WORLDWIDE PDB

PROTEIN DATA BANK

wwPDB EM Validation Summary Report ⓘ

Nov 26, 2022 – 12:24 PM EST

PDB ID	:	7STE
EMDB ID	:	EMD-25426
Title	:	Rad24-RFC ADP state
Authors	:	Castaneda, J.C.; Schrecker, M.; Remus, D.; Hite, R.K.
Deposited on	:	2021-11-12
Resolution	:	2.73 Å(reported)
Based on initial models	:	1SXJ, 3A1J

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

EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 2.73 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	Percentile Ranks	Value
Clashscore		3
Ramachandran outliers		0
Sidechain outliers		0.2%

Worse   *Better*

▮ Percentile relative to all structures
▯ Percentile relative to all EM structures
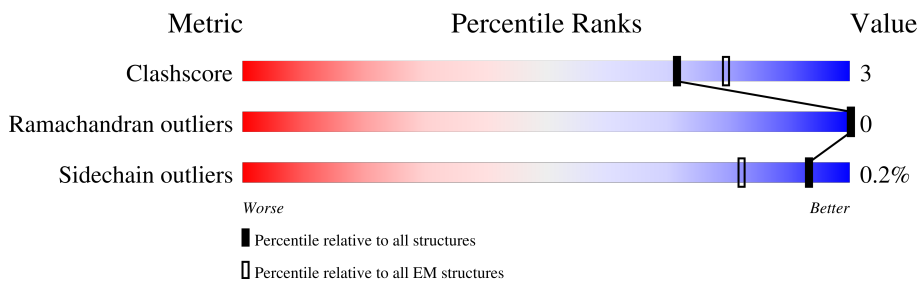
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=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 <=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	B	323	84% 13% ••
2	C	339	91% 5% •
3	D	353	84% 8% 7%
4	E	354	86% 10% •
5	A	696	14% 61% 6% 33%

2   Entry composition ⓘ

There are 8 unique types of molecules in this entry. The entry contains 28688 atoms, of which 14439 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 Replication factor C subunit 4.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	B	315	Total	C	H	N	O	S	0	0
			5028	1558	2556	441	460	13		

- Molecule 2 is a protein called Replication factor C subunit 3.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	C	324	Total	C	H	N	O	S	0	0
			5146	1613	2586	447	492	8		

- Molecule 3 is a protein called Replication factor C subunit 2.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	D	327	Total	C	H	N	O	S	0	0
			5218	1640	2625	446	497	10		

- Molecule 4 is a protein called Replication factor C subunit 5.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	E	340	Total	C	H	N	O	S	0	0
			5470	1694	2796	465	498	17		

- Molecule 5 is a protein called Checkpoint protein RAD24.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	A	468	Total	C	H	N	O	S	0	0
			7626	2427	3816	663	701	19		

There are 37 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	660	GLY	-	expression tag	UNP P32641
A	661	LEU	-	expression tag	UNP P32641
A	662	ASN	-	expression tag	UNP P32641

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Chain	Residue	Modelled	Actual	Comment	Reference
A	663	LEU	-	expression tag	UNP P32641
A	664	GLU	-	expression tag	UNP P32641
A	665	VAL	-	expression tag	UNP P32641
A	666	LEU	-	expression tag	UNP P32641
A	667	PHE	-	expression tag	UNP P32641
A	668	GLN	-	expression tag	UNP P32641
A	669	GLY	-	expression tag	UNP P32641
A	670	PRO	-	expression tag	UNP P32641
A	671	GLY	-	expression tag	UNP P32641
A	672	GLY	-	expression tag	UNP P32641
A	673	ASP	-	expression tag	UNP P32641
A	674	TYR	-	expression tag	UNP P32641
A	675	LYS	-	expression tag	UNP P32641
A	676	ASP	-	expression tag	UNP P32641
A	677	ASP	-	expression tag	UNP P32641
A	678	ASP	-	expression tag	UNP P32641
A	679	ASP	-	expression tag	UNP P32641
A	680	LYS	-	expression tag	UNP P32641
A	681	ASP	-	expression tag	UNP P32641
A	682	TYR	-	expression tag	UNP P32641
A	683	LYS	-	expression tag	UNP P32641
A	684	ASP	-	expression tag	UNP P32641
A	685	ASP	-	expression tag	UNP P32641
A	686	ASP	-	expression tag	UNP P32641
A	687	ASP	-	expression tag	UNP P32641
A	688	LYS	-	expression tag	UNP P32641
A	689	ASP	-	expression tag	UNP P32641
A	690	TYR	-	expression tag	UNP P32641
A	691	LYS	-	expression tag	UNP P32641
A	692	ASP	-	expression tag	UNP P32641
A	693	ASP	-	expression tag	UNP P32641
A	694	ASP	-	expression tag	UNP P32641
A	695	ASP	-	expression tag	UNP P32641
A	696	LYS	-	expression tag	UNP P32641

- Molecule 6 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).

| Mol	Chain	Residues	Atoms						AltConf
6	B	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	
6	C	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	
6	D	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	
6	E	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	

- Molecule 7 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).
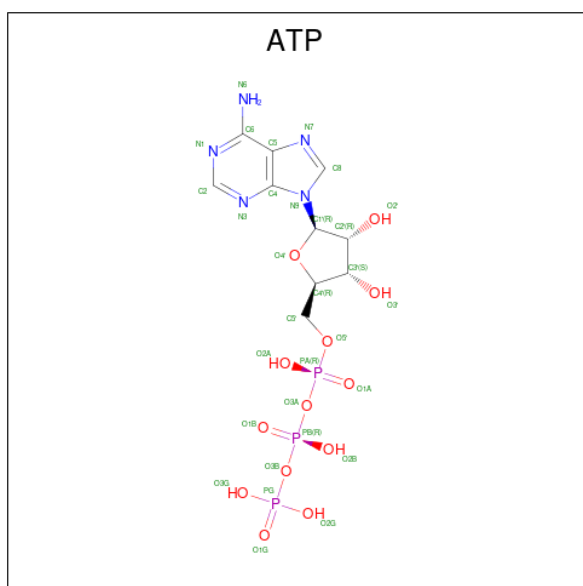
Mol	Chain	Residues	Atoms						AltConf
7	A	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	

- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

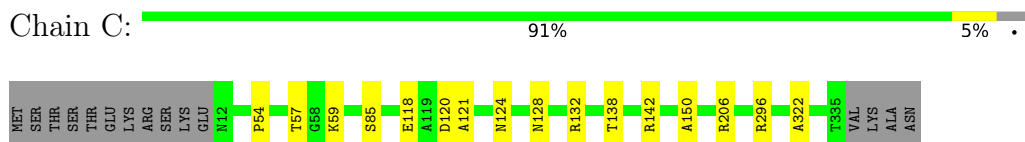| Mol	Chain	Residues	Atoms		AltConf
8	A	1	Total	Mg	0
			1	1	

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.
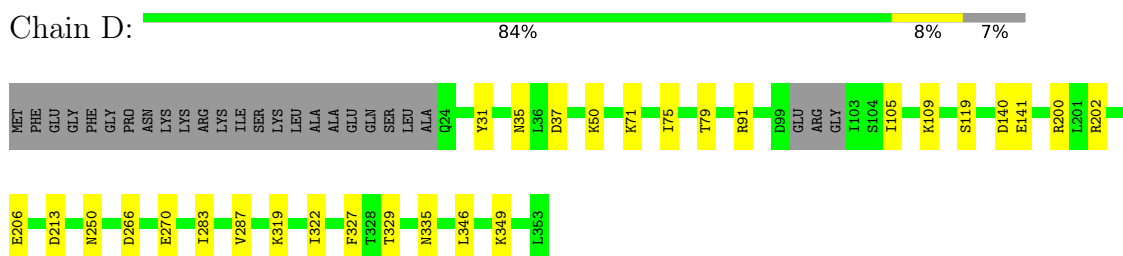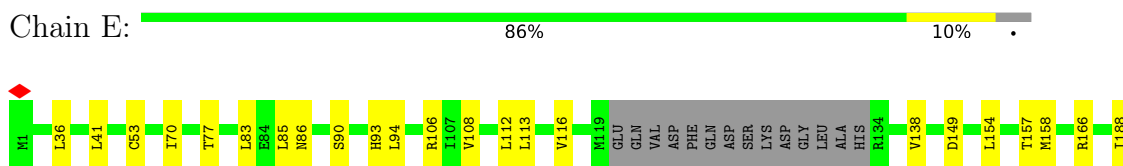
- Molecule 1: Replication factor C subunit 4
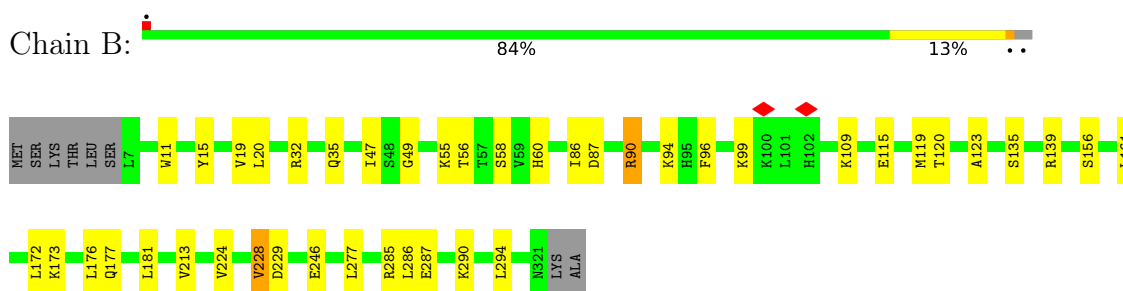
Chain B:

- Molecule 2: Replication factor C subunit 3

Chain C:
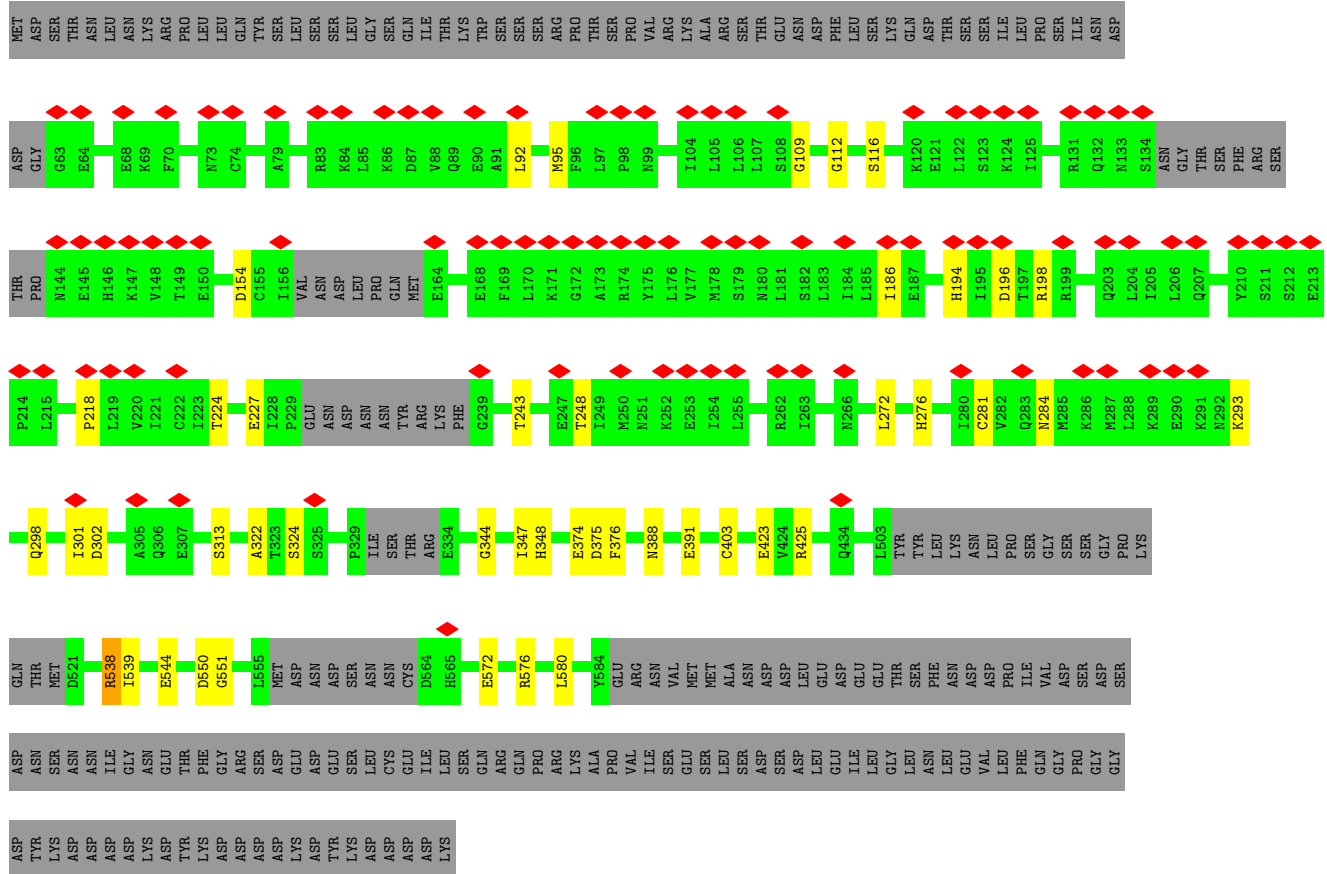

- Molecule 3: Replication factor C subunit 2

Chain D:

- Molecule 4: Replication factor C subunit 5

Chain E:

R189 C190 L202 V206 I211 R231 L237 L286 Y287 D288 E323 S333 I346 D354

• Molecule 5: Checkpoint protein RAD24

14%

Chain A: 61% 6% 33%

MET ASP SER THR ASN LEU ASN LYS ARG PRO LEU LEU GLN TYR SER LEU SER SER LEU GLY SER GLN ILE THR LYS TRP SER SER SER ARG PRO THR SER PRO VAL ARG LYS ALA ARG SER THR GLU ASN ASP PHE LEU SER LYS GLN ASP THR SER SER ILE LEU PRO SER ILE ASN ASP

ASP GLY G63 E64 E68 K69 F70 N73 C74 A79 R83 K84 L85 K86 D87 V88 Q89 E90 A91 L92 M95 F96 L97 P98 N99 I104 L105 L106 L107 S108 G109 G112 S116 K120 E121 L122 S123 K124 I125 R131 Q132 N133 S134 ASN GLY THR SER PHE ARG SER

THR PRO N144 E145 H146 K147 V148 T149 E150 D154 C155 I156 VAL ASN ASP LEU PRO GLN MET E164 E168 F169 L170 K171 G172 A173 R174 Y175 L176 V177 M178 S179 N180 L181 S182 L183 I184 L185 I186 E187 H194 I195 D196 T197 R198 R199 Q203 L204 I205 L206 Q207 Y210 S211 S212 E213

P214 L215 P218 L219 V220 I221 C222 I223 T224 E227 I228 P229 GLU ASN ASP ASN ASN TYR ARG LYS PHE G239 T243 E247 T248 I249 M250 N251 K252 E253 I254 L255 R262 I263 N266 L272 H276 I280 C281 V282 Q283 N284 M285 K286 M287 L288 K289 E290 K291 N292 K293

Q298 I301 D302 A305 Q306 E307 S313 A322 T323 S324 S325 P329 ILE SER THR ARG E334 G344 I347 H348 E374 D375 F376 N388 E391 C403 E423 V424 R425 Q434 L503 TYR TYR LEU LYS ASN LEU PRO SER GLY SER SER GLY PRO LYS

GLN THR MET D521 R538 I539 E544 D550 G551 L555 MET ASP ASN ASP SER ASN ASN CYS D564 H565 E572 R576 L580 Y584 GLU ARG ASN VAL MET ALA ASN ASP ASP LEU GLU ASP GLU THR SER PHE ASN ASP ASP PRO ILE VAL ASP SER ASP SER

ASP ASN SER ASN ILE GLY ASN GLU THR PHE GLY ARG SER ASP GLU ASP GLU SER LEU CYS GLU ILE LEU SER GLN ARG GLN PRO ARG LYS ALA PRO VAL ILE LEU SER GLU LEU SER ASP SER SER ASP LEU GLU ILE LEU GLY LEU LEU ASN LEU GLU VAL LEU PHE GLN GLY PRO GLY GLY

ASP TYR LYS ASP ASP ASP ASP LYS ASP TYR LYS ASP ASP ASP ASP LYS ASP TYR LYS ASP ASP ASP LYS

4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	183334	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/Å^2)$	66	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.020	Depositor
Minimum map value	-0.843	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.035	Depositor
Recommended contour level	0.09	Depositor
Map size (Å)	317.184, 317.184, 317.184	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.826, 0.826, 0.826	Depositor

5   Model quality ⓘ

5.1   Standard geometry ⓘ

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

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	B	0.23	0/2507	0.48	1/3381 (0.0%)
2	C	0.23	0/2600	0.45	0/3518
3	D	0.23	0/2637	0.44	0/3566
4	E	0.24	0/2711	0.46	0/3663
5	A	0.23	0/3884	0.44	0/5224
All	All	0.23	0/14339	0.45	1/19352 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	228	VAL	C-N-CA	5.06	134.35	121.70

There are no chirality outliers.

There are no planarity outliers.

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	B	2472	2556	2556	30	0
2	C	2560	2586	2586	11	0
3	D	2593	2625	2625	18	0
4	E	2674	2796	2796	20	0
5	A	3810	3816	3812	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	27	12	12	1	0
6	C	27	12	12	2	0
6	D	27	12	12	1	0
6	E	27	12	12	1	0
7	A	31	12	12	2	0
8	A	1	0	0	0	0
All	All	14249	14439	14435	99	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.

The worst 5 of 99 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)
1:B:115:GLU:OE1	2:C:132:ARG:NH2	2.09	0.85
3:D:31:TYR:O	3:D:200:ARG:NH2	2.12	0.83
4:E:36:LEU:O	4:E:166:ARG:NH1	2.12	0.81
1:B:135:SER:O	1:B:139:ARG:NH1	2.13	0.81
3:D:91:ARG:NH1	3:D:119:SER:OG	2.17	0.78

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	B	313/323 (97%)	304 (97%)	9 (3%)	0	100	100
2	C	322/339 (95%)	320 (99%)	2 (1%)	0	100	100
3	D	323/353 (92%)	319 (99%)	4 (1%)	0	100	100
4	E	336/354 (95%)	332 (99%)	4 (1%)	0	100	100
5	A	454/696 (65%)	438 (96%)	16 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1748/2065 (85%)	1713 (98%)	35 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2   Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	275/283 (97%)	273 (99%)	2 (1%)	84	90
2	C	280/295 (95%)	280 (100%)	0	100	100
3	D	292/312 (94%)	292 (100%)	0	100	100
4	E	309/324 (95%)	309 (100%)	0	100	100
5	A	426/645 (66%)	425 (100%)	1 (0%)	93	96
All	All	1582/1859 (85%)	1579 (100%)	3 (0%)	93	96

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	90	ARG
1	B	99	LYS
5	A	538	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	177	GLN
2	C	184	HIS
5	A	351	HIS

5.3.3   RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 1 is monoatomic - leaving 5 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	ADP	D	801	-	24,29,29	0.96	1 (4%)	29,45,45	1.53	4 (13%)
7	ATP	A	801	8	26,33,33	0.59	0	31,52,52	1.08	2 (6%)
6	ADP	C	401	-	24,29,29	0.94	1 (4%)	29,45,45	1.55	4 (13%)
6	ADP	E	401	-	24,29,29	0.95	1 (4%)	29,45,45	1.51	4 (13%)
6	ADP	B	401	-	24,29,29	0.95	1 (4%)	29,45,45	1.50	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
6	ADP	D	801	-	-	1/12/32/32	0/3/3/3
7	ATP	A	801	8	-	3/18/38/38	0/3/3/3
6	ADP	C	401	-	-	4/12/32/32	0/3/3/3
6	ADP	E	401	-	-	5/12/32/32	0/3/3/3
6	ADP	B	401	-	-	5/12/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	401	ADP	C5-C4	2.41	1.47	1.40
6	E	401	ADP	C5-C4	2.37	1.47	1.40
6	C	401	ADP	C5-C4	2.37	1.47	1.40
6	D	801	ADP	C5-C4	2.36	1.47	1.40

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	C	401	ADP	PA-O3A-PB	-3.78	119.86	132.83
6	D	801	ADP	PA-O3A-PB	-3.77	119.89	132.83
6	E	401	ADP	N3-C2-N1	-3.70	122.89	128.68
6	C	401	ADP	N3-C2-N1	-3.68	122.92	128.68
6	E	401	ADP	PA-O3A-PB	-3.67	120.22	132.83

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	401	ADP	C5'-O5'-PA-O2A
6	B	401	ADP	C5'-O5'-PA-O3A
6	E	401	ADP	C5'-O5'-PA-O1A
6	E	401	ADP	C5'-O5'-PA-O2A
7	A	801	ATP	O4'-C4'-C5'-O5'

There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	801	ADP	1	0
7	A	801	ATP	2	0
6	C	401	ADP	2	0
6	E	401	ADP	1	0
6	B	401	ADP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.

Ligand ADP D 801

Bond lengths — Bond angles — Torsions — Rings

Ligand ATP A 801

Bond lengths — Bond angles — Torsions — Rings

Ligand ADP C 401

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP E 401

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP B 401

Bond lengths

Bond angles

Torsions

Rings
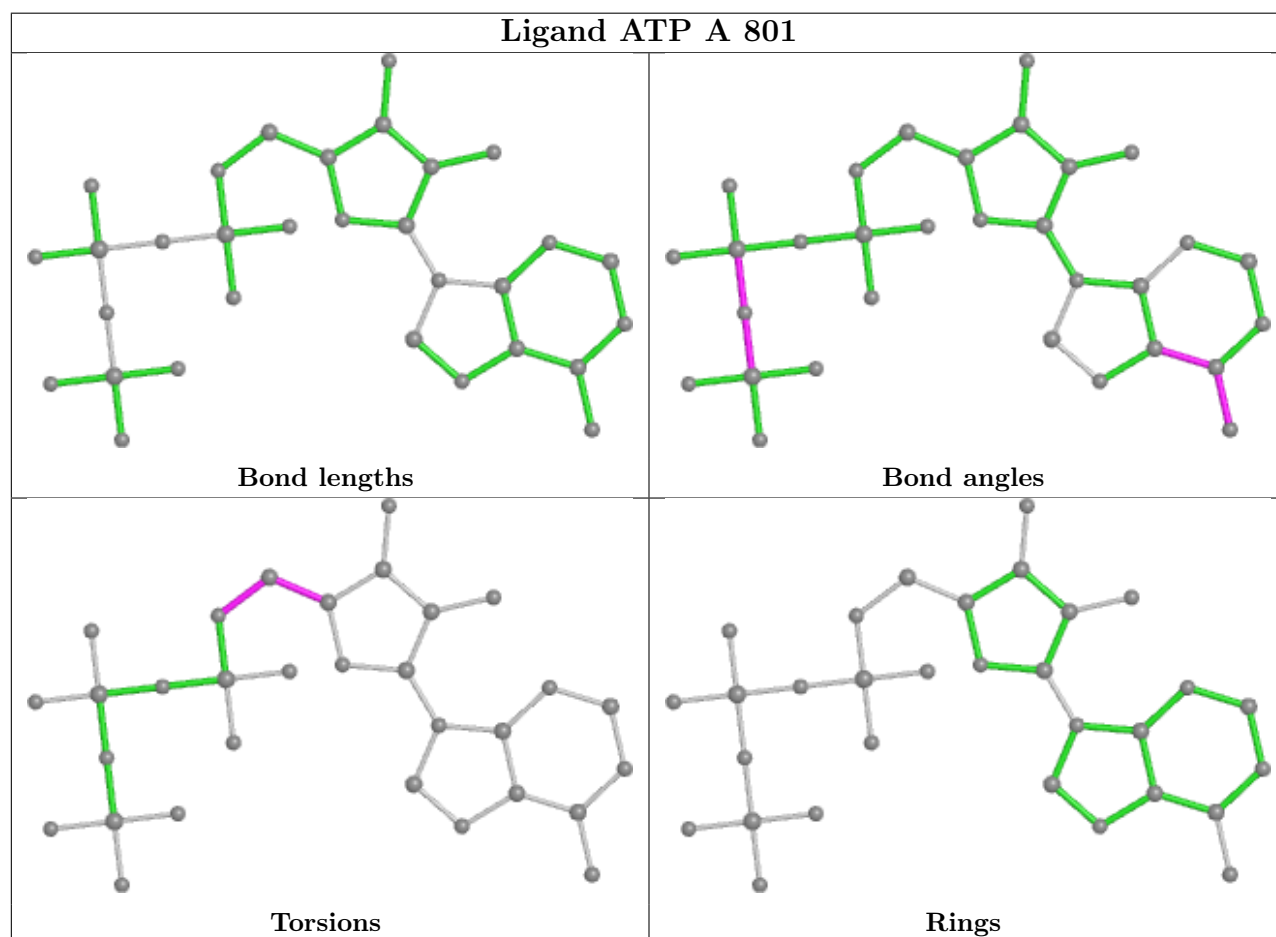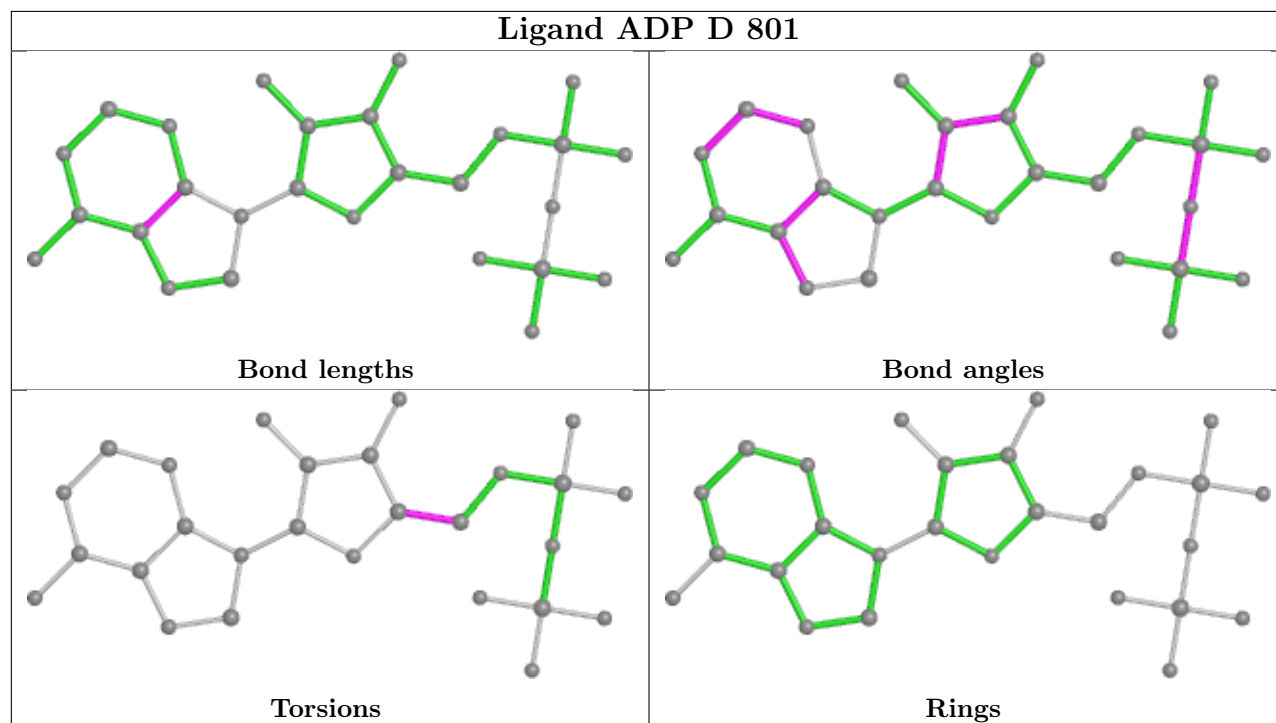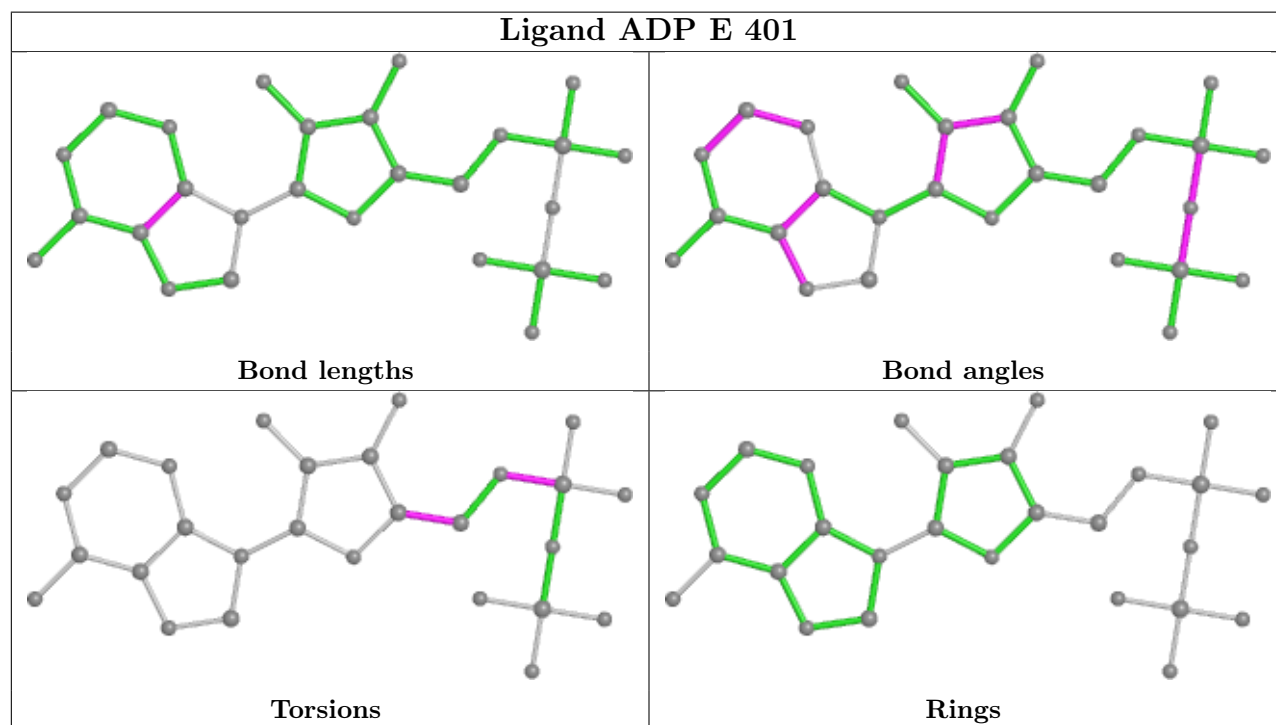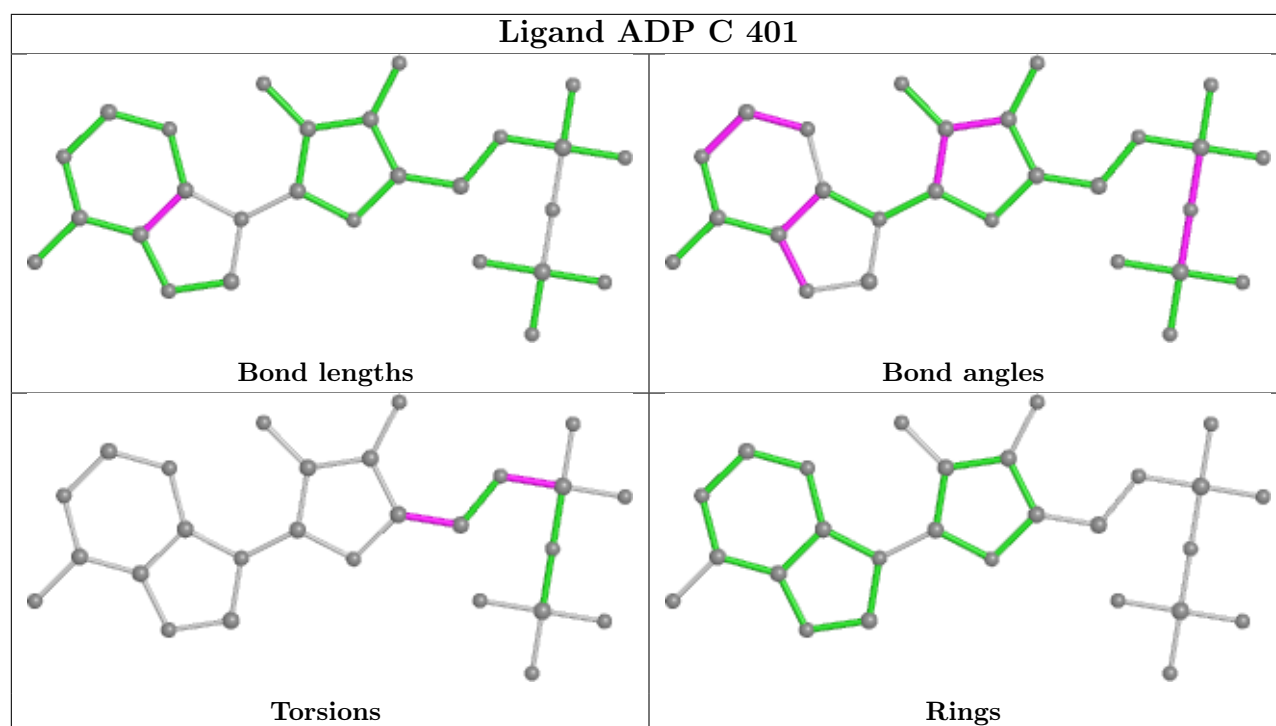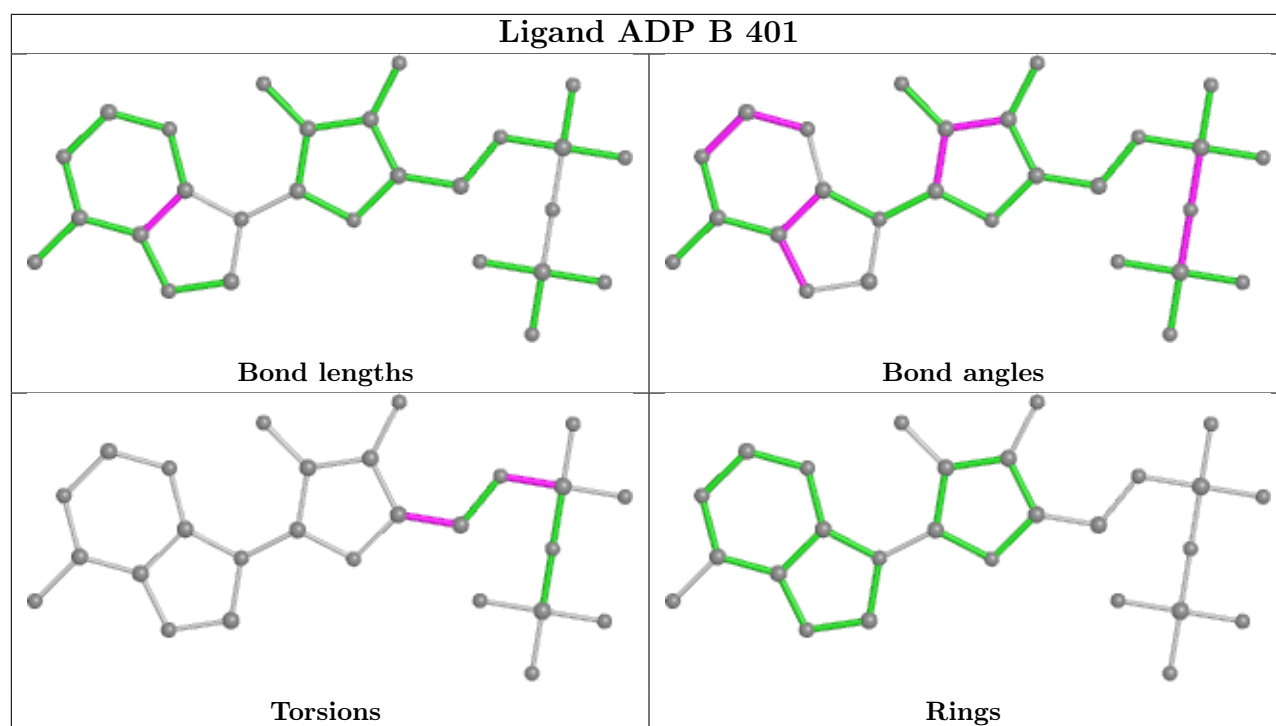
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-25426. 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 ⓘ

6.1.1 Primary map

| X | Y | Z |
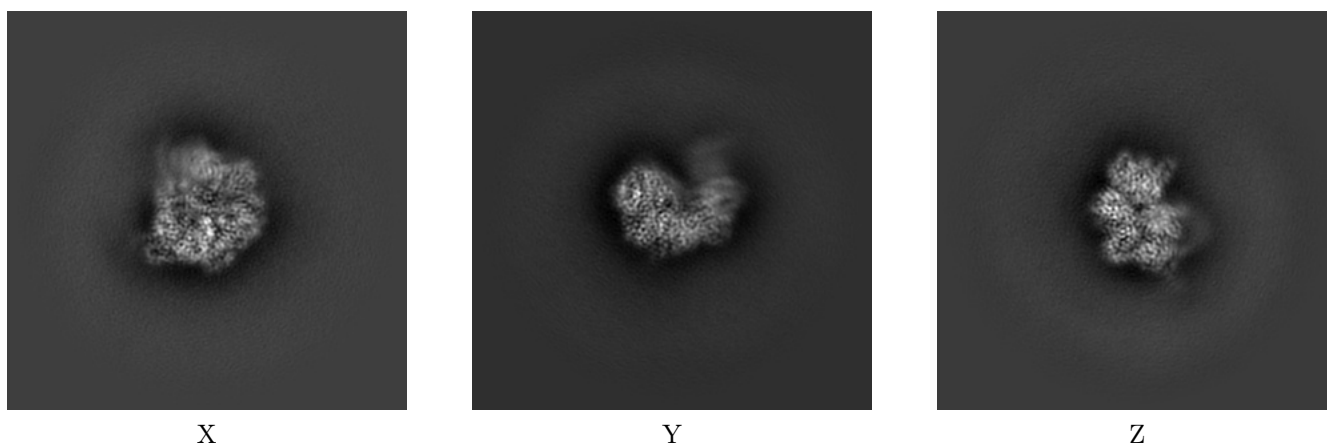
The images above show the map projected in three orthogonal directions.

6.2 Central slices ⓘ

6.2.1 Primary map

| X Index: 192 | Y Index: 192 | Z Index: 192 |
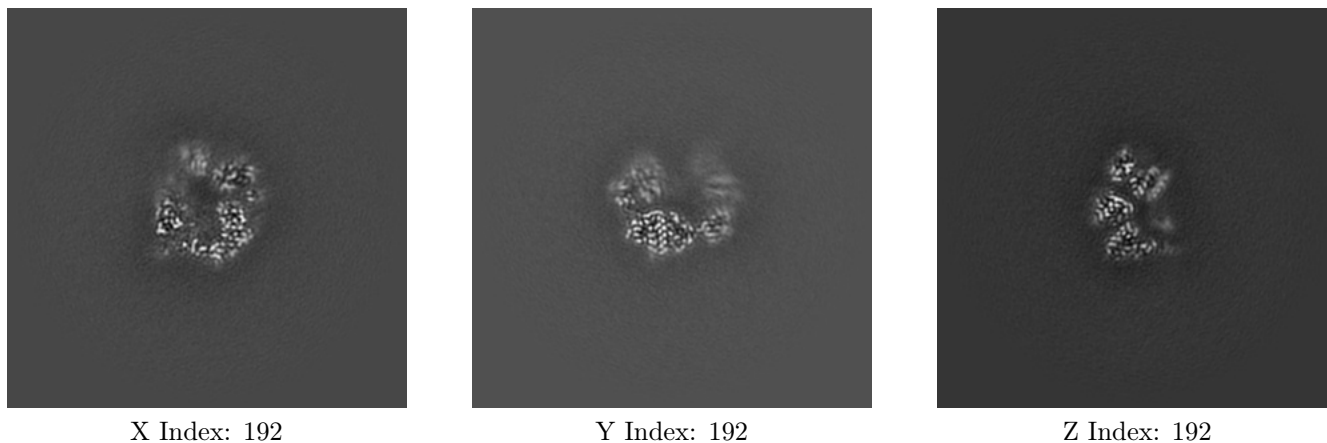
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map
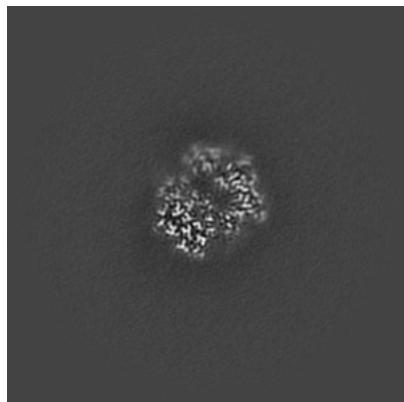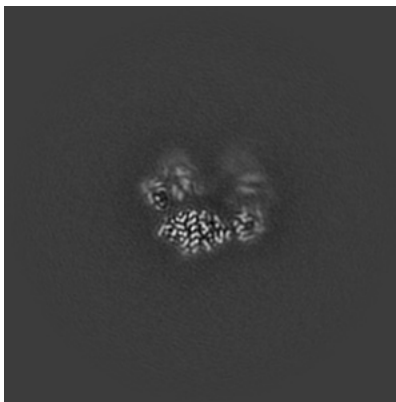
| X Index: 183 | Y Index: 194 | Z Index: 170 |
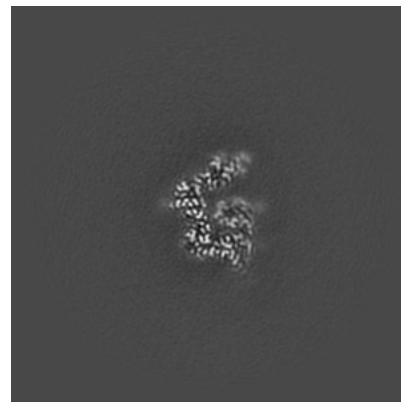
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

6.4.1 Primary map
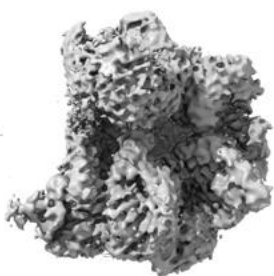
| X | Y | Z |
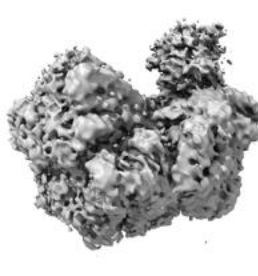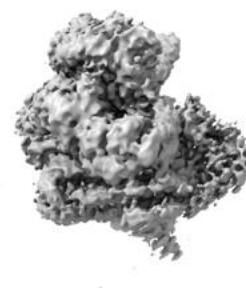
The images above show the 3D surface view of the map at the recommended contour level 0.09. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5   Mask visualisation ⓘ

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

7   Map analysis ⓘ

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

7.1   Map-value distribution ⓘ
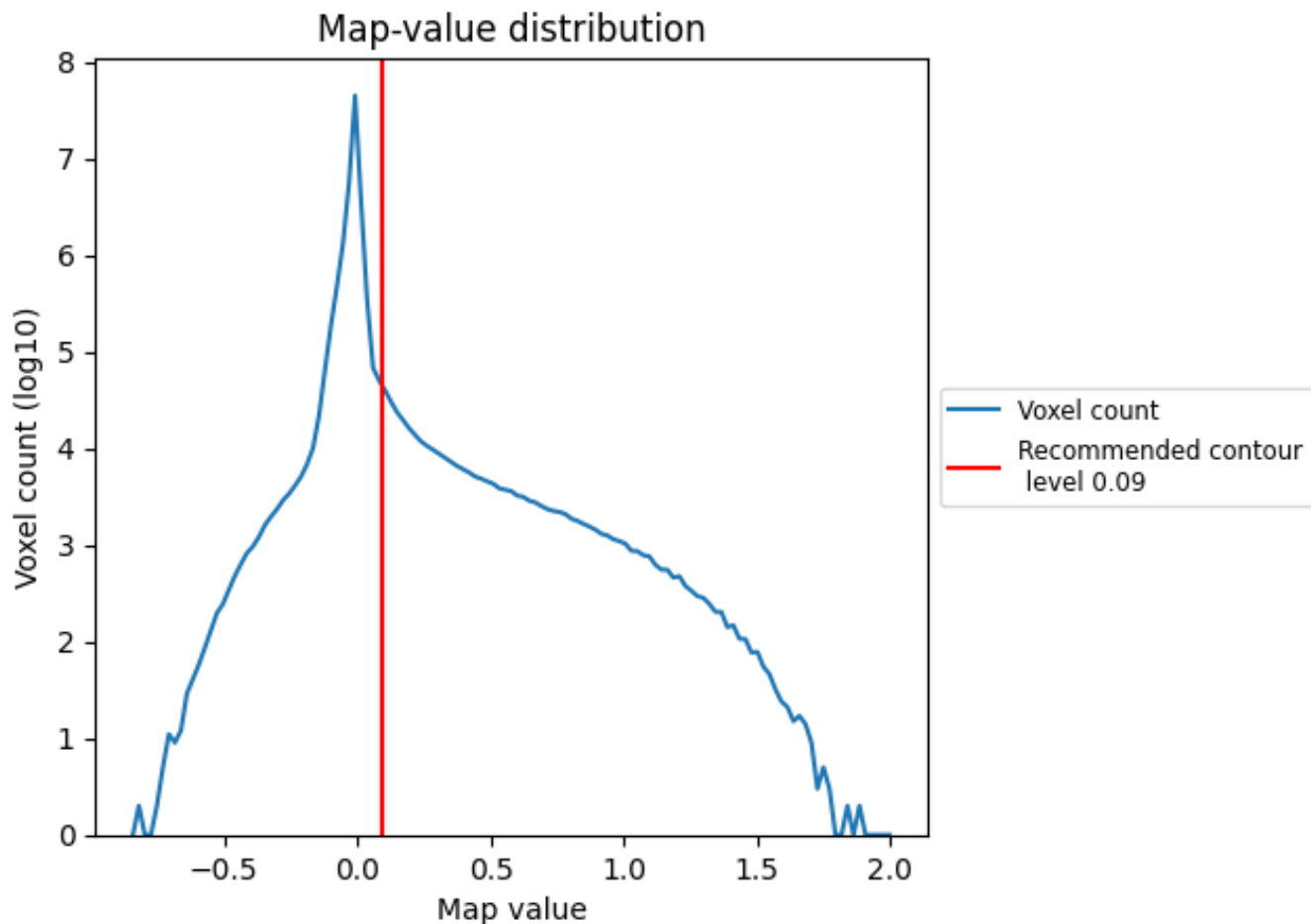
The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2 Volume estimate ⓘ
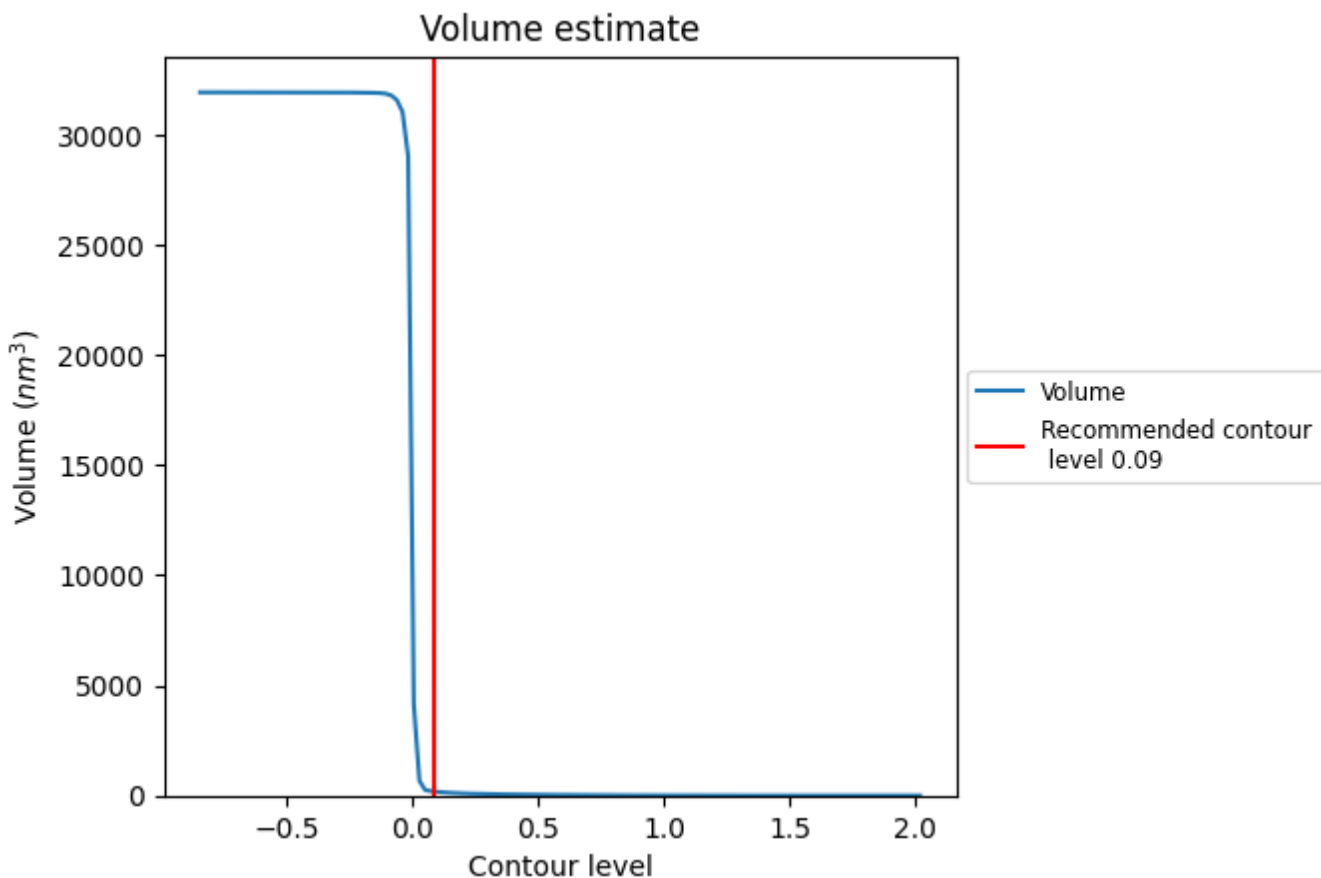
The volume at the recommended contour level is 182 nm^3; this corresponds to an approximate mass of 165 kDa.

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

7.3   Rotationally averaged power spectrum (i)
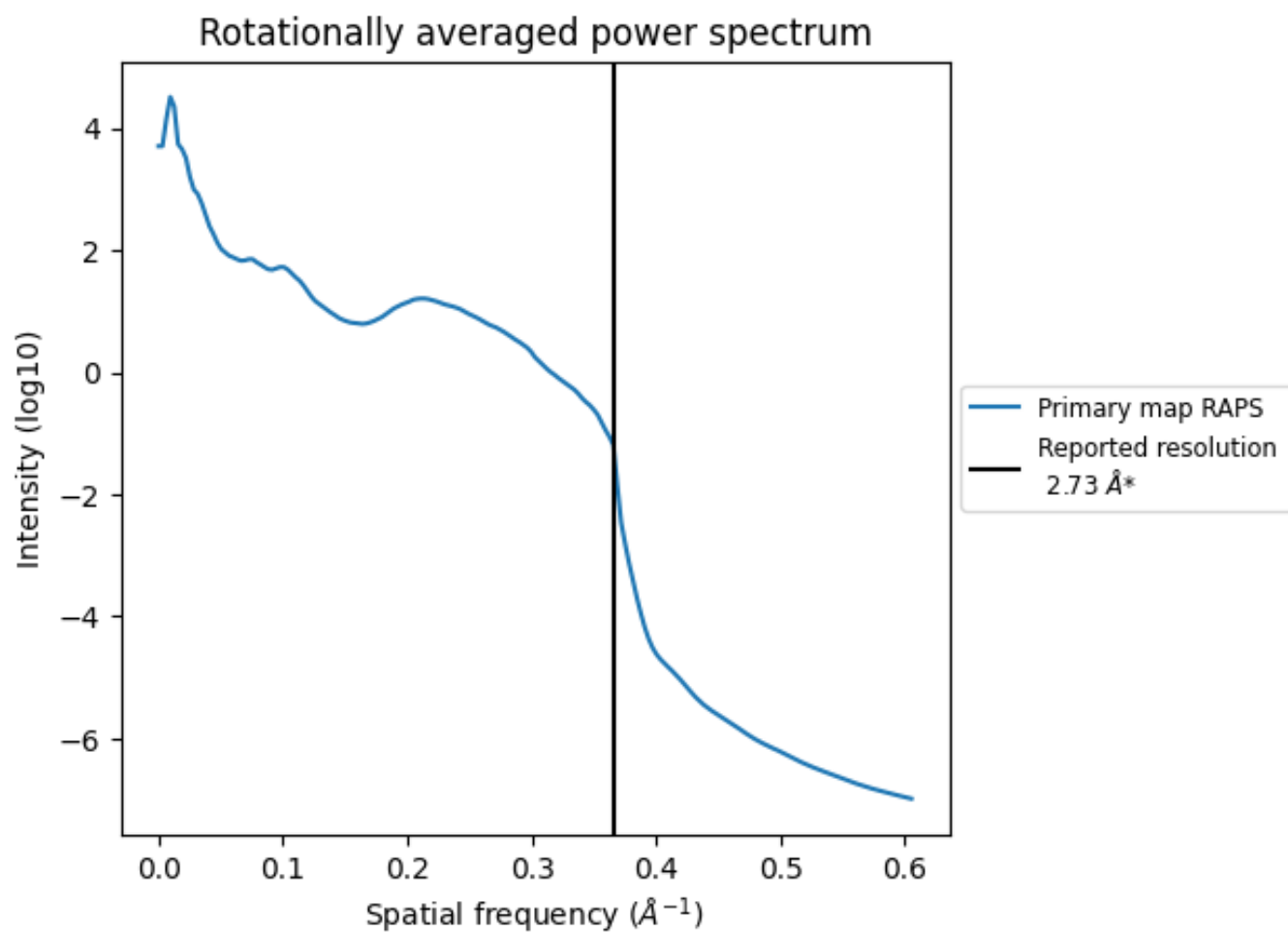
*Reported resolution corresponds to spatial frequency of 0.366 Å^{-1}

8 Fourier-Shell correlation ⓘ

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

9   Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-25426 and PDB model 7STE. Per-residue inclusion information can be found in section 3 on page 7.

9.1   Map-model overlay ⓘ

| X | Y | Z |
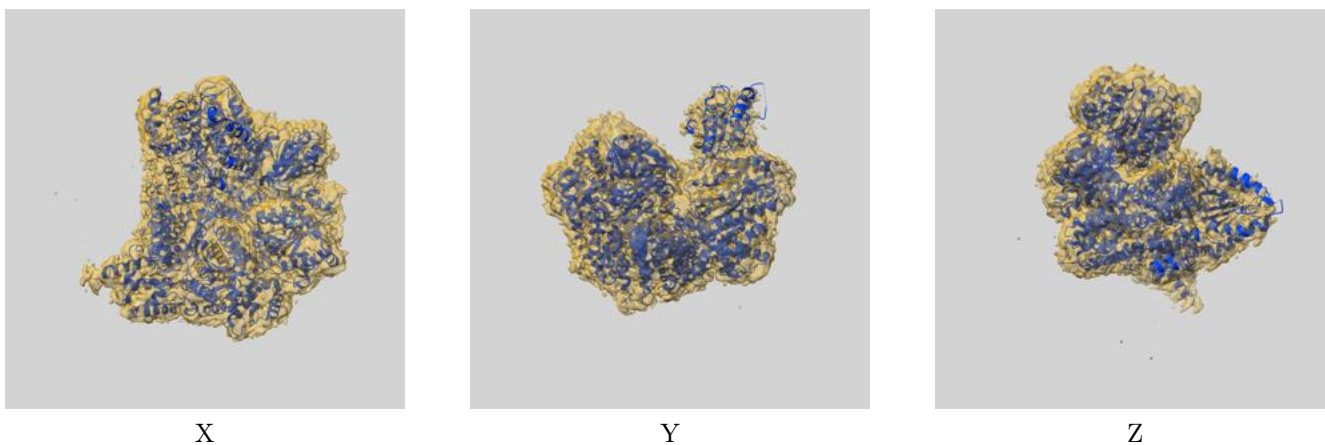
The images above show the 3D surface view of the map at the recommended contour level 0.09 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2   Q-score mapped to coordinate model ⓘ
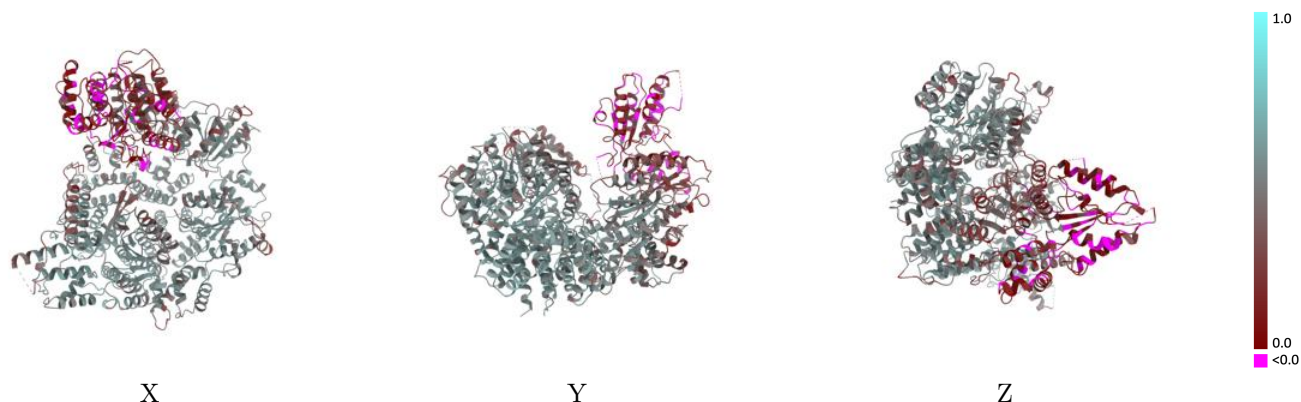
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 ⓘ
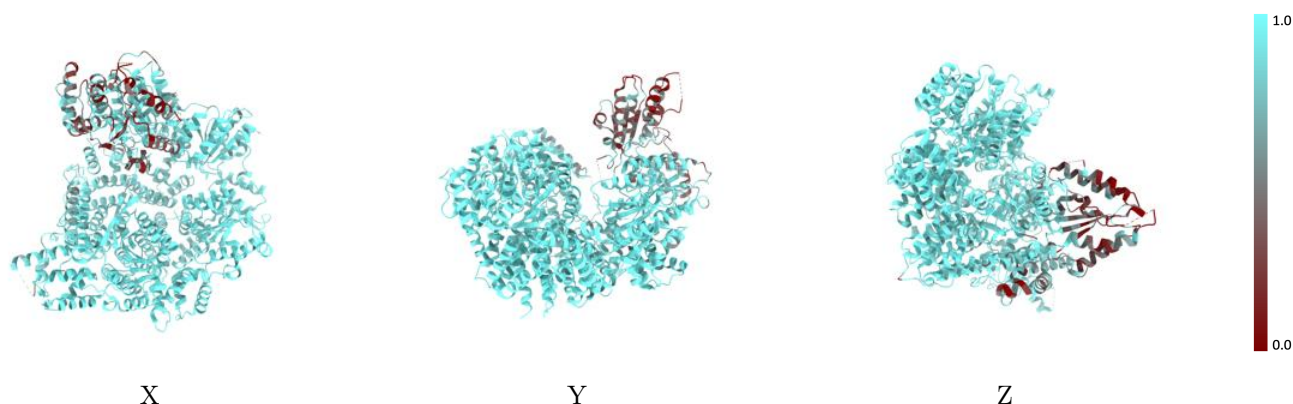
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.09).

9.4 Atom inclusion ⓘ
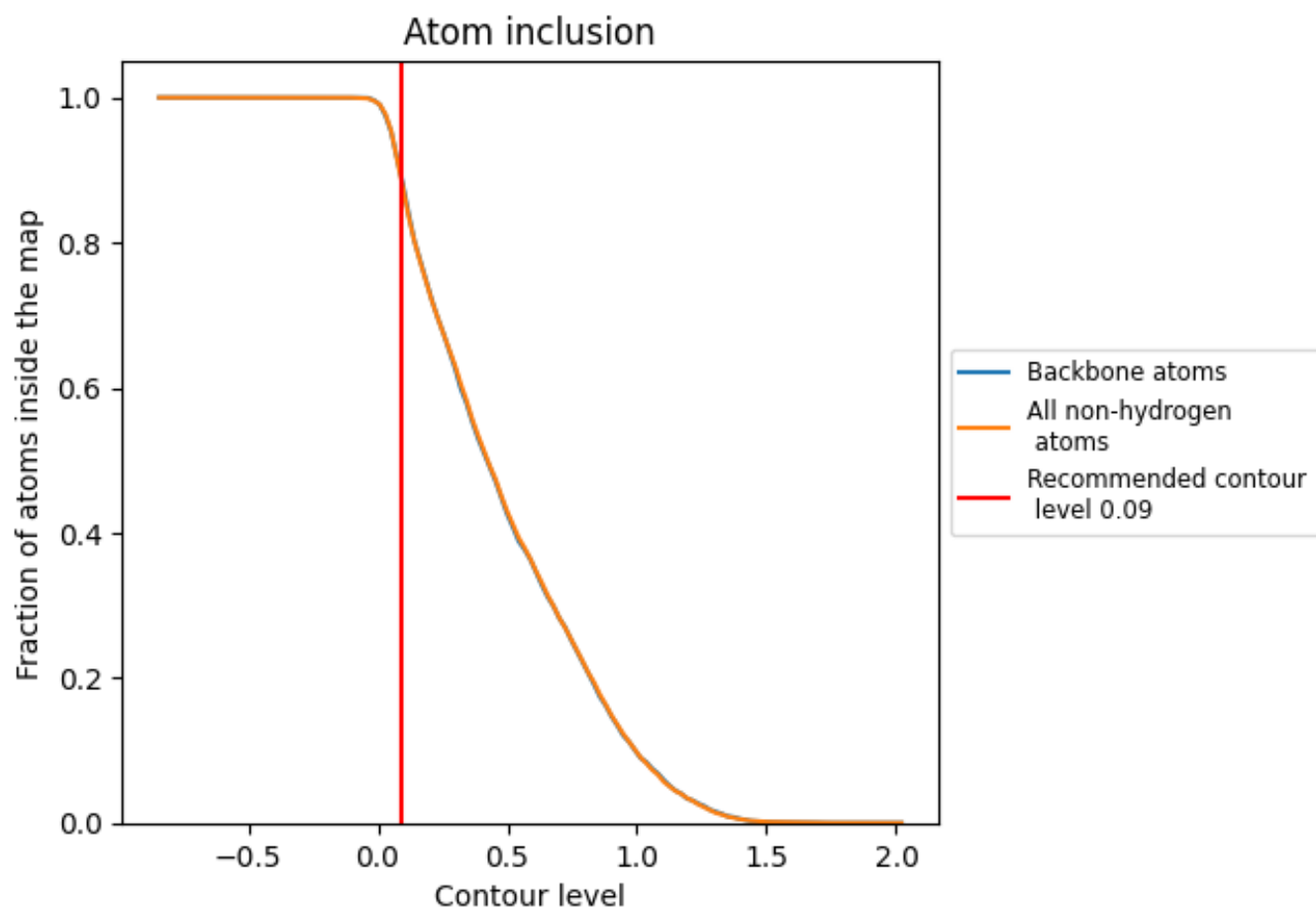
At the recommended contour level, 89% of all backbone atoms, 89% of all non-hydrogen atoms, are inside the map.

9.5   Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.09) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8893	0.4370
A	0.7051	0.2740
B	0.9276	0.3970
C	0.9775	0.5190
D	0.9798	0.5360
E	0.9691	0.5300

1.0

0.0
<0.0