wwPDB EM Validation Summary Report (i)

Nov 3, 2024 – 02:43 am GMT

PDB ID	:	4BOT
EMDB ID	:	EMD-2383
Title	:	The structure and super-organization of acetylcholine receptor- rapsyn complexes class E
Authors	:	Zuber, B.; Unwin, N.
Deposited on	:	2013-05-22
Resolution	:	42.00 Å(reported)
Based on initial model	:	2BG9

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

We welcome your comments at *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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

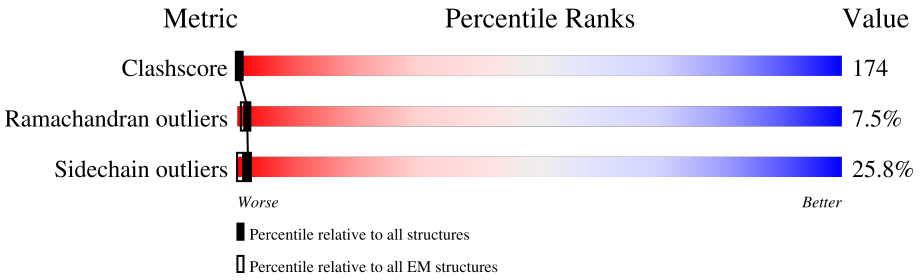
EMDB validation analysis	:	0.0.1.dev113
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 42.00 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=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	A	461	14% 6% 51% 20% · 20%
1	D	461	11% 7% 51% 21% · 20%
2	B	493	6% 5% 49% 19% · 25%
3	C	522	7% 7% 43% 19% · 29%
4	E	505	· 6% 46% 18% · 27%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 14924 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 ACETYLCHOLINE RECEPTOR SUBUNIT ALPHA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	370	Total	C	N	O	S	0	0
			2991	1954	478	540	19		
1	D	370	Total	C	N	O	S	0	0
			2991	1954	478	540	19		

- Molecule 2 is a protein called ACETYLCHOLINE RECEPTOR BETA SUBUNIT.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	370	Total	C	N	O	S	0	0
			2972	1938	465	554	15		

- Molecule 3 is a protein called ACETYLCHOLINE RECEPTOR DELTA SUBUNIT.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	370	Total	C	N	O	S	0	1
			2983	1944	489	536	14		

- Molecule 4 is a protein called ACETYLCHOLINE RECEPTOR GAMMA SUBUNIT.

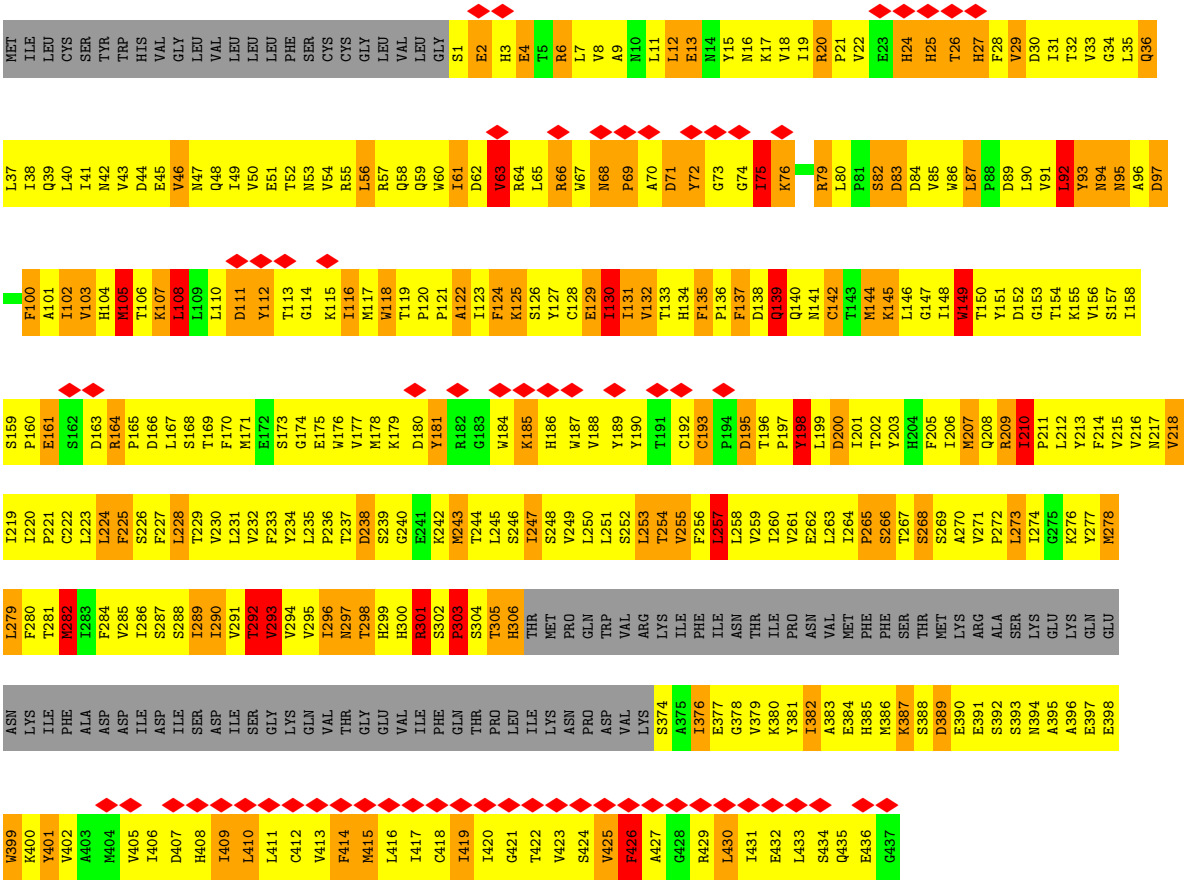
Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	371	Total	C	N	O	S	0	1
			2987	1948	478	551	10		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

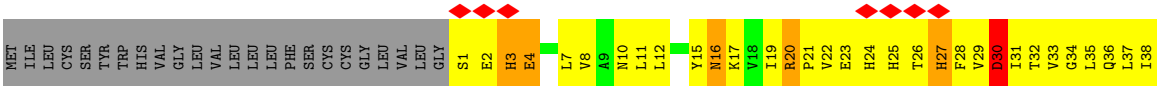
• Molecule 1: ACETYLCHOLINE RECEPTOR SUBUNIT ALPHA

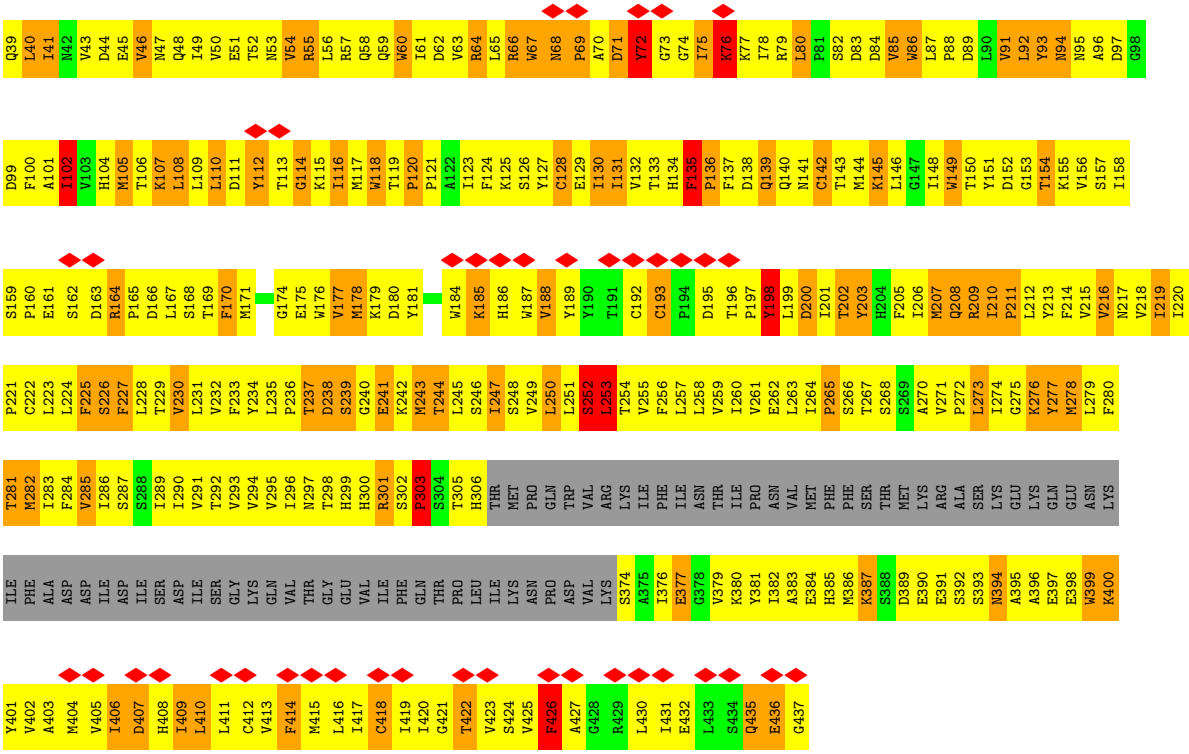
Chain A:



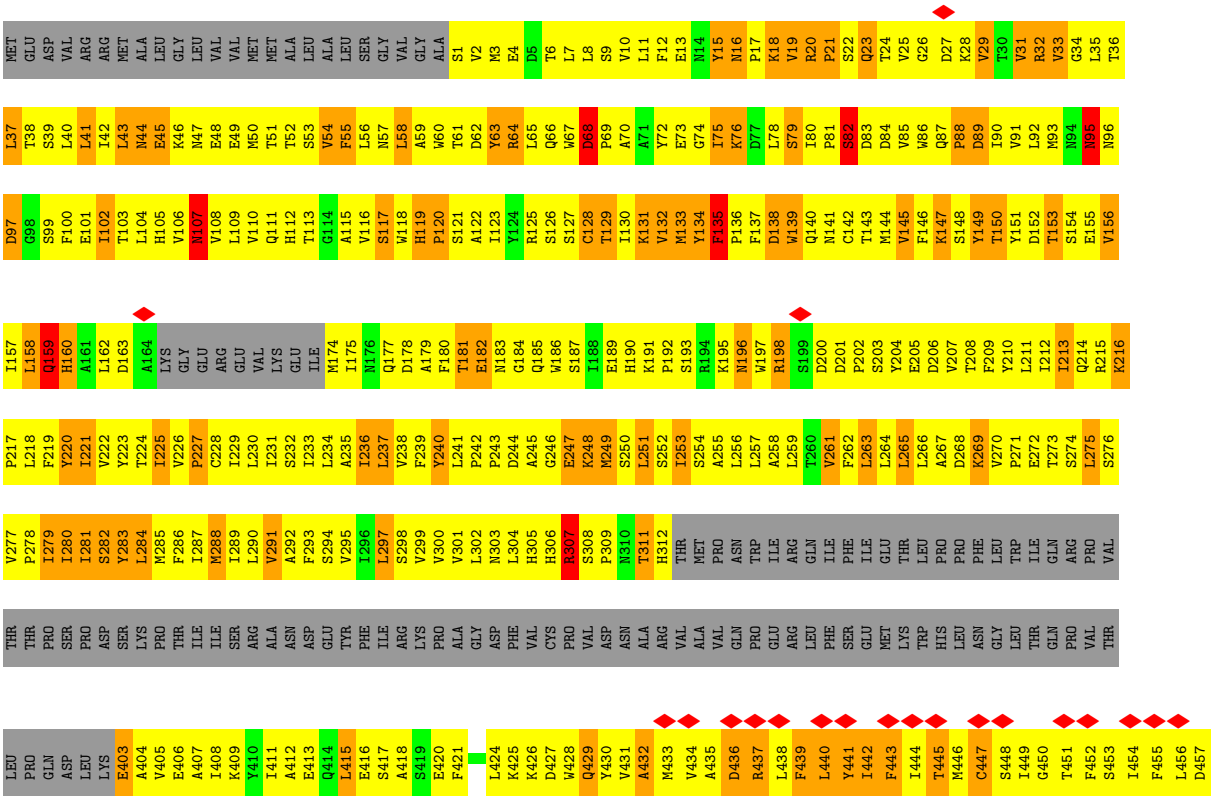
• Molecule 1: ACETYLCHOLINE RECEPTOR SUBUNIT ALPHA

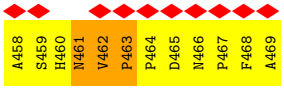
Chain D:





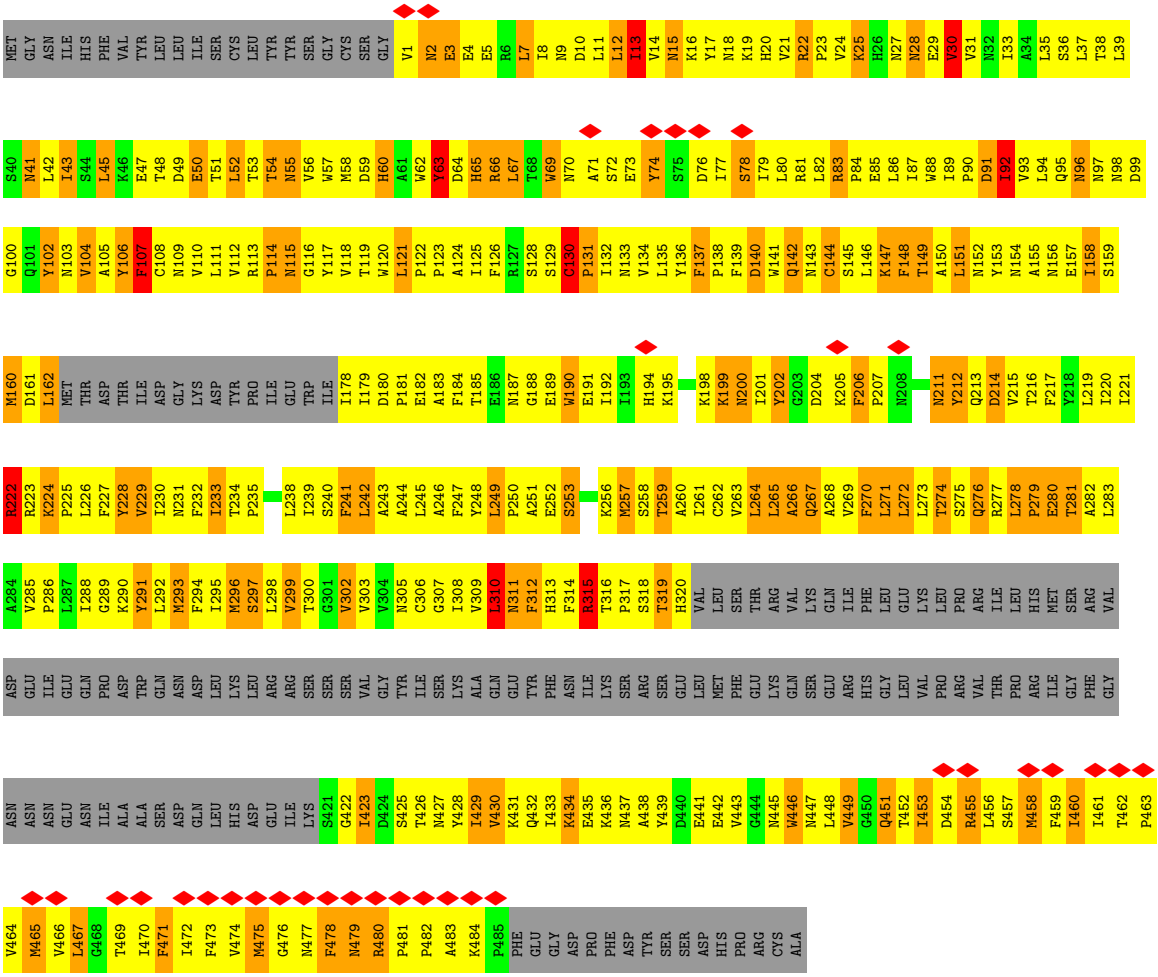
• Molecule 2: ACETYLCHOLINE RECEPTOR BETA SUBUNIT





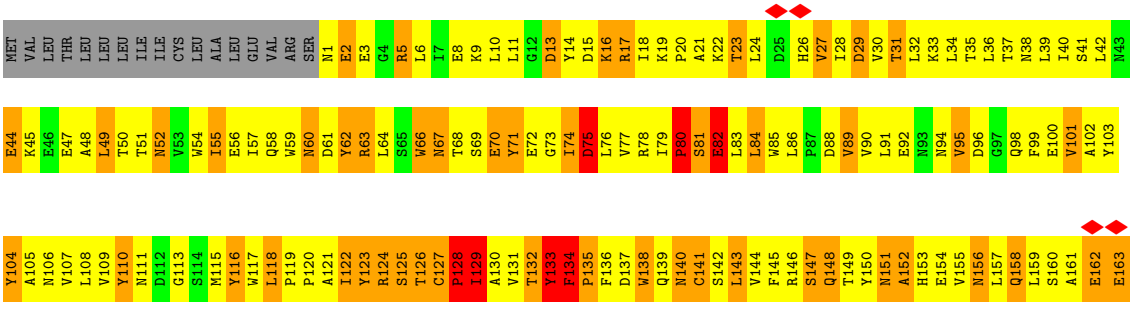
• Molecule 3: ACETYLCHOLINE RECEPTOR DELTA SUBUNIT

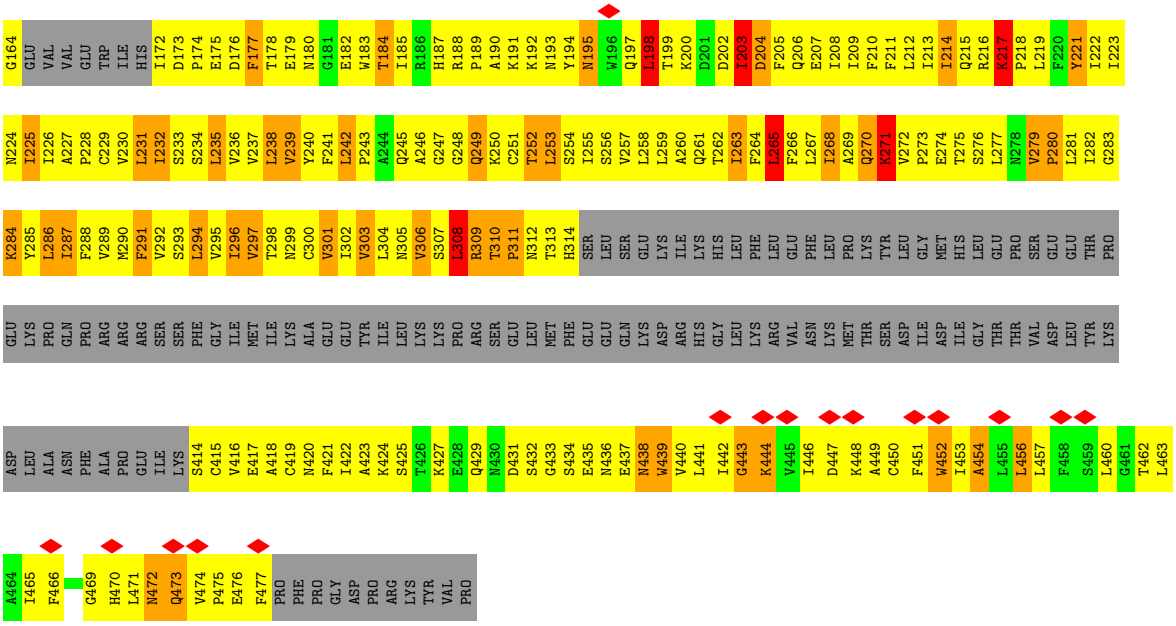
Chain C:



• Molecule 4: ACETYLCHOLINE RECEPTOR GAMMA SUBUNIT

Chain E:




G164 GLU VAL VAL GLU TRP ILE HIS I172 D173 P174 E175 D176 F177 T178 E179 N180 G181 E182 W183 T184 I185 R186 H187 R188 P189 A190 K191 K192 N193 Y194 N195 W196 Q197 L198 T199 K200 D201 D202 I203 D204 F205 Q206 E207 I208 I209 F210 F211 L212 I213 I214 Q215 R216 K217 P218 L219 F220 Y221 I222 I223
N224 I225 I226 A227 P228 C229 V230 L231 I232 S233 S234 L235 V236 V237 L238 V239 Y240 F241 L242 P243 A244 Q245 A246 G247 G248 Q249 K250 C251 T252 L253 S254 I255 S256 V257 L258 L259 A260 Q261 T262 I263 F264 L265 F266 L267 I268 A269 Q270 K271 V272 P273 E274 T275 S276 L277 N278 V279 P280 L281 I282 G283
K284 Y285 L286 I287 F288 V289 M290 F291 V292 S293 L294 V295 I296 V297 T298 N299 C300 V301 I302 V303 L304 N305 V306 S307 L308 R309 T310 P311 N312 T313 H314 SER LEU SER GLU LYS ILE LYS HIS LEU PHE LEU GLU PHE LEU PRO LYS TYR LEU GLY MET HIS LEU GLU PRO SER GLU GLU THR PRO
GLU LYS PRO GLN PRO ARG ARG ARG SER SER PHE GLY ILE MET ILE LYS ALA GLU GLU TYR ILE LEU LYS LYS PRO ARG SER GLU LEU MET PHE GLU GLU GLN LYS ASP ARG HIS GLY LEU LYS ARG VAL ASN LYS MET THR SER ASP ILE ASP ILE GLY THR THR VAL ASP LEU TYR LYS
ASP LEU ALA ASN PHE ALA PRO GLU ILE LYS S414 C415 V416 E417 A418 C419 N420 F421 I422 A423 K424 S425 T426 K427 E428 Q429 N430 D431 S432 G433 S434 E435 N436 E437 N438 W439 V440 L441 I442 G443 K444 V445 I446 D447 K448 A449 C450 F451 W452 I453 A454 L455 L456 L457 F458 S459 L460 G461 T462 L463
A464 I465 F466 G469 H470 L471 N472 Q473 V474 P475 E476 F477 PRO PHE PRO GLY ASP PRO ARG LYS TYR VAL PRO

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	TOMOGRAPHY	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of tilted images used	3564	Depositor
Resolution determination method	Not provided	
CTF correction method	Not provided	
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	3000	Depositor
Maximum defocus (nm)	6000	Depositor
Magnification	80213	Depositor
Image detector	GATAN ULTRASCAN 4000 (4k x 4k)	Depositor
Maximum voxel value	1.158	Depositor
Minimum voxel value	-0.778	Depositor
Average voxel value	0.000	Depositor
Voxel value standard deviation	0.068	Depositor
Recommended contour level	0.244	Depositor
Tomogram size (Å)	448.8, 448.8, 448.8	wwPDB
Tomogram dimensions	60, 60, 60	wwPDB
Tomogram angles (°)	90.0, 90.0, 90.0	wwPDB
Grid spacing (Å)	7.48, 7.48, 7.48	Depositor

5 Model quality

5.1 Standard geometry

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	0.72	3/3069 (0.1%)	1.03	10/4186 (0.2%)
1	D	0.74	2/3069 (0.1%)	1.01	6/4186 (0.1%)
2	B	0.76	2/3048 (0.1%)	0.99	4/4162 (0.1%)
3	C	0.74	2/3059 (0.1%)	1.03	9/4175 (0.2%)
4	E	0.74	6/3057 (0.2%)	1.01	9/4174 (0.2%)
All	All	0.74	15/15302 (0.1%)	1.01	38/20883 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	2
3	C	0	2
All	All	0	4

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	129	THR	C-N	-8.40	1.14	1.34
1	A	118	TRP	CB-CG	7.91	1.64	1.50
1	D	208	GLN	C-N	7.58	1.51	1.34
4	E	8	GLU	CB-CG	6.52	1.64	1.52
3	C	265	LEU	C-N	6.18	1.48	1.34

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	266	ALA	N-CA-CB	10.40	124.66	110.10
4	E	198	LEU	CA-CB-CG	7.18	131.82	115.30
3	C	315	ARG	NE-CZ-NH2	7.13	123.86	120.30
1	A	209	ARG	NE-CZ-NH2	6.96	123.78	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	263	ILE	CG1-CB-CG2	-6.67	96.73	111.40

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	63	TYR	Sidechain
3	C	74	TYR	Sidechain
1	D	277	TYR	Sidechain
1	D	72	TYR	Sidechain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2991	0	3005	1072	0
1	D	2991	0	3006	1056	0
2	B	2972	0	2952	1088	0
3	C	2983	0	2987	1159	0
4	E	2987	0	2994	1090	0
All	All	14924	0	14944	5204	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 174.

The worst 5 of 5204 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)
4:E:183:TRP:CB	4:E:216:ARG:HG2	1.33	1.53
2:B:134:TYR:CE1	2:B:213:ILE:HG13	1.44	1.51
1:A:167:LEU:HD12	1:A:178:MET:CB	1.43	1.48
1:A:167:LEU:CD1	1:A:178:MET:HB2	1.46	1.45
1:D:261:VAL:O	1:D:265:PRO:HD2	1.22	1.38

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	366/461 (79%)	288 (79%)	49 (13%)	29 (8%)	1 10
1	D	366/461 (79%)	294 (80%)	41 (11%)	31 (8%)	0 9
2	B	364/493 (74%)	274 (75%)	58 (16%)	32 (9%)	0 9
3	C	364/522 (70%)	288 (79%)	58 (16%)	18 (5%)	2 16
4	E	365/505 (72%)	281 (77%)	58 (16%)	26 (7%)	1 11
All	All	1825/2442 (75%)	1425 (78%)	264 (14%)	136 (8%)	1 10

5 of 136 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	GLU
1	A	27	HIS
1	A	76	LYS
1	A	83	ASP
1	A	102	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	343/427 (80%)	248 (72%)	95 (28%)	0 2
1	D	343/427 (80%)	258 (75%)	85 (25%)	0 3
2	B	340/449 (76%)	262 (77%)	78 (23%)	0 4
3	C	335/475 (70%)	243 (72%)	92 (28%)	0 2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	E	337/463 (73%)	249 (74%)	88 (26%)	0 3
All	All	1698/2241 (76%)	1260 (74%)	438 (26%)	2 3

5 of 438 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	274	THR
1	D	94	ASN
4	E	184	THR
3	C	296	MET
3	C	471	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 63 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	200	ASN
4	E	153	HIS
1	D	42	ASN
4	E	148	GLN
4	E	206	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	1

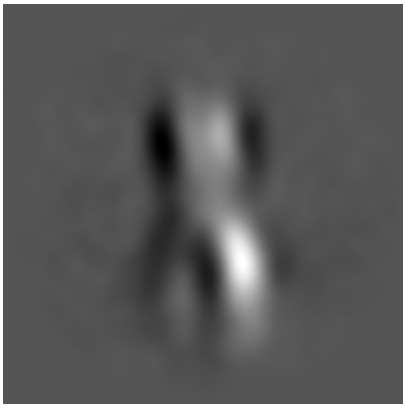
All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	129:THR	C	130:ILE	N	1.14

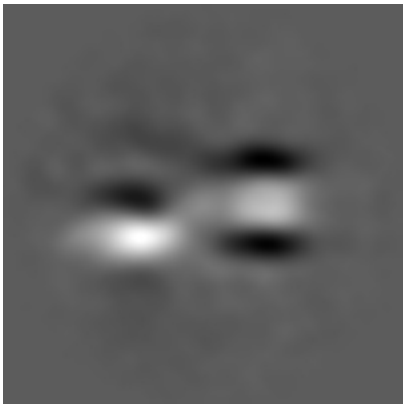
6 Tomogram visualisation

This section contains visualisations of the EMDB entry EMD-2383. These allow visual inspection of the internal detail of the tomogram and identification of artifacts.

6.1 Orthogonal projections



X



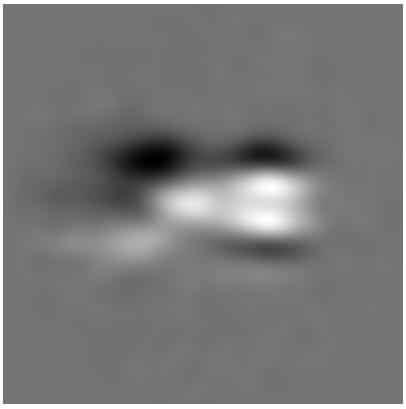
Y

Z

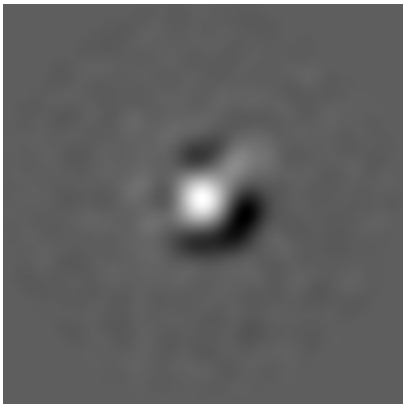
The images above show the tomogram projected in three orthogonal directions.

6.2 Central slices

X Index: 30



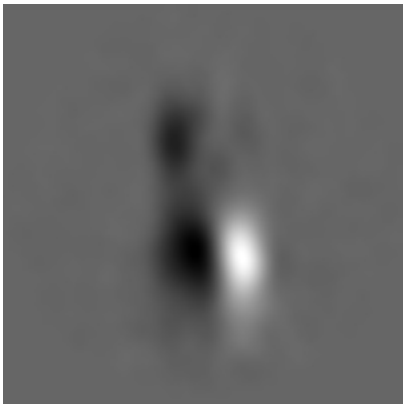
Y Index: 30



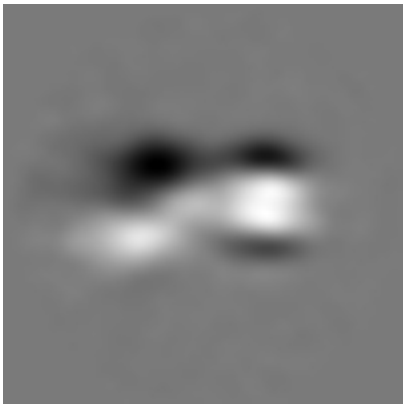
Z Index: 30

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

6.3 Largest variance slices (i)



X Index: 35

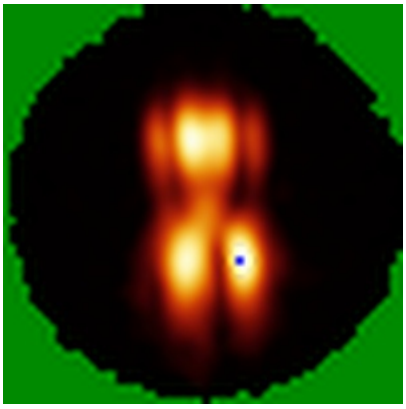


Y Index: 28

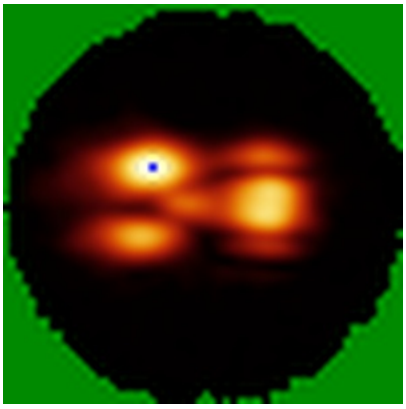
Z Index: 21

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

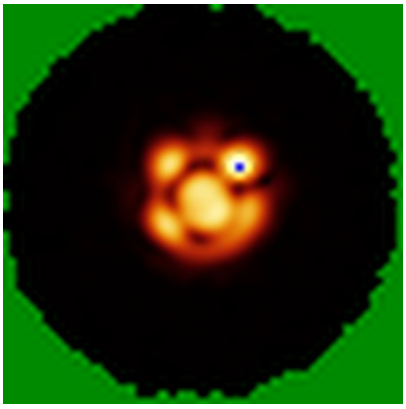
6.4 Orthogonal standard-deviation projections (False-color) (i)



X



Y



Z

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

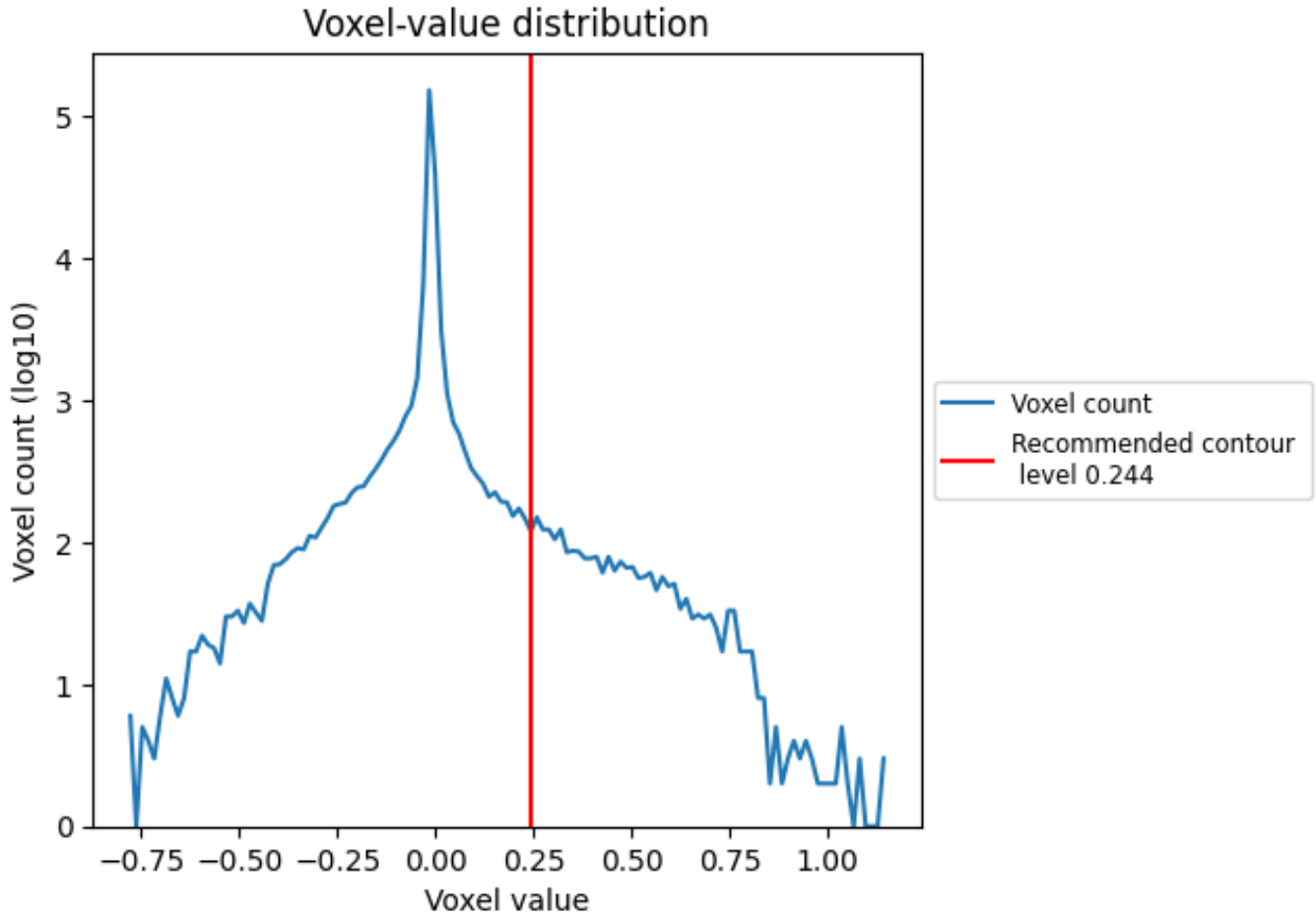
6.5 Mask visualisation (i)

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

7 Tomogram analysis (i)

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

7.1 Voxel-value distribution (i)



The voxel-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic.

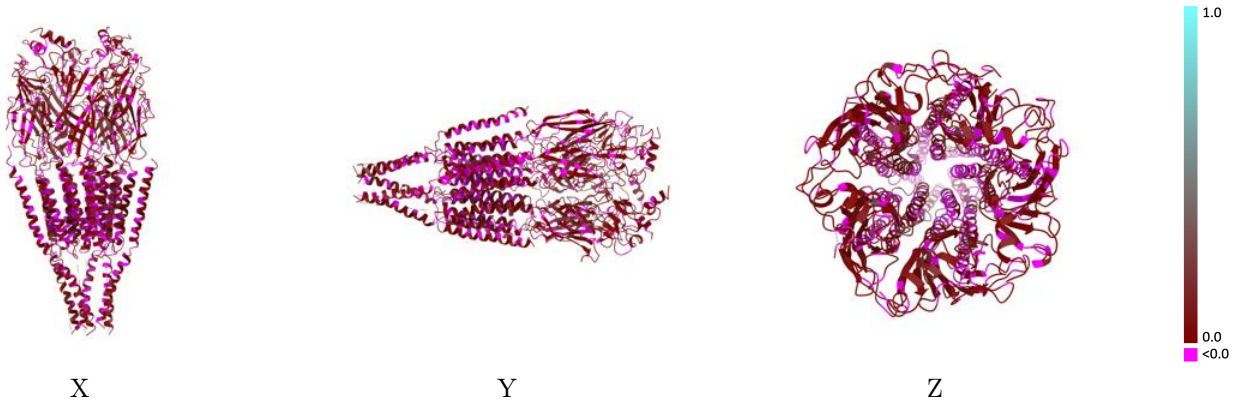
8 Map-model fit

This section contains information regarding the fit between EMDB map EMD-2383 and PDB model 4BOT. Per-residue inclusion information can be found in section 3 on page 4.

8.1 Map-model overlay

This section was not generated.

8.2 Q-score mapped to coordinate model



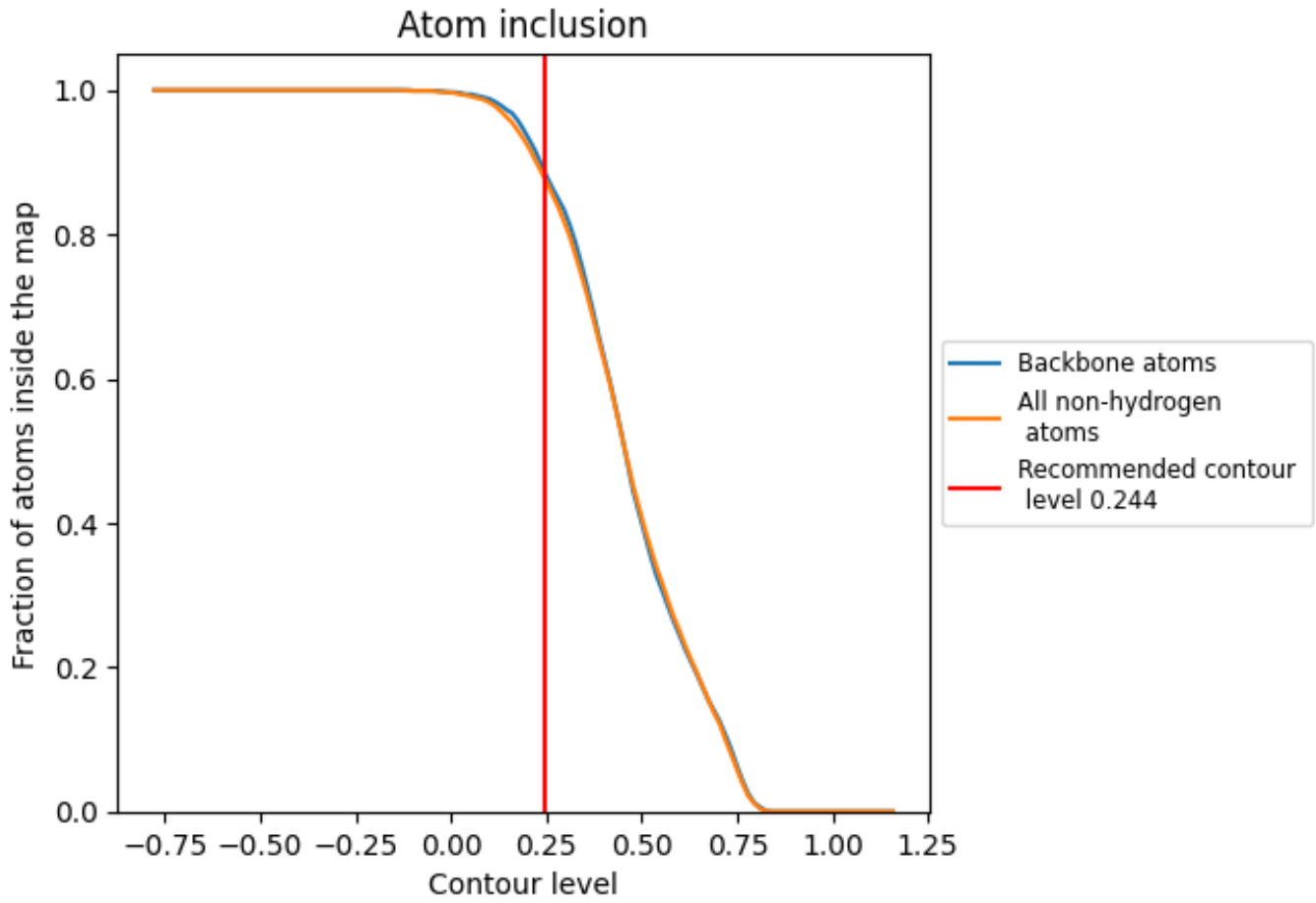
X Y Z

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.

8.3 Atom inclusion mapped to coordinate model

This section was not generated.

8.4 Atom inclusion (i)



At the recommended contour level, 89% of all backbone atoms, 88% of all non-hydrogen atoms, are inside the map.

8.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.244) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8790	0.0410
A	0.8140	0.0290
B	0.9120	0.0420
C	0.8950	0.0480
D	0.8500	0.0480
E	0.9260	0.0380