



wwPDB EM Validation Summary Report ⓘ

Oct 13, 2024 – 07:50 pm BST

PDB ID : 4BOR
EMDB ID : EMD-2382
Title : The structure and super-organization of acetylcholine receptor-rapsyn complexes class D
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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.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

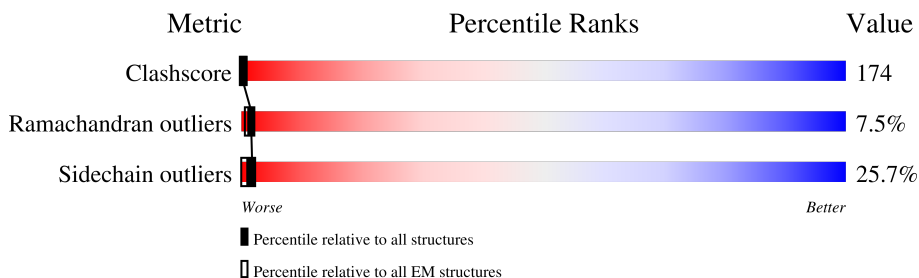
1 Overall quality at a glance

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 $\leq 5\%$. 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	461	<div> <div>12%</div> <div>6% 50% 20% . 20%</div> </div>
1	D	461	<div> <div>9%</div> <div>7% 51% 21% . 20%</div> </div>
2	B	493	<div> <div>8%</div> <div>5% 50% 19% . 25%</div> </div>
3	C	522	<div> <div>12%</div> <div>7% 43% 19% . 29%</div> </div>
4	E	505	<div> <div>13%</div> <div>6% 46% 18% . 27%</div> </div>

2 Entry composition

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		

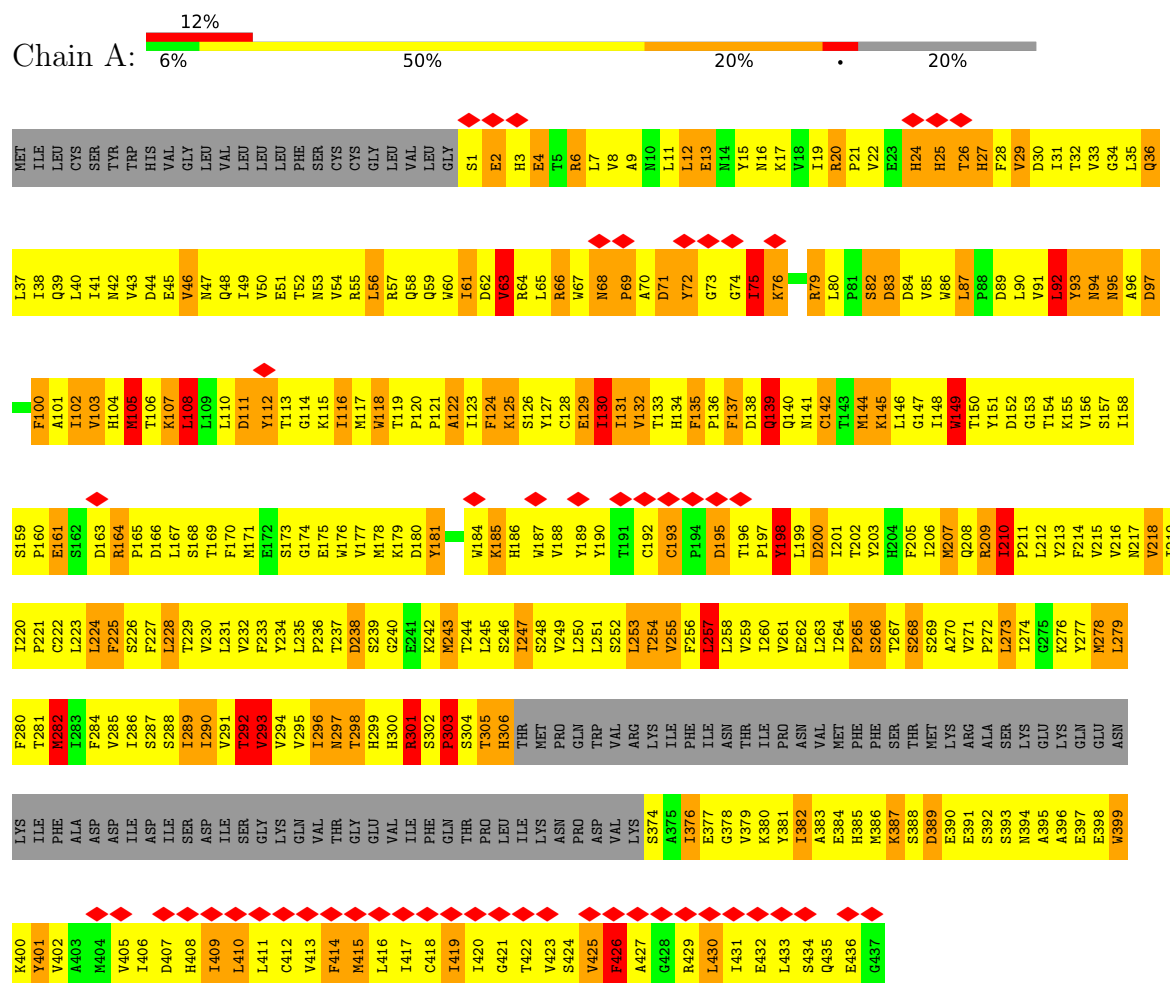
- Molecule 4 is a protein called ACETYLCHOLINE RECEPTOR GAMMA SUBUNIT.

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

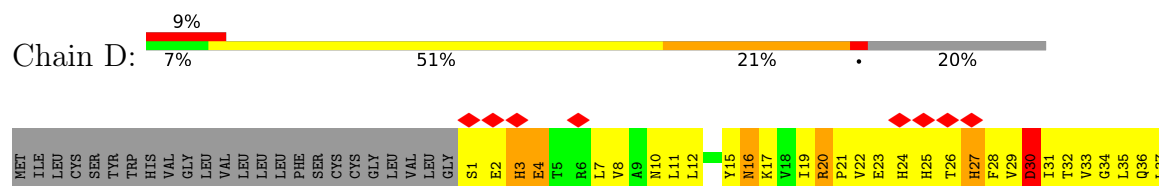
3 Residue-property plots

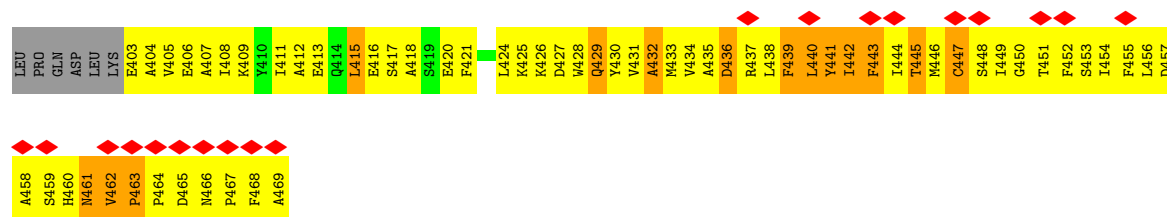
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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

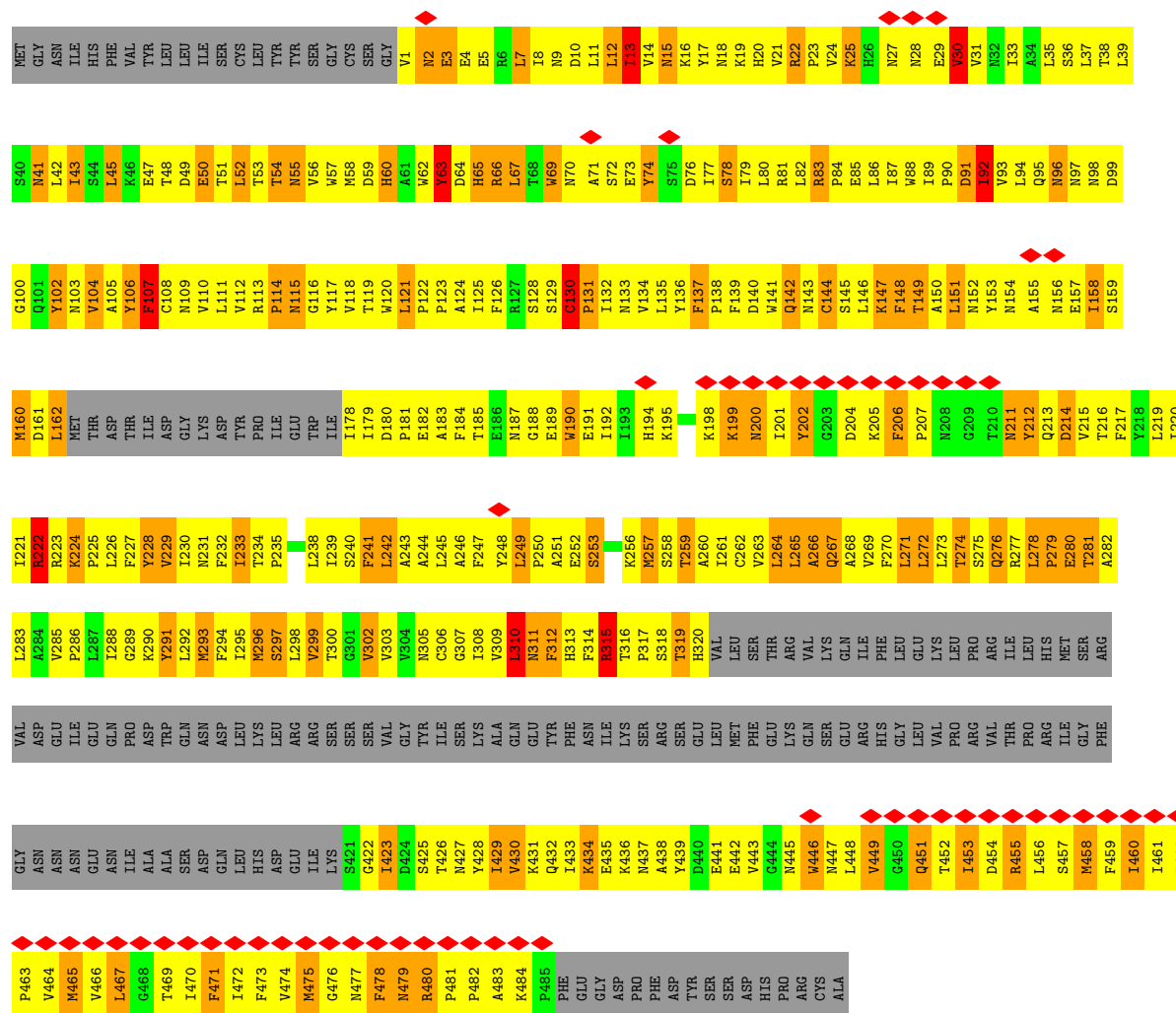


• Molecule 1: ACETYLCHOLINE RECEPTOR SUBUNIT ALPHA

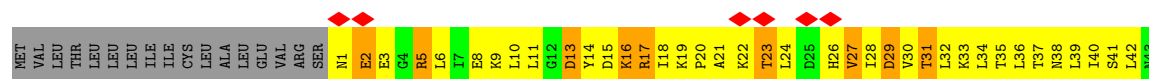




• Molecule 3: ACETYLCHOLINE RECEPTOR DELTA SUBUNIT



• Molecule 4: ACETYLCHOLINE RECEPTOR GAMMA SUBUNIT



A464	ASP	GLU	K284	M224	G164	Y104	E44
	LEU	LYS	Y285	T225	GLU	A105	K45
	ALA	PRO	L286	T226	VAL	N106	E46
	ASN	GLN	L287	A227	VAL	L107	E47
	PHE	PRO	F288	P228	GLU	L108	A48
	ALA	ARG	V289	C229	TRP	Y109	L49
	PRO	ARG	K290	L230	ILE	Y110	T50
	GLU	ARG	F291	L231	ILS	N111	T51
	ILE	SER	V292	T232	HIS	M112	N52
	LYS	SER	S293	S233	D173	G113	V53
L465	S414	PHE	L294	S234	P174	S114	W54
	C415	GLY	V295	L235	E175	M115	I55
	V416	ILE	T296	V236	D176	Y116	E56
	E417	MET	V297	V237	F177	W117	I57
	A418	ILE	T298	L238	T178	L118	Q58
	C419	LYS	N299	V239	E179	P119	W59
	N420	ALA	C300	V240	N180	P120	N60
	F421	GLU	V301	F241	G181	A121	D61
	L422	GLY	L302	L242	E182	I122	Y62
	A423	TYR	V303	P243	W183	Y123	R63
F466	K424	ILE	L304	A244	I184	R124	L64
	S425	LEU	Q305	Q245	I185	S125	S65
	T426	LYS	V306	A246	R186	T126	W66
	K427	LYS	S307	G247	H187	C127	N67
	E428	PRO	L308	G248	R188	P128	T68
	Q429	ARG	R309	Q249	P189	I129	S69
	W430	SER	T310	K250	A130	E70	E70
	D431	GLU	F311	C251	A131	V131	Y71
	S432	LEU	N312	T252	K191	T132	E72
	G433	MET	T313	L253	K192	Y133	G73
L467	S434	PHE	H314	S254	K193	F134	E74
	E435	GLY	SER	T255	N193	P135	I74
	N436	GLY	LEU	S256	N194	F136	D75
	E437	GLN	SER	V257	N195	D137	L76
	W438	LYS	GLU	L258	Y196	W138	V77
	Q439	ASP	LYS	L259	K197	Q139	R78
	V440	ARG	ILE	A260	L198	I79	I79
	L441	HIS	LYS	Q261	K200	C141	S81
	L442	GLY	HIS	T262	T199	S142	E82
	G443	LEU	LEU	L263	K201	L143	E83
V445	K444	LYS	PHE	F264	D201	L144	L83
	E445	ARG	LEU	L265	D202	V144	L84
	L446	VAL	GLU	F266	K203	F145	W85
	L447	ASN	PHE	L267	D204	R146	L86
	D447	LYS	LEU	L268	F205	S147	P87
	K448	MET	PRO	A269	T206	Q148	D88
	A449	THR	LYS	Q270	E207	T149	V89
	A450	ASP	TYR	K271	E208	Y150	V90
	F451	ILE	LEU	V272	L209	N151	L91
	L452	ILE	GLY	P273	F210	A152	E92
W452	F451	ASP	MET	E274	F211	H153	N93
	L452	ILE	HIS	T275	L212	E154	N94
	T453	GLY	LEU	S276	L213	N155	V95
	L453	THR	GLU	L277	I214	L157	D96
	A454	THR	PRO	K278	Q215	Q158	G97
	L455	VAL	SER	V279	R216	L159	Q98
	L456	ASP	GLU	P280	K217	F99	Q98
	L457	LEU	GLU	L281	P218	S160	E100
	F458	TYR	THR	L282	L219	A161	V101
	S459	LYS	PRO	G283	F220	E162	A102
L460	L460	LYS			Y221	E163	Y103
	G461				I223		
	L462						
	L463						
	L464						
	L465						
	L466						
	L467						
	L468						
	L469						

4 Experimental information

Property	Value	Source
EM reconstruction method	TOMOGRAPHY	Depositor
Imposed symmetry	POINT, Not provided	
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 ($e^-/\text{\AA}^2$)	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	1.112	Depositor
Minimum voxel value	-0.771	Depositor
Average voxel value	0.000	Depositor
Voxel value standard deviation	0.067	Depositor
Recommended contour level	0.278	Depositor
Tomogram size (\AA)	448.8, 448.8, 448.8	wwPDB
Tomogram dimensions	60, 60, 60	wwPDB
Tomogram angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Grid spacing (\AA)	7.48, 7.48, 7.48	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.73	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	-8.41	1.14	1.34
1	A	118	TRP	CB-CG	7.91	1.64	1.50
1	D	208	GLN	C-N	7.57	1.51	1.34
4	E	8	GLU	CB-CG	6.50	1.64	1.52
3	C	265	LEU	C-N	6.16	1.48	1.34

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	266	ALA	N-CA-CB	10.38	124.64	110.10
4	E	198	LEU	CA-CB-CG	7.19	131.83	115.30
3	C	315	ARG	NE-CZ-NH2	7.11	123.85	120.30
1	A	209	ARG	NE-CZ-NH2	6.92	123.76	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	263	ILE	CG1-CB-CG2	-6.66	96.75	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

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	1073	0
1	D	2991	0	3006	1063	0
2	B	2972	0	2952	1078	0
3	C	2983	0	2987	1156	0
4	E	2987	0	2994	1087	0
All	All	14924	0	14944	5194	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 5194 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	1.56
2:B:134:TYR:CE1	2:B:213:ILE:HG13	1.44	1.49
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	1.44
3:C:316:THR:CG2	3:C:317:PRO:HD2	1.53	1.37

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%)	273 (75%)	59 (16%)	32 (9%)	0	9
3	C	364/522 (70%)	289 (79%)	57 (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%)	244 (73%)	91 (27%)	0	3

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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%)	1261 (74%)	437 (26%)	2	3

5 of 437 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	276	GLN
1	D	105	MET
4	E	195	ASN
3	C	297	SER
3	C	475	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 64 such sidechains are listed below:

Mol	Chain	Res	Type
4	E	158	GLN
4	E	197	GLN
3	C	97	ASN
3	C	70	ASN
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

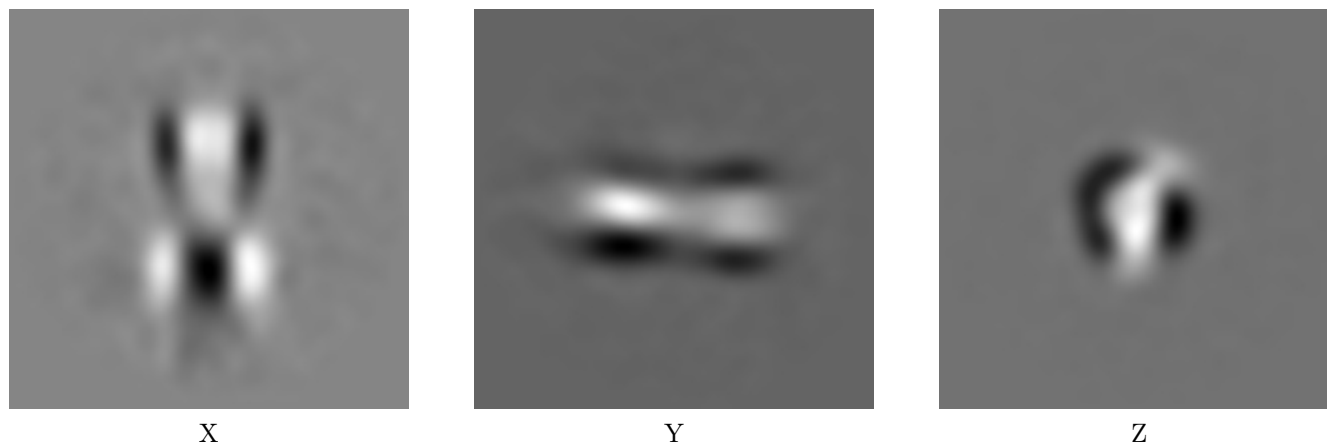
All chain breaks are listed below:

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 [i](#)

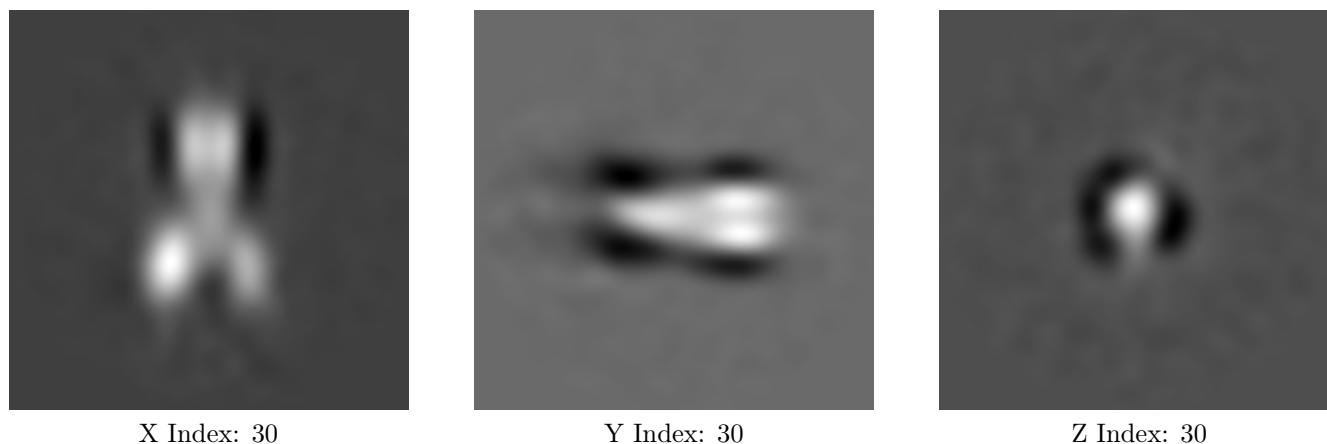
This section contains visualisations of the EMDB entry EMD-2382. These allow visual inspection of the internal detail of the tomogram and identification of artifacts.

6.1 Orthogonal projections [i](#)



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

6.2 Central slices [i](#)

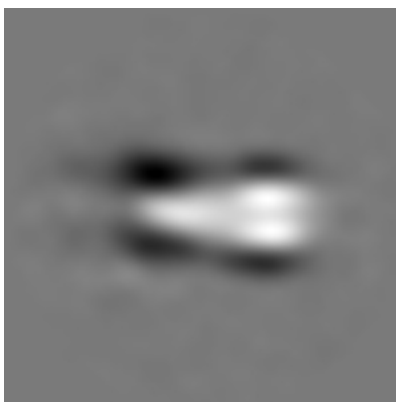


The images above show central slices of the tomogram in three orthogonal directions.

6.3 Largest variance slices [i](#)



X Index: 29



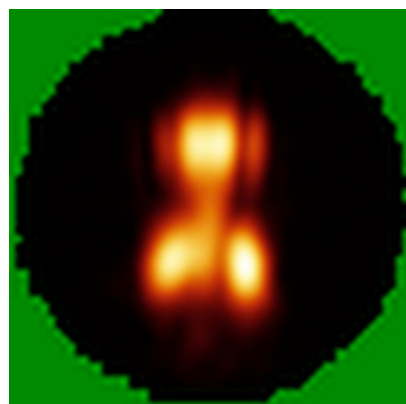
Y Index: 29



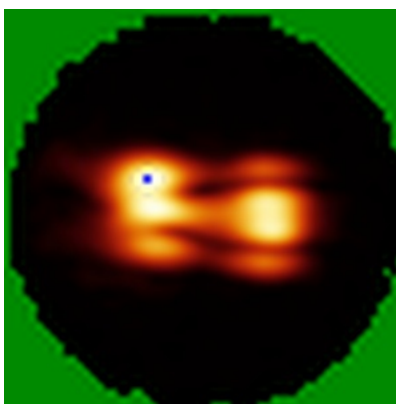
Z Index: 22

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

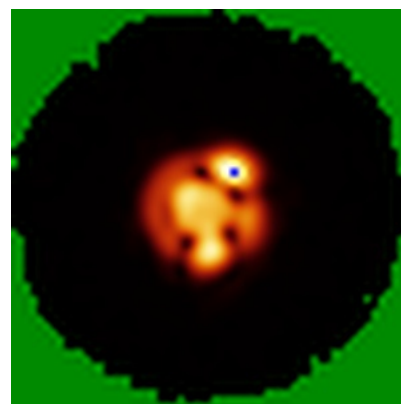
6.4 Orthogonal standard-deviation projections (False-color) [i](#)



X



Y



Z

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

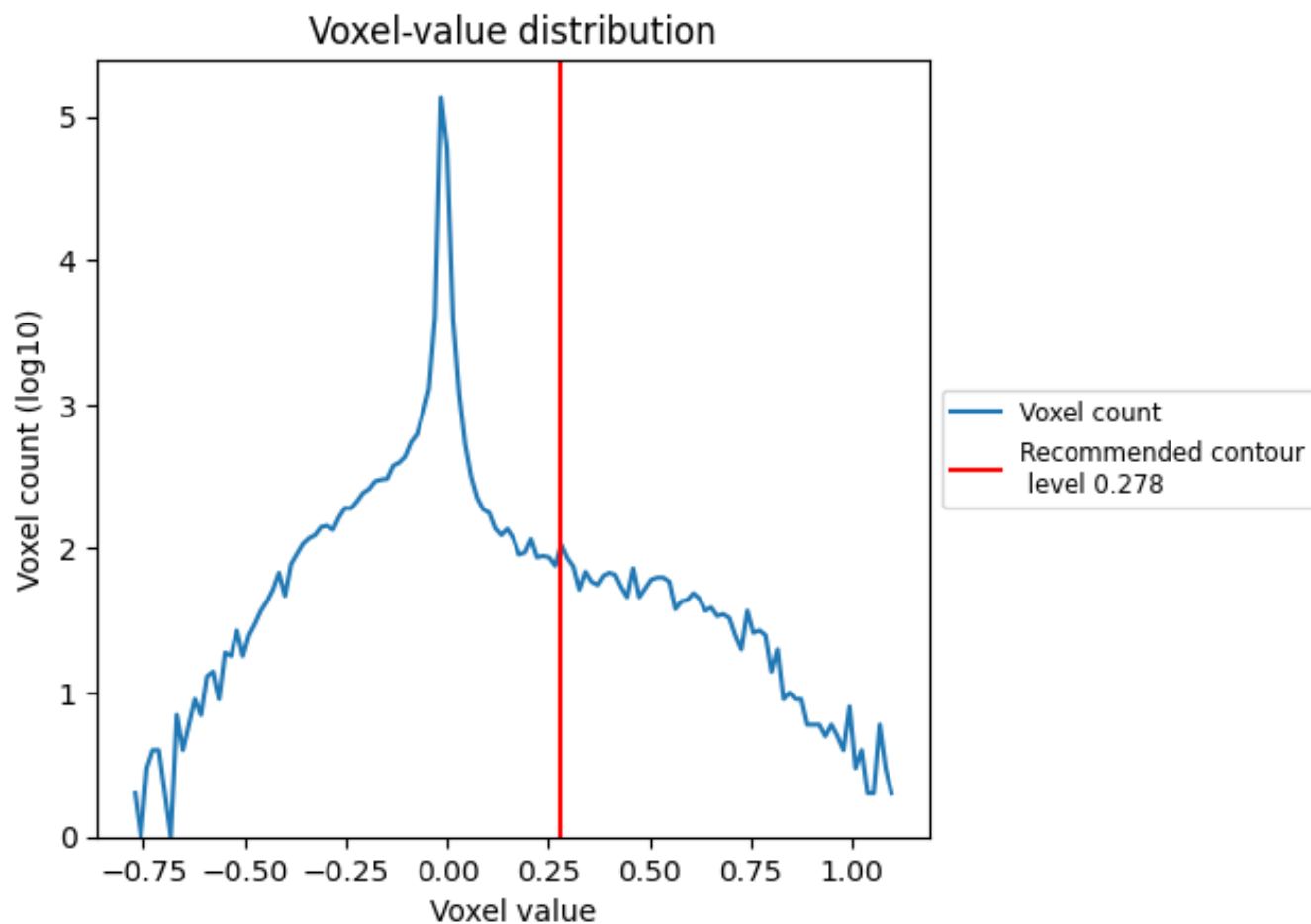
6.5 Mask visualisation [i](#)

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.

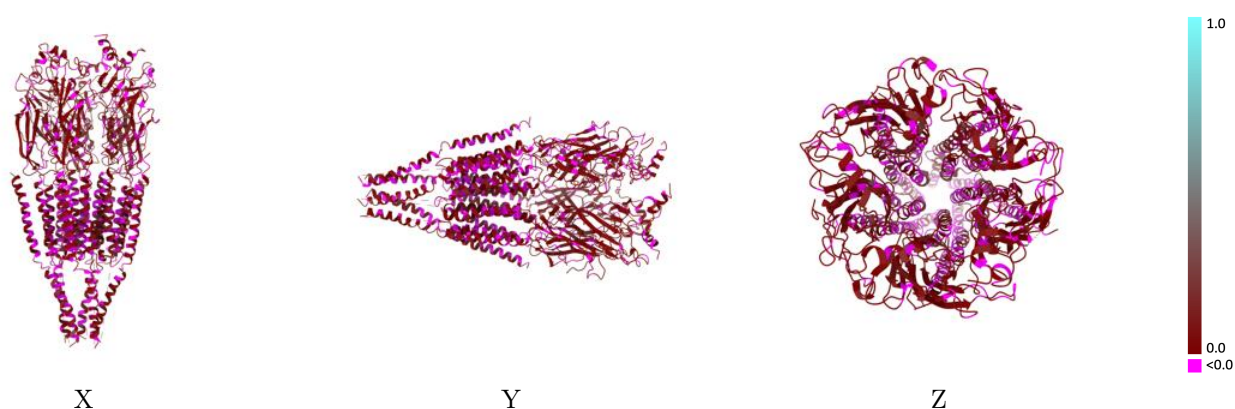
8 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-2382 and PDB model 4BOR. Per-residue inclusion information can be found in section [3](#) on page [4](#).

8.1 Map-model overlay [i](#)

This section was not generated.

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

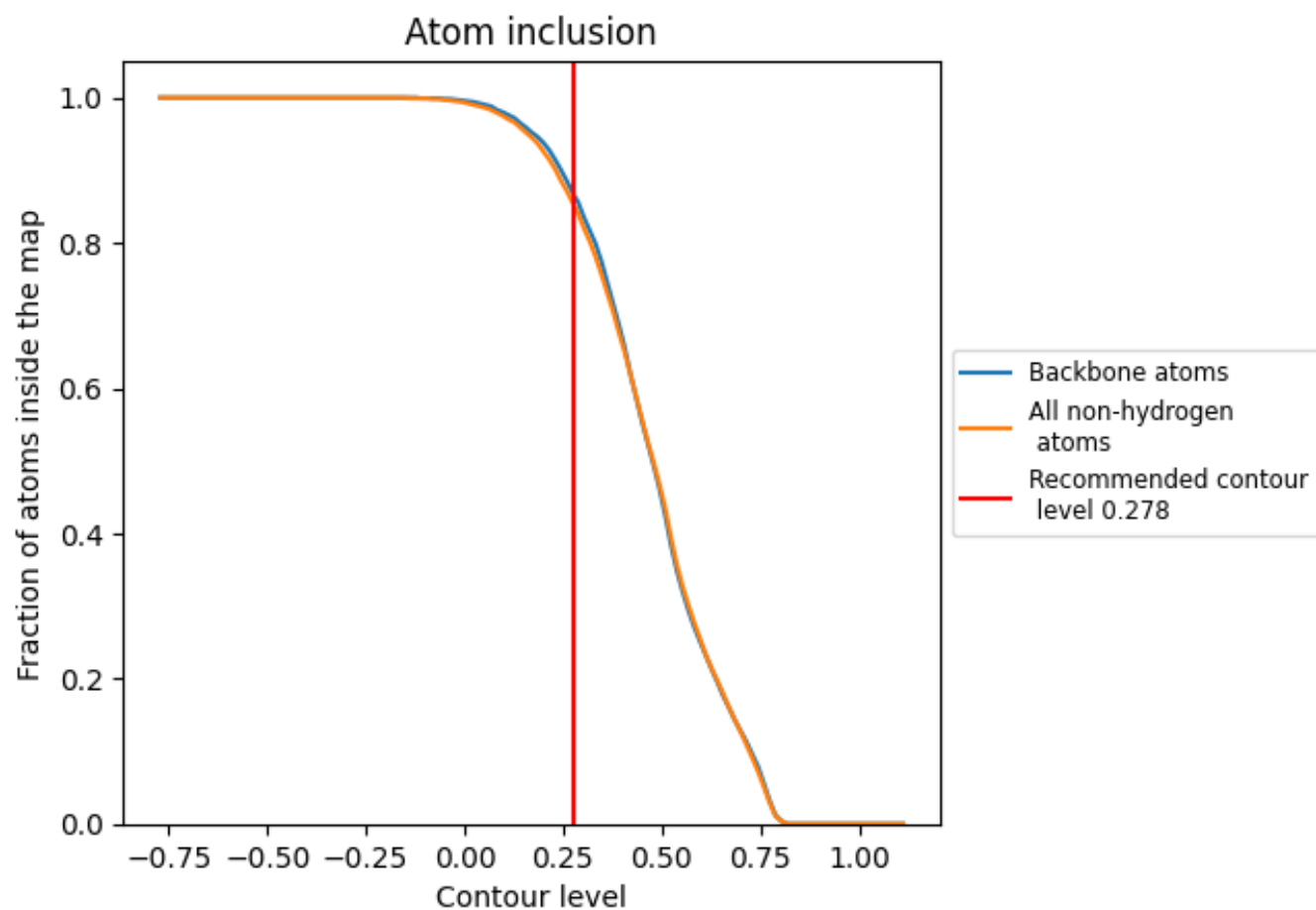


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

8.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 85% 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 (0.278) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8510	<div></div> 0.0430
A	<div></div> 0.8580	<div></div> 0.0460
B	<div></div> 0.8840	<div></div> 0.0460
C	<div></div> 0.8240	<div></div> 0.0320
D	<div></div> 0.8800	<div></div> 0.0470
E	<div></div> 0.8070	<div></div> 0.0460

