



## Full wwPDB EM Validation Report ⓘ

Nov 25, 2025 – 10:12 AM EST

PDB ID : 9PH4 / pdb\_00009ph4  
EMDB ID : EMD-71639  
Title : Cryo-EM structure of COP9 signalosome in complex with CSN5i-1a  
Authors : Shi, H.; Zheng, N.  
Deposited on : 2025-07-08  
Resolution : 3.00 Å (reported)  
Based on initial models : 5JOH, 4D10

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>.

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

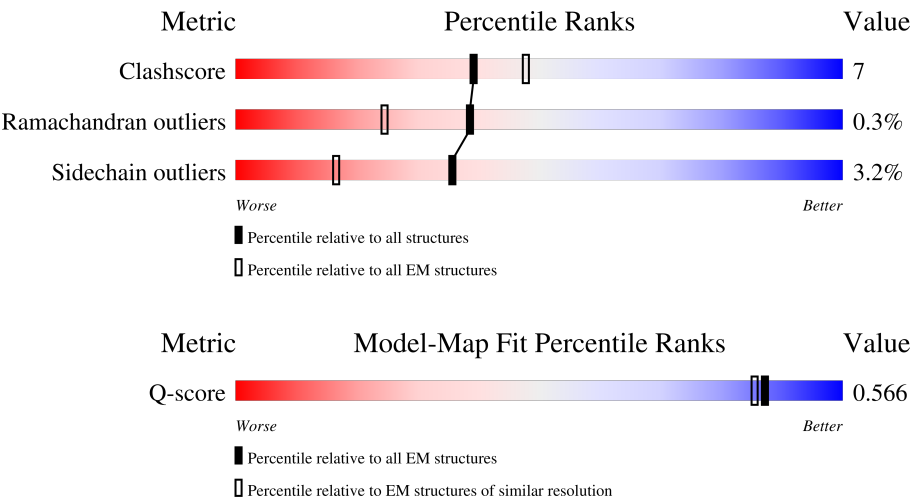
EMDB validation analysis : 0.0.1.dev129  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.46

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 3.00 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	14081 ( 2.50 - 3.50 )

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	491	<div><div>36%9%54%</div></div>
2	B	443	<div><div>20%37%7%56%</div></div>
3	C	423	<div><div>13%75%18%.</div></div>
4	D	406	<div><div>11%42%14%45%</div></div>

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Mol	Chain	Length	Quality of chain
5	E	334	<div><div>9%</div><div><div></div><div>70%</div><div>17%</div><div>12%</div></div></div>
6	F	327	<div><div>8%</div><div><div></div><div>63%</div><div>19%</div><div>17%</div></div></div>
7	G	264	<div><div>7%</div><div><div></div><div>70%</div><div>10%</div><div>19%</div></div></div>
8	H	209	<div><div>16%</div><div><div></div><div>69%</div><div>14%</div><div>17%</div></div></div>

## 2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 15982 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called COP9 signalosome complex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	224	Total	C	N	O	S	0	0
			1786	1141	310	322	13		

- Molecule 2 is a protein called COP9 signalosome complex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	193	Total	C	N	O	S	0	0
			1570	994	272	298	6		

- Molecule 3 is a protein called COP9 signalosome complex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	404	Total	C	N	O	S	0	0
			3216	2048	540	602	26		

- Molecule 4 is a protein called COP9 signalosome complex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	225	Total	C	N	O	S	0	0
			1805	1137	319	337	12		

- Molecule 5 is a protein called COP9 signalosome complex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	293	Total	C	N	O	S	0	0
			2336	1494	388	441	13		

- Molecule 6 is a protein called COP9 signalosome complex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	271	Total	C	N	O	S	0	0
			2173	1392	360	408	13		

- Molecule 7 is a protein called COP9 signalosome complex subunit 7b.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	213	Total	C	N	O	S	0	0
			1687	1070	287	324	6		

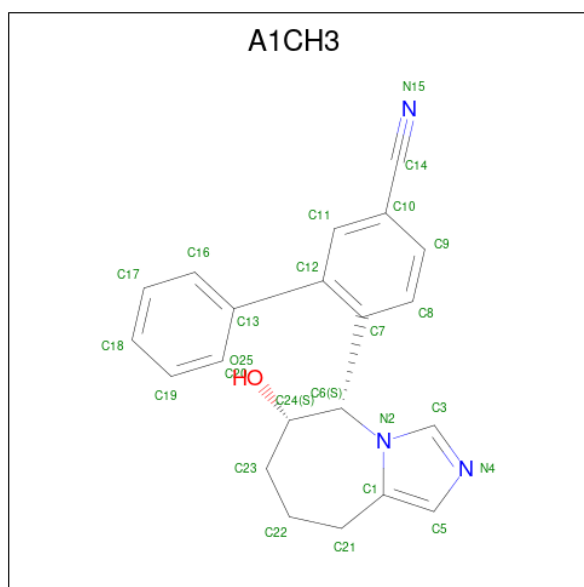
- Molecule 8 is a protein called COP9 signalosome complex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	173	Total	C	N	O	S	0	0
			1383	885	240	254	4		

- Molecule 9 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
9	E	1	Total	Zn	0
			1	1	

- Molecule 10 is 6-[(4R,5S,6S)-6-hydroxy-6,7,8,9-tetrahydro-5H-imidazo[1,5-a]azepin-5-yl][1,1'-biphenyl]-3-carbonitrile (CCD ID: A1CH3) (formula: C<sub>21</sub>H<sub>19</sub>N<sub>3</sub>O) (labeled as "Ligand of Interest" by depositor).

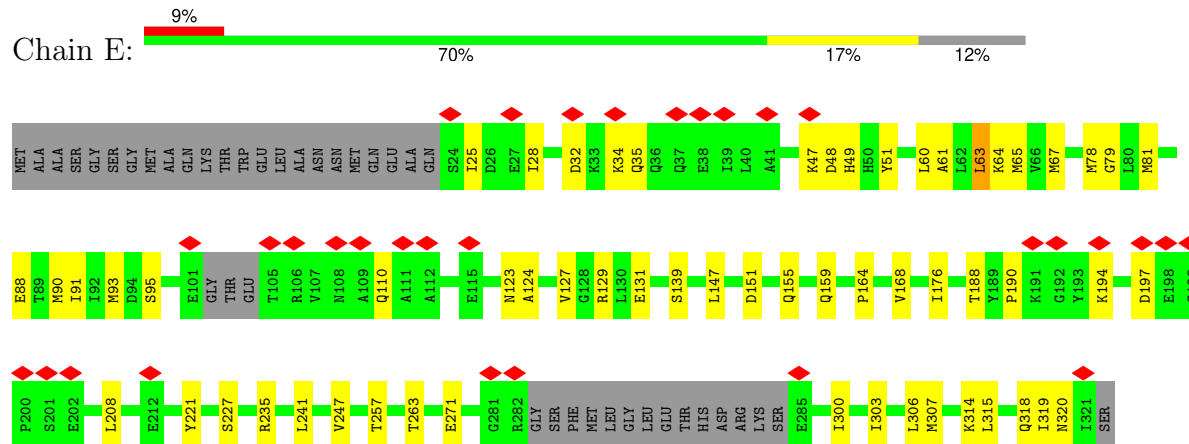


Mol	Chain	Residues	Atoms				AltConf
10	E	1	Total	C	N	O	0
			25	21	3	1	

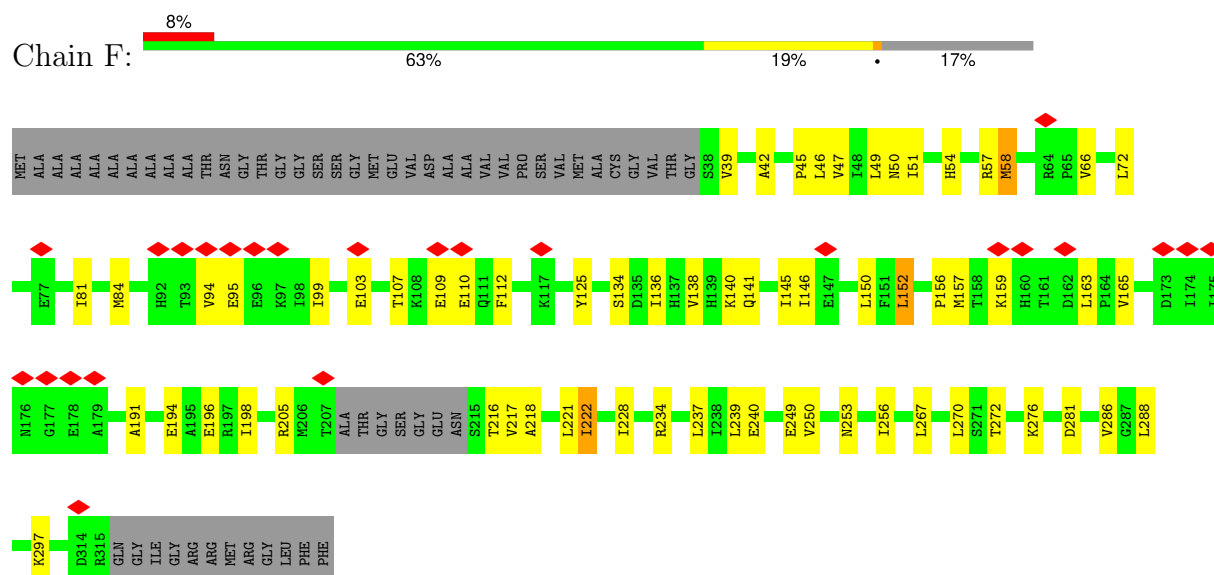




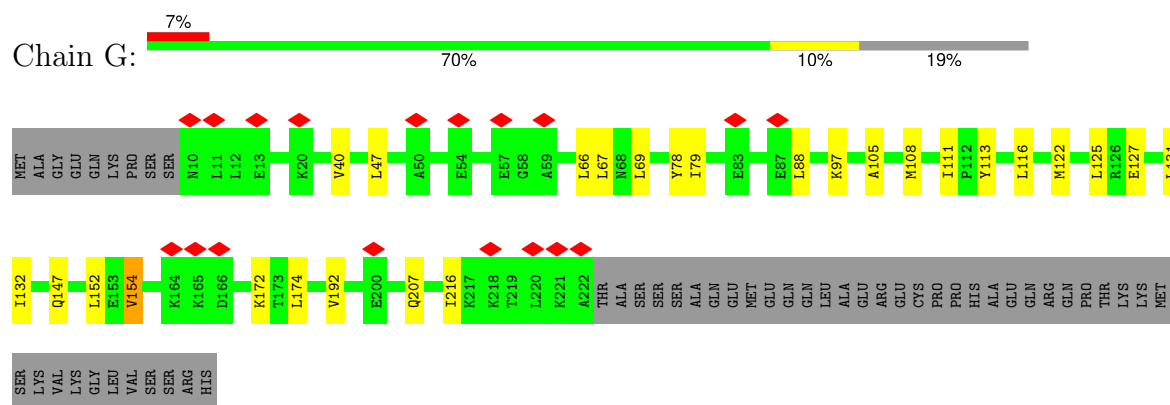
- Molecule 5: COP9 signalosome complex subunit 5



- Molecule 6: COP9 signalosome complex subunit 6



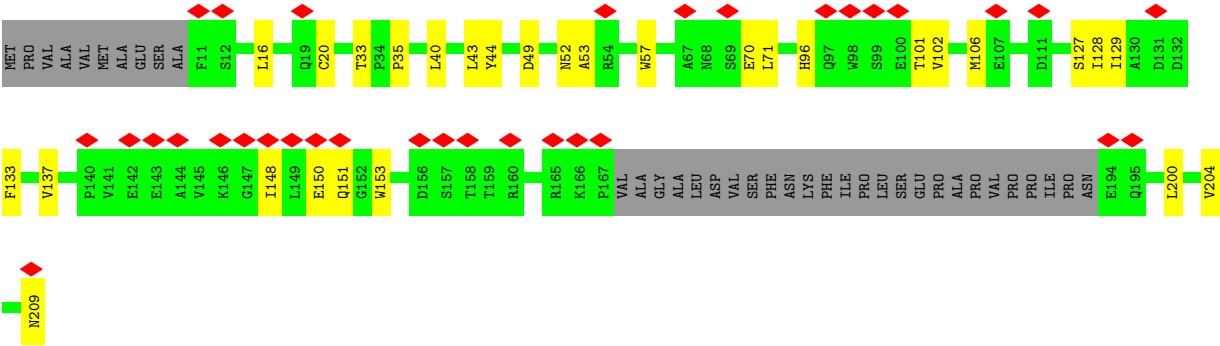
- Molecule 7: COP9 signalosome complex subunit 7b



- Molecule 8: COP9 signalosome complex subunit 8







## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	451908	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 ( $e^-/\text{\AA}^2$ )	60	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.984	Depositor
Minimum map value	-1.233	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.050	Depositor
Recommended contour level	0.308	Depositor
Map size (Å)	264.32, 264.32, 264.32	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.82600003, 0.82600003, 0.82600003	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, A1CH3

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	0.13	0/1815	0.32	0/2443
2	B	0.13	0/1598	0.34	0/2160
3	C	0.19	0/3275	0.37	1/4423 (0.0%)
4	D	0.13	0/1834	0.35	0/2470
5	E	0.13	0/2386	0.30	0/3223
6	F	0.12	0/2219	0.27	0/3007
7	G	0.11	0/1707	0.24	0/2309
8	H	0.13	0/1416	0.33	0/1924
All	All	0.14	0/16250	0.32	1/21959 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	74	PHE	N-CA-C	-5.48	99.13	110.80

There are no chirality outliers.

There are no planarity outliers.

### 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	1786	0	1839	30	0
2	B	1570	0	1576	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	3216	0	3238	60	0
4	D	1805	0	1812	32	0
5	E	2336	0	2315	39	0
6	F	2173	0	2164	45	0
7	G	1687	0	1730	15	0
8	H	1383	0	1366	21	0
9	E	1	0	0	0	0
10	E	25	0	0	0	0
All	All	15982	0	16040	225	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (225) 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:C:71:VAL:HG23	3:C:74:PHE:HA	1.58	0.85
5:E:78:MET:HE1	5:E:110:GLN:HB3	1.58	0.83
3:C:243:LYS:H	3:C:243:LYS:HD3	1.43	0.82
2:B:420:ARG:HE	5:E:263:THR:HG22	1.53	0.73
4:D:230:LEU:HD11	4:D:264:LEU:HB2	1.74	0.70
2:B:282:LEU:HD22	2:B:343:ILE:HD13	1.74	0.70
1:A:386:MET:HE1	1:A:401:GLU:HG2	1.73	0.69
5:E:176:ILE:HG23	6:F:194:GLU:HG2	1.74	0.69
4:D:281:PHE:HA	4:D:284:MET:HE2	1.75	0.68
3:C:71:VAL:HG11	3:C:76:THR:HB	1.74	0.68
7:G:66:LEU:HD11	7:G:88:LEU:HD21	1.76	0.68
6:F:145:ILE:HG22	6:F:146:ILE:HG23	1.77	0.67
4:D:201:PHE:HB3	4:D:235:LEU:HB3	1.76	0.66
6:F:156:PRO:HG2	6:F:157:MET:HE2	1.77	0.66
8:H:150:GLU:HG2	8:H:151:GLN:HE21	1.62	0.65
5:E:307:MET:HE1	6:F:217:VAL:HG13	1.79	0.64
6:F:103:GLU:O	6:F:107:THR:HG23	1.98	0.64
4:D:234:ILE:HD12	4:D:300:LEU:HD22	1.80	0.64
3:C:63:PHE:HE2	3:C:81:VAL:HG21	1.63	0.64
4:D:211:LEU:HA	4:D:214:LYS:HG2	1.80	0.64
5:E:300:ILE:HG12	8:H:204:VAL:HG13	1.80	0.62
7:G:47:LEU:HD13	7:G:67:LEU:HD23	1.80	0.62
4:D:400:MET:HE2	6:F:240:GLU:HG3	1.81	0.62
8:H:16:LEU:HG	8:H:43:LEU:HD11	1.80	0.62
7:G:108:MET:HE3	7:G:111:ILE:HG23	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:117:PRO:HB3	3:C:148:LEU:HD22	1.82	0.61
4:D:302:ARG:HH21	4:D:341:GLN:HE22	1.47	0.60
2:B:308:ILE:O	2:B:308:ILE:HD12	2.02	0.59
5:E:49:HIS:HE1	5:E:190:PRO:HG2	1.67	0.59
5:E:63:LEU:HD12	6:F:49:LEU:HD12	1.83	0.59
5:E:61:ALA:O	5:E:65:MET:HG3	2.04	0.58
3:C:52:GLN:HG2	3:C:84:PHE:HD1	1.69	0.58
4:D:207:ARG:O	4:D:211:LEU:HD23	2.02	0.58
3:C:217:SER:HB3	3:C:220:MET:HB2	1.86	0.57
6:F:81:ILE:HG21	6:F:150:LEU:HD11	1.86	0.57
5:E:63:LEU:O	5:E:67:MET:HG2	2.04	0.57
4:D:278:LEU:HD13	4:D:304:VAL:HG21	1.87	0.57
5:E:60:LEU:HD11	6:F:50:ASN:ND2	2.20	0.57
3:C:55:SER:HA	3:C:58:VAL:HB	1.85	0.56
5:E:90:MET:HE3	5:E:164:PRO:HB2	1.87	0.56
5:E:124:ALA:HB1	5:E:129:ARG:HB3	1.87	0.56
3:C:68:MET:O	3:C:69:PRO:C	2.47	0.56
3:C:71:VAL:CG1	3:C:76:THR:HB	2.35	0.55
3:C:322:MET:HE2	3:C:334:ALA:HB1	1.87	0.55
7:G:122:MET:HE2	7:G:127:GLU:HB3	1.88	0.55
3:C:68:MET:O	3:C:70:SER:N	2.40	0.55
3:C:203:TYR:O	3:C:207:GLN:HG2	2.06	0.55
4:D:321:PHE:O	4:D:322:GLU:HG3	2.05	0.55
3:C:353:GLN:HE21	8:H:129:ILE:H	1.55	0.55
5:E:67:MET:HG3	6:F:46:LEU:HD22	1.90	0.54
5:E:78:MET:HG2	5:E:79:GLY:N	2.21	0.54
1:A:400:LEU:O	1:A:404:LEU:HG	2.07	0.54
3:C:266:VAL:HG13	3:C:275:LEU:HD12	1.90	0.54
1:A:404:LEU:HA	1:A:407:LEU:HB2	1.89	0.54
3:C:73:ASP:O	3:C:74:PHE:HB3	2.06	0.54
2:B:277:LEU:HD21	2:B:303:LYS:HD3	1.89	0.54
1:A:404:LEU:HD22	1:A:424:LEU:HD22	1.88	0.54
3:C:118:LEU:HD12	3:C:121:ILE:HD12	1.90	0.54
3:C:131:MET:HE3	3:C:141:ILE:HD11	1.89	0.54
8:H:44:TYR:HB3	8:H:53:ALA:HB2	1.90	0.54
2:B:310:ALA:HB3	2:B:336:ASN:HD21	1.73	0.53
6:F:94:VAL:HG12	6:F:95:GLU:HG3	1.91	0.53
3:C:60:ALA:O	3:C:64:VAL:HG23	2.09	0.53
6:F:297:LYS:NZ	8:H:209:ASN:HD21	2.06	0.53
5:E:25:ILE:HD11	5:E:235:ARG:HH21	1.74	0.53
5:E:47:LYS:HD2	5:E:47:LYS:N	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:400:MET:HE3	4:D:404:MET:HE2	1.91	0.53
3:C:353:GLN:HE21	8:H:128:ILE:HA	1.74	0.53
3:C:88:CYS:SG	3:C:130:LYS:HD3	2.49	0.52
3:C:252:PHE:O	3:C:256:LEU:HD12	2.09	0.52
1:A:442:MET:HE2	2:B:428:THR:HG23	1.92	0.52
1:A:449:ARG:HH11	2:B:435:ASN:ND2	2.07	0.52
3:C:322:MET:HE1	3:C:338:VAL:HG23	1.91	0.52
5:E:48:ASP:HB3	5:E:51:TYR:HB2	1.92	0.52
5:E:315:LEU:HD11	6:F:228:ILE:HG12	1.91	0.52
3:C:97:THR:HG23	3:C:172:GLU:HA	1.91	0.52
3:C:63:PHE:CE2	3:C:81:VAL:HG21	2.45	0.52
6:F:218:ALA:O	6:F:222:ILE:HD13	2.09	0.51
8:H:20:CYS:HB3	8:H:40:LEU:HD13	1.92	0.51
8:H:49:ASP:OD1	8:H:52:ASN:HB2	2.10	0.51
1:A:387:HIS:C	1:A:389:MET:H	2.18	0.51
6:F:218:ALA:HA	7:G:192:VAL:HG22	1.93	0.51
3:C:205:TYR:HB3	3:C:227:TYR:HB2	1.94	0.50
5:E:188:THR:HG22	5:E:221:TYR:HB3	1.94	0.50
3:C:74:PHE:O	3:C:75:GLU:C	2.54	0.50
3:C:369:ASN:HD22	3:C:371:ALA:HB3	1.76	0.50
4:D:340:SER:O	4:D:344:THR:HG23	2.12	0.50
8:H:33:THR:OG1	8:H:35:PRO:HD2	2.12	0.49
6:F:109:GLU:HA	6:F:112:PHE:CD2	2.48	0.49
4:D:387:LYS:O	4:D:391:THR:HG23	2.11	0.49
4:D:362:GLU:H	4:D:362:GLU:CD	2.21	0.49
5:E:306:LEU:HD22	6:F:286:VAL:HB	1.95	0.49
3:C:56:LEU:HD22	3:C:93:ILE:HG22	1.95	0.49
3:C:353:GLN:NE2	8:H:128:ILE:HG13	2.26	0.49
1:A:386:MET:HE2	1:A:422:LYS:HG3	1.95	0.49
3:C:243:LYS:HD3	3:C:243:LYS:N	2.21	0.49
5:E:28:ILE:HD11	5:E:91:ILE:HG21	1.95	0.49
5:E:155:GLN:O	5:E:159:GLN:HG3	2.12	0.48
1:A:349:LYS:HZ1	1:A:363:ARG:NH1	2.11	0.48
7:G:113:TYR:CD2	7:G:125:LEU:HD11	2.47	0.48
8:H:70:GLU:OE1	8:H:102:VAL:HG11	2.14	0.48
7:G:105:ALA:HB1	7:G:154:VAL:HG21	1.96	0.48
2:B:363:ILE:HD12	2:B:411:LEU:HD22	1.96	0.47
5:E:32:ASP:HB3	5:E:35:GLN:HB3	1.96	0.47
6:F:72:LEU:HD21	6:F:125:TYR:HB3	1.96	0.47
3:C:71:VAL:CG2	3:C:74:PHE:HA	2.38	0.47
6:F:39:VAL:HG21	6:F:81:ILE:HD12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:99:ILE:HA	6:F:141:GLN:HE22	1.80	0.47
1:A:385:ASP:HB3	1:A:387:HIS:O	2.14	0.47
4:D:321:PHE:HB3	4:D:332:ALA:HB1	1.97	0.47
4:D:321:PHE:C	4:D:323:GLU:H	2.22	0.47
5:E:64:LYS:HG2	6:F:46:LEU:HD11	1.96	0.47
5:E:314:LYS:HA	5:E:318:GLN:HG3	1.97	0.47
5:E:49:HIS:CE1	5:E:190:PRO:HG2	2.49	0.46
6:F:152:LEU:HD21	6:F:165:VAL:HG13	1.97	0.46
3:C:367:TYR:HD2	3:C:372:MET:HG2	1.80	0.46
1:A:442:MET:HE3	1:A:442:MET:HB3	1.80	0.46
3:C:142:HIS:HB3	3:C:184:TYR:CD1	2.50	0.46
6:F:297:LYS:HZ1	8:H:209:ASN:HD21	1.62	0.46
1:A:320:LEU:HB3	1:A:327:ARG:HB2	1.97	0.46
1:A:449:ARG:HD2	2:B:435:ASN:ND2	2.30	0.46
2:B:291:ILE:HA	2:B:319:GLN:HE21	1.81	0.46
3:C:71:VAL:O	3:C:72:PRO:C	2.59	0.46
3:C:205:TYR:O	3:C:209:ILE:HG13	2.16	0.46
3:C:243:LYS:H	3:C:243:LYS:CD	2.21	0.46
3:C:249:VAL:HA	3:C:253:ILE:HD12	1.98	0.46
4:D:394:GLU:HA	4:D:398:GLN:HB2	1.98	0.46
3:C:368:ASN:HB3	6:F:281:ASP:OD1	2.16	0.46
3:C:221:LEU:HD12	3:C:253:ILE:HG23	1.98	0.46
1:A:244:ALA:HA	1:A:277:HIS:HB3	1.98	0.46
2:B:287:MET:O	2:B:288:LYS:HG2	2.16	0.46
3:C:284:GLU:HG2	3:C:285:THR:N	2.31	0.45
2:B:359:LEU:O	2:B:363:ILE:HG23	2.16	0.45
3:C:68:MET:HE2	3:C:68:MET:HB3	1.76	0.45
3:C:72:PRO:O	3:C:73:ASP:HB3	2.17	0.45
1:A:275:PHE:CE1	1:A:322:LEU:HD11	2.52	0.45
6:F:136:ILE:HG22	6:F:140:LYS:HD2	1.99	0.45
3:C:37:LYS:NZ	3:C:65:LYS:HE2	2.32	0.45
2:B:432:ASN:O	2:B:436:GLN:HG3	2.17	0.45
5:E:93:MET:HG3	5:E:131:GLU:CD	2.41	0.45
6:F:42:ALA:HB1	6:F:191:ALA:HB2	1.97	0.45
7:G:97:LYS:HB3	7:G:131:LEU:HD21	1.99	0.45
1:A:375:ILE:HD13	1:A:413:ILE:HG13	1.99	0.45
2:B:362:LEU:HD11	2:B:373:PHE:HE2	1.82	0.45
1:A:255:LEU:HD21	1:A:357:TYR:CD2	2.52	0.44
3:C:71:VAL:O	3:C:73:ASP:N	2.50	0.44
4:D:253:GLU:H	4:D:253:GLU:HG3	1.61	0.44
5:E:208:LEU:HD12	5:E:271:GLU:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:303:ILE:HG23	8:H:200:LEU:HD22	1.98	0.44
1:A:253:ALA:O	1:A:257:GLU:HG3	2.18	0.44
1:A:451:LYS:HB2	1:A:451:LYS:HE2	1.68	0.44
3:C:321:ASP:O	3:C:325:ARG:HG3	2.16	0.44
4:D:385:LEU:HG	6:F:234:ARG:HG2	2.00	0.44
2:B:424:LEU:HD13	6:F:288:LEU:HD23	1.98	0.44
6:F:45:PRO:HD2	6:F:196:GLU:CD	2.42	0.44
6:F:194:GLU:O	6:F:198:ILE:HG12	2.18	0.44
7:G:116:LEU:HD13	7:G:132:ILE:HD11	1.99	0.44
6:F:159:LYS:HD2	6:F:159:LYS:N	2.33	0.44
6:F:47:VAL:O	6:F:51:ILE:HG13	2.18	0.43
4:D:230:LEU:O	4:D:233:THR:HG23	2.18	0.43
5:E:194:LYS:HD3	5:E:194:LYS:HA	1.72	0.43
8:H:133:PHE:O	8:H:137:VAL:HG23	2.18	0.43
3:C:122:GLY:HA2	3:C:125:LYS:HD3	1.99	0.43
4:D:193:ARG:HH12	4:D:197:TYR:HD1	1.67	0.43
3:C:67:SER:O	3:C:68:MET:C	2.61	0.43
6:F:54:HIS:CD2	6:F:58:MET:HE3	2.53	0.43
3:C:353:GLN:NE2	8:H:129:ILE:H	2.16	0.43
1:A:384:ALA:O	1:A:423:ILE:HG23	2.18	0.43
5:E:319:ILE:HG13	6:F:267:LEU:HD22	1.99	0.43
1:A:395:THR:HB	1:A:399:ALA:HB3	2.01	0.43
7:G:172:LYS:HE2	7:G:172:LYS:HB2	1.87	0.43
5:E:129:ARG:NH1	6:F:57:ARG:HD2	2.34	0.43
5:E:306:LEU:HB2	6:F:286:VAL:HG11	2.01	0.43
5:E:81:MET:HA	5:E:95:SER:HA	2.00	0.43
3:C:374:HIS:O	3:C:378:GLN:HG2	2.19	0.42
4:D:193:ARG:NH1	4:D:197:TYR:HB2	2.34	0.42
1:A:464:ILE:O	3:C:212:PRO:HG2	2.19	0.42
1:A:345:LEU:HD23	1:A:345:LEU:HA	1.90	0.42
6:F:163:LEU:HG	6:F:165:VAL:HG23	2.00	0.42
8:H:96:HIS:NE2	8:H:106:MET:HE2	2.34	0.42
1:A:380:PRO:HG3	2:B:390:VAL:HG13	2.00	0.42
6:F:205:ARG:HD3	6:F:205:ARG:HA	1.74	0.42
1:A:377:TYR:CD1	1:A:389:MET:HE3	2.55	0.42
1:A:432:ARG:HG3	2:B:421:TYR:CZ	2.54	0.42
3:C:171:LYS:HB2	3:C:171:LYS:HE2	1.75	0.42
3:C:389:ARG:HH11	3:C:389:ARG:HG2	1.85	0.42
3:C:126:GLN:O	3:C:130:LYS:HB2	2.20	0.42
3:C:202:LEU:HD11	3:C:231:SER:HB2	2.01	0.42
8:H:148:ILE:HB	8:H:153:TRP:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:353:GLN:NE2	8:H:129:ILE:HG13	2.34	0.42
5:E:123:ASN:O	5:E:127:VAL:HG22	2.20	0.42
6:F:221:LEU:O	6:F:222:ILE:HD12	2.20	0.42
2:B:366:TYR:CE2	4:D:354:GLN:HG3	2.55	0.42
7:G:79:ILE:HD13	7:G:79:ILE:HA	1.88	0.41
5:E:34:LYS:HD2	5:E:34:LYS:HA	1.90	0.41
3:C:93:ILE:H	3:C:93:ILE:HG13	1.66	0.41
4:D:236:ALA:HB3	4:D:242:ARG:HE	1.84	0.41
4:D:293:THR:C	4:D:295:ASP:H	2.28	0.41
4:D:298:SER:HB3	4:D:301:ASP:HB2	2.01	0.41
5:E:129:ARG:HA	5:E:129:ARG:HD3	1.77	0.41
8:H:57:TRP:HZ3	8:H:71:LEU:HB3	1.84	0.41
2:B:323:ILE:HG23	2:B:327:GLU:OE1	2.21	0.41
6:F:109:GLU:HA	6:F:112:PHE:HD2	1.84	0.41
8:H:200:LEU:O	8:H:204:VAL:HG23	2.21	0.41
1:A:441:LEU:O	1:A:445:GLU:HG3	2.19	0.41
6:F:272:THR:O	6:F:276:LYS:HG3	2.20	0.41
4:D:370:TRP:HB2	6:F:270:LEU:HD23	2.03	0.41
7:G:111:ILE:HD12	7:G:152:LEU:HD23	2.03	0.41
7:G:122:MET:CE	7:G:127:GLU:HB3	2.50	0.41
3:C:271:ASN:HB3	3:C:274:GLU:HB2	2.03	0.41
4:D:227:LYS:HB2	4:D:258:LEU:HD22	2.02	0.41
1:A:409:LEU:HD23	1:A:409:LEU:HA	1.92	0.41
1:A:444:LYS:HE2	1:A:444:LYS:HB3	1.84	0.41
4:D:302:ARG:O	4:D:306:GLU:HG3	2.21	0.41
1:A:456:ARG:HD3	3:C:244:TYR:CE1	2.55	0.41
2:B:307:GLU:CD	2:B:307:GLU:H	2.29	0.40
3:C:293:GLY:O	3:C:297:GLN:HG3	2.21	0.40
6:F:134:SER:O	6:F:138:VAL:HG23	2.21	0.40
4:D:388:ILE:HG12	6:F:256:ILE:HD13	2.02	0.40
5:E:147:LEU:HD22	5:E:151:ASP:HB3	2.02	0.40
6:F:239:LEU:HB2	7:G:174:LEU:HB3	2.03	0.40
7:G:69:LEU:HD21	7:G:78:TYR:HB2	2.02	0.40
2:B:251:PHE:CE1	2:B:286:LEU:HD13	2.57	0.40
4:D:209:ASN:HB2	4:D:245:MET:HE1	2.02	0.40
4:D:378:CYS:HB2	5:E:247:VAL:HG13	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	222/491 (45%)	216 (97%)	6 (3%)	0	100	100
2	B	191/443 (43%)	179 (94%)	12 (6%)	0	100	100
3	C	402/423 (95%)	383 (95%)	15 (4%)	4 (1%)	13	46
4	D	223/406 (55%)	203 (91%)	19 (8%)	1 (0%)	30	66
5	E	287/334 (86%)	277 (96%)	9 (3%)	1 (0%)	37	70
6	F	267/327 (82%)	258 (97%)	9 (3%)	0	100	100
7	G	211/264 (80%)	210 (100%)	1 (0%)	0	100	100
8	H	169/209 (81%)	164 (97%)	5 (3%)	0	100	100
All	All	1972/2897 (68%)	1890 (96%)	76 (4%)	6 (0%)	38	70

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	74	PHE
3	C	175	ALA
5	E	197	ASP
3	C	72	PRO
4	D	219	GLU
3	C	69	PRO

### 5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	192/429 (45%)	187 (97%)	5 (3%)	41	72
2	B	177/405 (44%)	175 (99%)	2 (1%)	70	87
3	C	361/377 (96%)	347 (96%)	14 (4%)	27	61
4	D	190/347 (55%)	182 (96%)	8 (4%)	25	59
5	E	252/283 (89%)	244 (97%)	8 (3%)	34	67
6	F	244/276 (88%)	233 (96%)	11 (4%)	23	57
7	G	185/229 (81%)	180 (97%)	5 (3%)	40	71
8	H	144/173 (83%)	142 (99%)	2 (1%)	62	83
All	All	1745/2519 (69%)	1690 (97%)	55 (3%)	36	67

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	295	LEU
1	A	343	LYS
1	A	356	MET
1	A	417	VAL
1	A	467	LYS
2	B	323	ILE
2	B	325	GLU
3	C	38	ASN
3	C	51	VAL
3	C	54	HIS
3	C	68	MET
3	C	71	VAL
3	C	74	PHE
3	C	171	LYS
3	C	210	THR
3	C	220	MET
3	C	248	ILE
3	C	278	LEU
3	C	285	THR
3	C	355	ASP
3	C	358	VAL
4	D	211	LEU
4	D	224	GLU
4	D	231	HIS
4	D	267	MET
4	D	309	LEU
4	D	358	ILE

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Mol	Chain	Res	Type
4	D	365	GLU
4	D	376	SER
5	E	63	LEU
5	E	88	GLU
5	E	139	SER
5	E	168	VAL
5	E	227	SER
5	E	241	LEU
5	E	257	THR
5	E	320	ASN
6	F	58	MET
6	F	66	VAL
6	F	84	MET
6	F	110	GLU
6	F	152	LEU
6	F	216	THR
6	F	222	ILE
6	F	237	LEU
6	F	249	GLU
6	F	250	VAL
6	F	253	ASN
7	G	40	VAL
7	G	147	GLN
7	G	154	VAL
7	G	207	GLN
7	G	216	ILE
8	H	101	THR
8	H	127	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	288	ASN
1	A	463	GLN
2	B	297	GLN
2	B	313	ASN
2	B	333	ASN
2	B	336	ASN
2	B	435	ASN
3	C	327	GLN
3	C	353	GLN
3	C	369	ASN

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Mol	Chain	Res	Type
4	D	231	HIS
4	D	240	GLN
4	D	241	GLN
4	D	288	HIS
4	D	398	GLN
5	E	36	GLN
5	E	49	HIS
5	E	132	ASN
5	E	159	GLN
5	E	182	ASN
5	E	318	GLN
5	E	320	ASN
6	F	50	ASN
6	F	114	GLN
6	F	220	HIS
7	G	33	GLN
7	G	191	GLN
7	G	196	ASN
7	G	203	ASN
8	H	51	ASN
8	H	196	GLN
8	H	209	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

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

Of 2 ligands modelled in this entry, 1 is 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
10	A1CH3	E	402	9	23,28,28	1.12	1 (4%)	29,39,39	1.41	4 (13%)

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
10	A1CH3	E	402	9	-	4/10/24/24	0/3/4/4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	E	402	A1CH3	C10-C14	4.01	1.53	1.44

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	E	402	A1CH3	N4-C3-N2	-5.27	104.43	112.26
10	E	402	A1CH3	C5-N4-C3	2.20	109.20	105.72
10	E	402	A1CH3	C21-C1-C5	2.18	133.14	127.46
10	E	402	A1CH3	C11-C12-C7	2.05	120.45	118.92

There are no chirality outliers.

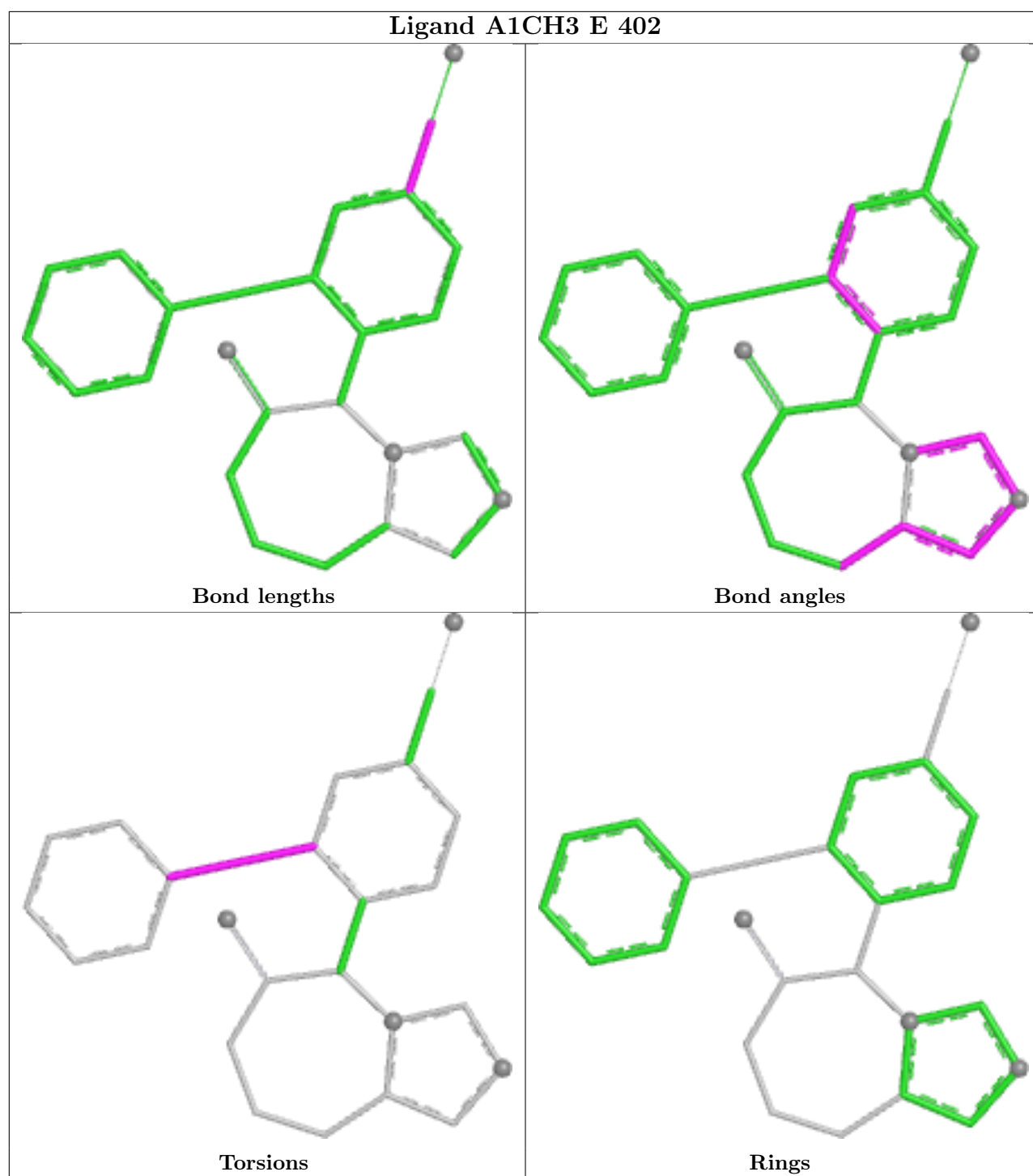
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	E	402	A1CH3	C7-C12-C13-C16
10	E	402	A1CH3	C7-C12-C13-C20
10	E	402	A1CH3	C11-C12-C13-C16
10	E	402	A1CH3	C11-C12-C13-C20

There are no ring outliers.

No monomer is involved in short contacts.

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



## 5.7 Other polymers [i](#)

There are no such residues in this entry.



## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

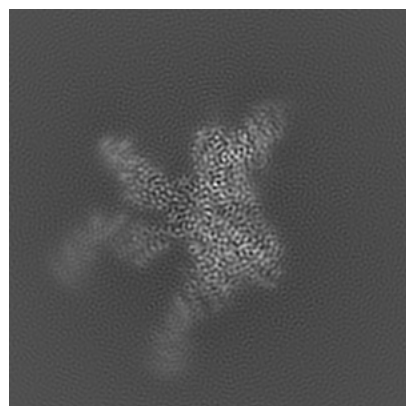
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-71639. These allow visual inspection of the internal detail of the map and identification of artifacts.

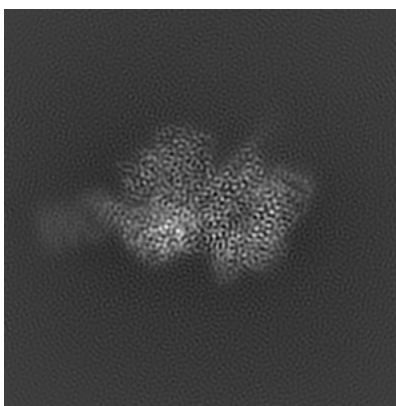
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

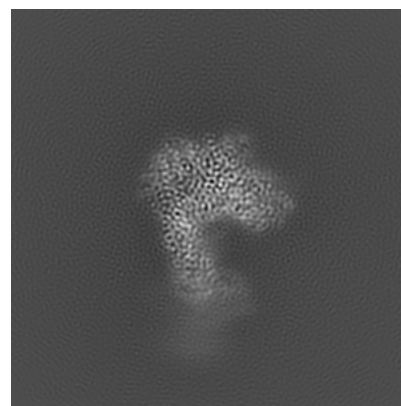
#### 6.1.1 Primary map



X

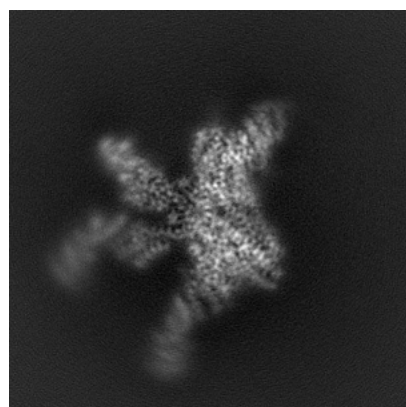


Y

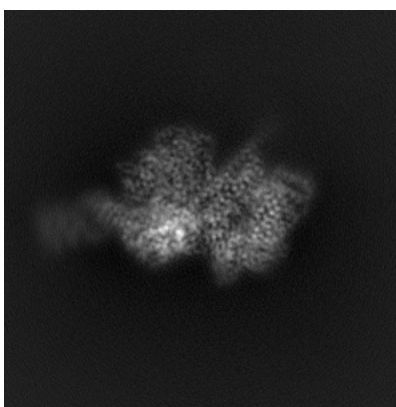


Z

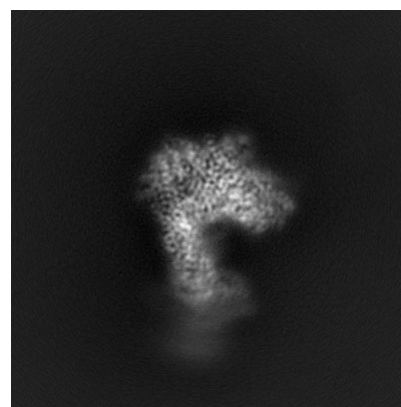
#### 6.1.2 Raw map



X



Y

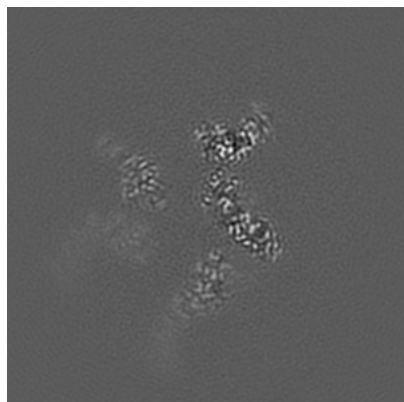


Z

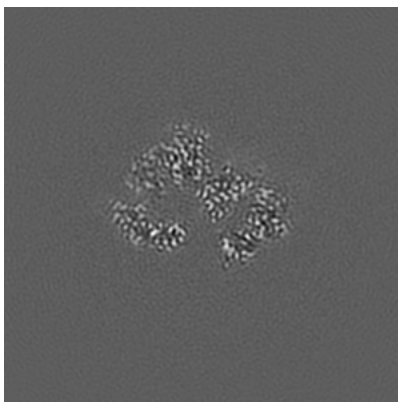
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

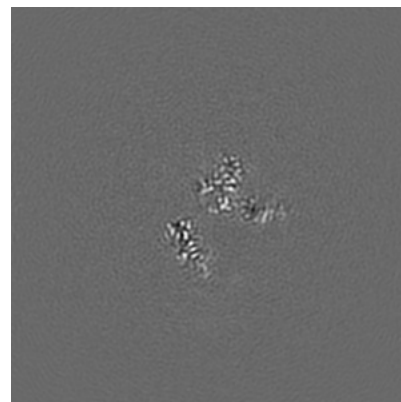
### 6.2.1 Primary map



X Index: 160

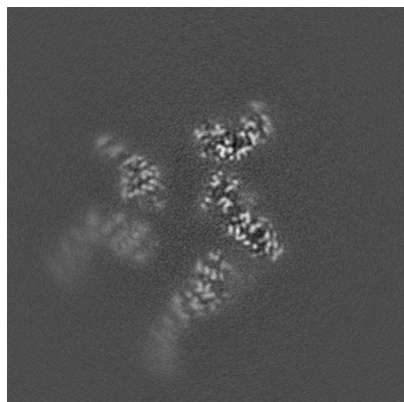


Y Index: 160

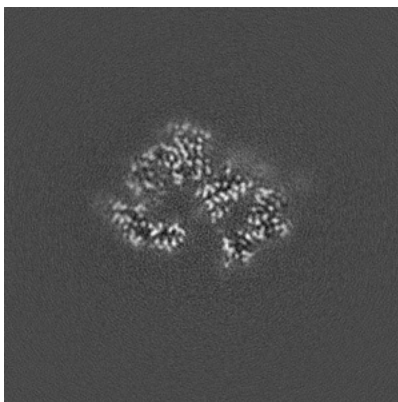


Z Index: 160

### 6.2.2 Raw map



X Index: 160



Y Index: 160

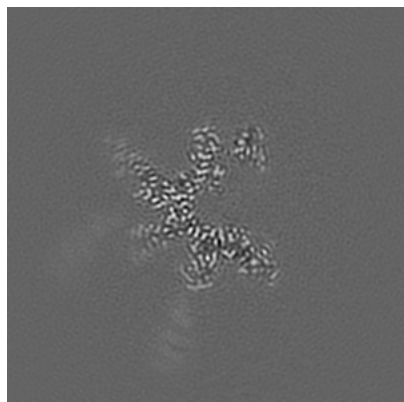


Z Index: 160

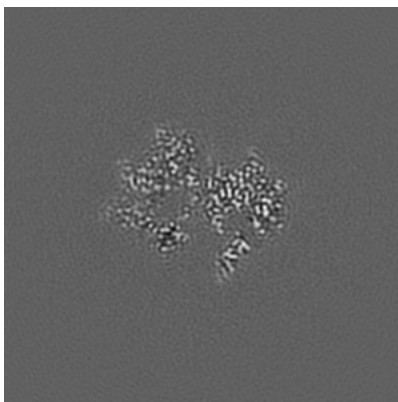
The images above show central slices of the map in three orthogonal directions.

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

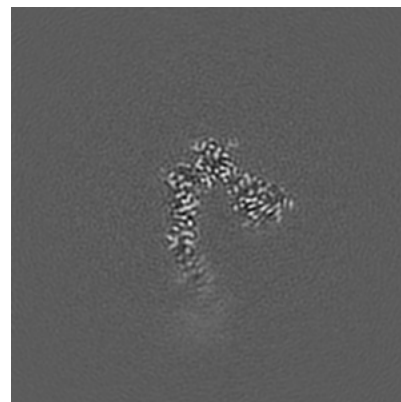
### 6.3.1 Primary map



X Index: 138

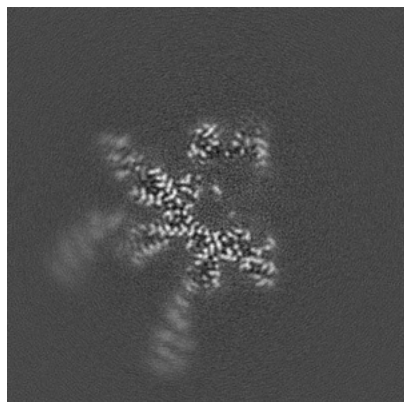


Y Index: 170

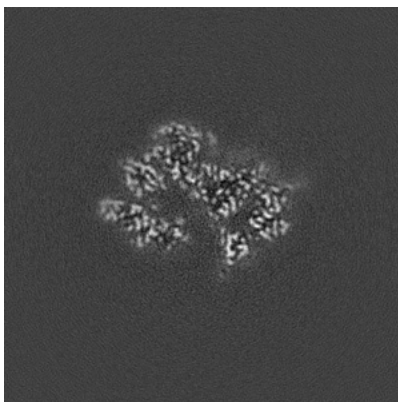


Z Index: 138

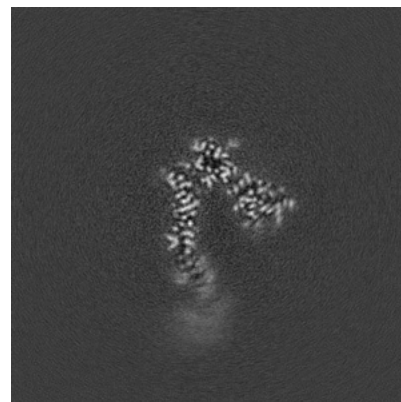
### 6.3.2 Raw map



X Index: 142



Y Index: 165



Z Index: 138

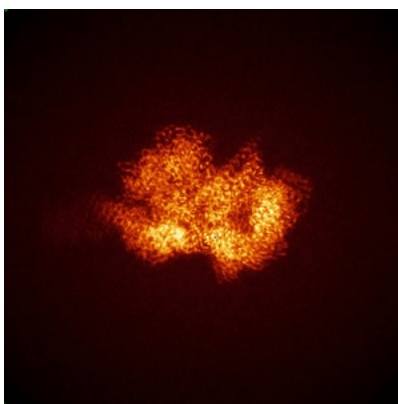
The images above show the largest variance slices of the map in three orthogonal directions.

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

### 6.4.1 Primary map



X

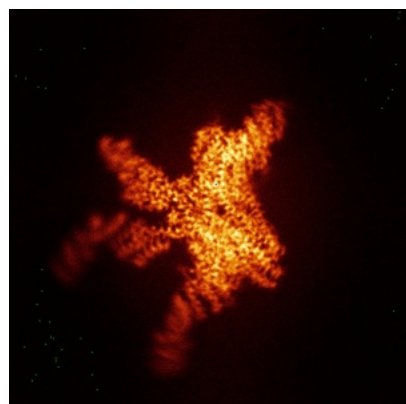


Y

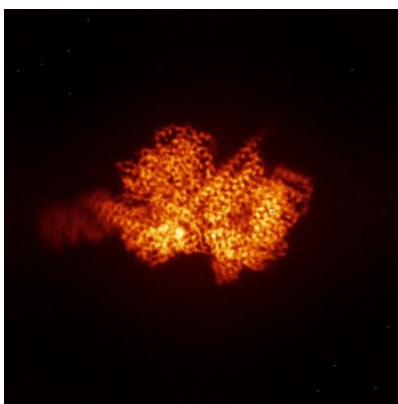


Z

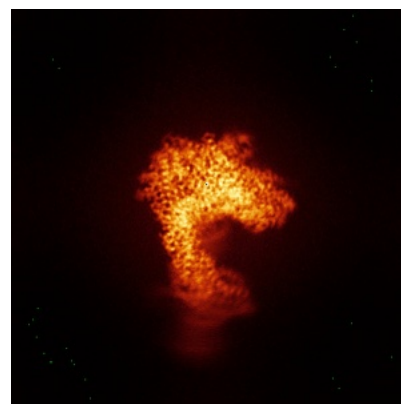
### 6.4.2 Raw map



X



Y



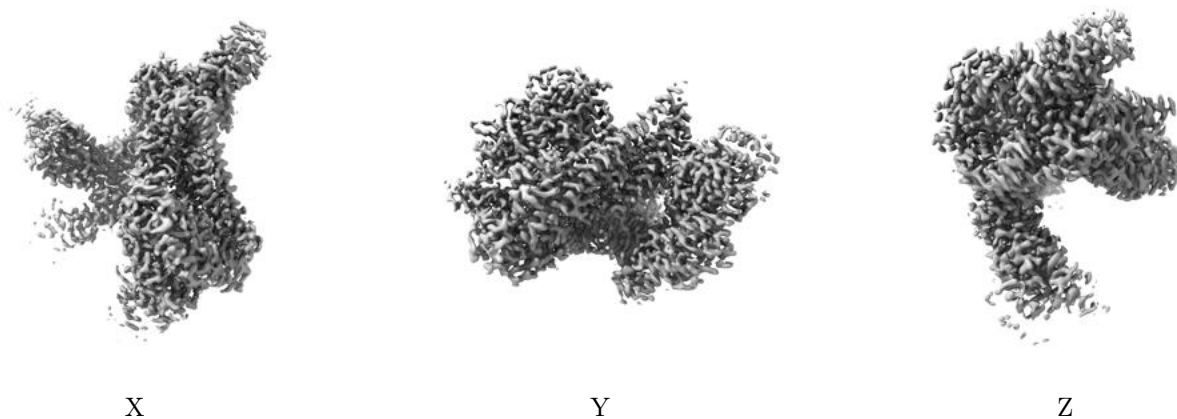
Z

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.



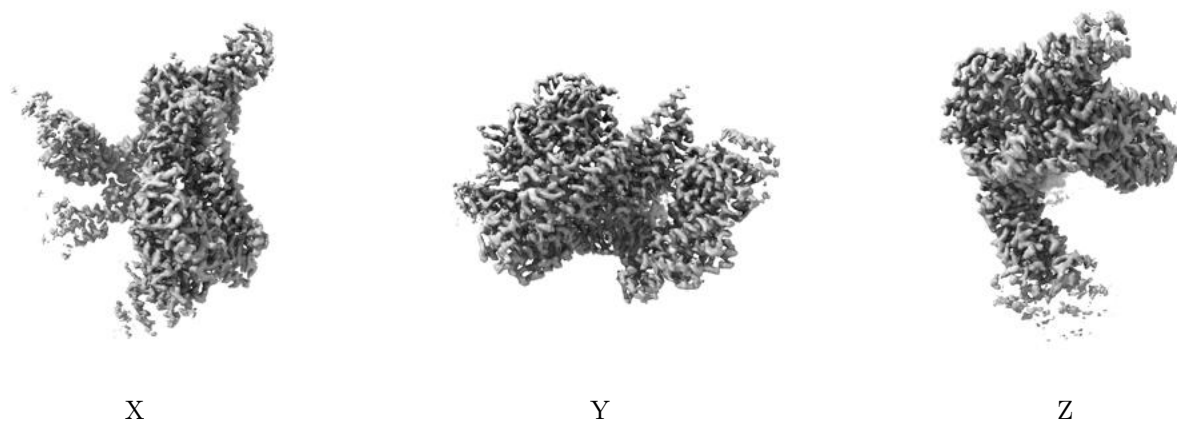
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.308. 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.

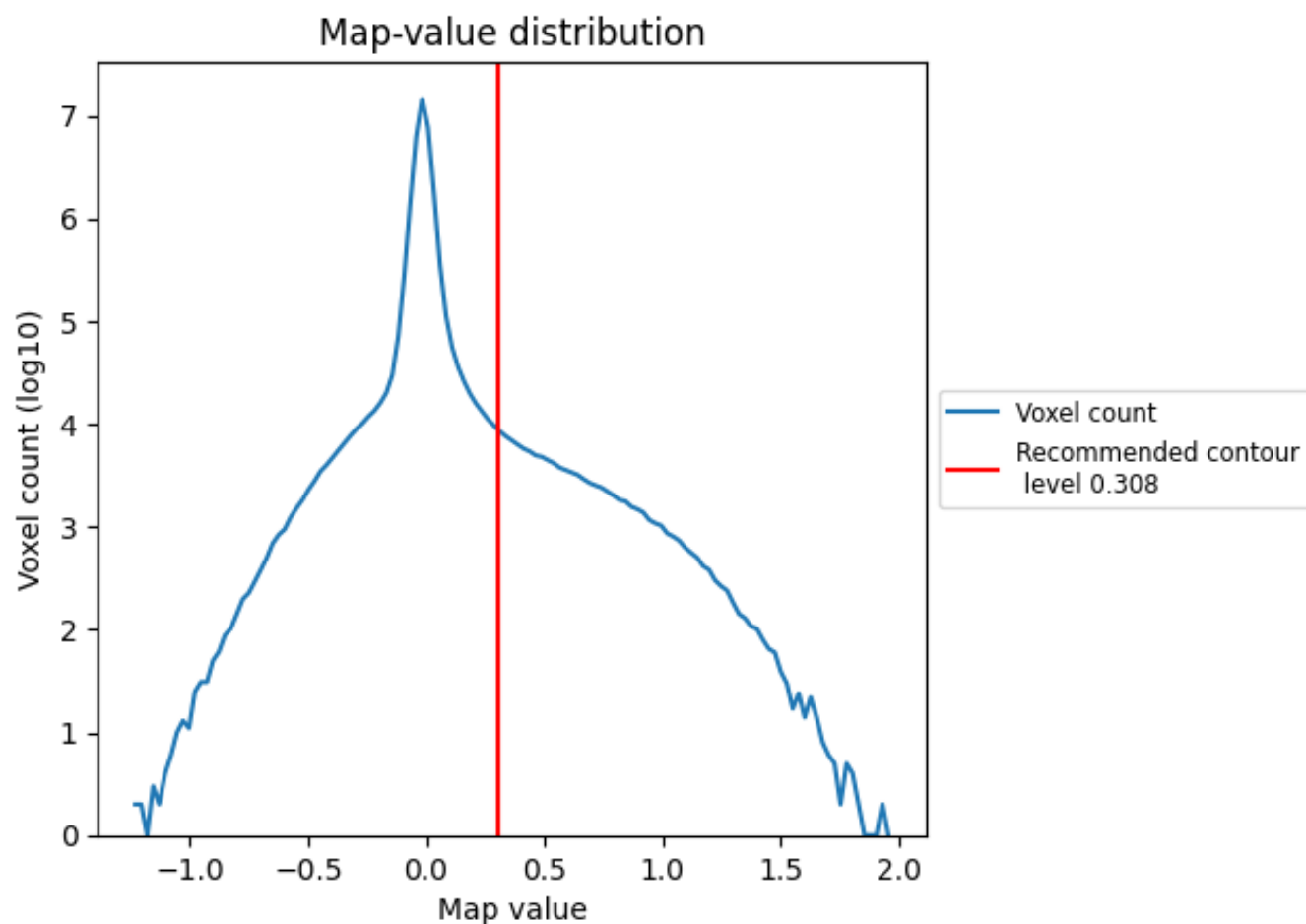
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

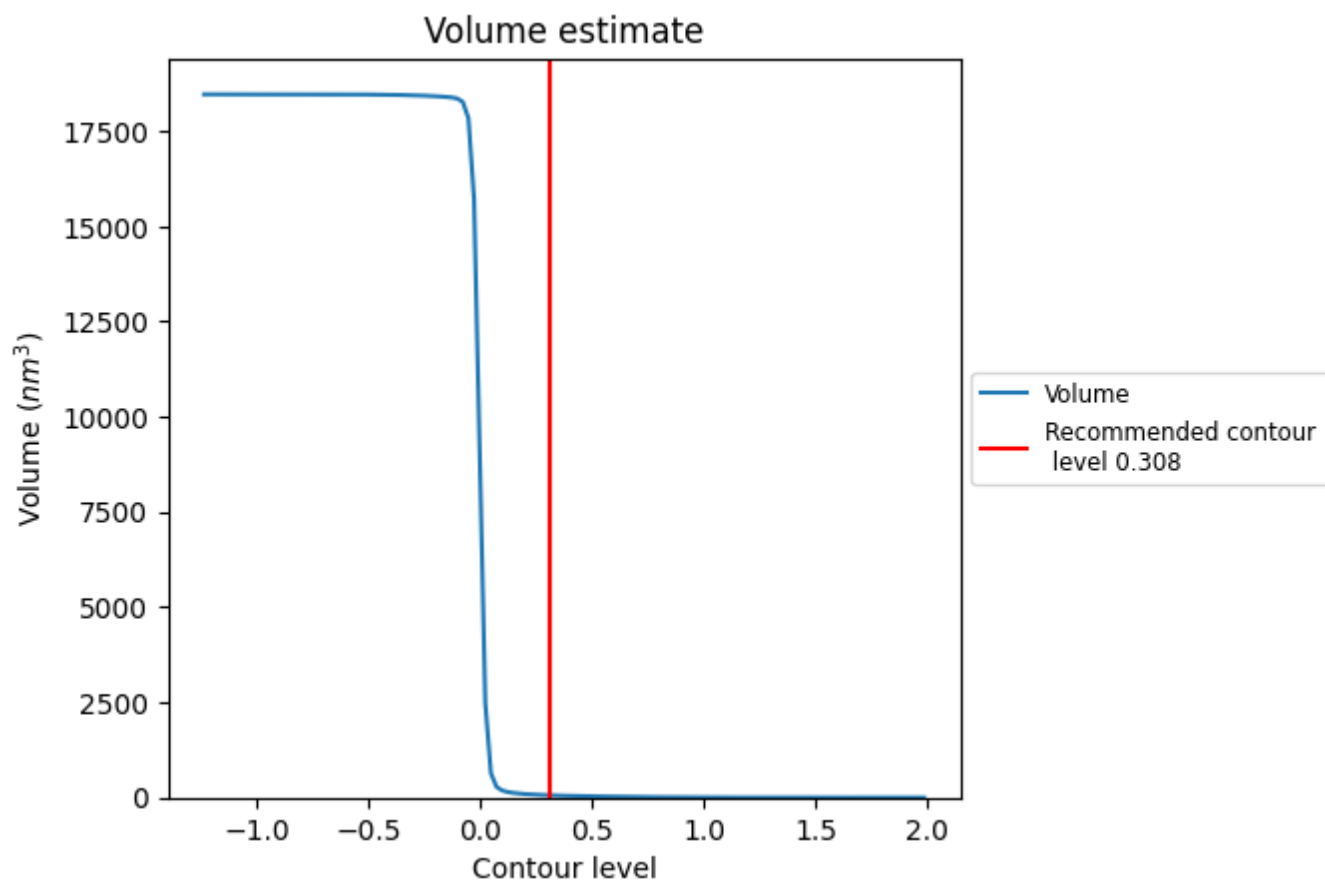
This section contains the results of statistical analysis of the map.

### 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](#)

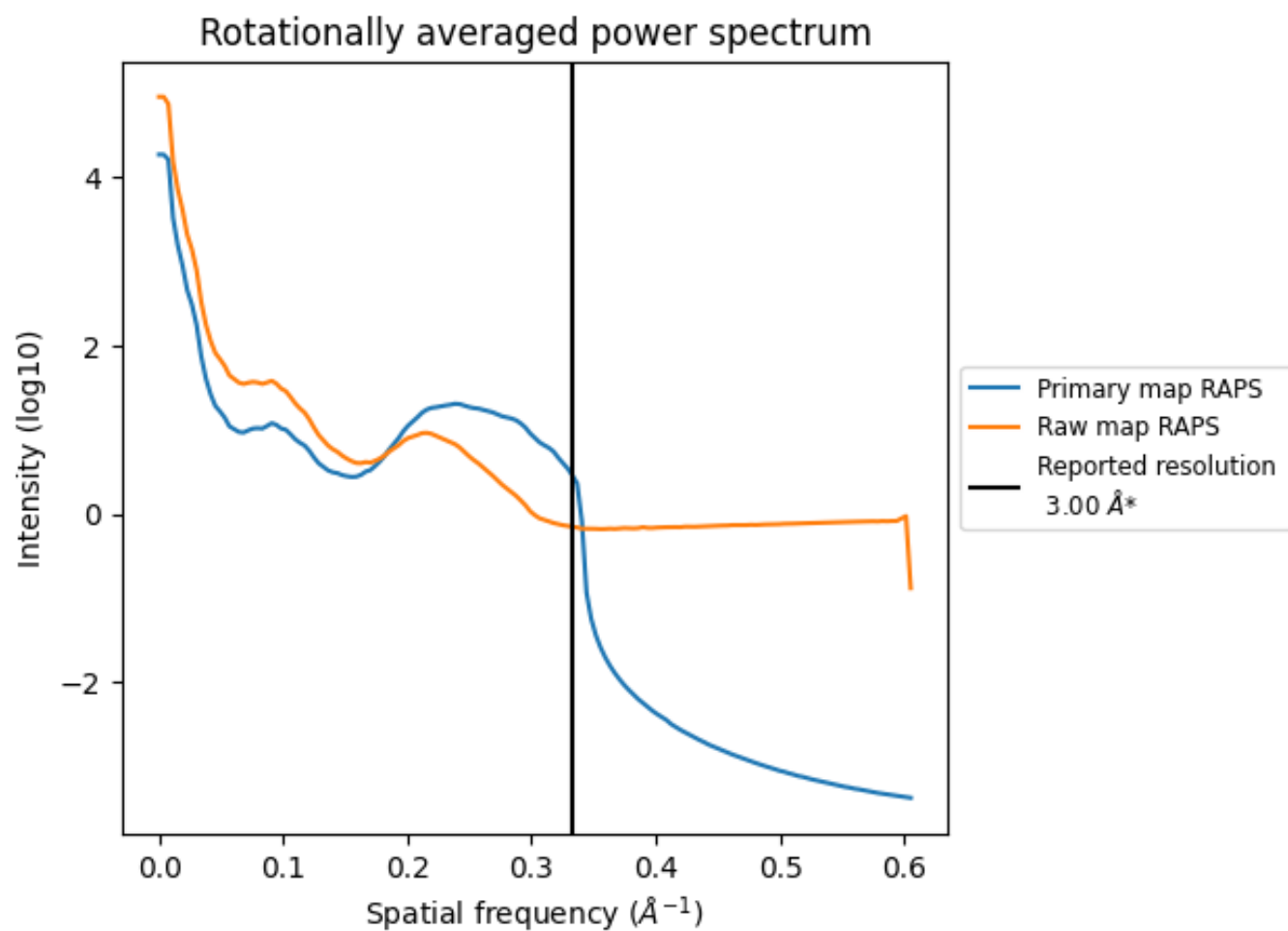


The volume at the recommended contour level is 60  $\text{nm}^3$ ; this corresponds to an approximate mass of 55 kDa.

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 ⓘ

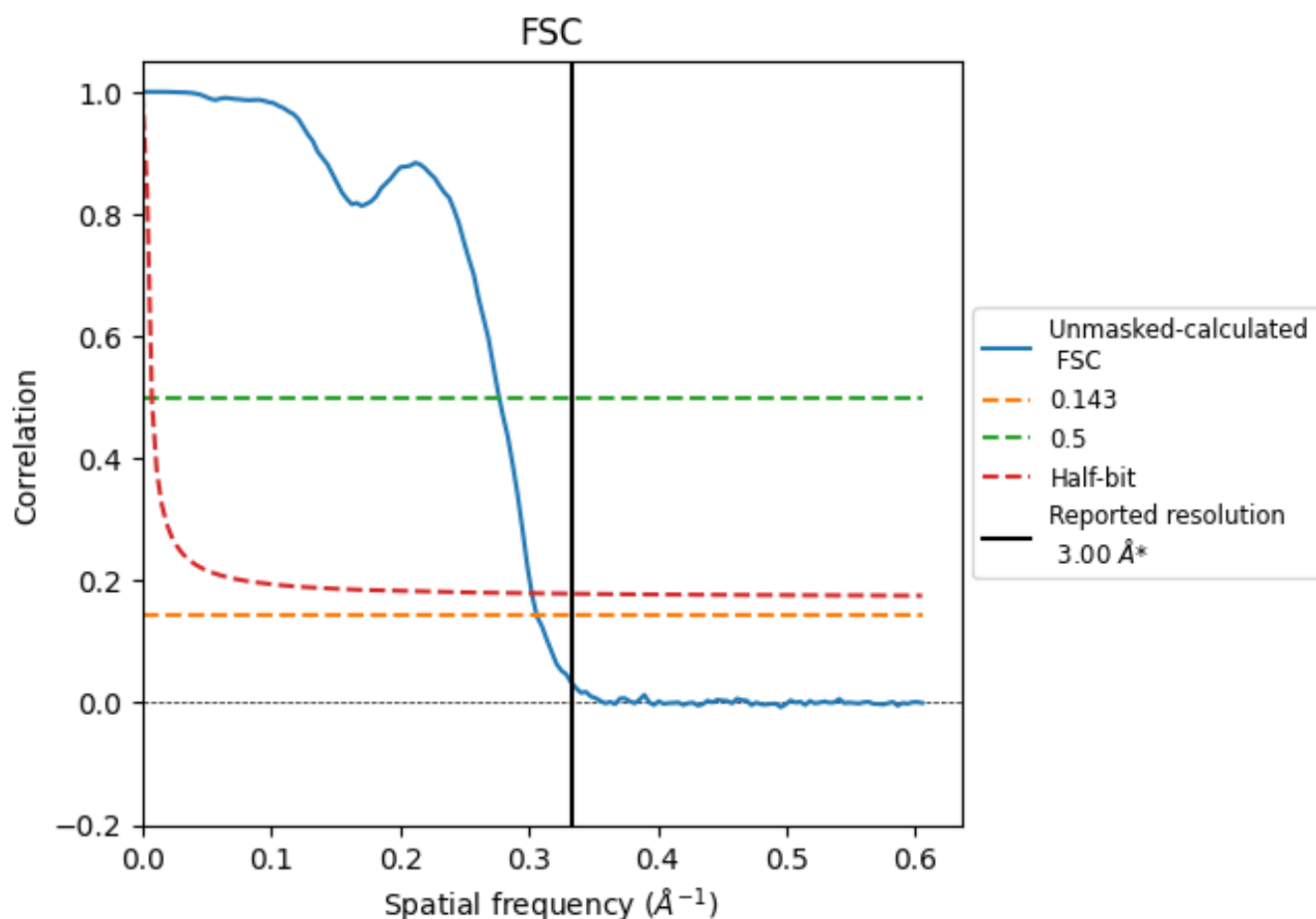


\*Reported resolution corresponds to spatial frequency of 0.333 Å<sup>-1</sup>

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

## 8.2 Resolution estimates [i](#)

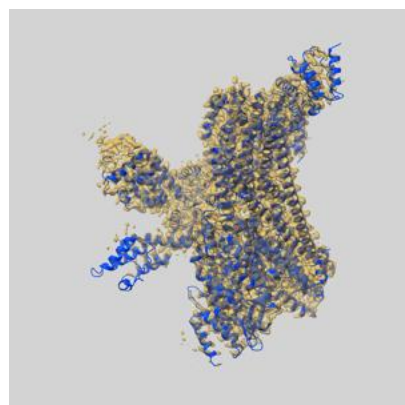
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.27	3.61	3.31

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

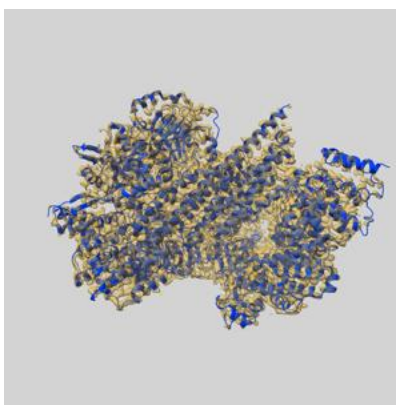
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-71639 and PDB model 9PH4. Per-residue inclusion information can be found in section [3](#) on page [6](#).

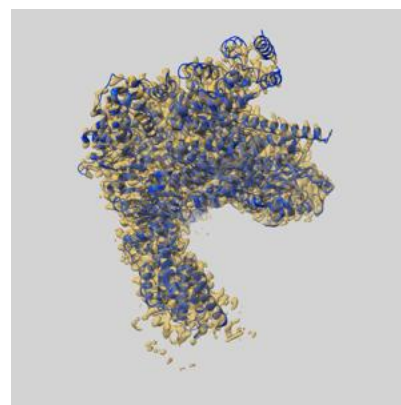
### 9.1 Map-model overlay [i](#)



X



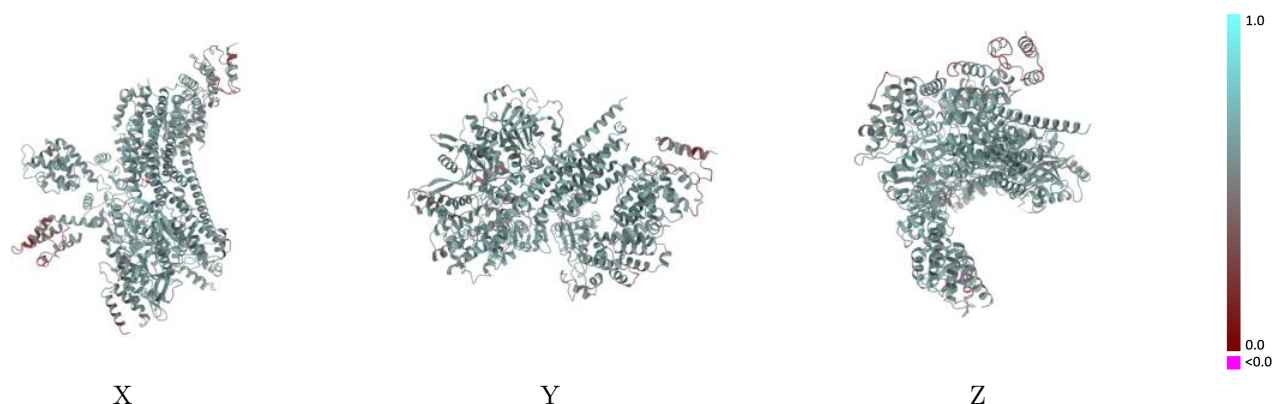
Y



Z

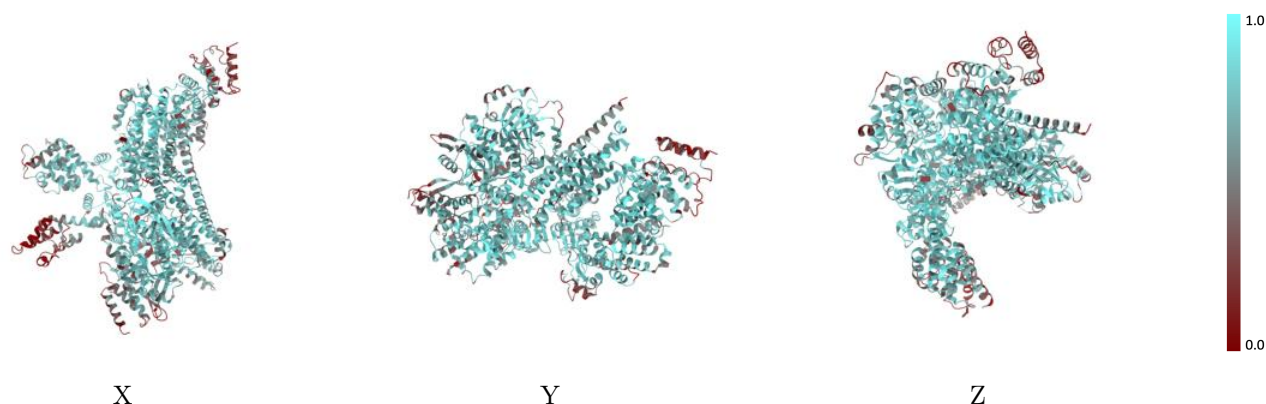
The images above show the 3D surface view of the map at the recommended contour level 0.308 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



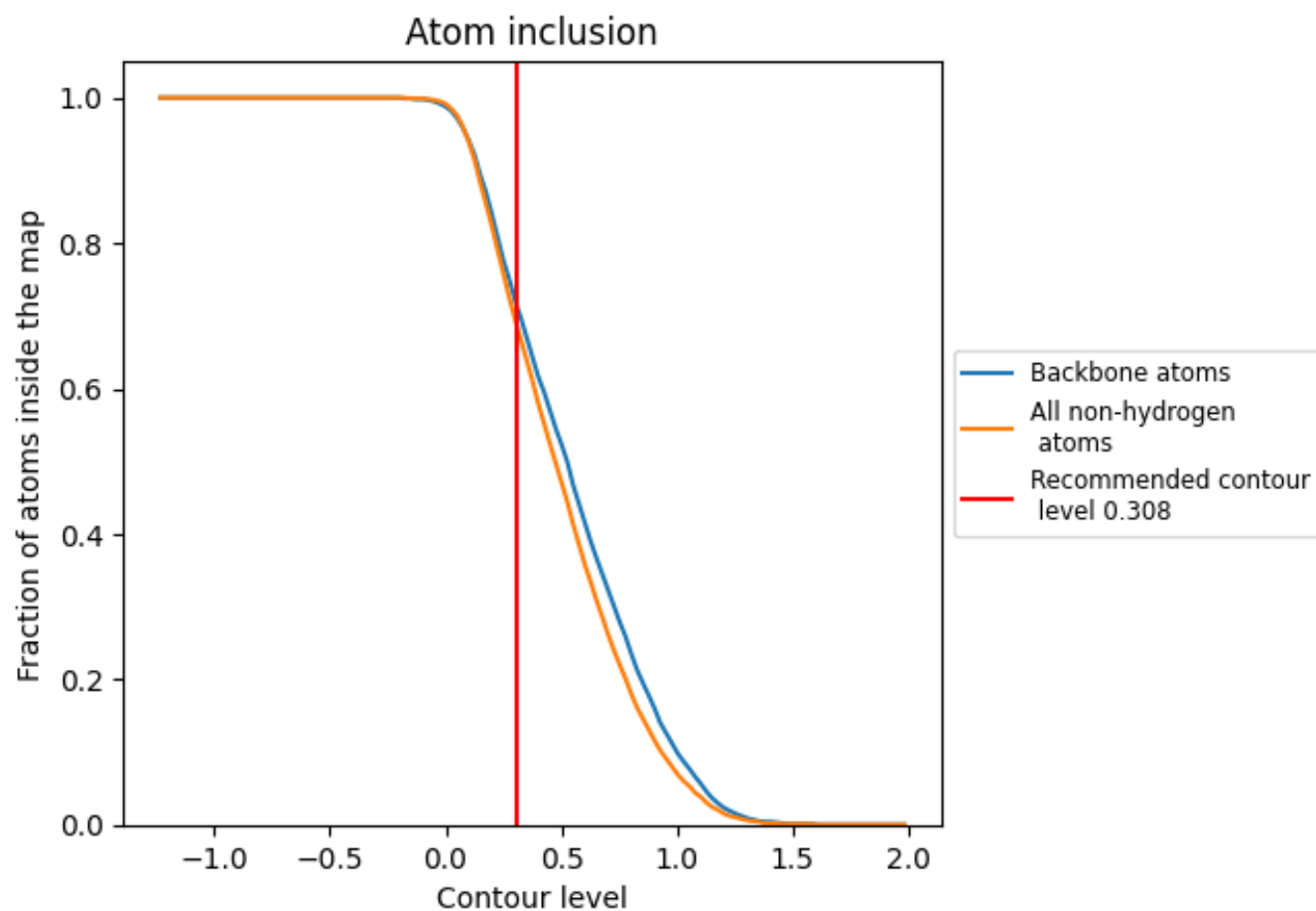
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.308).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 71% of all backbone atoms, 69% 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 (0.308) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.6860	<div><div></div></div> 0.5660
A	<div><div></div></div> 0.7520	<div><div></div></div> 0.5860
B	<div><div></div></div> 0.4600	<div><div></div></div> 0.4870
C	<div><div></div></div> 0.7050	<div><div></div></div> 0.5630
D	<div><div></div></div> 0.6490	<div><div></div></div> 0.5510
E	<div><div></div></div> 0.7480	<div><div></div></div> 0.5910
F	<div><div></div></div> 0.7280	<div><div></div></div> 0.5930
G	<div><div></div></div> 0.7140	<div><div></div></div> 0.5850
H	<div><div></div></div> 0.6520	<div><div></div></div> 0.5490

1.0

0.0

<0.0