:HD3	2:F:148:LYS:N	2.20	0.57
4:B:1322:GLN:O	4:B:1322:GLN:CD	2.43	0.56
4:B:1441:GLU:OE1	4:B:1441:GLU:N	2.37	0.56
4:B:822:VAL:HA	4:B:826:LEU:HD23	1.88	0.55
4:A:231:ALA:HB2	4:B:665:GLN:HB2	1.89	0.55
2:F:137:VAL:HG23	2:F:138:ASN:H	1.72	0.55
3:G:36:4HH:HJ3	3:G:37:LEU:N	2.22	0.54
1:C:328:ASP:OD1	1:C:328:ASP:O	2.25	0.54
4:A:1420:PHE:HA	4:A:1423:CYS:SG	2.48	0.54
4:B:1240:VAL:HG12	4:B:1244:ILE:HD13	1.89	0.54
4:B:1258:LEU:HD21	4:B:1380:MET:HG2	1.90	0.54
4:B:1423:CYS:SG	4:B:1430:LEU:HD11	2.48	0.53
4:B:1299:ASP:OD1	4:B:1300:LEU:N	2.42	0.53
4:A:65:GLU:O	4:A:65:GLU:HG3	2.08	0.53
4:A:1126:ASP:O	4:A:1127:ASN:OD1	2.27	0.53
4:A:1281:GLU:O	4:A:1285:ILE:HD12	2.08	0.53
2:E:7:GLU:OE1	2:E:7:GLU:N	2.38	0.52
4:A:236:GLU:OE2	4:A:1307:THR:HG21	2.08	0.52
4:A:828:VAL:HG12	4:A:828:VAL:O	2.08	0.52
3:G:36:4HH:CS	4:A:289:LEU:HD22	2.39	0.52
4:B:1161:VAL:HG12	4:B:1161:VAL:O	2.09	0.51
3:G:62:ILE:HG22	3:G:62:ILE:O	2.11	0.51
4:A:764:ASP:N	4:A:764:ASP:OD1	2.40	0.51
4:B:1246:LYS:HD2	4:B:1246:LYS:O	2.11	0.51
4:B:1395:LYS:O	4:B:1395:LYS:HD3	2.10	0.51
4:B:232:PHE:CZ	4:B:1240:VAL:HG11	2.46	0.51
4:B:273:ASP:OD1	4:B:273:ASP:C	2.49	0.51
4:B:828:VAL:HG12	4:B:828:VAL:O	2.10	0.51

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:140:ARG:HD2	2:E:140:ARG:O	2.11	0.51
4:B:217:LEU:HG	4:B:221:LEU:HD12	1.91	0.51
4:B:1319:LEU:HD12	4:B:1320:ASN:N	2.26	0.50
4:A:1361:GLU:OE1	4:A:1361:GLU:HA	2.12	0.50
1:C:158:ALA:HB3	1:C:159:PRO:HD3	1.94	0.50
1:C:370:GLN:OE1	1:C:370:GLN:O	2.29	0.50
4:A:1163:ASP:OD1	4:A:1164:ASN:N	2.45	0.50
4:A:1237:SER:OG	4:A:1238:LYS:N	2.45	0.50
4:B:1196:GLU:N	4:B:1196:GLU:OE1	2.45	0.50
3:I:36:4HH:O	3:I:40:VAL:HG23	2.12	0.49
4:A:1376:SER:O	4:A:1379:VAL:HG22	2.12	0.49
4:B:63:THR:HG21	4:B:1407:GLU:HG3	1.92	0.49
4:A:1211:ALA:O	4:A:1215:MET:HG2	2.13	0.49
1:C:358:LEU:HG	1:C:362:ILE:HD11	1.94	0.49
1:D:75:ASN:HD21	2:E:146:LEU:HB2	1.78	0.48
1:D:79:ASN:CG	2:E:142:SER:HB3	2.33	0.48
2:E:41:LEU:HD21	4:B:244:ILE:HD13	1.94	0.48
4:B:799:GLU:C	4:B:799:GLU:OE1	2.51	0.48
3:I:48:GLU:OE1	4:B:1107:ARG:CZ	2.59	0.48
4:A:200:LEU:HD12	4:A:1378:LEU:HD22	1.94	0.48
4:A:732:GLU:OE1	4:A:732:GLU:N	2.46	0.48
4:B:782:ALA:O	4:B:785:ASN:N	2.47	0.48
3:I:48:GLU:CD	4:B:1107:ARG:HE	2.13	0.48
4:B:1322:GLN:O	4:B:1322:GLN:OE1	2.32	0.48
4:B:1376:SER:O	4:B:1379:VAL:HG22	2.13	0.48
2:F:56:GLU:OE1	2:F:56:GLU:HA	2.13	0.48
2:F:180:ILE:HG23	2:F:184:VAL:HG21	1.96	0.48
3:G:2:THR:OG1	3:G:3:ILE:N	2.45	0.48
2:E:124:LEU:C	2:E:124:LEU:HD23	2.34	0.47
4:B:674:MET:HE3	4:B:674:MET:HA	1.96	0.47
4:B:774:GLU:N	4:B:774:GLU:OE1	2.48	0.47
1:C:391:LEU:HD13	1:C:428:TYR:CD2	2.50	0.47
1:C:391:LEU:HD13	1:C:428:TYR:CE2	2.49	0.47
3:G:11:ILE:HG23	3:G:12:GLY:N	2.29	0.47
4:B:665:GLN:C	4:B:665:GLN:OE1	2.53	0.47
4:B:1117:TRP:O	4:B:1121:MET:HG2	2.14	0.47
1:C:375:PRO:HA	1:C:440:TYR:OH	2.15	0.47
4:A:588:GLU:O	4:A:592:GLN:HG3	2.15	0.47
4:B:1275:LEU:HD12	4:B:1347:ASP:O	2.15	0.47
4:B:664:SER:OG	4:B:665:GLN:HG3	2.15	0.47
4:B:824:LYS:HG2	4:B:824:LYS:O	2.15	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:1161:VAL:O	4:B:1161:VAL:CG1	2.62	0.47
3:I:41:GLU:OE2	4:B:285:LEU:HD13	2.15	0.46
4:B:94:ASN:OD1	4:B:95:SER:N	2.47	0.46
2:F:39:ASP:OD1	2:F:39:ASP:N	2.49	0.46
3:G:57:GLU:OE1	3:G:57:GLU:N	2.45	0.46
4:A:8:ARG:HH21	4:A:8:ARG:HG3	1.80	0.46
2:E:49:ASP:OD2	4:B:1320:ASN:ND2	2.49	0.46
3:G:28:PHE:CE1	3:G:65:VAL:HG22	2.51	0.46
4:B:91:ASP:C	4:B:91:ASP:OD1	2.54	0.46
4:B:542:PHE:CD2	4:B:876:LEU:HD21	2.51	0.46
3:G:36:4HH:ON	3:G:40:VAL:HG23	2.14	0.46
4:A:12:LEU:HD21	4:A:46:ALA:HB2	1.97	0.46
4:B:1257:MET:SD	4:B:1257:MET:C	2.95	0.46
3:G:36:4HH:OM	3:G:37:LEU:HA	2.17	0.45
4:A:62:ASN:OD1	4:A:63:THR:N	2.48	0.45
4:B:782:ALA:O	4:B:785:ASN:CB	2.65	0.45
4:A:765:ARG:HH11	4:B:748:VAL:HG23	1.81	0.45
2:E:5:HIS:CD2	2:E:7:GLU:OE1	2.69	0.45
2:F:121:TYR:CZ	2:F:125:ILE:HD11	2.52	0.45
1:D:158:ALA:HB3	1:D:159:PRO:HD3	1.97	0.45
4:A:349:LYS:HE3	4:A:353:TYR:CZ	2.51	0.45
4:A:589:GLN:O	4:A:593:LYS:N	2.40	0.45
4:A:1121:MET:HA	4:A:1124:VAL:HG12	1.99	0.45
4:B:679:GLU:OE1	4:B:679:GLU:HA	2.17	0.45
4:B:732:GLU:H	4:B:732:GLU:CD	2.18	0.45
2:F:16:GLN:C	2:F:16:GLN:OE1	2.55	0.45
4:A:1285:ILE:HD12	4:A:1285:ILE:H	1.81	0.45
4:B:784:GLU:HA	4:B:787:LEU:HG	1.98	0.45
4:A:1213:GLU:OE1	4:B:813:ARG:NE	2.50	0.45
4:B:691:ASP:OD1	4:B:780:ARG:HB3	2.17	0.45
2:F:137:VAL:HG23	2:F:138:ASN:N	2.31	0.44
4:A:247:GLU:HA	4:A:247:GLU:OE1	2.17	0.44
4:B:839:ARG:HG2	4:B:839:ARG:HH21	1.82	0.44
1:C:355:ASN:OD1	1:C:355:ASN:N	2.48	0.44
1:C:426:ASN:OD1	1:C:430:ALA:HB3	2.16	0.44
4:B:1104:TYR:CE1	4:B:1107:ARG:NH1	2.86	0.44
4:B:1375:MET:HG2	4:B:1419:LEU:HD11	1.98	0.44
1:C:399:ARG:O	1:C:403:ASP:OD2	2.36	0.44
3:I:64:THR:HG22	3:I:65:VAL:N	2.33	0.43
4:A:640:ARG:O	4:A:643:THR:HG22	2.17	0.43
1:C:356:ASP:C	1:C:356:ASP:OD1	2.55	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:358:LEU:HA	1:C:361:MET:SD	2.59	0.43
4:A:1274:ARG:HG3	4:A:1357:TRP:CZ3	2.53	0.43
2:F:108:ARG:NH1	4:A:1285:ILE:HD11	2.34	0.43
4:A:152:GLU:OE1	4:A:152:GLU:N	2.51	0.43
4:B:1436:GLU:O	4:B:1438:ILE:HG23	2.19	0.43
2:E:180:ILE:HG22	2:E:181:THR:N	2.33	0.43
4:B:605:LEU:O	4:B:609:ASP:OD2	2.37	0.43
4:B:750:ASN:HB3	4:B:761:LYS:HB3	2.00	0.43
1:C:292:ASP:CG	1:C:295:ARG:HA	2.39	0.43
1:C:120:PHE:CZ	1:C:218:LEU:HD12	2.54	0.43
4:A:51:LEU:O	4:A:52:ILE:HD13	2.18	0.43
4:B:594:ILE:HD12	4:B:845:HIS:CE1	2.54	0.43
4:B:184:ILE:HG23	4:B:185:PRO:HD2	2.00	0.43
4:B:745:ASP:OD1	4:B:745:ASP:N	2.51	0.43
4:B:782:ALA:O	4:B:785:ASN:HB3	2.18	0.42
2:F:25:GLU:O	2:F:29:GLN:HG3	2.19	0.42
3:G:36:4HH:CT	4:A:292:ARG:HD3	2.49	0.42
4:A:1373:THR:O	4:A:1377:ILE:HG12	2.19	0.42
4:B:775:LEU:N	4:B:775:LEU:HD22	2.34	0.42
3:I:40:VAL:O	3:I:43:VAL:HG12	2.19	0.42
4:B:1247:THR:O	4:B:1251:GLU:OE1	2.37	0.42
4:A:782:ALA:O	4:A:783:ARG:HD3	2.19	0.42
4:A:1202:ILE:O	4:A:1202:ILE:HG22	2.20	0.42
1:C:108:ILE:CD1	1:D:176:ARG:HD2	2.50	0.42
1:C:201:ILE:HD13	1:C:289:ILE:HD11	2.02	0.42
4:A:1199:ARG:O	4:A:1199:ARG:HG2	2.19	0.42
2:F:25:GLU:CD	2:F:25:GLU:H	2.23	0.41
4:A:12:LEU:HD22	4:A:15:TRP:CG	2.55	0.41
4:B:1126:ASP:O	4:B:1127:ASN:HB3	2.20	0.41
4:B:1411:LEU:HB2	4:B:1416:ILE:HD11	2.02	0.41
3:G:64:THR:HG23	3:G:67:ALA:H	1.85	0.41
4:B:1227:THR:O	4:B:1230:GLU:HG3	2.21	0.41
4:A:594:ILE:HD12	4:A:845:HIS:CE1	2.55	0.41
4:A:1235:ILE:HG21	4:B:675:ILE:HD13	2.01	0.41
4:B:288:ALA:HB2	4:B:1106:ILE:HG22	2.03	0.41
1:C:4:TYR:CD1	1:D:115:ILE:HG22	2.56	0.41
4:A:767:TRP:CE3	4:B:717:LEU:HD13	2.55	0.41
4:B:1240:VAL:CG1	4:B:1244:ILE:HD13	2.50	0.41
4:A:12:LEU:HD21	4:A:46:ALA:CB	2.50	0.41
4:A:45:ALA:HB1	4:A:60:PHE:CE2	2.55	0.41
4:A:788:GLU:O	4:A:792:LEU:HD13	2.21	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:606:ALA:HA	4:B:609:ASP:OD2	2.20	0.41
1:C:357:GLN:O	1:C:361:MET:SD	2.78	0.41
3:I:15:LEU:HD22	3:I:34:ALA:HB2	2.03	0.41
4:A:46:ALA:O	4:A:49:THR:HG22	2.20	0.41
4:B:141:GLY:O	4:B:143:ARG:NH1	2.54	0.41
4:B:695:ILE:N	4:B:695:ILE:HD12	2.35	0.41
2:E:41:LEU:HD21	4:B:244:ILE:CD1	2.51	0.41
2:E:108:ARG:NH1	2:E:111:ASN:HD21	2.19	0.41
4:A:87:TYR:CD2	4:A:136:LEU:HD23	2.56	0.41
4:A:1118:CYS:SG	4:A:1122:ARG:NH1	2.92	0.41
4:A:1407:GLU:OE1	4:A:1407:GLU:HA	2.21	0.41
4:B:1335:GLU:HA	4:B:1338:LEU:HG	2.03	0.41
2:F:90:GLU:HA	2:F:90:GLU:OE1	2.20	0.40
3:I:29:VAL:HG13	3:I:30:GLU:N	2.36	0.40
4:B:1331:GLN:OE1	4:B:1331:GLN:N	2.54	0.40
4:B:1338:LEU:N	4:B:1338:LEU:HD23	2.36	0.40
2:F:182:GLU:OE1	2:F:182:GLU:N	2.48	0.40
3:G:36:4HH:CB	3:G:36:4HH:CJ	2.90	0.40
4:A:87:TYR:CG	4:A:136:LEU:HD23	2.56	0.40
4:B:1307:THR:OG1	4:B:1310:GLU:HG3	2.22	0.40
3:G:7:VAL:O	3:G:11:ILE:HG22	2.21	0.40
2:F:190:ASP:OD1	2:F:190:ASP:C	2.60	0.40
1:C:440:TYR:N	1:C:440:TYR:CD1	2.90	0.40
2:F:42:ASP:OD1	2:F:43:ASN:N	2.54	0.40
3:G:54:ILE:O	4:A:292:ARG:NH1	2.55	0.40
4:A:1387:GLU:OE1	4:A:1388:GLU:N	2.54	0.40
4:B:148:LEU:HA	4:B:149:PRO:HD3	1.96	0.40
4:B:604:TRP:CH2	4:B:608:GLN:HG3	2.56	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	C	438/440 (100%)	425 (97%)	13 (3%)	0	100	100
1	D	288/440 (66%)	281 (98%)	7 (2%)	0	100	100
2	E	210/240 (88%)	206 (98%)	4 (2%)	0	100	100
2	F	196/240 (82%)	191 (97%)	5 (3%)	0	100	100
3	G	69/78 (88%)	68 (99%)	1 (1%)	0	100	100
3	I	69/78 (88%)	66 (96%)	3 (4%)	0	100	100
4	A	1465/1482 (99%)	1423 (97%)	42 (3%)	0	100	100
4	B	1465/1482 (99%)	1414 (96%)	51 (4%)	0	100	100
All	All	4200/4480 (94%)	4074 (97%)	126 (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	C	376/376 (100%)	364 (97%)	12 (3%)	34	55
1	D	247/376 (66%)	238 (96%)	9 (4%)	30	52
2	E	189/212 (89%)	186 (98%)	3 (2%)	58	74
2	F	177/212 (84%)	174 (98%)	3 (2%)	56	73
3	G	62/66 (94%)	62 (100%)	0	100	100
3	I	62/66 (94%)	62 (100%)	0	100	100
4	A	1269/1281 (99%)	1260 (99%)	9 (1%)	81	87
4	B	1269/1281 (99%)	1257 (99%)	12 (1%)	75	83
All	All	3651/3870 (94%)	3603 (99%)	48 (1%)	64	77

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	2	SER
1	C	92	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	94	LEU
1	C	132	VAL
1	C	209	SER
1	C	250	ASP
1	C	287	THR
1	C	300	ARG
1	C	361	MET
1	C	370	GLN
1	C	428	TYR
1	C	438	ASP
1	D	2	SER
1	D	92	SER
1	D	94	LEU
1	D	132	VAL
1	D	173	MET
1	D	209	SER
1	D	279	ARG
1	D	286	ARG
1	D	287	THR
2	E	147	ASP
2	E	169	TYR
2	E	181	THR
2	F	39	ASP
2	F	152	GLN
2	F	190	ASP
4	A	24	ASP
4	A	319	GLN
4	A	732	GLU
4	A	747	SER
4	A	783	ARG
4	A	1060	ARG
4	A	1131	ARG
4	A	1165	GLU
4	A	1204	ARG
4	B	62	ASN
4	B	211	SER
4	B	250	ARG
4	B	665	GLN
4	B	673	ARG
4	B	687	SER
4	B	1127	ASN
4	B	1131	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
4	B	1152	LYS
4	B	1213	GLU
4	B	1322	GLN
4	B	1347	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	128	GLN
1	C	198	GLN
1	D	75	ASN
1	D	128	GLN
2	E	111	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	4HH	I	36	3	21,26,27	0.47	0	27,35,37	1.73	3 (11%)
3	4HH	G	36	3	21,26,27	0.45	0	27,35,37	3.13	4 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	4HH	I	36	3	-	6/32/35/37	-
3	4HH	G	36	3	-	5/32/35/37	-

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	36	4HH	O1P-P-OG	11.65	161.87	107.75
3	G	36	4HH	OG-P-O2P	-8.86	74.45	109.07
3	G	36	4HH	P-OG-CB	6.12	157.55	121.68
3	I	36	4HH	P-OG-CB	-5.39	90.07	121.68
3	I	36	4HH	O1P-P-OG	4.64	129.28	107.75
3	I	36	4HH	OG-CB-CA	4.47	112.49	108.14
3	G	36	4HH	OG-CB-CA	2.81	110.88	108.14

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	I	36	4HH	N-CA-CB-OG
3	I	36	4HH	CB-OG-P-O1P
3	G	36	4HH	CJ-O3P-P-OG
3	G	36	4HH	CB-OG-P-O3P
3	I	36	4HH	CO-CP-CQ-NR
3	I	36	4HH	CO-CP-CQ-OR
3	I	36	4HH	CB-OG-P-O3P
3	G	36	4HH	ON-CL3-CM-OM
3	I	36	4HH	ON-CL3-CM-OM
3	G	36	4HH	CT-CS-NR-CQ
3	G	36	4HH	CB-OG-P-O2P

There are no ring outliers.

2 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	I	36	4HH	1	0
3	G	36	4HH	14	0



## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	$\# Z  > 2$
6	ATP	A	1502	5	26,33,33	0.62	0	31,52,52	1.12	3 (9%)
6	ATP	B	1502	5	26,33,33	0.64	0	31,52,52	1.13	3 (9%)

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	ATP	A	1502	5	-	1/18/38/38	0/3/3/3
6	ATP	B	1502	5	-	2/18/38/38	0/3/3/3

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	1502	ATP	C5-C6-N6	2.39	123.98	120.35
6	A	1502	ATP	C5-C6-N6	2.34	123.91	120.35
6	A	1502	ATP	O2'-C2'-C3'	-2.31	104.33	111.82
6	B	1502	ATP	O2'-C2'-C3'	-2.20	104.72	111.82
6	B	1502	ATP	O3'-C3'-C2'	-2.15	104.86	111.82
6	A	1502	ATP	O3'-C3'-C2'	-2.05	105.19	111.82

There are no chirality outliers.

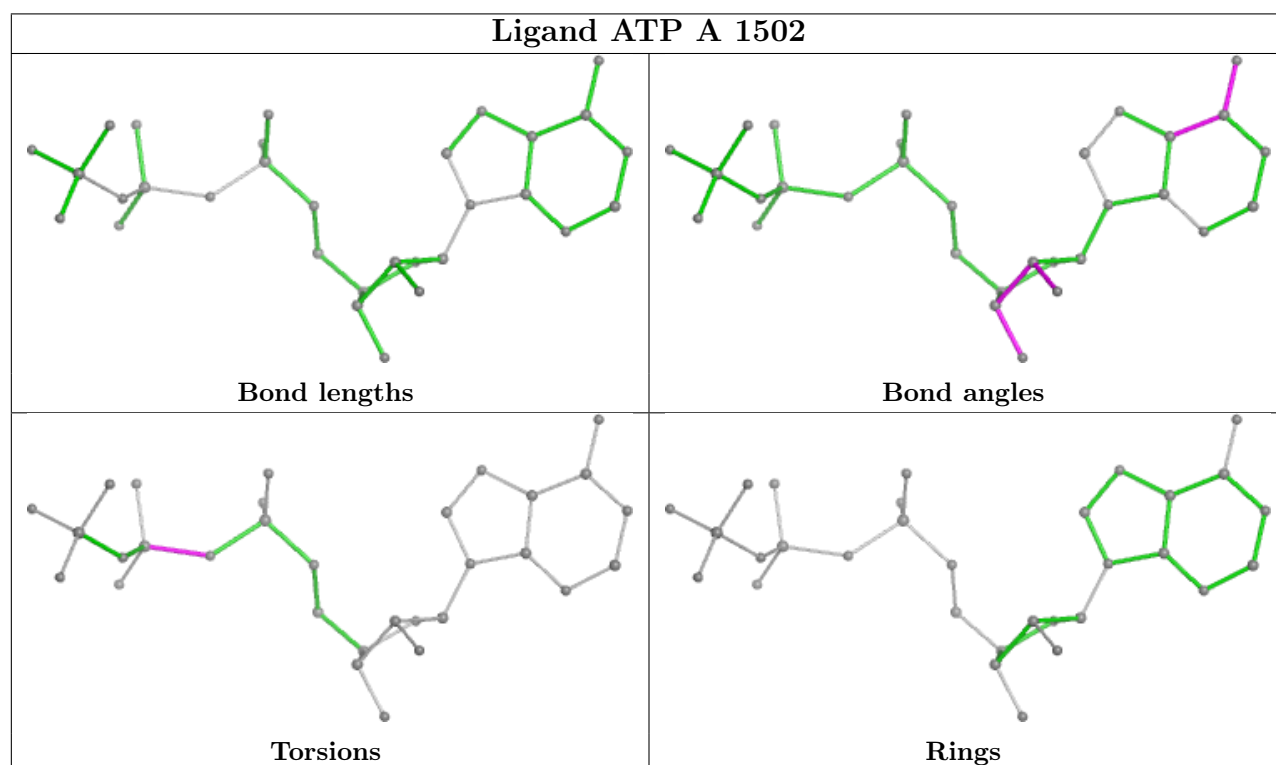
All (3) torsion outliers are listed below:

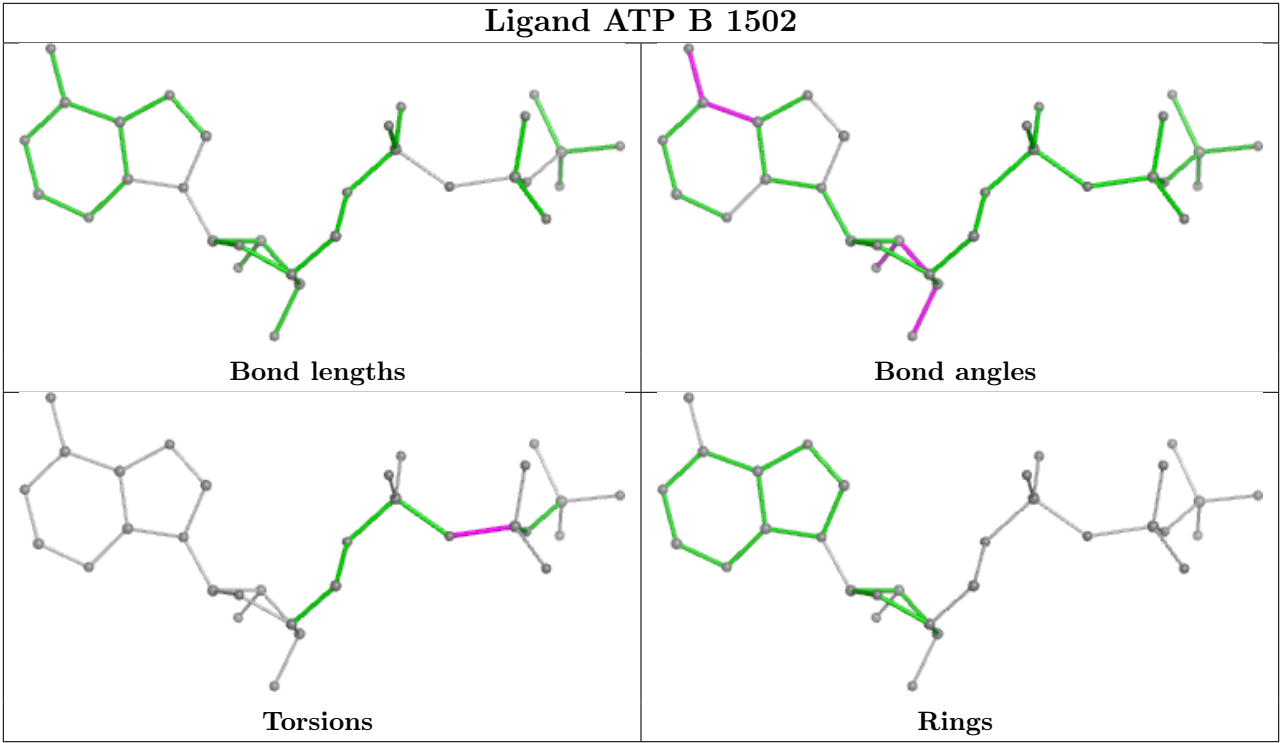
Mol	Chain	Res	Type	Atoms
6	A	1502	ATP	PA-O3A-PB-O2B
6	B	1502	ATP	PA-O3A-PB-O1B
6	B	1502	ATP	PA-O3A-PB-O2B

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	295:ARG	C	296:ILE	N	1.04

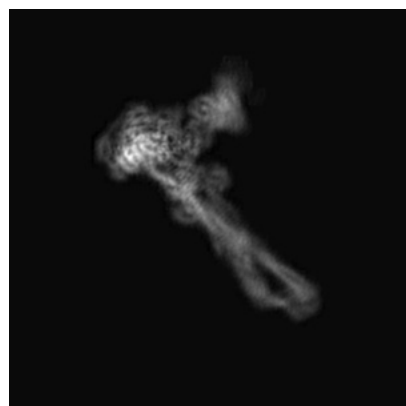
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-51443. These allow visual inspection of the internal detail of the map and identification of artifacts.

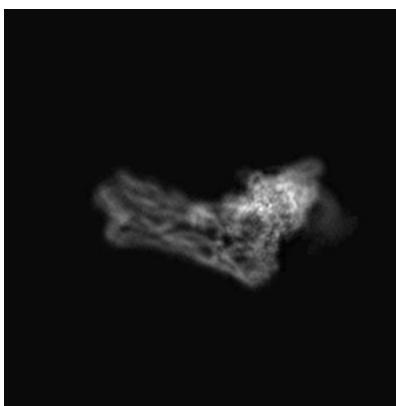
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

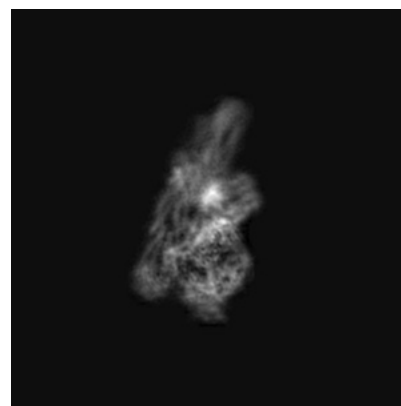
#### 6.1.1 Primary map



X



Y

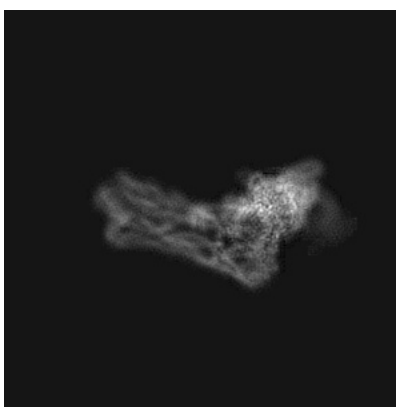


Z

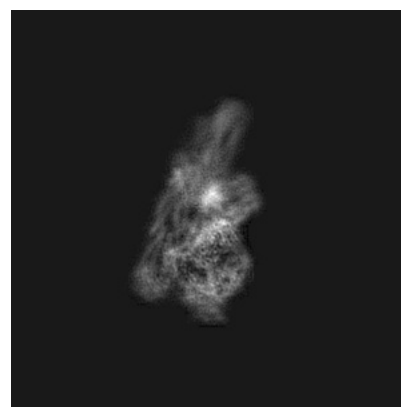
#### 6.1.2 Raw map



X



Y

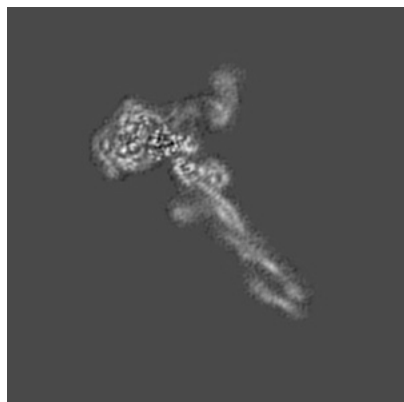


Z

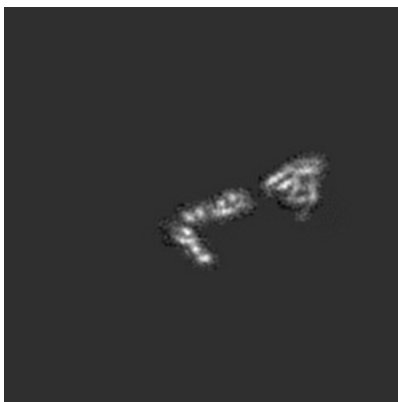
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

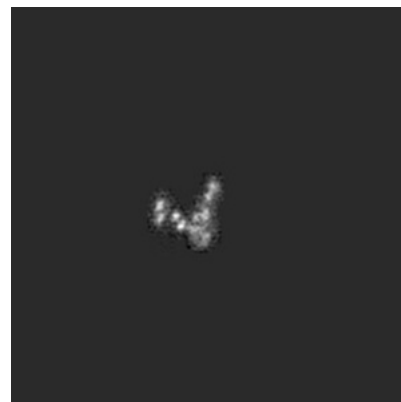
### 6.2.1 Primary map



X Index: 156

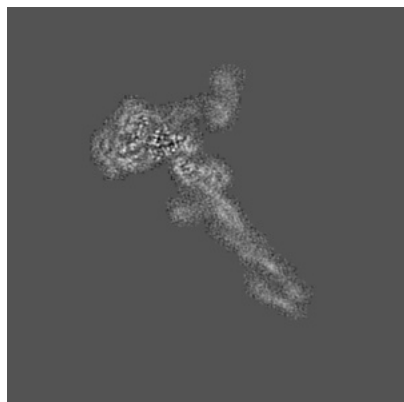


Y Index: 156

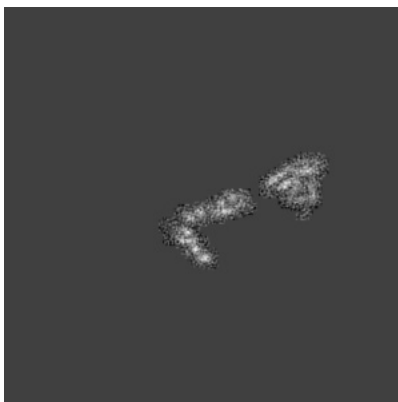


Z Index: 156

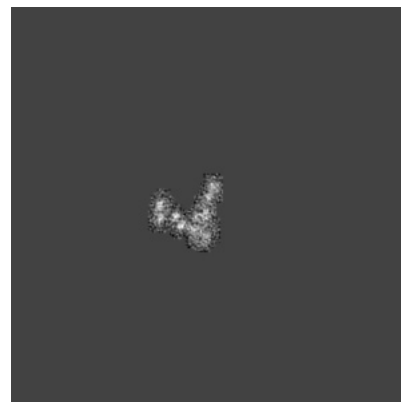
### 6.2.2 Raw map



X Index: 156



Y Index: 156

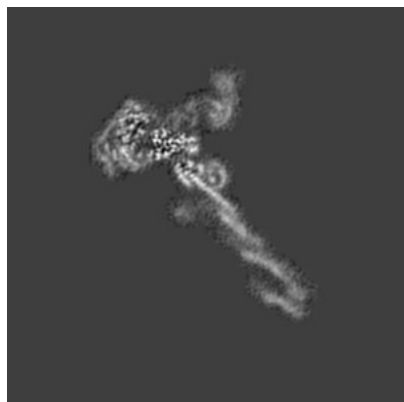


Z Index: 156

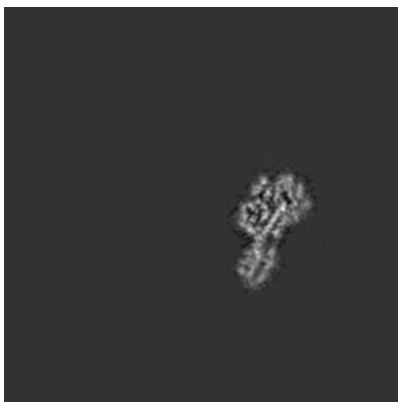
The images above show central slices of the map in three orthogonal directions.

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

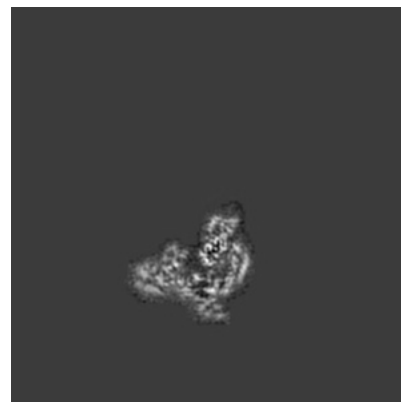
### 6.3.1 Primary map



X Index: 158

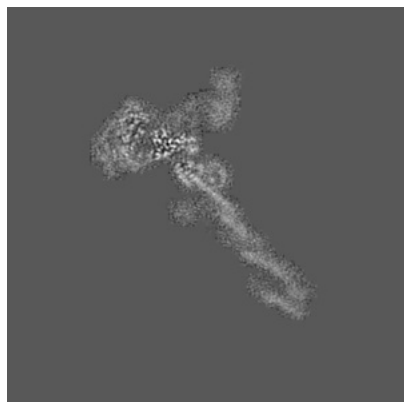


Y Index: 96



Z Index: 199

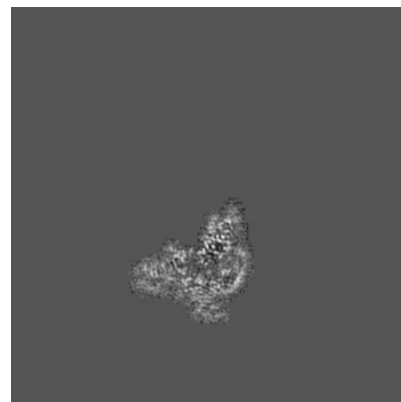
### 6.3.2 Raw map



X Index: 158



Y Index: 97

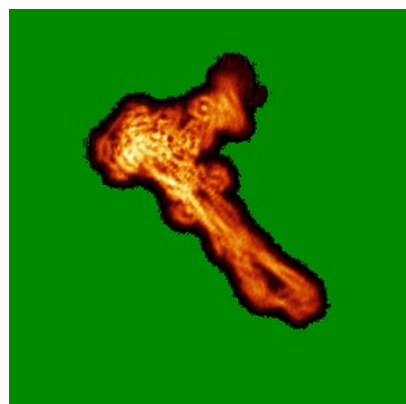


Z Index: 202

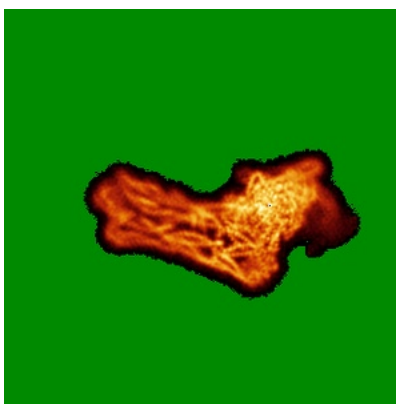
The images above show the largest variance slices of the map in three orthogonal directions.

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

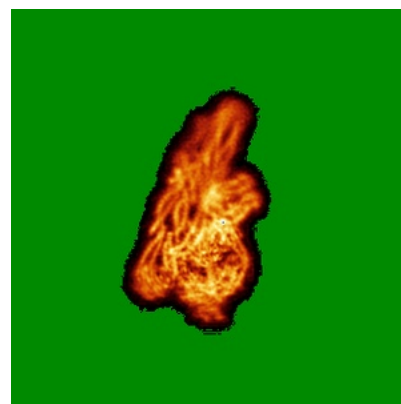
### 6.4.1 Primary map



X

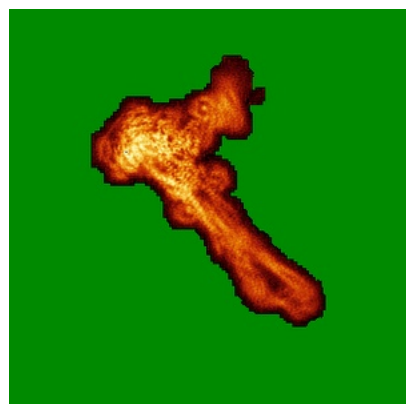


Y

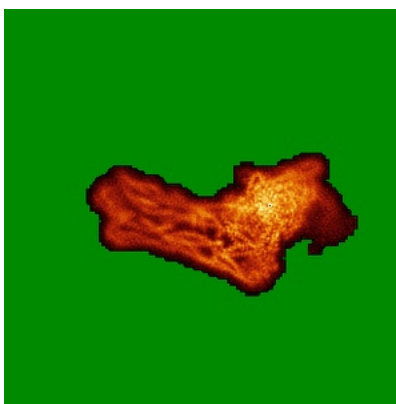


Z

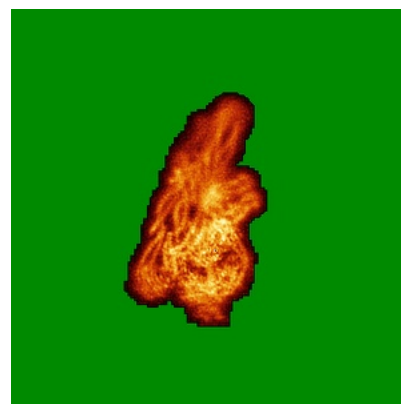
### 6.4.2 Raw map



X



Y

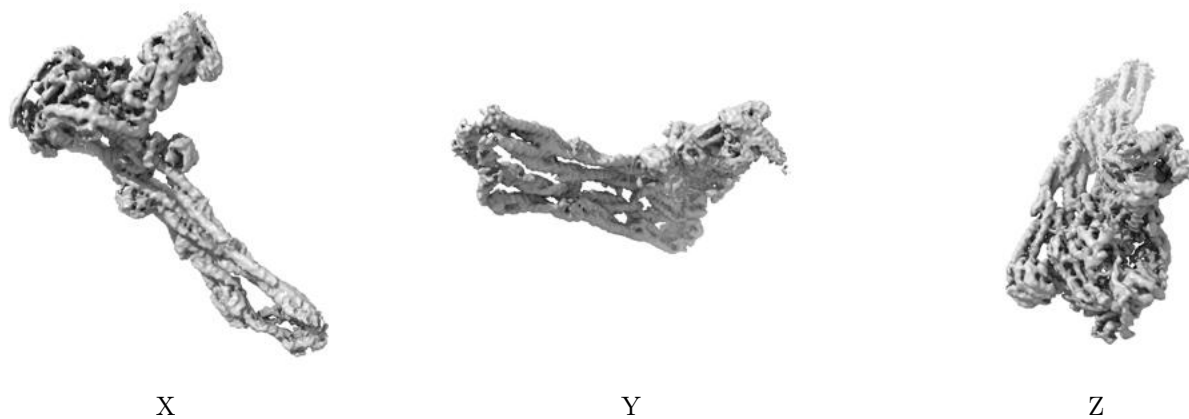


Z

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 0.012. 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](#)

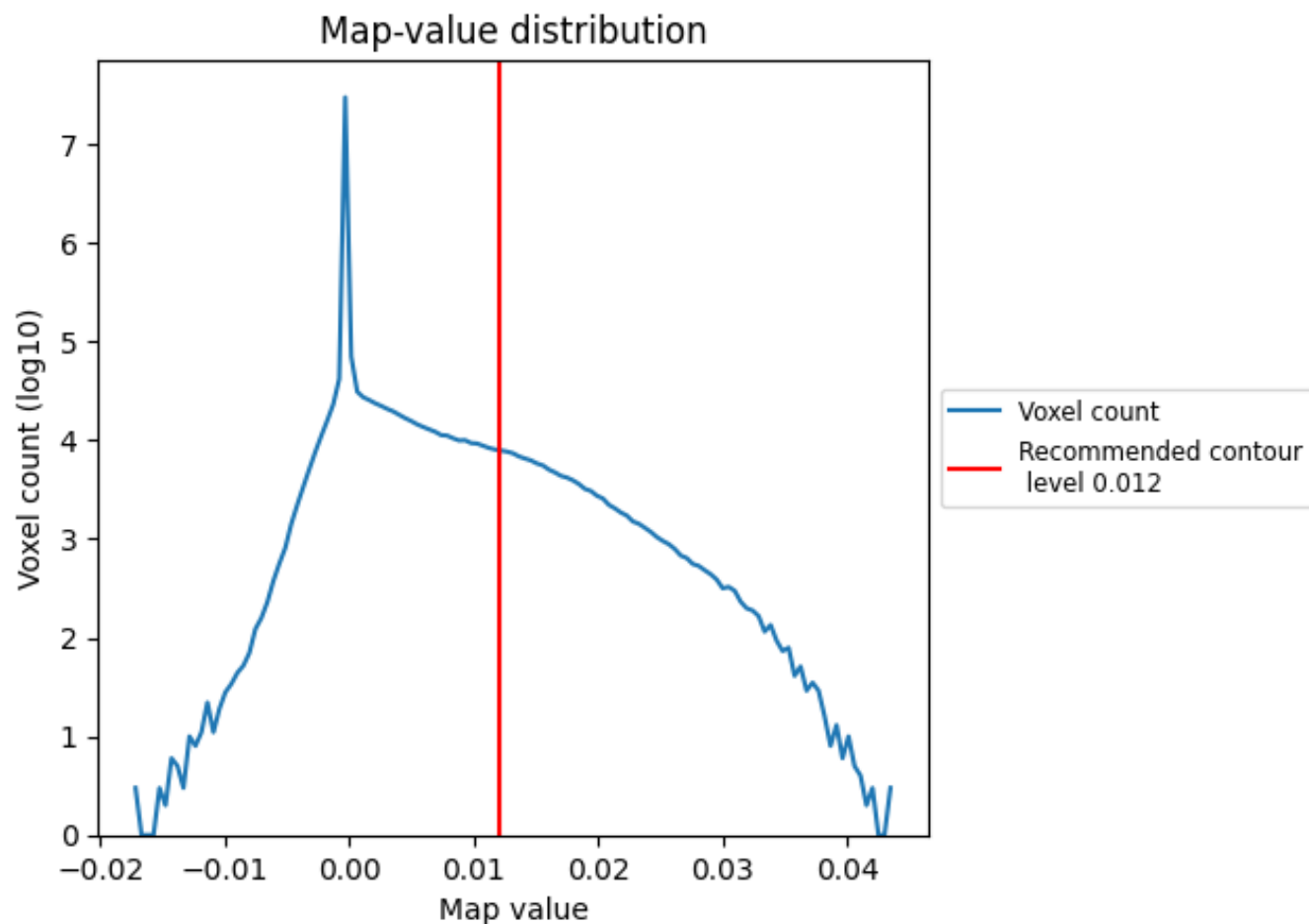
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

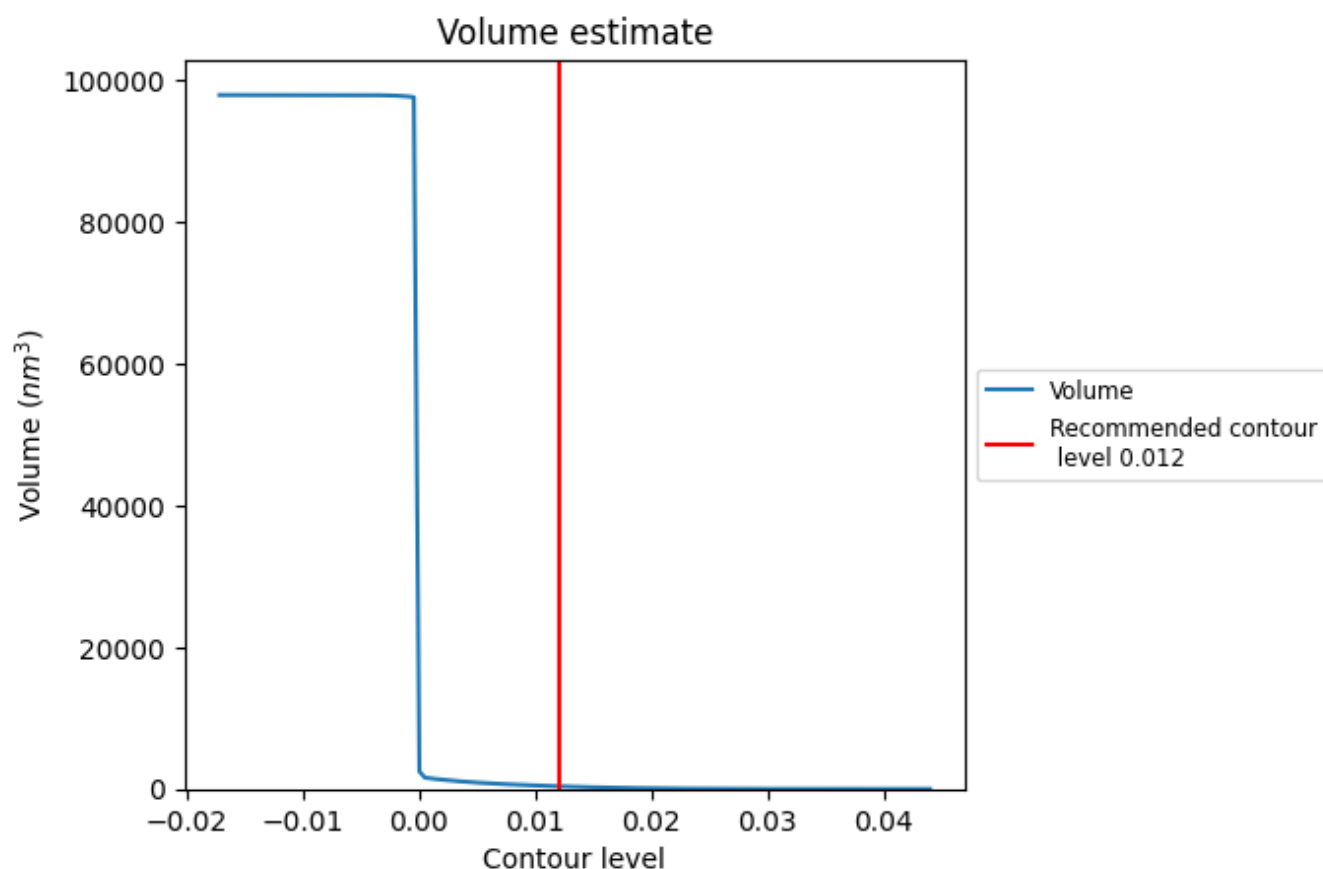
This section contains the results of statistical analysis of the map.

### 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.

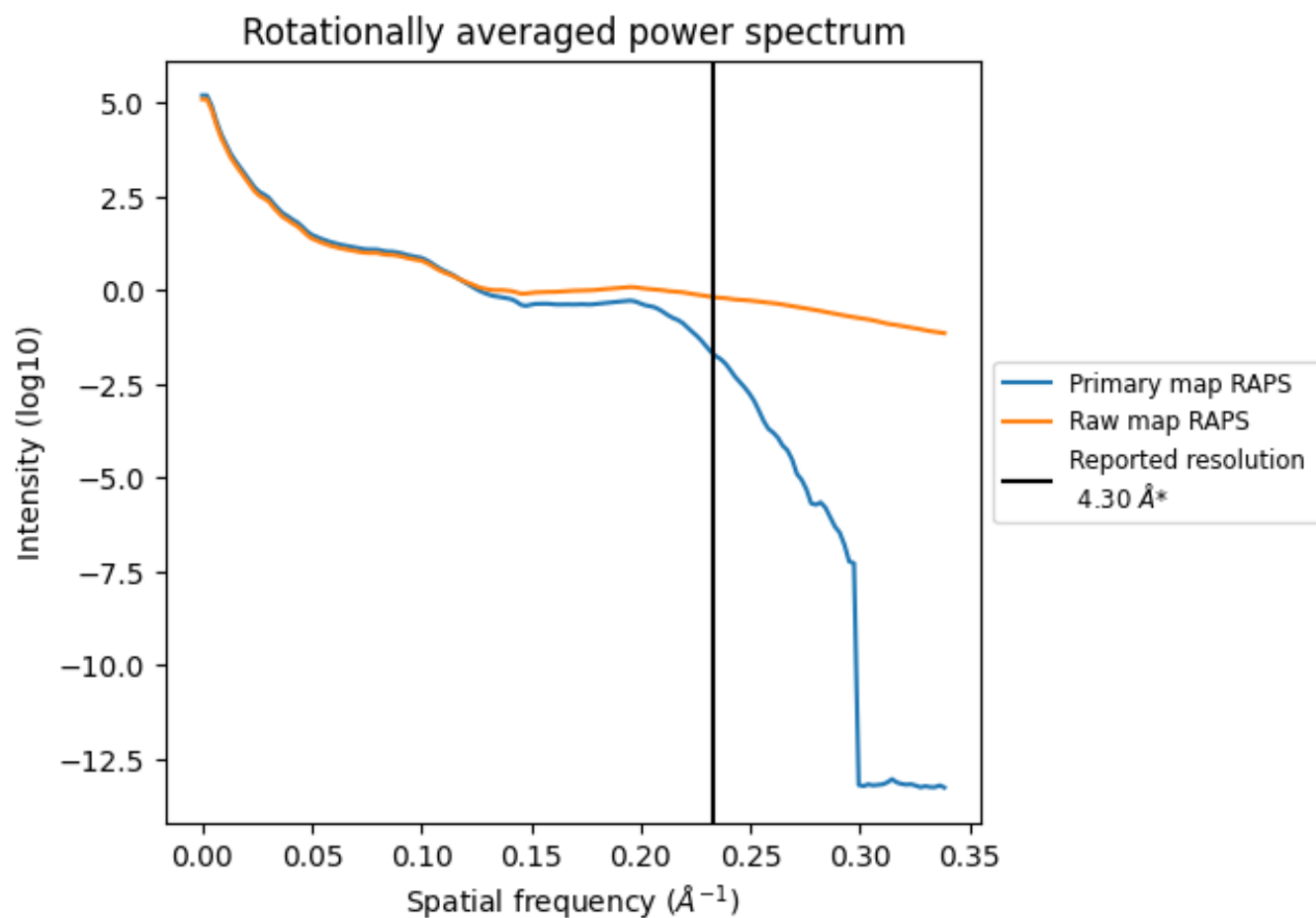
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 378 nm<sup>3</sup>; this corresponds to an approximate mass of 342 kDa.

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

### 7.3 Rotationally averaged power spectrum ⓘ

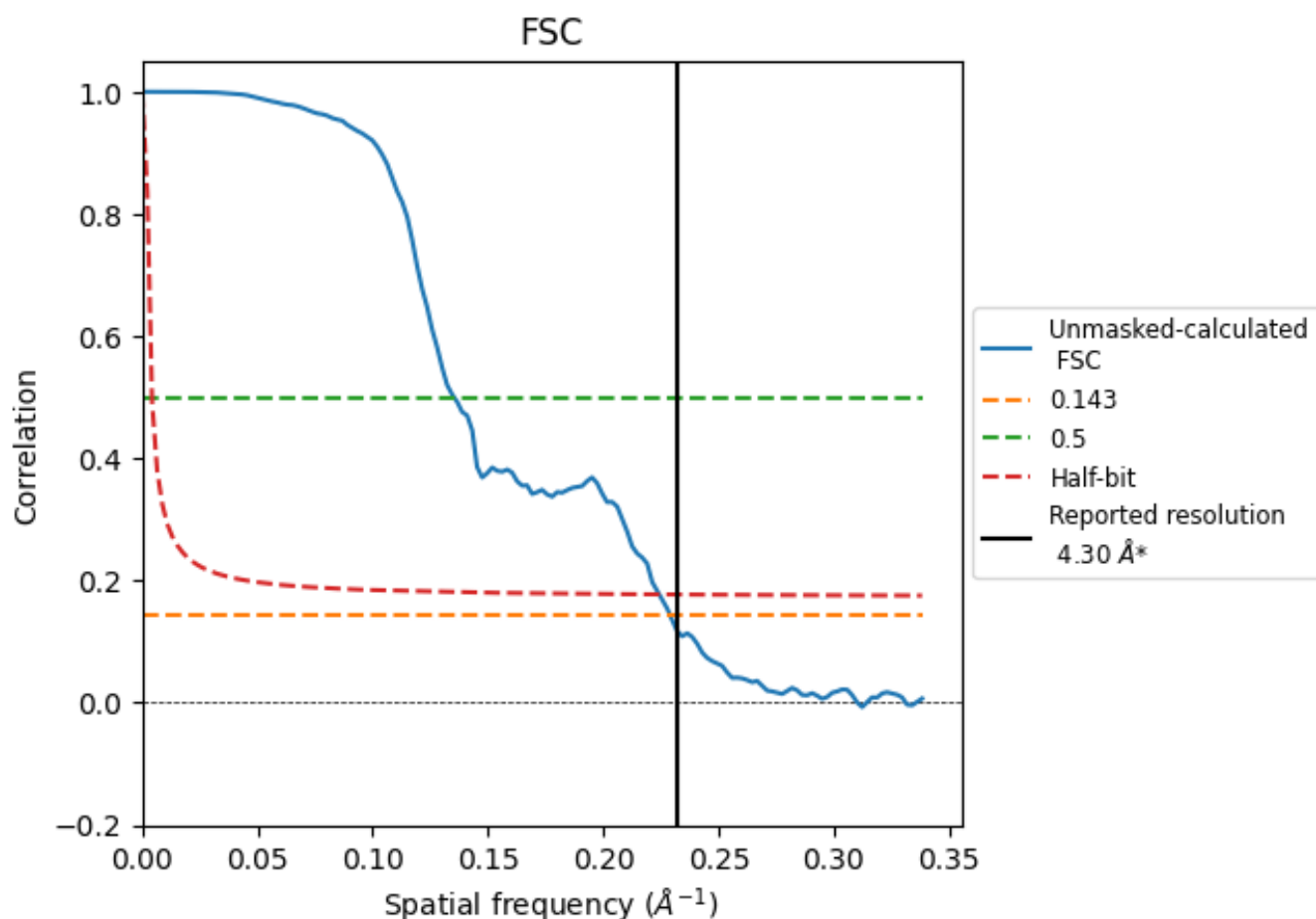


\*Reported resolution corresponds to spatial frequency of 0.233 Å<sup>-1</sup>

## 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 0.233  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

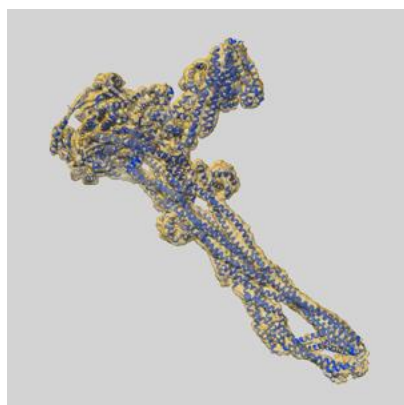
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.36	7.39	4.46

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

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

This section contains information regarding the fit between EMDB map EMD-51443 and PDB model 9GM7. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

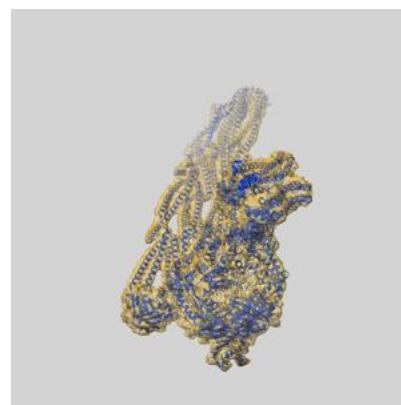
### 9.1 Map-model overlay [i](#)



X



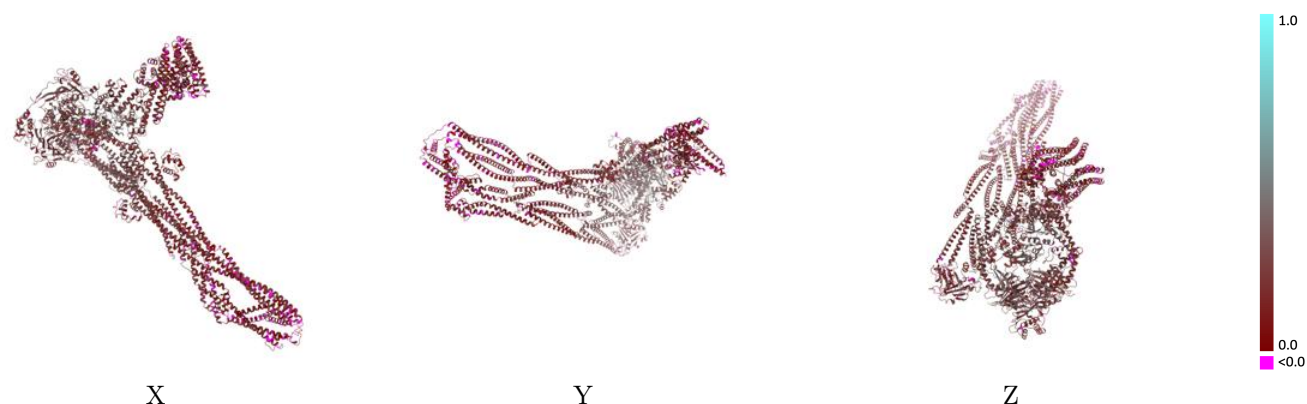
Y



Z

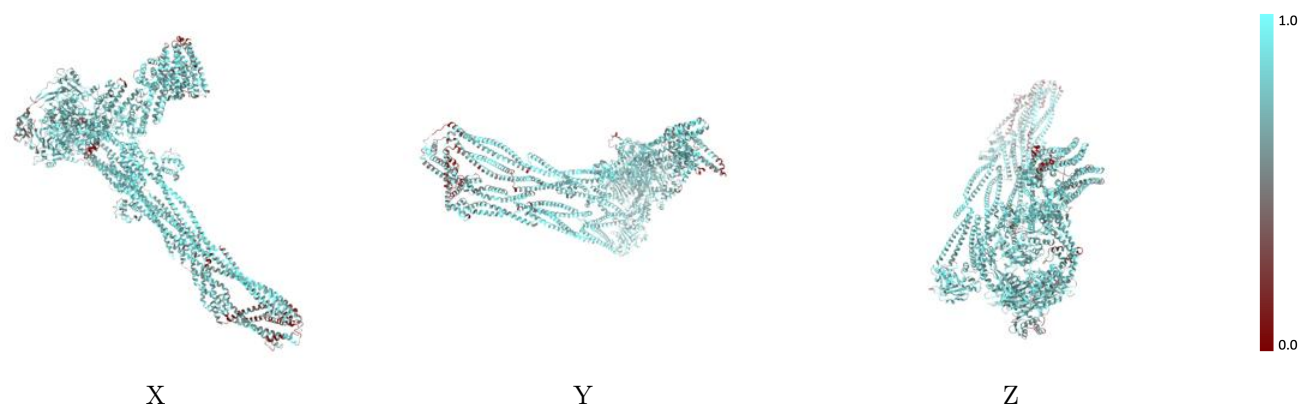
The images above show the 3D surface view of the map at the recommended contour level 0.012 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



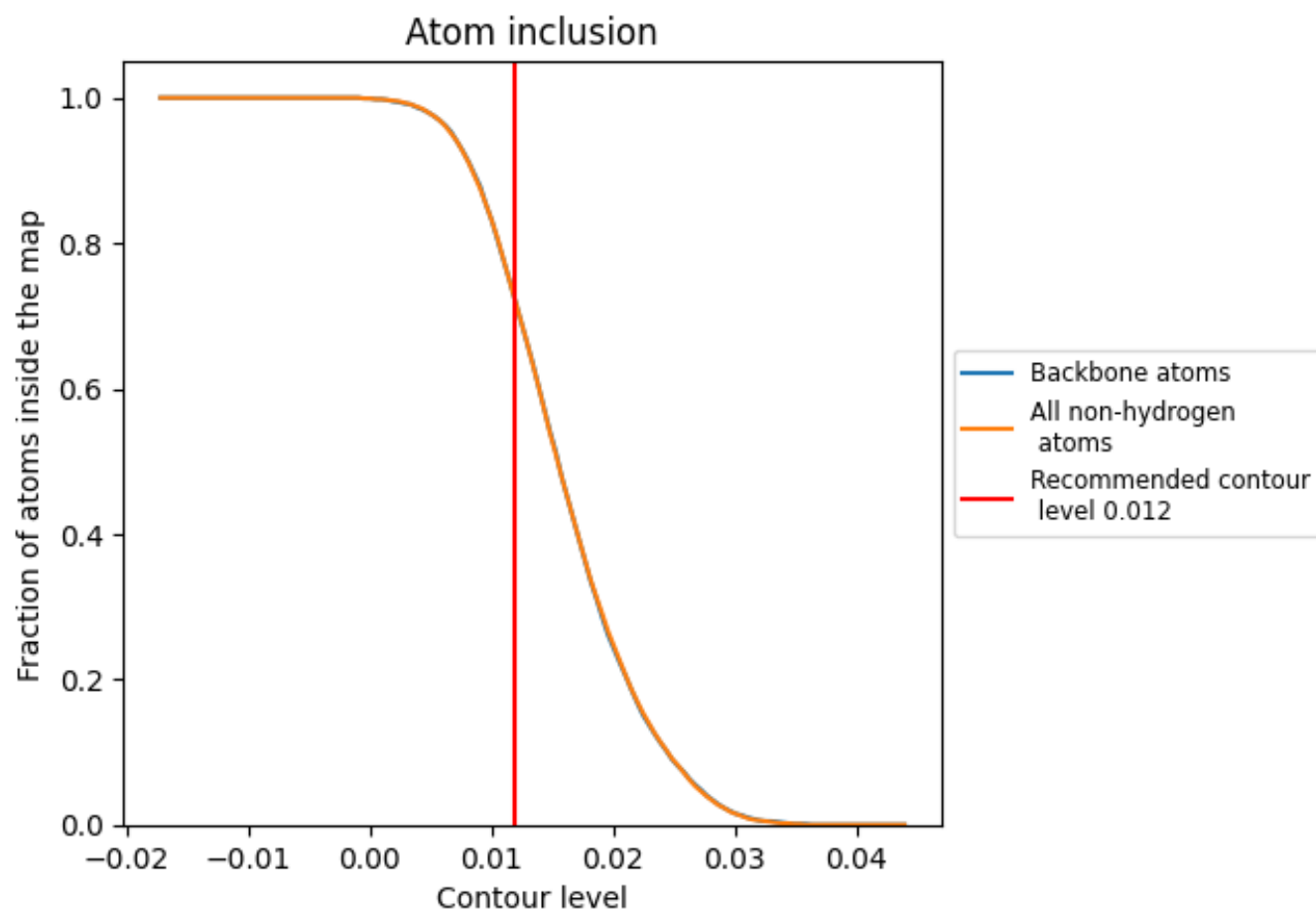
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.012).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 72% of all backbone atoms, 72% 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 (0.012) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.7200	<div><div></div></div> 0.2210
A	<div><div></div></div> 0.7380	<div><div></div></div> 0.2220
B	<div><div></div></div> 0.7450	<div><div></div></div> 0.2190
C	<div><div></div></div> 0.6790	<div><div></div></div> 0.1900
D	<div><div></div></div> 0.6750	<div><div></div></div> 0.1470
E	<div><div></div></div> 0.7830	<div><div></div></div> 0.3280
F	<div><div></div></div> 0.7630	<div><div></div></div> 0.3060
G	<div><div></div></div> 0.6930	<div><div></div></div> 0.1900
I	<div><div></div></div> 0.7410	<div><div></div></div> 0.1730

1.0

0.0

<0.0