



## Full wwPDB EM Validation Report ⓘ

Nov 13, 2025 – 12:08 PM EST

PDB ID : 9OTY / pdb\_00009oty  
EMDB ID : EMD-70862  
Title : DDB1-CRBN with CK1 alpha, SB-405483, and DEG-47: composite map and model submission  
Authors : Rizvi, Z.; Lander, G.C.  
Deposited on : 2025-05-27  
Resolution : 3.00 Å (reported)  
Based on initial models : 5fqd, .

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

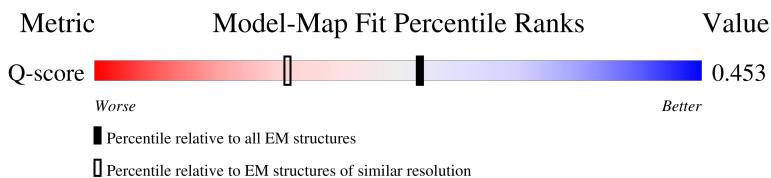
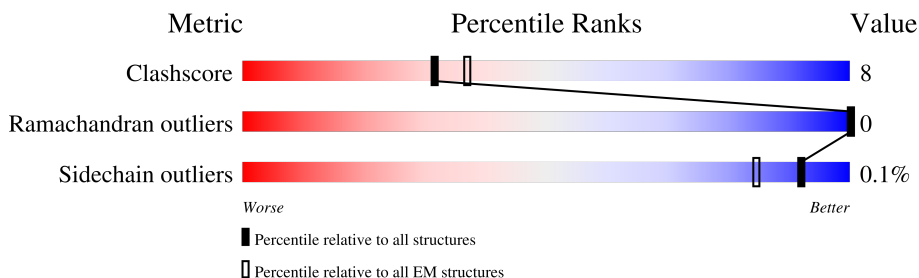
# 1 Overall quality at a glance

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	830	
2	B	382	
3	C	294	

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11542 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 DNA damage-binding protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	802	Total	C	N	O	S	0	0
			6326	4017	1067	1207	35		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1141	TRP	-	expression tag	UNP Q16531
A	1142	SER	-	expression tag	UNP Q16531
A	1143	HIS	-	expression tag	UNP Q16531
A	1144	PRO	-	expression tag	UNP Q16531
A	1145	GLN	-	expression tag	UNP Q16531
A	1146	PHE	-	expression tag	UNP Q16531
A	1147	GLU	-	expression tag	UNP Q16531
A	1148	LYS	-	expression tag	UNP Q16531

- Molecule 2 is a protein called Protein cereblon.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	375	Total	C	N	O	S	0	0
			3026	1934	517	552	23		

- Molecule 3 is a protein called Casein kinase I isoform alpha.

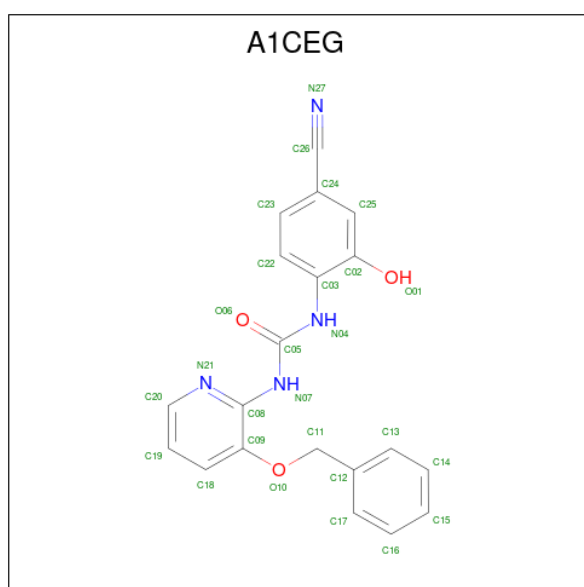
Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	261	Total	C	N	O	S	0	0
			2135	1376	370	376	13		

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
4	B	1	Total	Zn	0
			1	1	

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- Molecule 6 is N-[3-(benzyloxy)pyridin-2-yl]-N'-(4-cyano-2-hydroxyphenyl)urea (CCD ID: A1CEG) (formula:  $C_{20}H_{16}N_4O_3$ ) (labeled as "Ligand of Interest" by depositor).

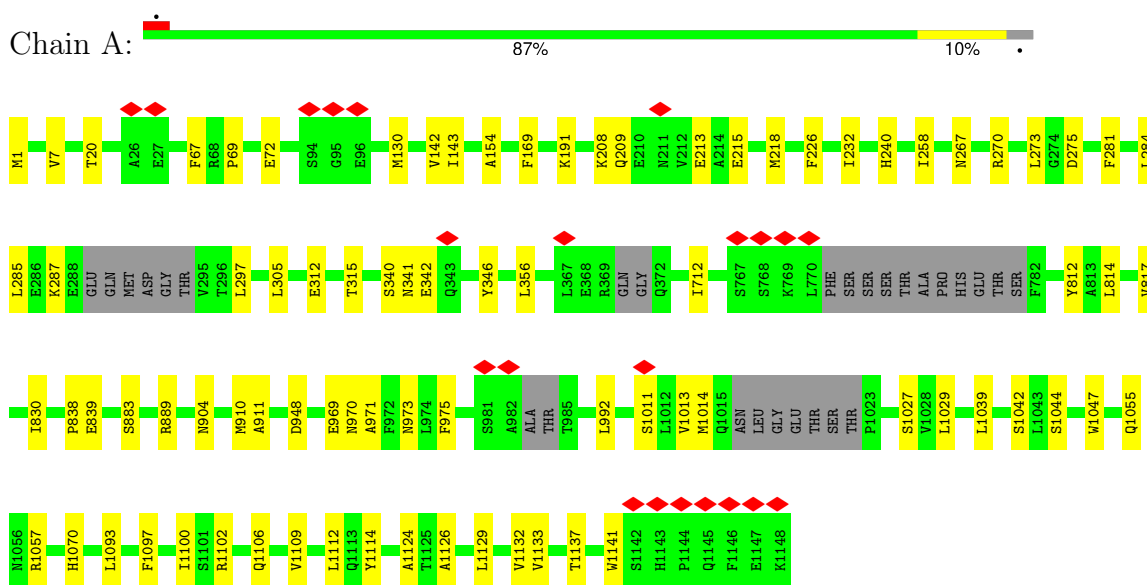


Mol	Chain	Residues	Atoms				AltConf
6	B	1	Total	C	N	O	0
			27	20	4	3	

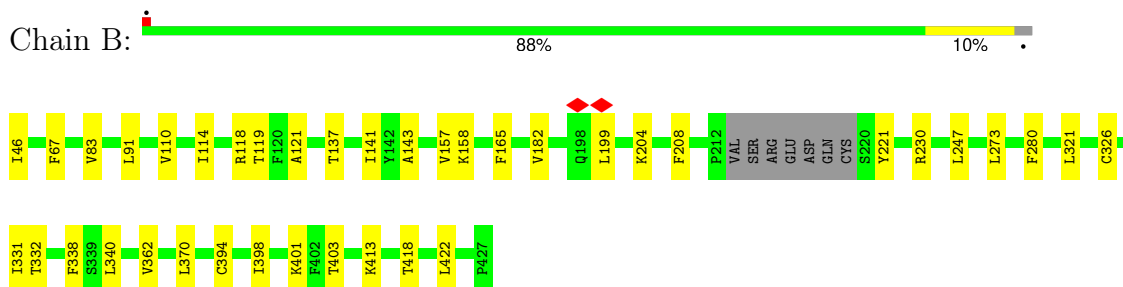
### 3 Residue-property plots

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.

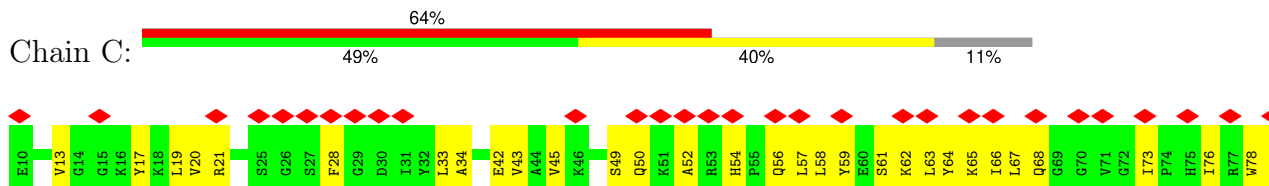
#### • Molecule 1: DNA damage-binding protein 1



#### • Molecule 2: Protein cereblon



#### • Molecule 3: Casein kinase I isoform alpha





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	328293	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1200	Depositor
Magnification	189189	Depositor
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	0.495	Depositor
Minimum map value	-0.129	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.0346	Depositor
Map size ( $\text{\AA}$ )	222.0, 222.0, 222.0	wwPDB
Map dimensions	300, 300, 300	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, A1CEG, A1CEH

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	0/6439	0.31	0/8701
2	B	0.15	0/3099	0.35	0/4204
3	C	0.26	0/2176	0.68	0/2916
All	All	0.17	0/11714	0.41	0/15821

There are no bond length outliers.

There are no bond angle outliers.

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	6326	0	6304	57	0
2	B	3026	0	3024	23	0
3	C	2135	0	2143	120	0
4	B	1	0	0	0	0
5	B	27	0	0	0	0
6	B	27	0	0	0	0
All	All	11542	0	11471	195	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (195) 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:201:ARG:HB3	3:C:266:LEU:HB2	1.48	0.95
3:C:123:ARG:HH21	3:C:153:LEU:HB3	1.40	0.86
3:C:93:LEU:HD13	3:C:156:ILE:HD13	1.59	0.85
3:C:65:LYS:O	3:C:68:GLN:HG3	1.76	0.84
3:C:256:PHE:HA	3:C:259:TYR:HD2	1.41	0.83
1:A:1057:ARG:HH12	1:A:1112:LEU:HB2	1.45	0.81
1:A:342:GLU:H	1:A:346:TYR:HE2	1.28	0.81
3:C:61:SER:HB3	3:C:88:LEU:HD21	1.64	0.79
3:C:123:ARG:NH2	3:C:153:LEU:HB3	2.02	0.75
1:A:1057:ARG:NH1	1:A:1112:LEU:HB2	2.02	0.74
3:C:124:ILE:HD12	3:C:207:LEU:HD11	1.69	0.74
3:C:229:LYS:HA	3:C:232:LYS:HG2	1.70	0.73
3:C:63:LEU:HD13	3:C:161:ALA:HB3	1.70	0.72
3:C:121:ILE:HG22	3:C:278:ARG:NE	2.05	0.70
3:C:259:TYR:HE1	3:C:280:LEU:HD13	1.56	0.70
1:A:1011:SER:HA	1:A:1027:SER:HB3	1.72	0.70
3:C:274:TYR:HB2	3:C:278:ARG:HH12	1.54	0.70
3:C:45:VAL:HG22	3:C:89:VAL:HG22	1.75	0.69
3:C:245:VAL:HG12	3:C:257:ALA:HB1	1.76	0.67
3:C:199:SER:H	3:C:202:ASP:HB2	1.59	0.67
3:C:97:LEU:HG	3:C:101:PHE:CE2	2.29	0.67
3:C:263:CYS:SG	3:C:277:LEU:HD13	2.34	0.67
1:A:1109:VAL:HG12	1:A:1129:LEU:HD12	1.75	0.66
3:C:50:GLN:HE21	3:C:81:GLN:NE2	1.94	0.66
3:C:20:VAL:HG13	3:C:21:ARG:HG2	1.80	0.63
3:C:123:ARG:HH12	3:C:142:PHE:HD1	1.47	0.62
3:C:43:VAL:HG11	3:C:89:VAL:HG13	1.82	0.62
3:C:67:LEU:HD13	3:C:73:ILE:HB	1.80	0.62
3:C:179:LYS:H	3:C:195:GLY:HA2	1.63	0.61
1:A:69:PRO:HG2	1:A:72:GLU:HG3	1.81	0.61
3:C:97:LEU:HG	3:C:101:PHE:HE2	1.66	0.61
3:C:256:PHE:HA	3:C:259:TYR:CD2	2.31	0.61
1:A:1114:TYR:HB2	1:A:1124:ALA:HB2	1.82	0.60
3:C:50:GLN:HE21	3:C:81:GLN:HE21	1.46	0.60
1:A:1014:MET:HB3	1:A:1141:TRP:HD1	1.67	0.59
1:A:1055:GLN:HG3	1:A:1093:LEU:HD23	1.85	0.58
3:C:278:ARG:O	3:C:282:ARG:HG2	2.03	0.58
3:C:124:ILE:HG12	3:C:134:HIS:CE1	2.39	0.57
1:A:1:MET:HG2	1:A:1042:SER:HB3	1.86	0.57
3:C:156:ILE:HG22	3:C:157:ASP:H	1.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:338:PHE:HE2	2:B:340:LEU:HD13	1.70	0.57
3:C:125:GLU:HG3	3:C:278:ARG:NE	2.19	0.57
3:C:56:GLN:HA	3:C:59:TYR:HD2	1.69	0.56
2:B:403:THR:HG22	2:B:413:LYS:HG3	1.87	0.56
1:A:969:GLU:HB2	1:A:973:ASN:HB2	1.88	0.55
3:C:232:LYS:O	3:C:236:ILE:HD12	2.06	0.55
3:C:121:ILE:HG22	3:C:278:ARG:HE	1.71	0.55
3:C:139:PRO:HA	3:C:142:PHE:CD2	2.41	0.55
3:C:274:TYR:HB2	3:C:278:ARG:NH1	2.20	0.55
1:A:191:LYS:HG3	1:A:208:LYS:HD3	1.88	0.55
3:C:116:LEU:HD22	3:C:153:LEU:HD21	1.89	0.55
2:B:321:LEU:HD13	2:B:422:LEU:HD13	1.89	0.54
3:C:273:ASP:HA	3:C:276:TYR:CD2	2.42	0.54
2:B:46:ILE:HD11	2:B:338:PHE:HD2	1.71	0.54
2:B:67:PHE:CD1	2:B:118:ARG:NH1	2.76	0.54
1:A:218:MET:HB2	1:A:232:ILE:HB	1.90	0.54
1:A:20:THR:HG23	1:A:315:THR:HG21	1.90	0.54
3:C:274:TYR:HD2	3:C:278:ARG:NH1	2.06	0.54
1:A:130:MET:HE2	1:A:169:PHE:HZ	1.73	0.53
3:C:116:LEU:HG	3:C:296:PHE:CE1	2.44	0.53
3:C:139:PRO:HA	3:C:142:PHE:CE2	2.44	0.53
3:C:57:LEU:HG	3:C:88:LEU:HG	1.90	0.53
2:B:143:ALA:HB3	2:B:158:LYS:HB2	1.89	0.53
2:B:331:ILE:HG22	2:B:332:THR:HG23	1.91	0.52
3:C:56:GLN:HA	3:C:59:TYR:CD2	2.44	0.52
3:C:117:ALA:O	3:C:121:ILE:HG13	2.09	0.52
1:A:948:ASP:HB2	1:A:992:LEU:HB2	1.92	0.52
1:A:213:GLU:HG2	1:A:215:GLU:H	1.75	0.52
1:A:342:GLU:HB2	1:A:346:TYR:OH	2.09	0.52
3:C:131:ASN:HA	3:C:170:ARG:HD3	1.92	0.52
3:C:125:GLU:HG3	3:C:278:ARG:CZ	2.40	0.51
1:A:270:ARG:HG2	1:A:284:LEU:HD23	1.92	0.51
3:C:266:LEU:HD21	3:C:273:ASP:HB3	1.92	0.51
1:A:838:PRO:HB2	2:B:221:TYR:OH	2.10	0.51
1:A:1055:GLN:HE21	1:A:1070:HIS:CE1	2.28	0.51
2:B:332:THR:HG21	2:B:362:VAL:HG21	1.93	0.51
3:C:99:ASP:O	3:C:103:PHE:HD2	1.93	0.51
3:C:124:ILE:HG23	3:C:134:HIS:HE1	1.76	0.51
3:C:127:VAL:HG13	3:C:132:PHE:CZ	2.47	0.50
3:C:208:GLY:O	3:C:212:MET:HG2	2.12	0.50
1:A:1112:LEU:HD23	1:A:1129:LEU:HD11	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:156:ILE:HG22	3:C:157:ASP:N	2.26	0.50
3:C:43:VAL:HG13	3:C:90:MET:O	2.11	0.50
3:C:121:ILE:CG2	3:C:278:ARG:HG2	2.42	0.49
3:C:255:GLU:O	3:C:258:MET:HG3	2.12	0.49
3:C:63:LEU:HD12	3:C:158:PHE:O	2.11	0.49
3:C:98:GLU:HB2	3:C:139:PRO:C	2.37	0.49
1:A:356:LEU:HD21	1:A:712:ILE:HD13	1.94	0.49
3:C:17:TYR:HB3	3:C:34:ALA:HB1	1.95	0.49
3:C:164:TYR:CD1	3:C:172:HIS:HA	2.48	0.49
3:C:202:ASP:O	3:C:205:GLU:HG3	2.13	0.49
2:B:326:CYS:SG	2:B:394:CYS:HB3	2.53	0.48
3:C:124:ILE:CD1	3:C:207:LEU:HD11	2.38	0.48
1:A:273:LEU:HB2	1:A:281:PHE:HB2	1.94	0.48
1:A:1055:GLN:HE21	1:A:1070:HIS:HE1	1.61	0.48
3:C:196:ILE:H	3:C:196:ILE:HD12	1.78	0.48
3:C:173:ILE:HD11	3:C:197:GLU:OE2	2.12	0.48
3:C:133:ILE:HD13	3:C:164:TYR:CE2	2.48	0.48
3:C:274:TYR:HA	3:C:277:LEU:HD12	1.96	0.48
1:A:218:MET:HG2	2:B:204:LYS:HE3	1.95	0.48
2:B:370:LEU:HD21	2:B:401:LYS:HD3	1.95	0.48
3:C:205:GLU:HB3	3:C:264:ARG:HG2	1.95	0.47
2:B:83:VAL:HG22	2:B:121:ALA:HB3	1.96	0.47
3:C:121:ILE:HG22	3:C:278:ARG:HG2	1.96	0.47
3:C:207:LEU:O	3:C:211:LEU:HG	2.14	0.47
3:C:61:SER:CB	3:C:88:LEU:HD21	2.41	0.47
3:C:58:LEU:HD11	3:C:62:LYS:HE3	1.95	0.47
2:B:208:PHE:CE1	2:B:230:ARG:HB3	2.49	0.47
3:C:13:VAL:HB	3:C:17:TYR:HB2	1.95	0.47
1:A:143:ILE:HG12	1:A:154:ALA:HB2	1.97	0.47
3:C:49:SER:HB3	3:C:52:ALA:HB2	1.97	0.47
3:C:79:TYR:CD1	3:C:88:LEU:HD23	2.49	0.47
3:C:96:SER:HA	3:C:143:LEU:HG	1.97	0.46
1:A:305:LEU:O	1:A:346:TYR:HA	2.16	0.46
3:C:123:ARG:HE	3:C:153:LEU:HB3	1.80	0.46
3:C:202:ASP:HA	3:C:205:GLU:HG2	1.98	0.46
1:A:226:PHE:CZ	1:A:287:LYS:HB3	2.51	0.46
3:C:256:PHE:O	3:C:260:LEU:HG	2.15	0.46
3:C:43:VAL:CG1	3:C:89:VAL:HG13	2.46	0.45
3:C:134:HIS:HE2	3:C:137:ILE:HD11	1.80	0.45
3:C:119:GLN:CB	3:C:153:LEU:HD12	2.46	0.45
3:C:123:ARG:CZ	3:C:153:LEU:HB3	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:148:ARG:HG3	3:C:149:HIS:CD2	2.52	0.45
1:A:1027:SER:OG	1:A:1039:LEU:HD11	2.16	0.45
3:C:130:LYS:HD3	3:C:130:LYS:HA	1.84	0.45
3:C:134:HIS:HD2	3:C:137:ILE:HG13	1.82	0.45
3:C:61:SER:O	3:C:65:LYS:HG3	2.17	0.45
1:A:270:ARG:HG2	1:A:284:LEU:CD2	2.46	0.45
3:C:62:LYS:O	3:C:66:ILE:HG23	2.17	0.45
1:A:209:GLN:OE1	1:A:240:HIS:CD2	2.70	0.45
1:A:910:MET:HE1	2:B:247:LEU:HD13	1.98	0.45
1:A:1102:ARG:O	1:A:1106:GLN:HG2	2.17	0.45
1:A:312:GLU:OE1	2:B:199:LEU:HD12	2.17	0.44
3:C:120:MET:HB3	3:C:120:MET:HE3	1.66	0.44
1:A:969:GLU:HG2	1:A:975:PHE:CD1	2.51	0.44
3:C:63:LEU:HA	3:C:66:ILE:HG12	1.99	0.44
1:A:341:ASN:H	1:A:346:TYR:HD2	1.65	0.44
3:C:20:VAL:HG12	3:C:33:LEU:O	2.18	0.44
3:C:123:ARG:HH11	3:C:155:LEU:HB2	1.82	0.44
2:B:165:PHE:HB2	2:B:182:VAL:HG13	1.99	0.44
3:C:28:PHE:HD1	3:C:54:HIS:CB	2.30	0.44
3:C:78:TRP:HZ3	3:C:87:VAL:CG1	2.30	0.44
1:A:285:LEU:HB3	1:A:297:LEU:HD11	2.00	0.44
1:A:1133:VAL:O	1:A:1137:THR:HG23	2.17	0.44
3:C:78:TRP:HZ3	3:C:87:VAL:HG13	1.83	0.44
3:C:123:ARG:NE	3:C:153:LEU:HB3	2.32	0.44
3:C:123:ARG:NH1	3:C:155:LEU:HB2	2.33	0.44
3:C:76:ILE:HA	3:C:90:MET:HG2	2.00	0.44
3:C:118:ASP:HB3	3:C:281:PHE:CD2	2.52	0.44
3:C:134:HIS:NE2	3:C:137:ILE:HD11	2.33	0.43
1:A:812:TYR:HE2	1:A:814:LEU:HD23	1.84	0.43
1:A:1013:VAL:HG21	1:A:1029:LEU:HD11	2.00	0.43
3:C:235:LYS:O	3:C:238:GLU:HG3	2.19	0.43
1:A:889:ARG:HG3	1:A:904:ASN:ND2	2.33	0.42
1:A:839:GLU:HA	2:B:221:TYR:HE1	1.84	0.42
3:C:33:LEU:HD11	3:C:42:GLU:HB3	2.01	0.42
3:C:119:GLN:O	3:C:123:ARG:HG3	2.18	0.42
1:A:340:SER:HB2	1:A:346:TYR:CD2	2.54	0.42
2:B:141:ILE:HG23	2:B:157:VAL:HG13	2.02	0.42
3:C:258:MET:O	3:C:262:TYR:HD2	2.03	0.42
1:A:267:ASN:HD22	1:A:267:ASN:H	1.68	0.42
1:A:1044:SER:OG	1:A:1047:TRP:HD1	2.03	0.42
3:C:13:VAL:HG23	3:C:19:LEU:HD11	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:97:LEU:HB2	3:C:142:PHE:HB2	2.00	0.42
3:C:115:MET:HG3	3:C:296:PHE:CZ	2.54	0.42
3:C:206:SER:O	3:C:210:VAL:HG23	2.20	0.42
1:A:258:ILE:HD13	1:A:275:ASP:HB3	2.01	0.41
3:C:156:ILE:CG2	3:C:157:ASP:H	2.31	0.41
1:A:130:MET:HE3	1:A:142:VAL:HG13	2.03	0.41
3:C:118:ASP:HB3	3:C:281:PHE:CE2	2.54	0.41
3:C:155:LEU:C	3:C:156:ILE:HG13	2.46	0.41
3:C:273:ASP:O	3:C:277:LEU:HG	2.20	0.41
3:C:50:GLN:HG2	3:C:81:GLN:NE2	2.36	0.41
3:C:64:TYR:OH	3:C:156:ILE:HG23	2.20	0.41
1:A:7:VAL:HG12	1:A:1039:LEU:HB3	2.02	0.41
2:B:91:LEU:O	2:B:137:THR:HG21	2.21	0.41
3:C:63:LEU:HA	3:C:63:LEU:HD23	1.57	0.41
3:C:116:LEU:HG	3:C:296:PHE:CD1	2.56	0.41
1:A:1047:TRP:HZ3	1:A:1132:VAL:HG13	1.85	0.41
3:C:50:GLN:HG2	3:C:81:GLN:HE21	1.85	0.41
1:A:67:PHE:CD2	1:A:69:PRO:HD3	2.55	0.41
2:B:110:VAL:O	2:B:114:ILE:HG12	2.20	0.41
3:C:79:TYR:CG	3:C:80:GLY:N	2.88	0.41
3:C:280:LEU:O	3:C:284:LEU:HG	2.21	0.41
1:A:1109:VAL:HG11	1:A:1126:ALA:HA	2.02	0.40
3:C:259:TYR:O	3:C:263:CYS:SG	2.79	0.40
1:A:817:VAL:HG22	1:A:830:ILE:HB	2.03	0.40
3:C:66:ILE:HB	3:C:165:ARG:CZ	2.51	0.40
3:C:120:MET:SD	3:C:153:LEU:HD13	2.61	0.40
1:A:1044:SER:HG	1:A:1047:TRP:HD1	1.69	0.40
1:A:883:SER:OG	1:A:911:ALA:HB3	2.21	0.40
1:A:970:ASN:CG	1:A:971:ALA:H	2.29	0.40
2:B:398:ILE:O	2:B:418:THR:HG22	2.21	0.40
1:A:1097:PHE:O	1:A:1100:ILE:HG12	2.21	0.40
2:B:273:LEU:HD13	2:B:280:PHE:CE2	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	A	788/830 (95%)	762 (97%)	26 (3%)	0	100	100
2	B	371/382 (97%)	363 (98%)	8 (2%)	0	100	100
3	C	247/294 (84%)	232 (94%)	15 (6%)	0	100	100
All	All	1406/1506 (93%)	1357 (96%)	49 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	702/726 (97%)	702 (100%)	0	100	100
2	B	339/346 (98%)	338 (100%)	1 (0%)	91	96
3	C	227/261 (87%)	227 (100%)	0	100	100
All	All	1268/1333 (95%)	1267 (100%)	1 (0%)	92	98

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	119	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	183	GLN
1	A	240	HIS
1	A	343	GLN
1	A	711	HIS
1	A	790	ASN

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Mol	Chain	Res	Type
1	A	810	ASN
1	A	826	ASN
1	A	904	ASN
1	A	907	ASN
1	A	990	GLN
1	A	1070	HIS
1	A	1113	GLN
1	A	1140	HIS
2	B	73	HIS
2	B	198	GLN
2	B	228	GLN
2	B	233	HIS
2	B	367	ASN
3	C	39	ASN
3	C	54	HIS
3	C	81	GLN
3	C	141	ASN
3	C	171	GLN
3	C	261	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 3 ligands modelled in this entry, 1 is 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	A1CEG	B	503	-	29,29,29	2.52	9 (31%)	35,38,38	1.29	5 (14%)
5	A1CEH	B	502	-	30,30,30	2.95	11 (36%)	43,43,43	2.98	9 (20%)

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	A1CEG	B	503	-	-	2/15/15/15	0/3/3/3
5	A1CEH	B	502	-	-	6/12/37/37	0/4/4/4

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	502	A1CEH	C25-N16	8.93	1.45	1.36
5	B	502	A1CEH	C20-N22	7.61	1.50	1.37
5	B	502	A1CEH	C23-N22	7.11	1.50	1.37
6	B	503	A1CEG	C08-N07	5.98	1.52	1.39
6	B	503	A1CEG	C03-N04	5.40	1.52	1.41
6	B	503	A1CEG	C05-N07	5.32	1.49	1.37
6	B	503	A1CEG	C24-C26	4.90	1.55	1.44
6	B	503	A1CEG	O01-C02	4.71	1.45	1.36
5	B	502	A1CEH	C13-C25	3.59	1.54	1.48
5	B	502	A1CEH	C02-N01	3.18	1.44	1.35
6	B	503	A1CEG	O06-C05	-3.07	1.16	1.23
5	B	502	A1CEH	C15-C14	2.73	1.53	1.50
6	B	503	A1CEG	O10-C09	2.68	1.42	1.37
5	B	502	A1CEH	O24-C23	-2.46	1.18	1.23
5	B	502	A1CEH	C18-C19	-2.28	1.48	1.53
5	B	502	A1CEH	O21-C20	-2.24	1.18	1.23
5	B	502	A1CEH	C18-C17	-2.24	1.47	1.53
6	B	503	A1CEG	C25-C02	2.06	1.41	1.38
6	B	503	A1CEG	C23-C22	2.05	1.42	1.38
5	B	502	A1CEH	C15-N16	-2.05	1.44	1.47

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	502	A1CEH	C15-N16-C25	-11.90	108.13	113.15
5	B	502	A1CEH	C14-C15-N16	10.62	107.96	102.31
5	B	502	A1CEH	C23-C17-N16	-6.37	104.43	110.32
6	B	503	A1CEG	N07-C05-N04	4.03	120.24	112.44
5	B	502	A1CEH	C18-C17-N16	-3.82	109.85	114.03
5	B	502	A1CEH	C17-N16-C25	3.78	127.63	121.86
5	B	502	A1CEH	C20-N22-C23	-3.33	122.30	126.69
6	B	503	A1CEG	O06-C05-N07	-3.00	118.31	123.64
6	B	503	A1CEG	C20-N21-C08	2.69	121.98	116.74
5	B	502	A1CEH	C15-C14-C13	-2.37	108.24	109.73
5	B	502	A1CEH	C17-C23-N22	-2.35	112.80	116.24
6	B	503	A1CEG	C11-O10-C09	-2.27	113.26	117.76
6	B	503	A1CEG	O10-C09-C18	-2.05	119.47	123.95
5	B	502	A1CEH	C13-C25-N16	2.01	107.69	106.42

There are no chirality outliers.

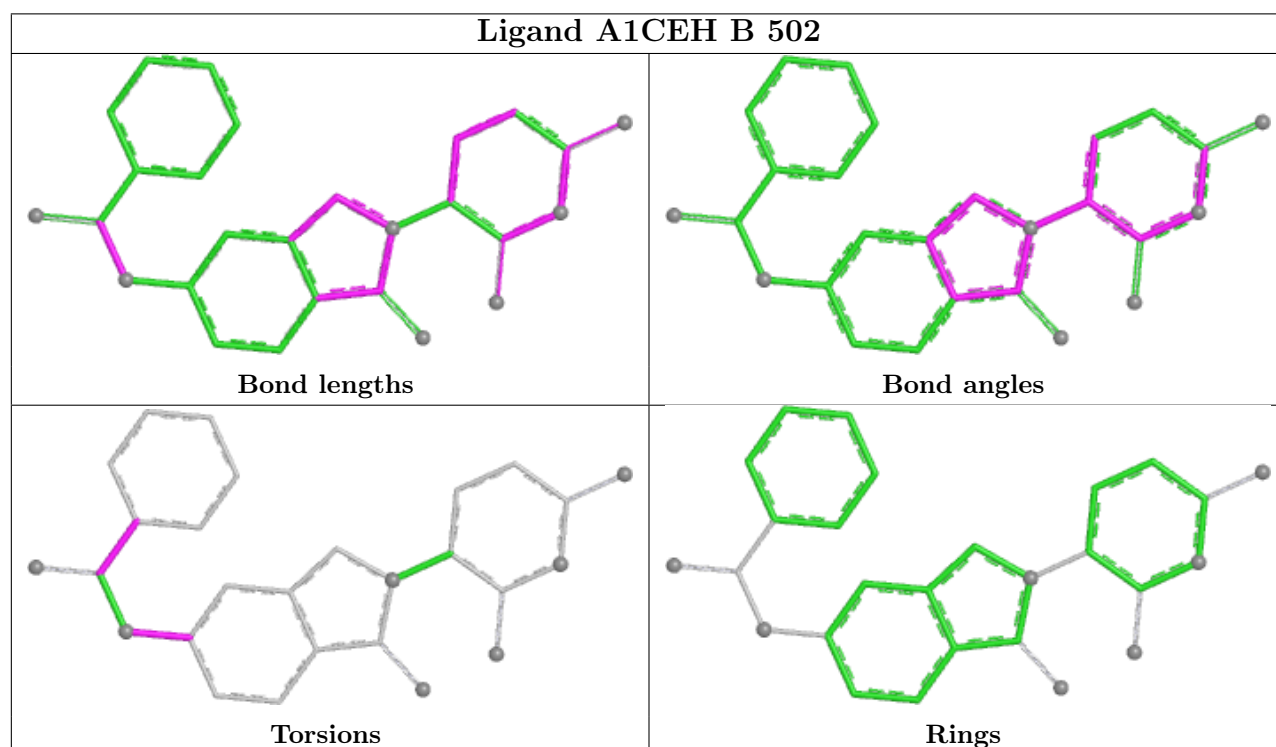
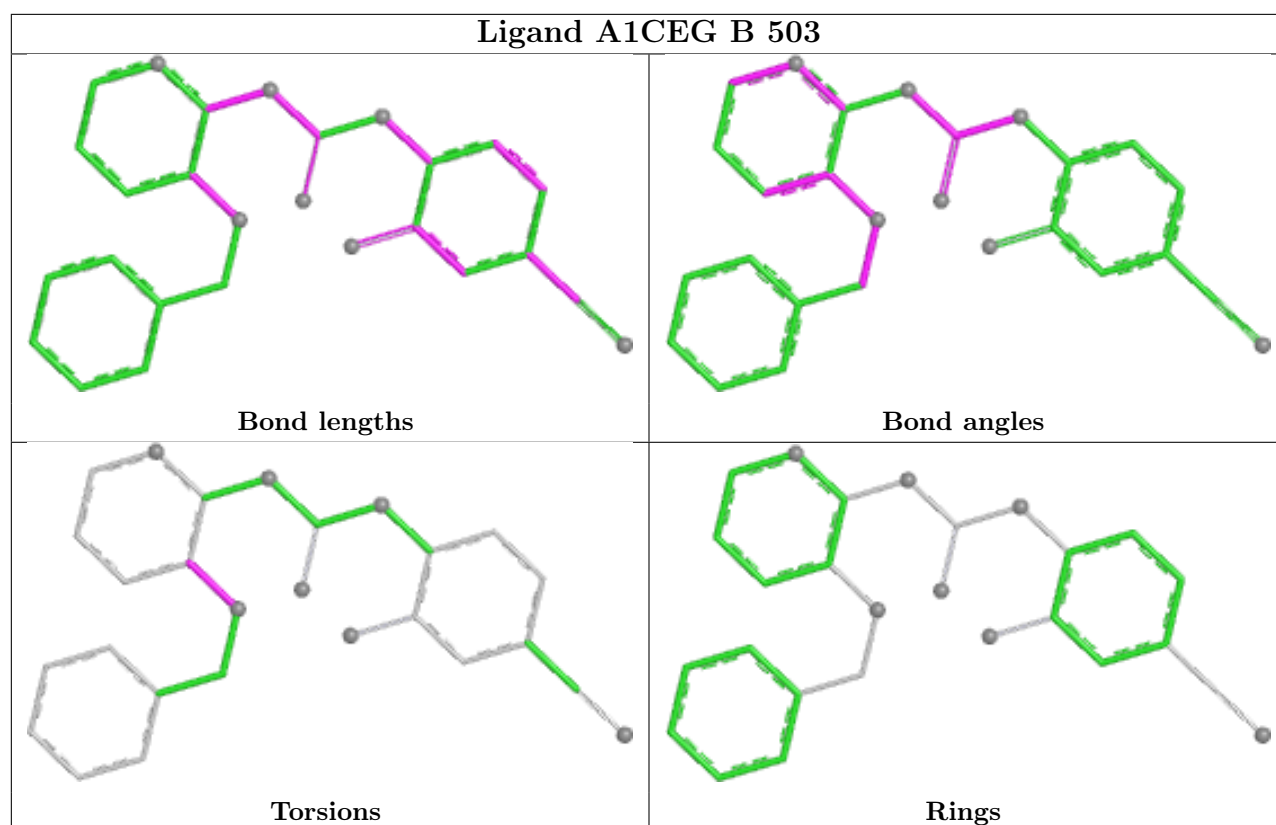
All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	502	A1CEH	O03-C02-C04-C05
5	B	502	A1CEH	O03-C02-C04-C09
5	B	502	A1CEH	N01-C02-C04-C05
5	B	502	A1CEH	N01-C02-C04-C09
5	B	502	A1CEH	C11-C10-N01-C02
5	B	502	A1CEH	C27-C10-N01-C02
6	B	503	A1CEG	C08-C09-O10-C11
6	B	503	A1CEG	C18-C09-O10-C11

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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	391:ARG	C	710:LEU	N	6.27

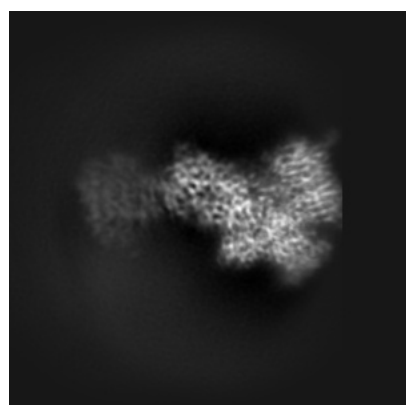
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-70862. These allow visual inspection of the internal detail of the map and identification of artifacts.

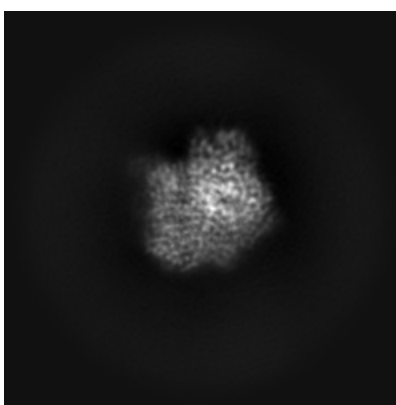
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

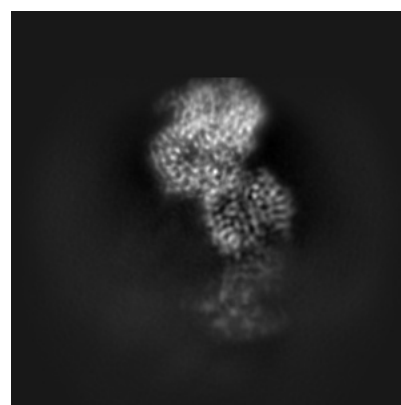
#### 6.1.1 Primary map



X



Y

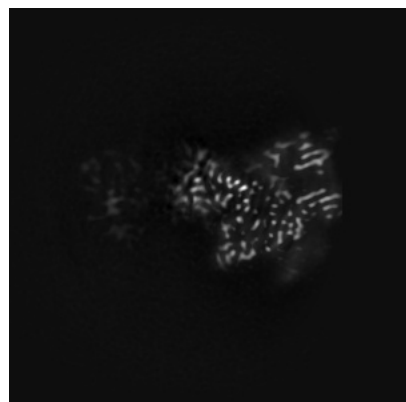


Z

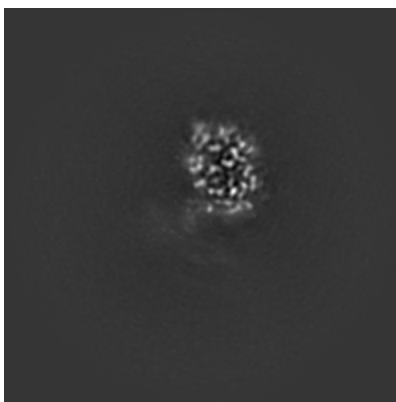
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

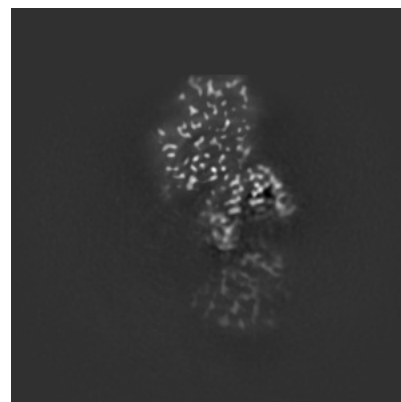
#### 6.2.1 Primary map



X Index: 150



Y Index: 150

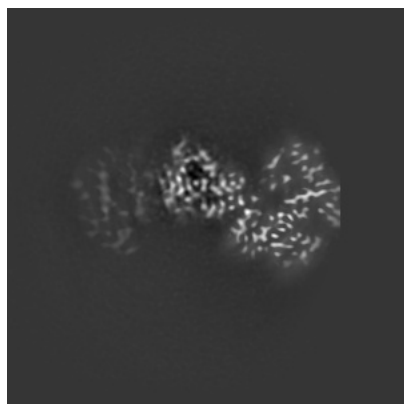


Z Index: 150

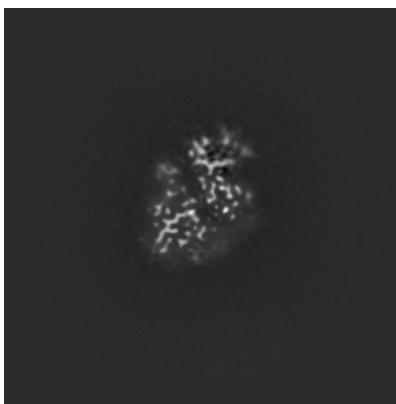
The images above show central slices of the map in three orthogonal directions.

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

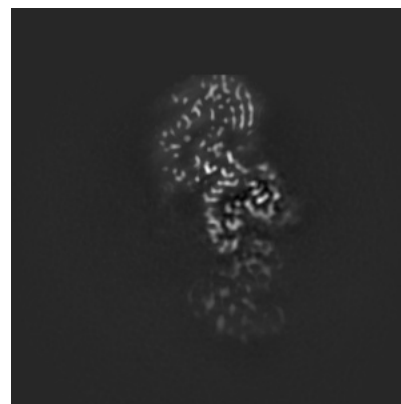
### 6.3.1 Primary map



X Index: 166



Y Index: 167

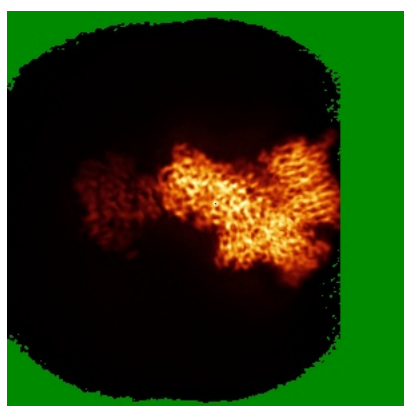


Z Index: 156

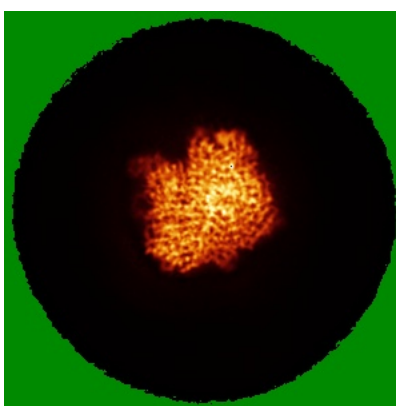
The images above show the largest variance slices of the map in three orthogonal directions.

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

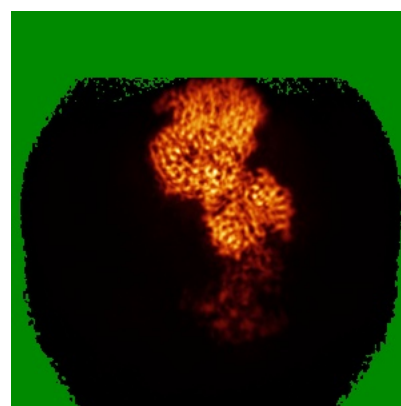
### 6.4.1 Primary map



X



Y

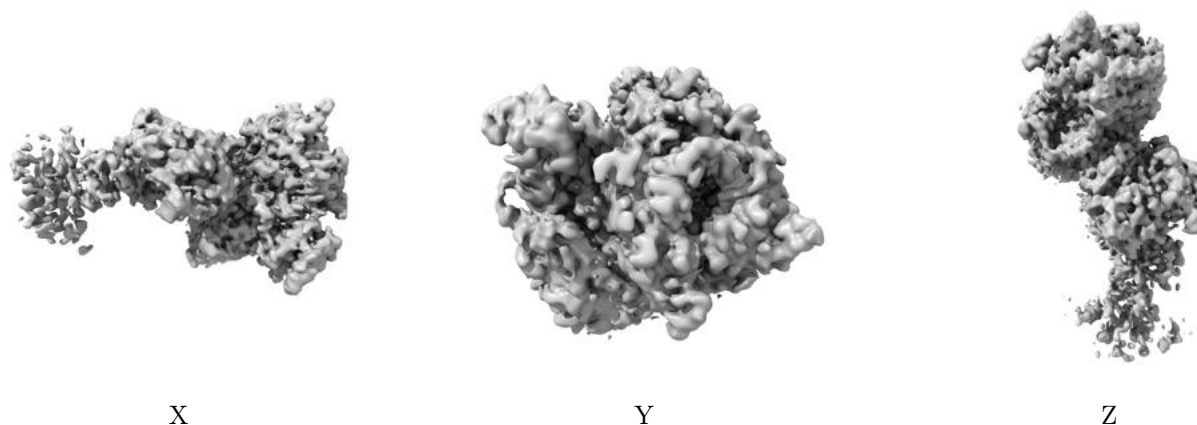


Z

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 0.0346. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

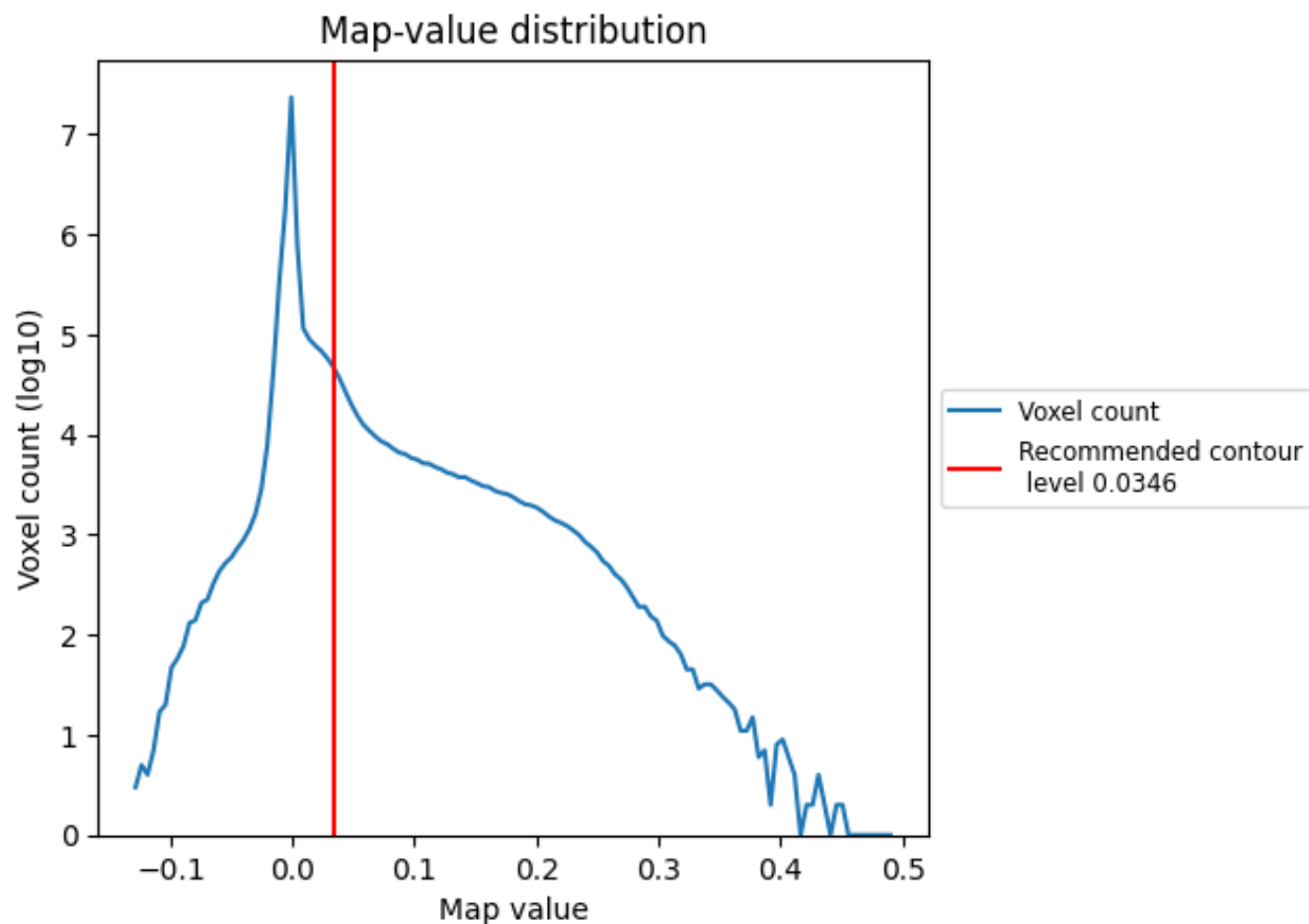
## 6.6 Mask visualisation [i](#)

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.

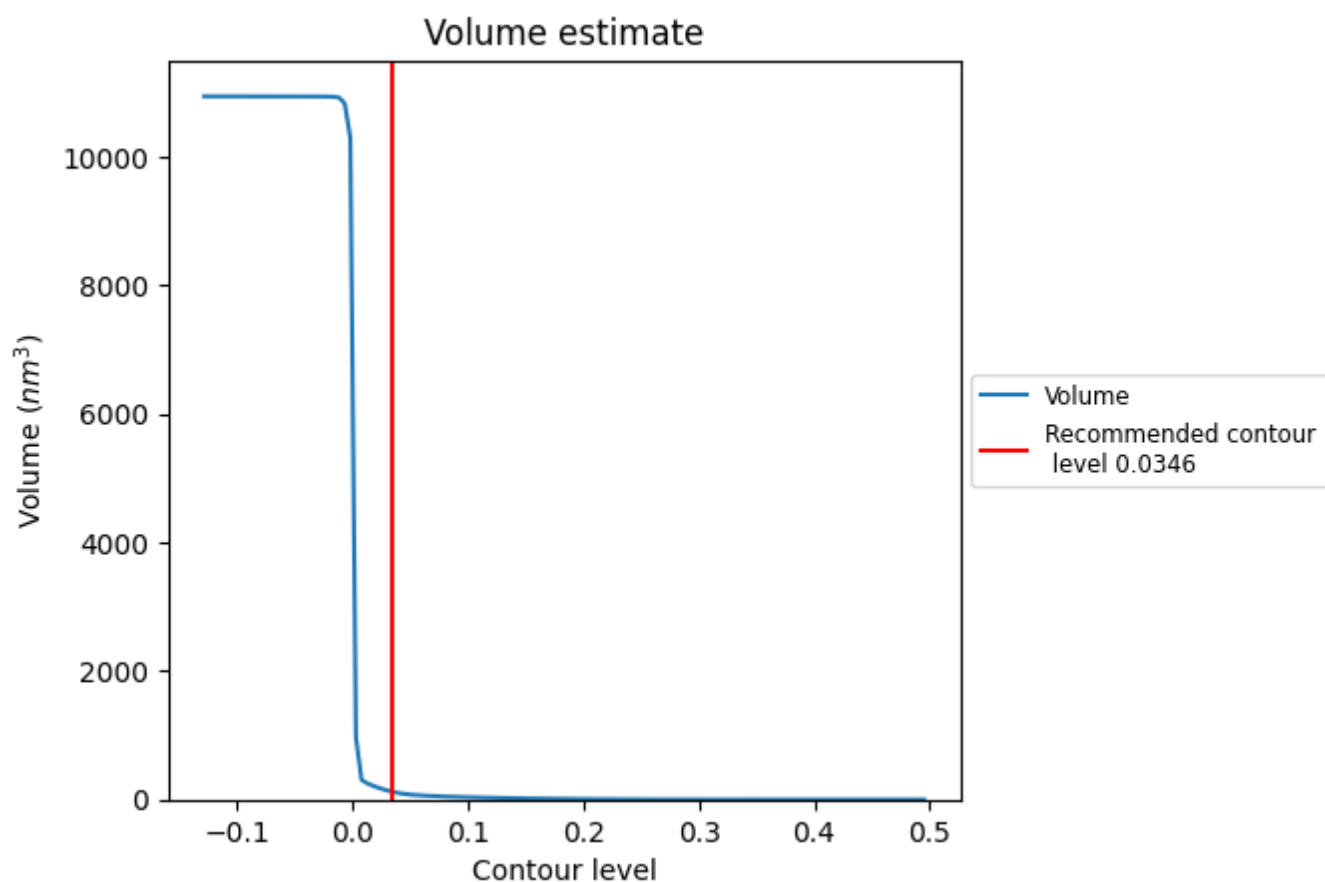
### 7.1 Map-value distribution [i](#)



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.



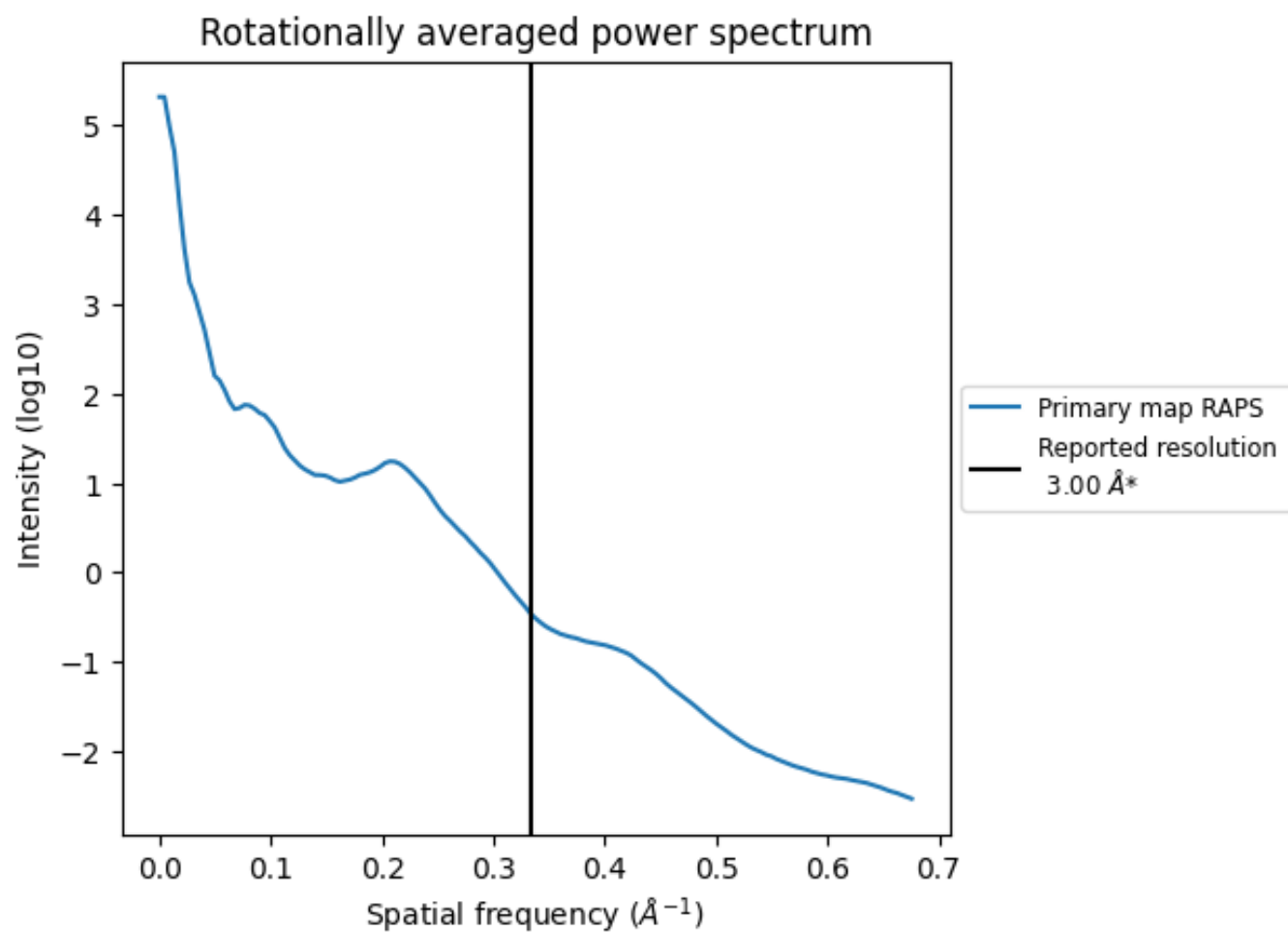
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 121 nm<sup>3</sup>; this corresponds to an approximate mass of 109 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>

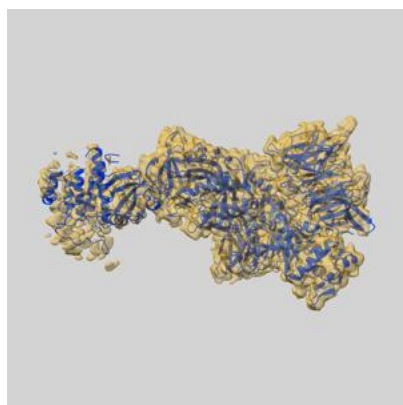
## 8 Fourier-Shell correlation ⓘ

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

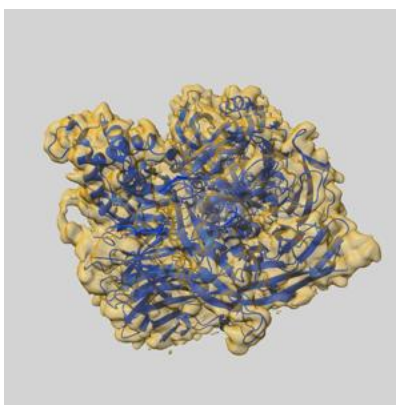
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-70862 and PDB model 9OTY. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

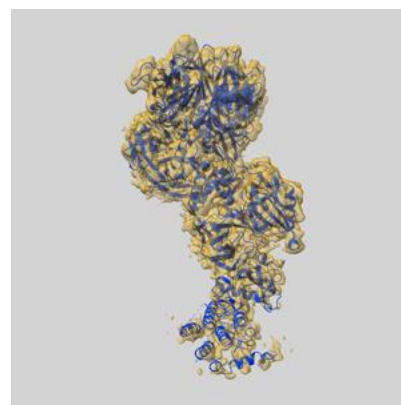
### 9.1 Map-model overlay [i](#)



X



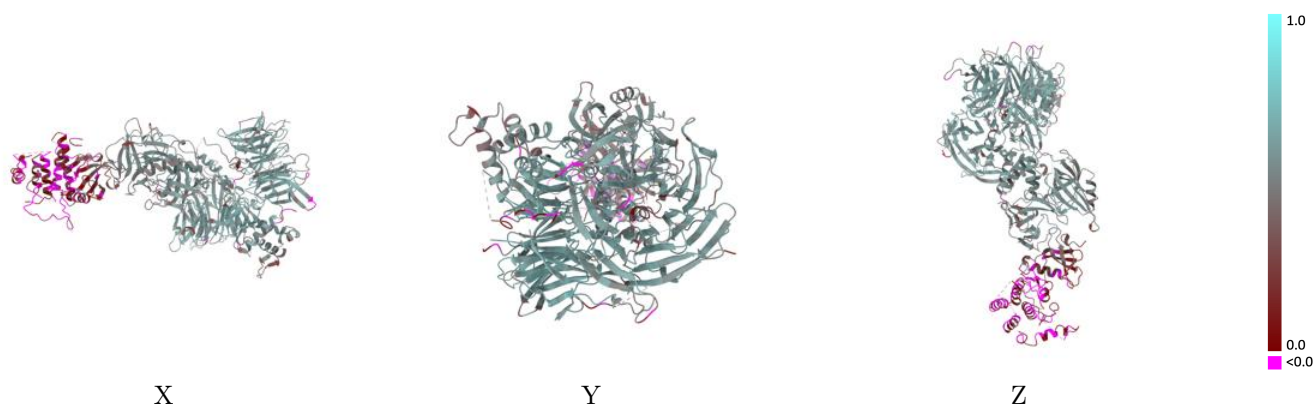
Y



Z

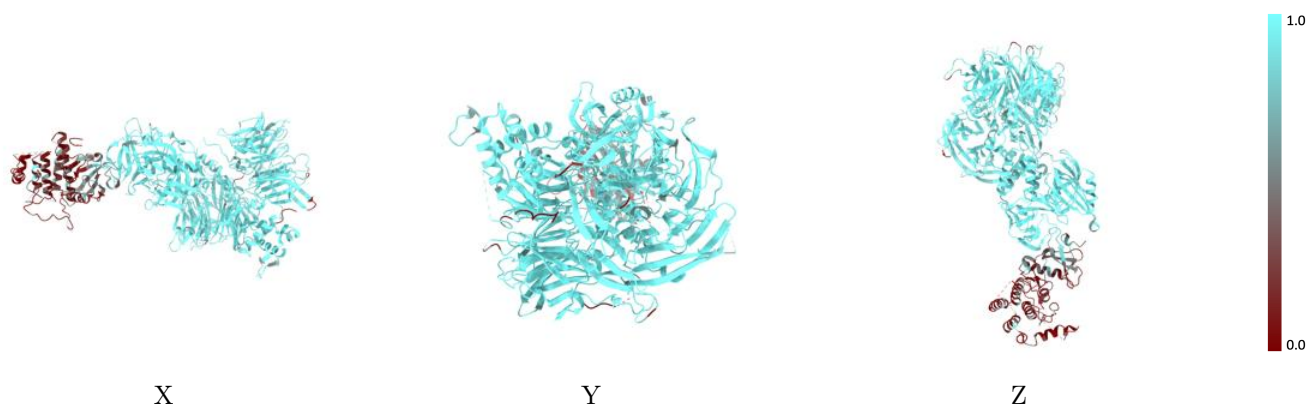
The images above show the 3D surface view of the map at the recommended contour level 0.0346 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



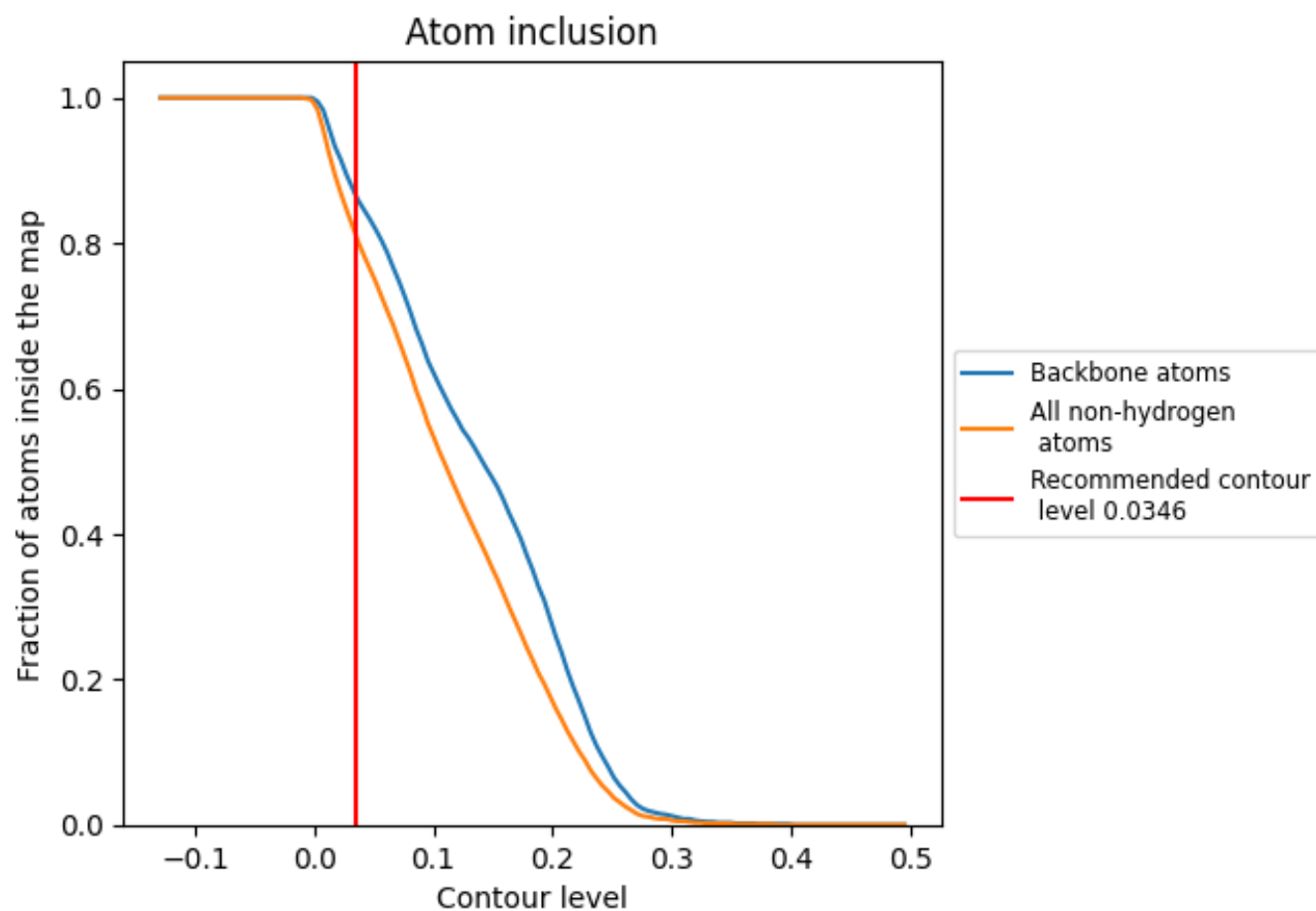
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0346).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 81% 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 (0.0346) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8130	<div></div> 0.4530
A	<div></div> 0.9340	<div></div> 0.5510
B	<div></div> 0.9440	<div></div> 0.5040
C	<div></div> 0.2620	<div></div> 0.0910

