



wwPDB EM Validation Summary Report ⓘ

Nov 1, 2022 – 04:42 PM EDT

PDB ID : 5IPU
EMDB ID : EMD-8105
Title : Cryo-EM structure of GluN1/GluN2B NMDA receptor in the DCKA/D-APV-bound conformation, state 6
Authors : Zhu, S.; Stein, A.R.; Yoshioka, C.; Lee, C.H.; Goehring, A.; Mchaourab, S.H.; Gouaux, E.
Deposited on : 2016-03-09
Resolution : 15.40 Å(reported)

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.dev43
MolProbity : 4.02b-467
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

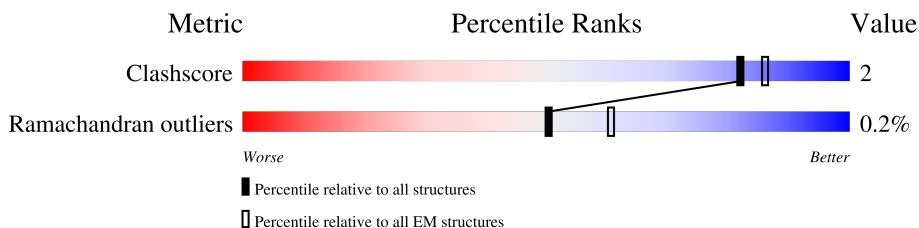
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY





The reported resolution of this entry is 15.40 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	158937	4297
Ramachandran outliers	154571	4023

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	822	
1	C	822	
2	B	825	
2	D	825	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10156 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 N-methyl-D-aspartate receptor subunit NR1-8a.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	653	Total	C	N	O	0	0
			2612	1306	653	653		
1	C	626	Total	C	N	O	0	0
			2504	1252	626	626		

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	51	PHE	LYS	engineered mutation	UNP C0KD18
A	52	PHE	ARG	engineered mutation	UNP C0KD18
A	300	GLN	ASN	engineered mutation	UNP C0KD18
A	350	GLN	ASN	engineered mutation	UNP C0KD18
A	368	ASP	ASN	engineered mutation	UNP C0KD18
A	440	ASP	ASN	engineered mutation	UNP C0KD18
A	469	ASP	ASN	engineered mutation	UNP C0KD18
A	493	ALA	LYS	engineered mutation	UNP C0KD18
A	494	ALA	LYS	engineered mutation	UNP C0KD18
A	495	ALA	GLU	engineered mutation	UNP C0KD18
A	?	-	LYS	deletion	UNP C0KD18
A	?	-	VAL	deletion	UNP C0KD18
A	?	-	ASN	deletion	UNP C0KD18
A	?	-	SER	deletion	UNP C0KD18
A	?	-	GLU	deletion	UNP C0KD18
A	?	-	GLU	deletion	UNP C0KD18
A	?	-	GLU	deletion	UNP C0KD18
A	?	-	GLU	deletion	UNP C0KD18
A	602	ARG	GLY	engineered mutation	UNP C0KD18
A	609	LEU	ILE	engineered mutation	UNP C0KD18
A	648	ARG	ASP	engineered mutation	UNP C0KD18
A	761	GLU	ASN	engineered mutation	UNP C0KD18
A	829	SER	-	expression tag	UNP C0KD18
A	830	ARG	-	expression tag	UNP C0KD18
A	831	ALA	-	expression tag	UNP C0KD18
A	832	GLU	-	expression tag	UNP C0KD18

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Chain	Residue	Modelled	Actual	Comment	Reference
A	833	ALA	-	expression tag	UNP C0KD18
A	834	LYS	-	expression tag	UNP C0KD18
A	835	ARG	-	expression tag	UNP C0KD18
A	836	MET	-	expression tag	UNP C0KD18
A	837	LYS	-	expression tag	UNP C0KD18
A	838	GLY	-	expression tag	UNP C0KD18
A	839	LEU	-	expression tag	UNP C0KD18
A	840	GLU	-	expression tag	UNP C0KD18
A	841	VAL	-	expression tag	UNP C0KD18
A	842	LEU	-	expression tag	UNP C0KD18
A	843	PHE	-	expression tag	UNP C0KD18
A	844	GLN	-	expression tag	UNP C0KD18
C	51	PHE	LYS	engineered mutation	UNP C0KD18
C	52	PHE	ARG	engineered mutation	UNP C0KD18
C	300	GLN	ASN	engineered mutation	UNP C0KD18
C	350	GLN	ASN	engineered mutation	UNP C0KD18
C	368	ASP	ASN	engineered mutation	UNP C0KD18
C	440	ASP	ASN	engineered mutation	UNP C0KD18
C	469	ASP	ASN	engineered mutation	UNP C0KD18
C	493	ALA	LYS	engineered mutation	UNP C0KD18
C	494	ALA	LYS	engineered mutation	UNP C0KD18
C	495	ALA	GLU	engineered mutation	UNP C0KD18
C	?	-	LYS	deletion	UNP C0KD18
C	?	-	VAL	deletion	UNP C0KD18
C	?	-	ASN	deletion	UNP C0KD18
C	?	-	SER	deletion	UNP C0KD18
C	?	-	GLU	deletion	UNP C0KD18
C	?	-	GLU	deletion	UNP C0KD18
C	?	-	GLU	deletion	UNP C0KD18
C	?	-	GLU	deletion	UNP C0KD18
C	602	ARG	GLY	engineered mutation	UNP C0KD18
C	609	LEU	ILE	engineered mutation	UNP C0KD18
C	648	ARG	ASP	engineered mutation	UNP C0KD18
C	761	GLU	ASN	engineered mutation	UNP C0KD18
C	829	SER	-	expression tag	UNP C0KD18
C	830	ARG	-	expression tag	UNP C0KD18
C	831	ALA	-	expression tag	UNP C0KD18
C	832	GLU	-	expression tag	UNP C0KD18
C	833	ALA	-	expression tag	UNP C0KD18
C	834	LYS	-	expression tag	UNP C0KD18
C	835	ARG	-	expression tag	UNP C0KD18
C	836	MET	-	expression tag	UNP C0KD18

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Chain	Residue	Modelled	Actual	Comment	Reference
C	837	LYS	-	expression tag	UNP C0KD18
C	838	GLY	-	expression tag	UNP C0KD18
C	839	LEU	-	expression tag	UNP C0KD18
C	840	GLU	-	expression tag	UNP C0KD18
C	841	VAL	-	expression tag	UNP C0KD18
C	842	LEU	-	expression tag	UNP C0KD18
C	843	PHE	-	expression tag	UNP C0KD18
C	844	GLN	-	expression tag	UNP C0KD18

- Molecule 2 is a protein called Ionotropic glutamate receptor subunit NR2B.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	B	633	Total	C	N	O	0	0
			2532	1266	633	633		
2	D	627	Total	C	N	O	0	0
			2508	1254	627	627		

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	20	SER	MET	engineered mutation	UNP A7XY94
B	21	ARG	GLY	engineered mutation	UNP A7XY94
B	22	ALA	CYS	engineered mutation	UNP A7XY94
B	64	GLU	ALA	engineered mutation	UNP A7XY94
B	69	GLN	ASN	engineered mutation	UNP A7XY94
B	343	ASP	ASN	engineered mutation	UNP A7XY94
B	?	-	LYS	deletion	UNP A7XY94
B	?	-	TYR	deletion	UNP A7XY94
B	?	-	TYR	deletion	UNP A7XY94
B	?	-	VAL	deletion	UNP A7XY94
B	486	VAL	THR	engineered mutation	UNP A7XY94
B	?	-	ARG	deletion	UNP A7XY94
B	?	-	CYS	deletion	UNP A7XY94
B	?	-	LEU	deletion	UNP A7XY94
B	?	-	ALA	deletion	UNP A7XY94
B	?	-	ASP	deletion	UNP A7XY94
B	?	-	GLY	deletion	UNP A7XY94
B	?	-	ARG	deletion	UNP A7XY94
B	?	-	GLU	deletion	UNP A7XY94
B	?	-	PRO	deletion	UNP A7XY94
B	?	-	GLY	deletion	UNP A7XY94
B	601	LEU	VAL	engineered mutation	UNP A7XY94

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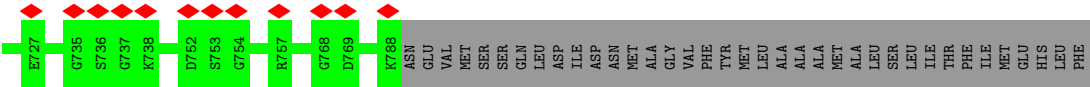
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Chain	Residue	Modelled	Actual	Comment	Reference
B	640	ARG	GLU	engineered mutation	UNP A7XY94
B	641	ARG	GLU	engineered mutation	UNP A7XY94
D	20	SER	MET	engineered mutation	UNP A7XY94
D	21	ARG	GLY	engineered mutation	UNP A7XY94
D	22	ALA	CYS	engineered mutation	UNP A7XY94
D	64	GLU	ALA	engineered mutation	UNP A7XY94
D	69	GLN	ASN	engineered mutation	UNP A7XY94
D	343	ASP	ASN	engineered mutation	UNP A7XY94
D	?	-	LYS	deletion	UNP A7XY94
D	?	-	TYR	deletion	UNP A7XY94
D	?	-	TYR	deletion	UNP A7XY94
D	?	-	VAL	deletion	UNP A7XY94
D	486	VAL	THR	engineered mutation	UNP A7XY94
D	?	-	ARG	deletion	UNP A7XY94
D	?	-	CYS	deletion	UNP A7XY94
D	?	-	LEU	deletion	UNP A7XY94
D	?	-	ALA	deletion	UNP A7XY94
D	?	-	ASP	deletion	UNP A7XY94
D	?	-	GLY	deletion	UNP A7XY94
D	?	-	ARG	deletion	UNP A7XY94
D	?	-	GLU	deletion	UNP A7XY94
D	?	-	PRO	deletion	UNP A7XY94
D	?	-	GLY	deletion	UNP A7XY94
D	601	LEU	VAL	engineered mutation	UNP A7XY94
D	640	ARG	GLU	engineered mutation	UNP A7XY94
D	641	ARG	GLU	engineered mutation	UNP A7XY94

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.

- Chain A:
-
- 6% 77% 21%
- D23 P24 G30 R56 T63 I90 L91 A97 P98 T99 D100 H101 K131 S132 A191 D192 K193 Q200 L220 L221 E299 Q300 P319 E342 N358 R359 G365 Q374 N375 D376 R377 G384 T386 E387 Y392 G404
- T415 S416 D417 G418 E441 T442 I443 P444 G445 R446 L464 M468 G480 K481 F482 G483 E486 R487 V487 A493 N497 G498 M499 M500 G501 S505 N519 K542 E543 I544 P544 R545 T546 A547 S548 G549 A550 T551 A552 S553 A554 A555 A556 A557 A558 A559 A560 A561 A562 A563 A564 A565 A566 A567 A568 A569 A570 A571 A572 A573 A574 A575 A576 A577 A578 A579 A580 A581 A582 A583 A584 A585 A586 A587 A588 A589 A590 A591 A592 A593 A594 A595 A596 A597 A598 A599 A600 A601 A602 A603 A604 A605 A606 A607 A608 A609 A610 A611 A612 A613 A614 A615 A616 A617 A618 A619 A620 A621 A622 A623 A624 A625 A626 A627 A628 A629 A630 A631 A632 A633 A634 A635 A636 A637 A638 A639 A640 A641 A642 A643 A644 A645 A646 A647 A648 A649 A650 A651 A652 A653 A654 A655 A656 A657 A658 A659 A660 A661 A662 A663 A664 A665 A666 A667 A668 A669 A670 A671 A672 A673 A674 A675 A676 A677 A678 A679 A680 A681 A682 A683 A684 A685 A686 A687 A688 A689 A690 A691 A692 A693 A694 A695 A696 A697 A698 A699 A700 A701 A702 A703 A704 A705 A706 A707 A708 A709 A710 A711 A712 A713 A714 A715 A716 A717 A718 A719 A720 A721 A722 A723 A724 A725 A726 A727 A728 A729 A730 A731 A732 A733 A734 A735 A736 A737 A738 A739 A740 A741 A742 A743 A744 A745 A746 A747 A748 A749 A750 A751 A752 A753 A754 A755 A756 A757 A758 A759 A760 A761 A762 A763 A764 A765 A766 A767 A768 A769 A770 A771 A772 A773 A774 A775 A776 A777 A778 A779 A780 A781 A782 A783 A784 A785 A786 A787 A788 A789 A790 A791 A792 A793 A794 A795 A796 A797 A798 A799 A800 A801 A802 A803 A804 A805 A806 A807 A808 A809 A810 A811 A812 A813 A814 A815 A816 A817 A818 A819 A820 A821 A822 A823 A824 A825 A826 A827 A828 A829 A830 A831 A832 A833 A834 A835 A836 A837 A838 A839 A840 A841 A842 A843 A844 A845 A846 A847 A848 A849 A850 A851 A852 A853 A854 A855 A856 A857 A858 A859 A860 A861 A862 A863 A864 A865 A866 A867 A868 A869 A870 A871 A872 A873 A874 A875 A876 A877 A878 A879 A880 A881 A882 A883 A884 A885 A886 A887 A888 A889 A890 A891 A892 A893 A894 A895 A896 A897 A898 A899 A900 A901 A902 A903 A904 A905 A906 A907 A908 A909 A910 A911 A912 A913 A914 A915 A916 A917 A918 A919 A920 A921 A922 A923 A924 A925 A926 A927 A928 A929 A930 A931 A932 A933 A934 A935 A936 A937 A938 A939 A940 A941 A942 A943 A944 A945 A946 A947 A948 A949 A950 A951 A952 A953 A954 A955 A956 A957 A958 A959 A960 A961 A962 A963 A964 A965 A966 A967 A968 A969 A970 A971 A972 A973 A974 A975 A976 A977 A978 A979 A980 A981 A982 A983 A984 A985 A986 A987 A988 A989 A990 A991 A992 A993 A994 A995 A996 A997 A998 A999 A1000

- Chain C:
-
- 74% 7% 24%
- Sequence logo for Chain C. The y-axis represents information content in bits (0.00 to 0.25). The x-axis lists amino acids. Red diamonds indicate positions with high conservation. A bar chart at the top shows the overall conservation score for each position, with a 7% threshold line.



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	18309	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 ($e^-/\text{\AA}^2$)	10.5	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.139	Depositor
Minimum map value	-0.041	Depositor
Average map value	0.007	Depositor
Map value standard deviation	0.021	Depositor
Recommended contour level	0.052	Depositor
Map size (Å)	236.47003, 215.07004, 204.37003	wwPDB
Map dimensions	221, 201, 191	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0700002, 1.0700002, 1.0700002	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	0.29	0/2608	0.62	0/3253
1	C	0.29	0/2500	0.63	1/3118 (0.0%)
2	B	0.30	0/2528	0.74	4/3153 (0.1%)
2	D	0.32	0/2504	0.67	1/3123 (0.0%)
All	All	0.30	0/10140	0.67	6/12647 (0.0%)

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	A	0	1
2	B	0	1
All	All	0	2

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	409	PHE	N-CA-C	-14.47	71.94	111.00
2	B	410	VAL	N-CA-C	9.32	136.17	111.00
2	B	37	VAL	C-N-CA	-6.65	108.33	122.30
1	C	123	THR	N-CA-C	5.60	126.12	111.00
2	B	42	GLU	N-CA-C	-5.21	96.92	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	542	LYS	Peptide
2	B	246	GLY	Peptide

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	2612	0	699	8	0
1	C	2504	0	664	7	0
2	B	2532	0	687	8	0
2	D	2508	0	685	9	0
All	All	10156	0	2735	32	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 2.

The worst 5 of 32 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:C:660:PRO:O	1:C:664:ASN:N	2.15	0.77
2:D:50:GLU:O	2:D:53:ASP:N	2.20	0.75
1:A:660:PRO:O	1:A:664:ASN:N	2.22	0.71
1:C:464:LEU:O	1:C:468:MET:N	2.20	0.71
1:A:464:LEU:O	1:A:468:MET:N	2.23	0.71

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	645/822 (78%)	626 (97%)	19 (3%)	0	100	100
1	C	618/822 (75%)	597 (97%)	21 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	625/825 (76%)	592 (95%)	29 (5%)	4 (1%)	25	66
2	D	619/825 (75%)	592 (96%)	26 (4%)	1 (0%)	47	81
All	All	2507/3294 (76%)	2407 (96%)	95 (4%)	5 (0%)	50	81

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	407	ALA
2	B	408	PRO
2	D	408	PRO
2	B	397	GLU
2	B	43	VAL

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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 monosaccharides 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 ⓘ

There are no chain breaks in this entry.

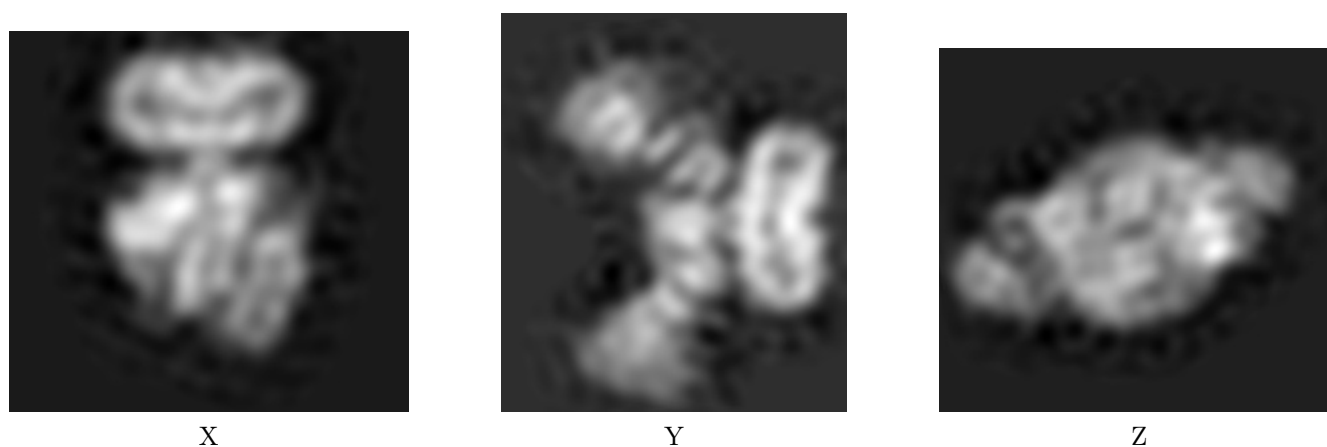
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8105. 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](#)

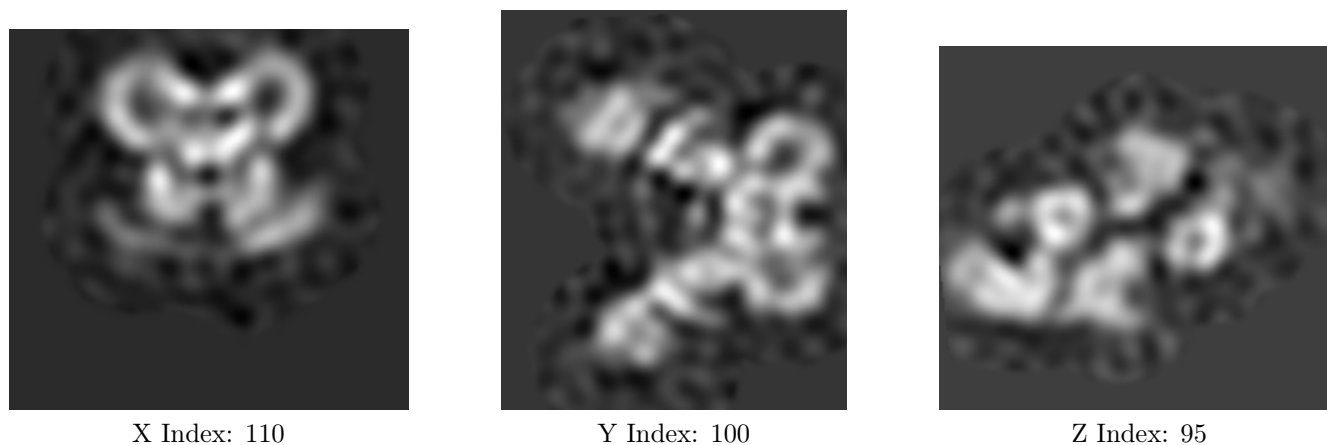
6.1.1 Primary map



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

6.2 Central slices [i](#)

6.2.1 Primary map



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: 109



Y Index: 89



Z Index: 140

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

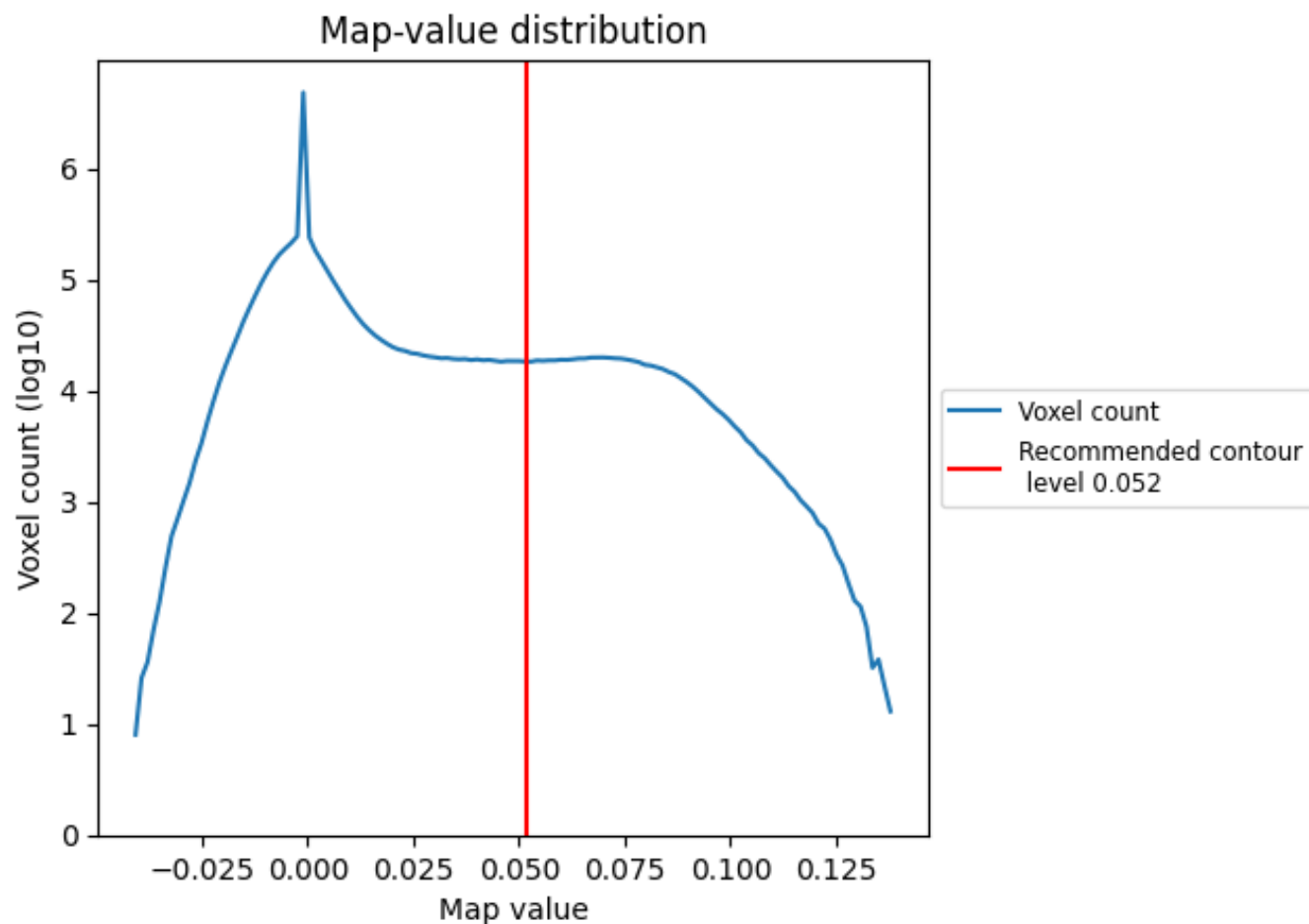
6.5 Mask visualisation

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

7 Map analysis [i](#)

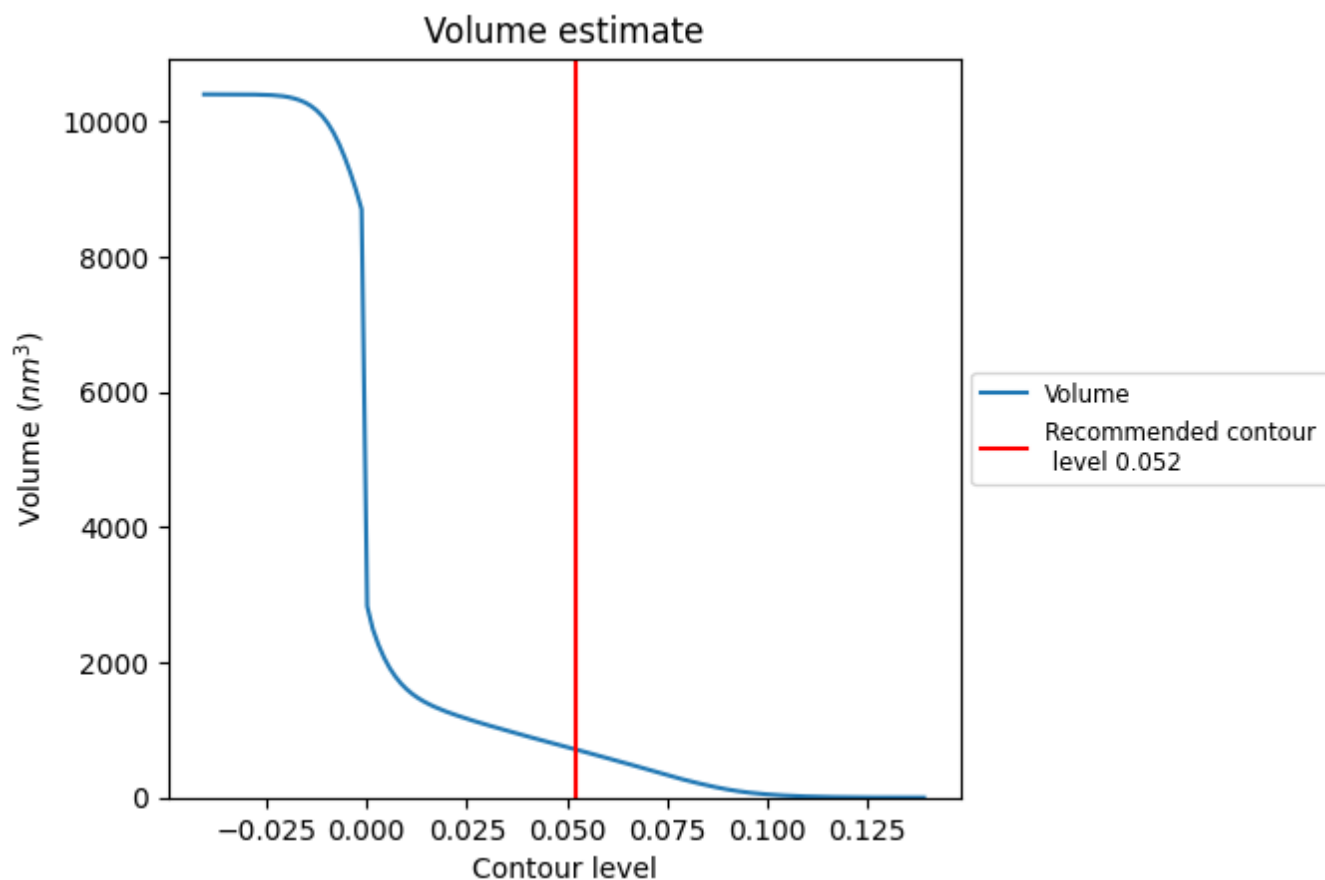
This section contains the results of statistical analysis of the map.

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 714 nm³; this corresponds to an approximate mass of 645 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](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

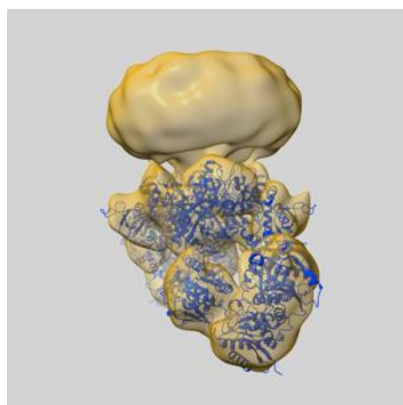
8 Fourier-Shell correlation

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

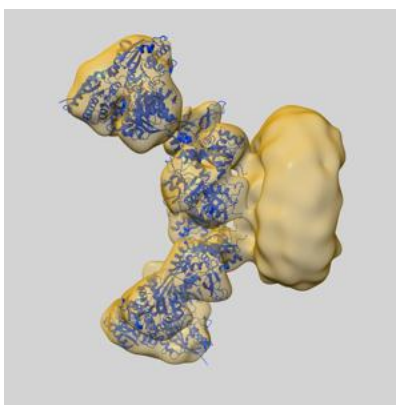
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-8105 and PDB model 5IPU. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

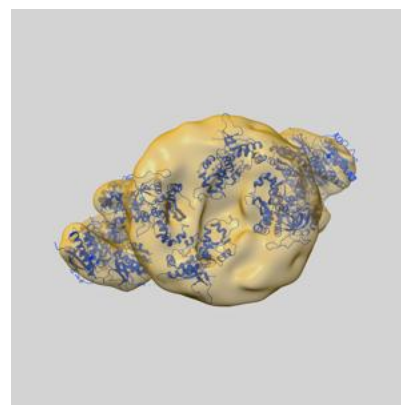
9.1 Map-model overlay [i](#)



X



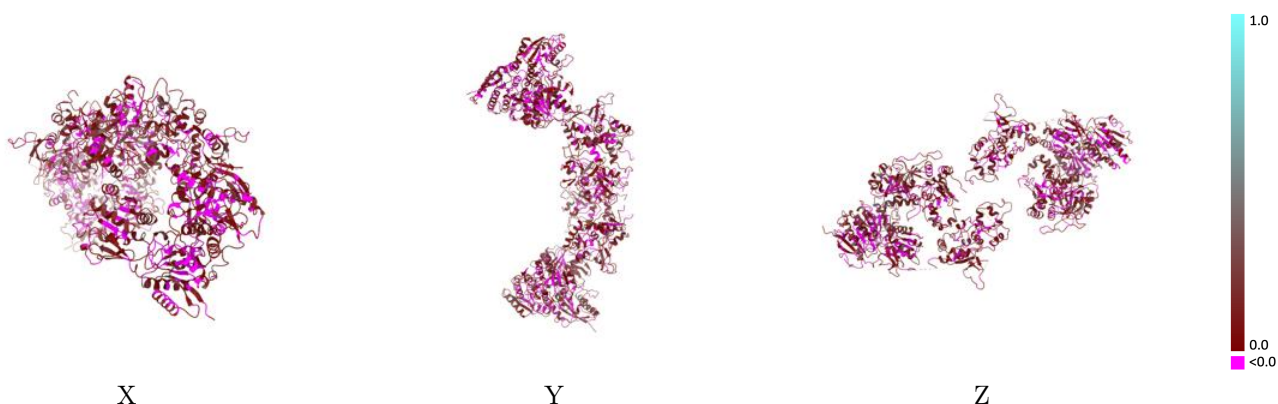
Y



Z

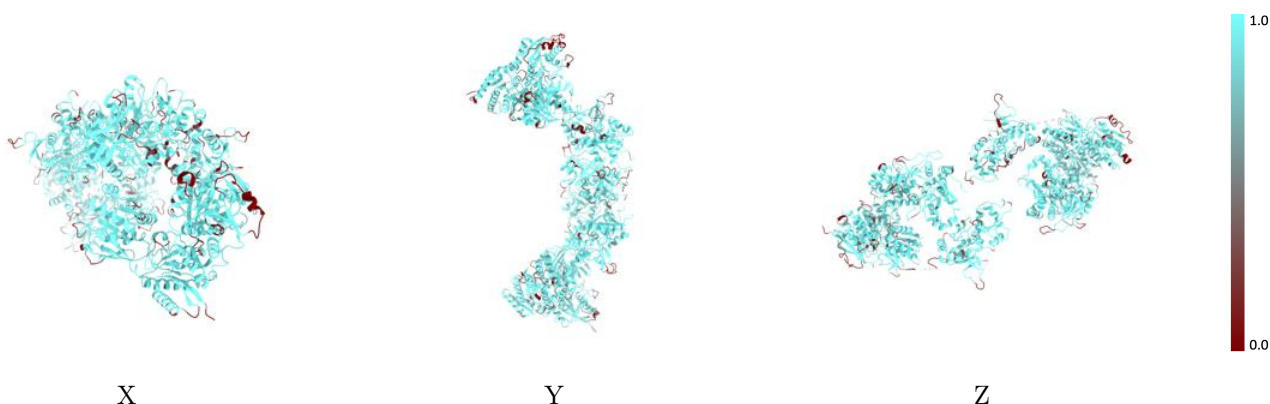
The images above show the 3D surface view of the map at the recommended contour level 0.052 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



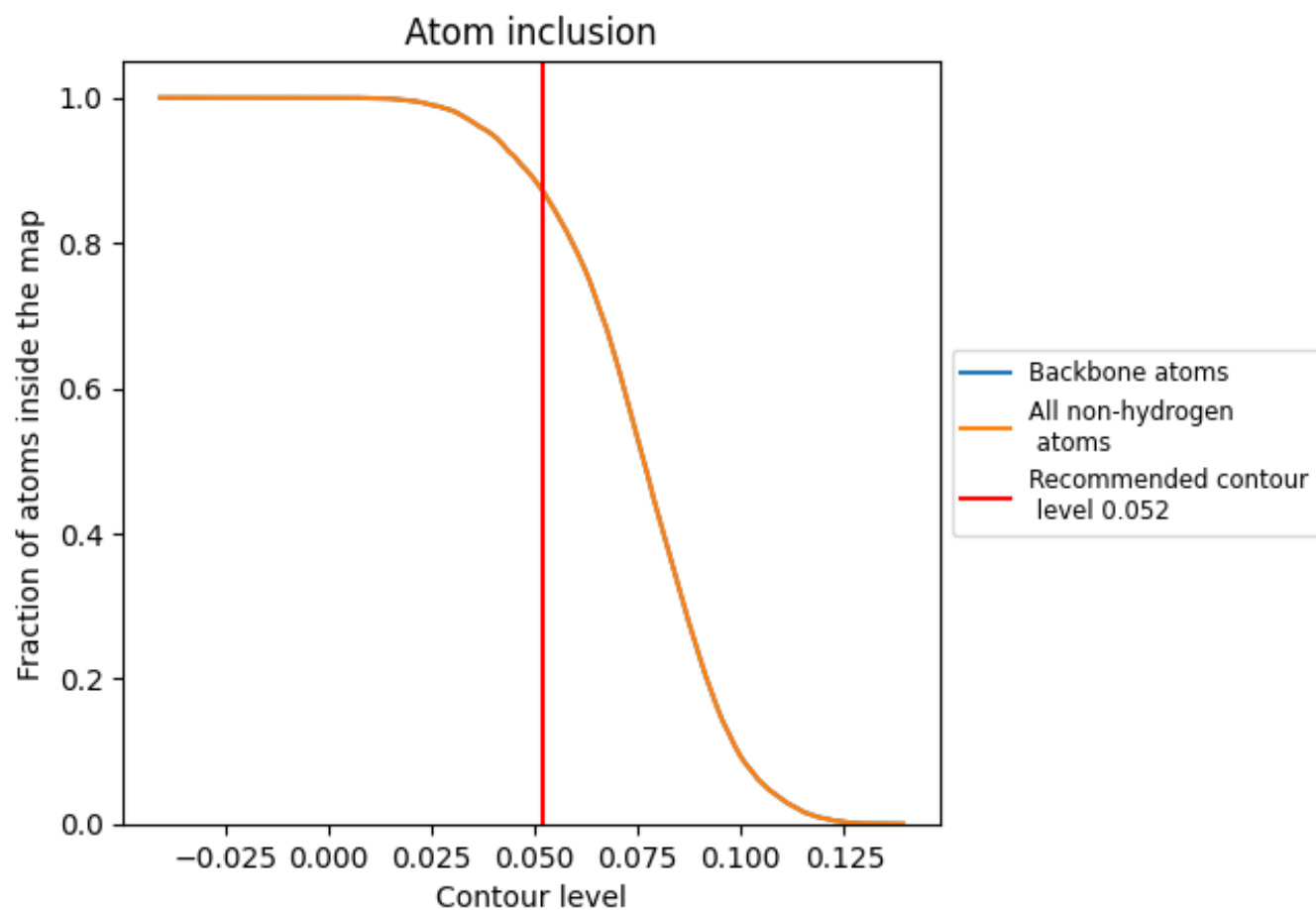
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.052).

9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 87% 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 (0.052) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8716	<div></div> 0.0830
A	<div></div> 0.9096	<div></div> 0.0920
B	<div></div> 0.8590	<div></div> 0.0830
C	<div></div> 0.8946	<div></div> 0.0830
D	<div></div> 0.8218	<div></div> 0.0750

