



Full wwPDB EM Validation Report ⓘ

Mar 7, 2026 – 01:56 AM UTC

PDB ID : 5IOU / pdb_00005iou
EMDB ID : EMD-8097
Title : Cryo-EM structure of GluN1/GluN2B NMDA receptor in the glutamate/glycine-bound conformation
Authors : Zhu, S.; Stein, A.R.; Yoshioka, C.; Lee, C.H.; Goehring, A.; Mchaourab, S.H.; Gouaux, E.
Deposited on : 2016-03-09
Resolution : 7.00 Å(reported)

This is a Full wwPDB EM Validation 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:

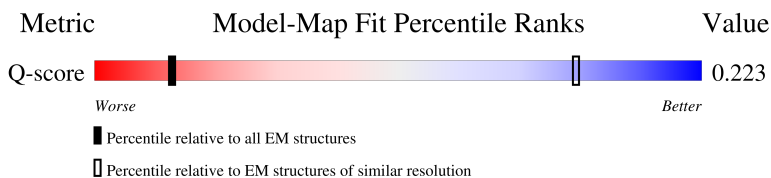
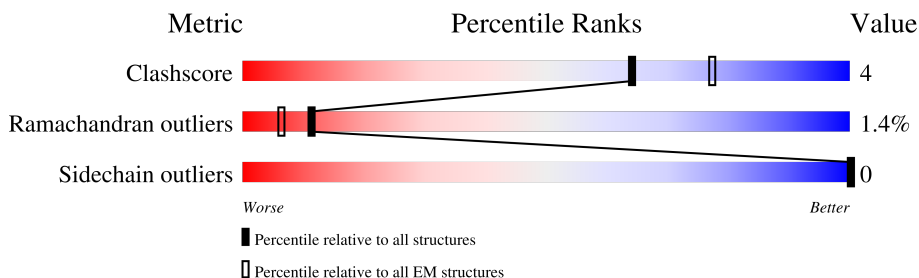
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 7.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	483 (6.50 - 7.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 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	14% 92% 5% ..
1	C	822	13% 93% 5% .
2	B	825	15% 88% 8% ..
2	D	825	16% 87% 9% .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15824 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	803	Total	C	N	O	0	0
			3963	2358	803	802		
1	C	803	Total	C	N	O	0	0
			3963	2358	803	802		

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	797	Total	C	N	O	0	0
			3934	2341	797	796		
2	D	797	Total	C	N	O	0	0
			3934	2341	797	796		

There are 48 discrepancies between the modelled and reference sequences:

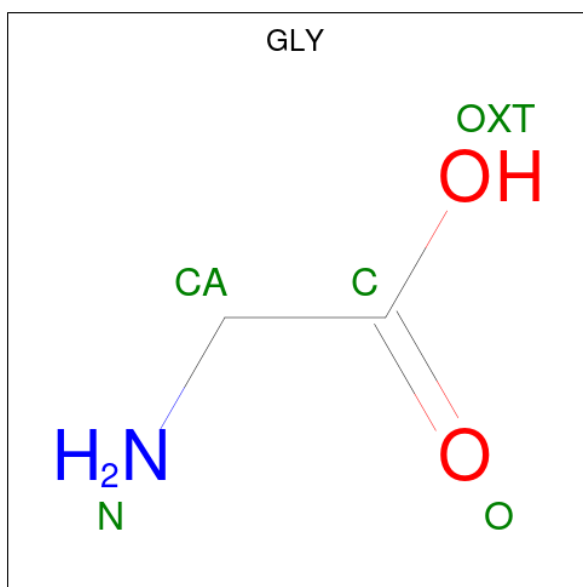
Chain	Residue	Modelled	Actual	Comment	Reference
B	20	SER	MET	engineered mutation	UNP A7XY94
B	21	ARG	GLY	engineered mutation	UNP A7XY94
B	22	ALA	CYS	engineered mutation	UNP A7XY94
B	64	GLU	ALA	engineered mutation	UNP A7XY94
B	69	GLN	ASN	engineered mutation	UNP A7XY94
B	343	ASP	ASN	engineered mutation	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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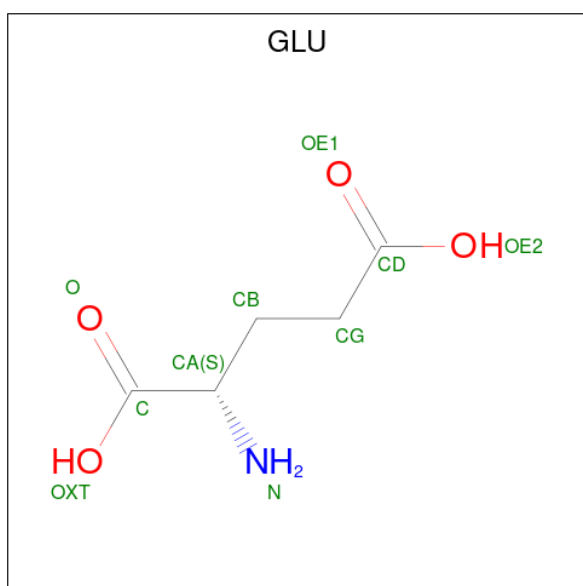
Chain	Residue	Modelled	Actual	Comment	Reference
B	640	ARG	GLU	engineered mutation	UNP A7XY94
B	641	ARG	GLU	engineered mutation	UNP A7XY94
D	20	SER	MET	engineered mutation	UNP A7XY94
D	21	ARG	GLY	engineered mutation	UNP A7XY94
D	22	ALA	CYS	engineered mutation	UNP A7XY94
D	64	GLU	ALA	engineered mutation	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

- Molecule 3 is GLYCINE (CCD ID: GLY) (formula: $C_2H_5NO_2$).



Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	N	O	0
			5	2	1	2	
3	C	1	Total	C	N	O	0
			5	2	1	2	

- Molecule 4 is GLUTAMIC ACID (CCD ID: GLU) (formula: C₅H₉NO₄).

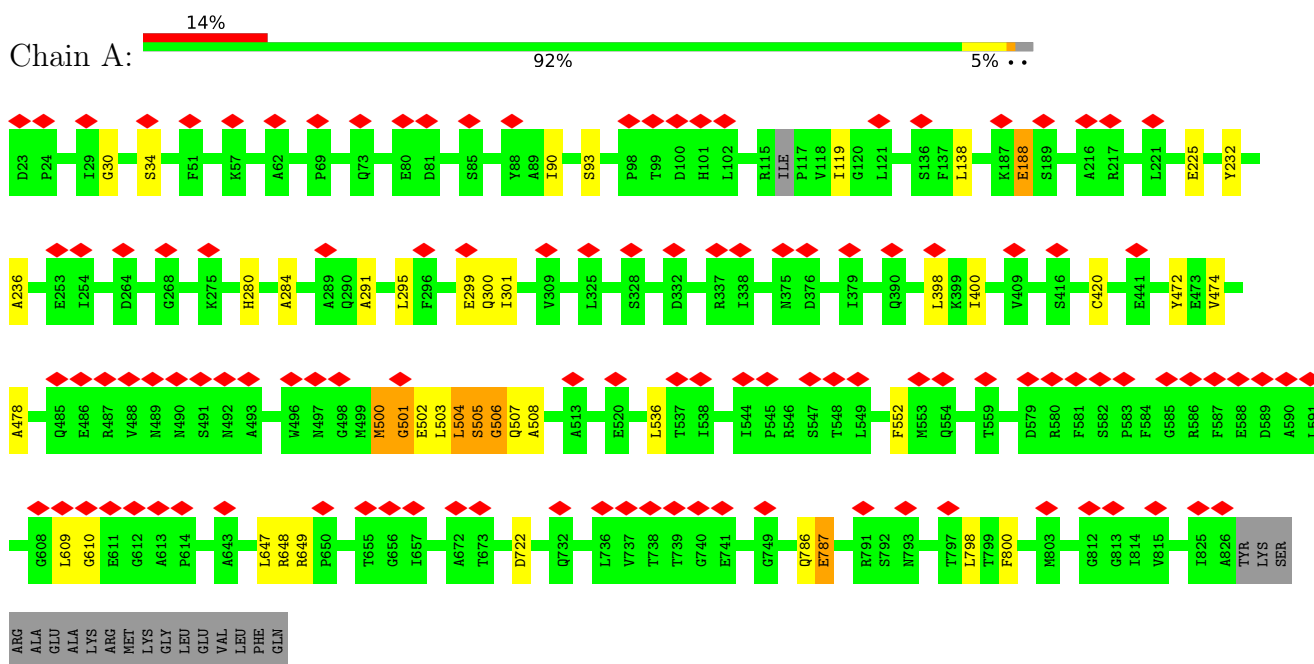


Mol	Chain	Residues	Atoms				AltConf
4	B	1	Total	C	N	O	0
			10	5	1	4	
4	D	1	Total	C	N	O	0
			10	5	1	4	

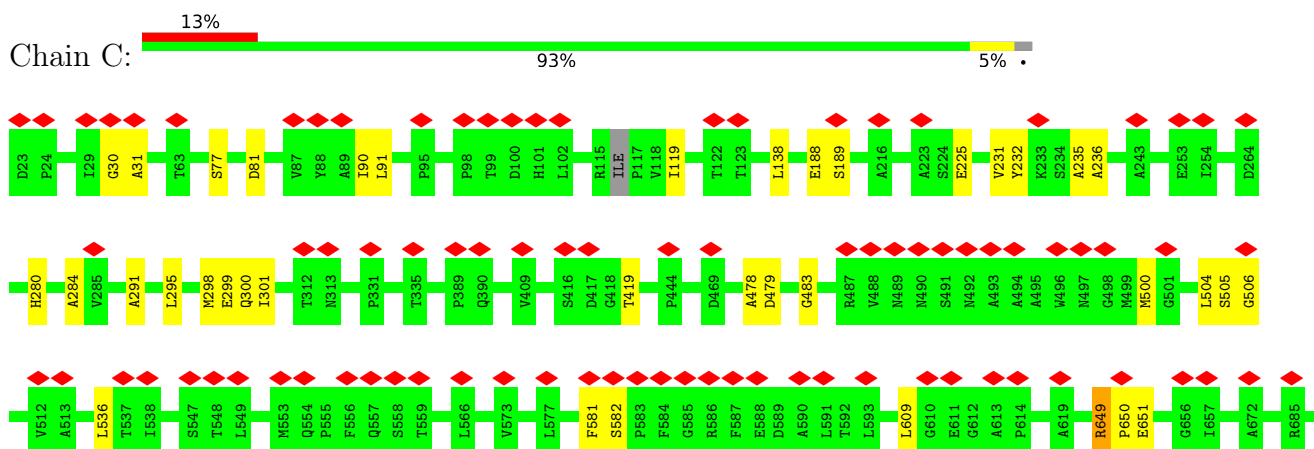
3 Residue-property plots [i](#)

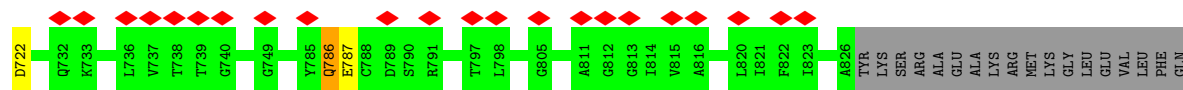
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: N-methyl-D-aspartate receptor subunit NR1-8a

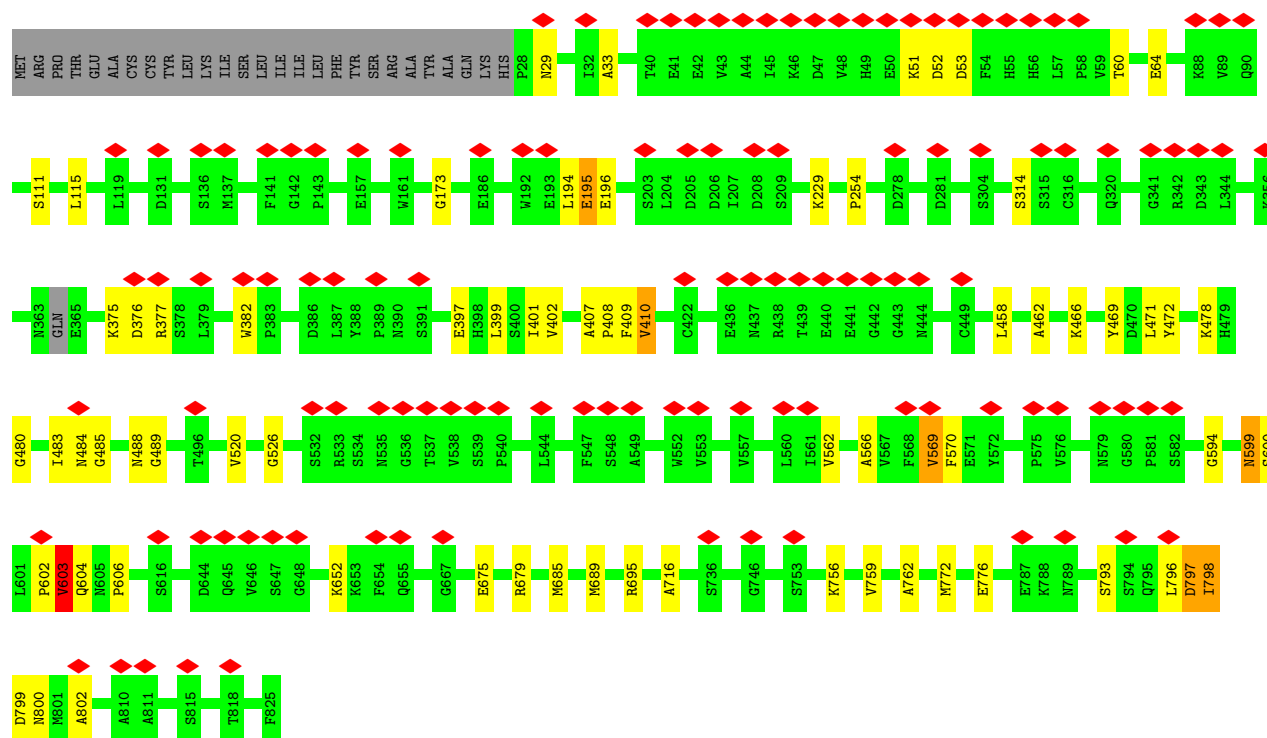
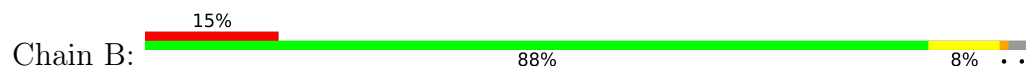


- Molecule 1: N-methyl-D-aspartate receptor subunit NR1-8a

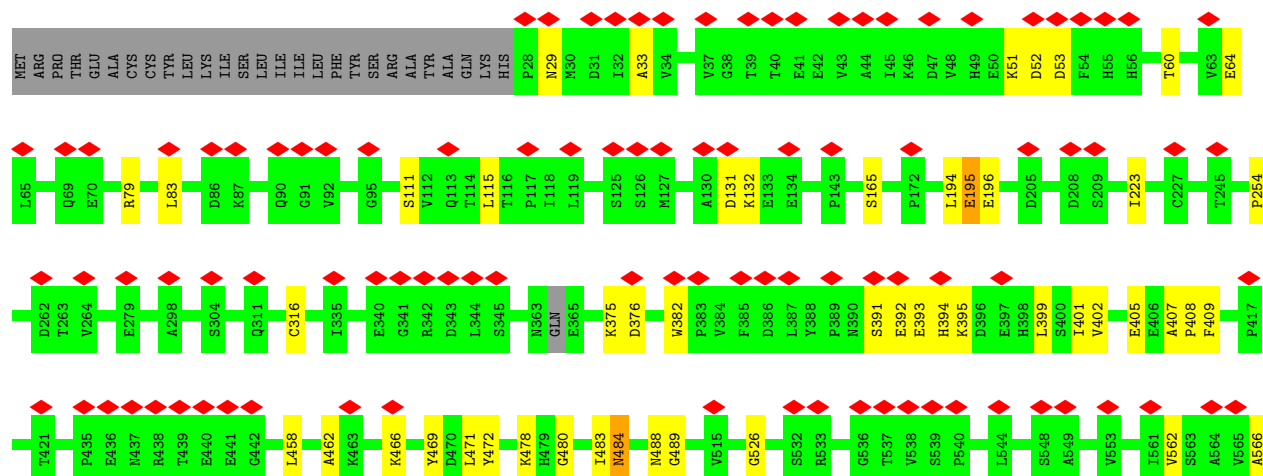
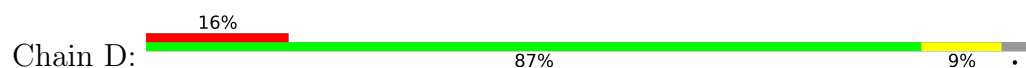


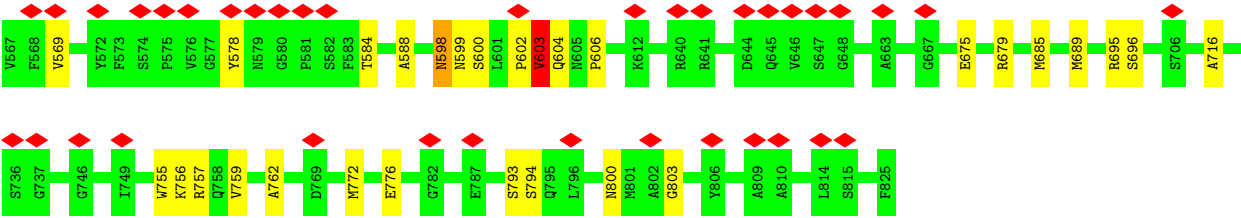


• Molecule 2: Ionotropic glutamate receptor subunit NR2B



• Molecule 2: Ionotropic glutamate receptor subunit NR2B





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	116968	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 ($e^-/\text{\AA}^2$)	8.7	Depositor
Minimum defocus (nm)	2500	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.132	Depositor
Minimum map value	-0.070	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.022	Depositor
Map size ($\text{\AA}$)	236.47003, 215.07004, 204.37003	wwPDB
Map dimensions	221, 201, 191	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.0700002, 1.0700002, 1.0700002	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	0.12	0/3961	0.94	19/5512 (0.3%)
1	C	0.15	1/3961 (0.0%)	0.91	26/5512 (0.5%)
2	B	0.12	0/3932	0.68	21/5472 (0.4%)
2	D	0.12	0/3932	0.72	22/5472 (0.4%)
All	All	0.13	1/15786 (0.0%)	0.82	88/21968 (0.4%)

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
1	C	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	786	GLN	C-N	-7.29	1.23	1.33

All (88) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	609	LEU	CB-CA-C	-31.10	72.86	111.43
1	C	299	GLU	N-CA-C	30.45	153.59	114.31
1	A	504	LEU	CB-CA-C	-23.20	74.65	112.00
1	A	786	GLN	N-CA-C	20.84	140.64	112.30
1	A	786	GLN	CB-CA-C	-20.29	77.58	110.85
1	A	188	GLU	N-CA-C	19.99	153.38	110.80
1	C	188	GLU	N-CA-C	19.98	137.01	111.24
2	D	794	SER	N-CA-C	19.66	136.60	111.24
1	C	504	LEU	CB-CA-C	-18.41	80.56	110.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	299	GLU	N-CA-CB	-17.10	88.16	110.90
1	C	298	MET	N-CA-C	-16.93	84.70	108.07
2	B	599	ASN	CB-CA-C	-16.74	77.11	110.42
2	D	195	GLU	N-CA-C	-15.82	86.84	109.31
2	B	195	GLU	N-CA-C	-15.75	86.95	109.31
1	A	188	GLU	CA-C-N	15.05	148.10	122.82
1	A	188	GLU	C-N-CA	15.05	148.10	122.82
1	C	504	LEU	N-CA-C	14.80	129.59	112.72
2	D	793	SER	N-CA-C	-14.63	88.04	108.23
1	A	505	SER	N-CA-CB	-13.92	90.18	110.79
1	C	478	ALA	N-CA-C	13.81	129.06	111.24
2	B	600	SER	N-CA-CB	-13.81	85.19	110.32
1	C	505	SER	N-CA-CB	-12.46	90.89	109.82
1	C	189	SER	N-CA-C	-12.12	90.65	109.07
2	B	520	VAL	N-CA-C	11.88	118.85	108.63
1	A	300	GLN	N-CA-CB	-11.65	92.45	110.39
2	D	794	SER	N-CA-CB	-11.01	93.89	110.07
2	D	196	GLU	N-CA-CB	-10.70	92.51	110.16
2	B	196	GLU	N-CA-CB	-10.66	92.58	110.16
2	B	798	ILE	N-CA-C	-10.46	87.59	109.34
1	A	505	SER	N-CA-C	-10.45	98.04	112.25
1	A	188	GLU	CB-CA-C	-9.88	90.75	110.42
2	B	196	GLU	N-CA-C	9.84	125.79	109.46
2	D	196	GLU	N-CA-C	9.77	125.68	109.46
2	D	484	ASN	N-CA-C	-9.48	93.90	108.31
1	C	189	SER	N-CA-CB	9.15	126.95	111.66
2	D	316	CYS	N-CA-C	9.03	121.05	111.03
1	C	787	GLU	N-CA-CB	-8.98	95.31	110.49
2	B	797	ASP	N-CA-C	-8.95	91.74	110.80
2	D	394	HIS	N-CA-C	8.93	129.82	110.80
2	D	395	LYS	N-CA-C	-8.39	96.64	109.14
1	C	225	GLU	N-CA-C	8.36	120.17	111.14
1	A	225	GLU	N-CA-C	8.29	120.09	111.14
2	B	466	LYS	N-CA-C	8.17	120.47	110.91
2	D	466	LYS	N-CA-C	8.11	122.23	111.28
1	C	299	GLU	CB-CA-C	-7.61	96.24	109.02
1	C	786	GLN	O-C-N	-7.53	112.94	122.43
1	A	610	GLY	N-CA-C	7.38	130.68	113.18
1	C	300	GLN	N-CA-C	-7.37	95.10	110.80
1	C	188	GLU	CB-CA-C	-7.34	98.75	110.86
1	C	786	GLN	CB-CA-C	-7.33	96.94	111.60
1	C	479	ASP	N-CA-CB	7.31	122.37	110.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	797	ASP	CB-CA-C	7.30	124.94	110.42
1	C	478	ALA	CB-CA-C	-7.16	99.04	110.86
2	B	604	GLN	N-CA-CB	-7.01	98.64	110.49
2	D	604	GLN	N-CA-CB	-7.00	98.66	110.49
1	A	93	SER	N-CA-C	6.97	119.98	108.48
2	D	131	ASP	N-CA-C	6.89	121.17	111.52
2	D	394	HIS	CB-CA-C	-6.84	96.81	110.42
2	D	695	ARG	CB-CA-C	6.81	123.98	110.42
2	D	603	VAL	N-CA-C	-6.70	95.41	109.34
2	B	603	VAL	N-CA-C	-6.67	95.46	109.34
2	D	395	LYS	N-CA-CB	6.59	122.30	111.62
2	B	569	VAL	CB-CA-C	6.41	121.80	111.29
1	A	787	GLU	N-CA-CB	6.30	121.14	110.49
1	C	300	GLN	N-CA-CB	-6.21	99.99	110.49
2	B	570	PHE	N-CA-C	6.13	121.82	113.97
1	A	420	CYS	N-CA-C	6.07	118.17	110.33
2	B	695	ARG	CB-CA-C	5.96	122.28	110.42
2	D	696	SER	N-CA-CB	-5.95	100.44	110.49
1	C	582	SER	N-CA-C	5.94	118.89	110.40
1	A	34	SER	N-CA-C	5.83	119.88	111.02
1	C	581	PHE	N-CA-C	-5.78	101.17	108.45
1	C	787	GLU	N-CA-C	5.60	122.72	110.80
1	C	479	ASP	N-CA-C	-5.56	100.91	108.24
1	C	786	GLN	N-CA-C	-5.44	101.96	110.17
2	B	229	LYS	N-CA-C	5.37	118.16	111.24
2	B	652	LYS	N-CA-C	5.35	119.30	112.34
1	A	300	GLN	N-CA-C	-5.20	100.47	110.56
2	D	407	ALA	CA-C-N	-5.20	113.34	119.84
2	D	407	ALA	C-N-CA	-5.20	113.34	119.84
2	B	407	ALA	CA-C-N	-5.14	113.41	119.84
2	B	407	ALA	C-N-CA	-5.14	113.41	119.84
2	B	798	ILE	N-CA-CB	5.12	119.69	111.23
1	A	500	MET	N-CA-C	5.11	116.08	108.31
2	B	520	VAL	N-CA-CB	-5.11	104.77	110.23
2	D	132	LYS	N-CA-C	5.07	117.36	109.60
2	D	578	TYR	N-CA-C	5.05	117.68	111.82
1	C	419	THR	CB-CA-C	-5.01	102.85	112.43

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	188	GLU	Peptide
1	C	786	GLN	Mainchain

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	3963	0	1809	21	0
1	C	3963	0	1809	13	0
2	B	3934	0	1748	31	0
2	D	3934	0	1748	29	0
3	A	5	0	2	0	0
3	C	5	0	2	0	0
4	B	10	0	5	0	0
4	D	10	0	5	0	0
All	All	15824	0	7128	94	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 4.

All (94) 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)
2:B:594:GLY:O	2:B:599:ASN:CA	1.66	1.40
1:C:649:ARG:O	1:C:651:GLU:N	1.74	1.20
2:B:594:GLY:C	2:B:599:ASN:HA	1.81	1.06
2:B:594:GLY:O	2:B:599:ASN:HA	0.82	0.99
1:A:503:LEU:O	1:A:508:ALA:HB3	1.65	0.96
1:A:400:ILE:O	1:A:474:VAL:HA	1.67	0.94
2:B:594:GLY:O	2:B:599:ASN:N	2.02	0.92
2:D:29:ASN:HA	2:D:60:THR:O	1.70	0.91
2:B:29:ASN:HA	2:B:60:THR:O	1.70	0.90
1:A:119:ILE:HA	1:A:138:LEU:O	1.76	0.85
1:C:119:ILE:HA	1:C:138:LEU:O	1.77	0.85
2:B:409:PHE:O	2:B:410:VAL:CB	2.35	0.74
2:B:796:LEU:O	2:B:797:ASP:C	2.31	0.74
1:A:398:LEU:O	1:A:472:TYR:HA	1.88	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:399:LEU:O	2:D:469:TYR:HA	1.90	0.71
2:B:799:ASP:O	2:B:802:ALA:N	2.26	0.69
1:A:647:LEU:O	1:A:649:ARG:N	2.26	0.69
2:B:480:GLY:HA2	2:B:488:ASN:O	1.93	0.67
2:D:480:GLY:HA2	2:D:488:ASN:O	1.96	0.65
1:A:647:LEU:C	1:A:649:ARG:H	2.05	0.64
2:D:755:TRP:O	2:D:757:ARG:N	2.32	0.63
1:C:30:GLY:O	1:C:90:ILE:HA	1.99	0.62
2:D:401:ILE:O	2:D:471:LEU:HA	2.01	0.61
2:B:399:LEU:O	2:B:469:TYR:HA	2.00	0.61
1:A:30:GLY:O	1:A:90:ILE:HA	2.03	0.59
1:A:500:MET:O	1:A:502:GLU:N	2.37	0.58
2:D:480:GLY:HA2	2:D:489:GLY:HA3	1.85	0.57
2:D:562:VAL:O	2:D:566:ALA:CB	2.53	0.57
2:B:480:GLY:HA2	2:B:489:GLY:HA3	1.86	0.56
1:A:505:SER:C	1:A:507:GLN:H	2.14	0.56
1:A:500:MET:C	1:A:502:GLU:N	2.64	0.55
1:A:536:LEU:HA	1:A:722:ASP:HA	1.89	0.54
2:D:375:LYS:O	2:D:376:ASP:C	2.50	0.54
2:B:562:VAL:O	2:B:566:ALA:CB	2.56	0.54
2:B:796:LEU:O	2:B:798:ILE:N	2.40	0.54
2:B:799:ASP:O	2:B:800:ASN:C	2.50	0.54
1:C:536:LEU:HA	1:C:722:ASP:HA	1.89	0.53
2:B:194:LEU:C	2:B:195:GLU:O	2.48	0.53
2:D:598:ASN:O	2:D:600:SER:N	2.42	0.53
1:A:291:ALA:O	1:A:295:LEU:CB	2.57	0.53
2:D:602:PRO:O	2:D:603:VAL:C	2.52	0.53
2:B:562:VAL:O	2:B:566:ALA:HB3	2.08	0.53
1:C:483:GLY:HA2	1:C:500:MET:H	1.73	0.52
2:B:401:ILE:O	2:B:471:LEU:HA	2.09	0.52
2:B:375:LYS:O	2:B:377:ARG:N	2.42	0.52
2:B:458:LEU:O	2:B:462:ALA:HB2	2.10	0.52
2:D:562:VAL:O	2:D:566:ALA:HB3	2.10	0.52
1:A:504:LEU:C	1:A:506:GLY:H	2.17	0.52
2:B:602:PRO:O	2:B:603:VAL:C	2.52	0.51
2:D:33:ALA:HA	2:D:64:GLU:O	2.10	0.51
2:D:458:LEU:O	2:D:462:ALA:HB2	2.11	0.51
2:B:33:ALA:HA	2:B:64:GLU:O	2.11	0.51
2:B:772:MET:O	2:B:776:GLU:CB	2.59	0.51
2:D:772:MET:O	2:D:776:GLU:CB	2.58	0.51
2:D:483:ILE:O	2:D:484:ASN:C	2.54	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:685:MET:O	2:D:689:MET:CB	2.60	0.50
1:C:291:ALA:O	1:C:295:LEU:CB	2.59	0.50
2:B:685:MET:O	2:B:689:MET:CB	2.60	0.49
1:A:500:MET:O	1:A:501:GLY:C	2.55	0.49
1:C:280:HIS:O	1:C:284:ALA:HB2	2.14	0.47
1:C:232:TYR:O	1:C:236:ALA:HB2	2.14	0.47
1:A:232:TYR:O	1:A:236:ALA:HB2	2.15	0.47
1:A:280:HIS:O	1:A:284:ALA:HB2	2.15	0.46
2:D:51:LYS:O	2:D:53:ASP:N	2.48	0.46
2:B:51:LYS:O	2:B:53:ASP:N	2.48	0.45
2:D:165:SER:O	2:D:223:ILE:HA	2.17	0.45
2:D:759:VAL:O	2:D:762:ALA:HB3	2.16	0.45
1:C:31:ALA:HA	1:C:91:LEU:H	1.82	0.45
2:D:391:SER:C	2:D:393:GLU:N	2.73	0.45
2:D:458:LEU:O	2:D:462:ALA:CB	2.65	0.45
2:B:458:LEU:O	2:B:462:ALA:CB	2.65	0.44
2:D:584:THR:O	2:D:588:ALA:HB2	2.17	0.44
2:B:483:ILE:O	2:B:485:GLY:N	2.50	0.44
1:A:647:LEU:C	1:A:649:ARG:N	2.71	0.44
2:B:759:VAL:O	2:B:762:ALA:HB3	2.18	0.44
2:B:402:VAL:HA	2:B:472:TYR:O	2.18	0.43
1:A:505:SER:C	1:A:507:GLN:N	2.75	0.43
2:D:194:LEU:C	2:D:195:GLU:O	2.54	0.43
2:D:79:ARG:O	2:D:83:LEU:CB	2.66	0.43
1:A:798:LEU:O	1:A:800:PHE:N	2.45	0.43
2:D:800:ASN:O	2:D:803:GLY:N	2.53	0.42
1:C:232:TYR:O	1:C:236:ALA:CB	2.68	0.42
2:D:402:VAL:HA	2:D:472:TYR:O	2.20	0.42
1:C:231:VAL:O	1:C:235:ALA:HB3	2.20	0.41
2:D:526:GLY:O	2:D:716:ALA:N	2.53	0.41
2:D:111:SER:O	2:D:115:LEU:N	2.48	0.41
2:D:675:GLU:O	2:D:679:ARG:CB	2.68	0.41
1:A:232:TYR:O	1:A:236:ALA:CB	2.69	0.41
1:C:649:ARG:C	1:C:651:GLU:N	2.58	0.41
2:B:526:GLY:O	2:B:716:ALA:N	2.54	0.41
2:B:675:GLU:O	2:B:679:ARG:CB	2.69	0.41
2:B:111:SER:O	2:B:115:LEU:N	2.47	0.40
1:A:505:SER:O	1:A:507:GLN:N	2.54	0.40
1:C:77:SER:O	1:C:81:ASP:CB	2.69	0.40

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	799/822 (97%)	685 (86%)	106 (13%)	8 (1%)	12	48
1	C	799/822 (97%)	688 (86%)	106 (13%)	5 (1%)	21	59
2	B	793/825 (96%)	676 (85%)	101 (13%)	16 (2%)	6	31
2	D	793/825 (96%)	676 (85%)	103 (13%)	14 (2%)	6	34
All	All	3184/3294 (97%)	2725 (86%)	416 (13%)	43 (1%)	11	40

All (43) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	648	ARG
1	C	649	ARG
1	C	650	PRO
2	B	376	ASP
2	B	410	VAL
2	D	408	PRO
2	D	756	LYS
1	A	552	PHE
1	A	787	GLU
2	B	254	PRO
2	B	397	GLU
2	B	484	ASN
2	D	254	PRO
2	D	409	PHE
2	D	599	ASN
1	A	478	ALA
1	A	501	GLY
2	B	52	ASP
2	B	478	LYS
2	B	603	VAL
2	B	606	PRO
2	B	756	LYS

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Mol	Chain	Res	Type
2	D	52	ASP
2	D	478	LYS
2	D	598	ASN
2	D	606	PRO
1	C	609	LEU
2	B	314	SER
2	B	793	SER
2	D	569	VAL
2	D	603	VAL
1	A	301	ILE
1	C	301	ILE
2	D	392	GLU
1	A	299	GLU
1	A	506	GLY
2	B	382	TRP
2	D	382	TRP
2	D	405	GLU
2	B	173	GLY
2	B	569	VAL
1	C	506	GLY
2	B	408	PRO

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 oligosaccharides in this entry.

5.6 Ligand geometry

4 ligands are modelled in this entry.

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
3	GLY	A	901	-	4,4,4	1.14	1 (25%)	3,4,4	1.62	1 (33%)
4	GLU	D	901	-	8,9,9	1.12	1 (12%)	8,11,11	1.18	1 (12%)
3	GLY	C	1001	-	4,4,4	1.15	1 (25%)	3,4,4	1.65	1 (33%)
4	GLU	B	2001	-	8,9,9	1.12	1 (12%)	8,11,11	1.17	1 (12%)

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
3	GLY	A	901	-	-	0/2/2/2	-
4	GLU	D	901	-	-	2/9/9/9	-
3	GLY	C	1001	-	-	0/2/2/2	-
4	GLU	B	2001	-	-	2/9/9/9	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	901	GLU	OXT-C	-2.25	1.23	1.30
4	B	2001	GLU	OXT-C	-2.24	1.23	1.30
3	C	1001	GLY	OXT-C	-2.20	1.23	1.30
3	A	901	GLY	OXT-C	-2.17	1.23	1.30

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	901	GLU	OXT-C-O	-2.69	117.98	124.08
4	B	2001	GLU	OXT-C-O	-2.67	118.03	124.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1001	GLY	OXT-C-O	-2.08	118.00	123.33
3	A	901	GLY	OXT-C-O	-2.06	118.04	123.33

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	901	GLU	OE2-CD-CG-CB
4	D	901	GLU	OE1-CD-CG-CB
4	B	2001	GLU	OE1-CD-CG-CB
4	B	2001	GLU	OE2-CD-CG-CB

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

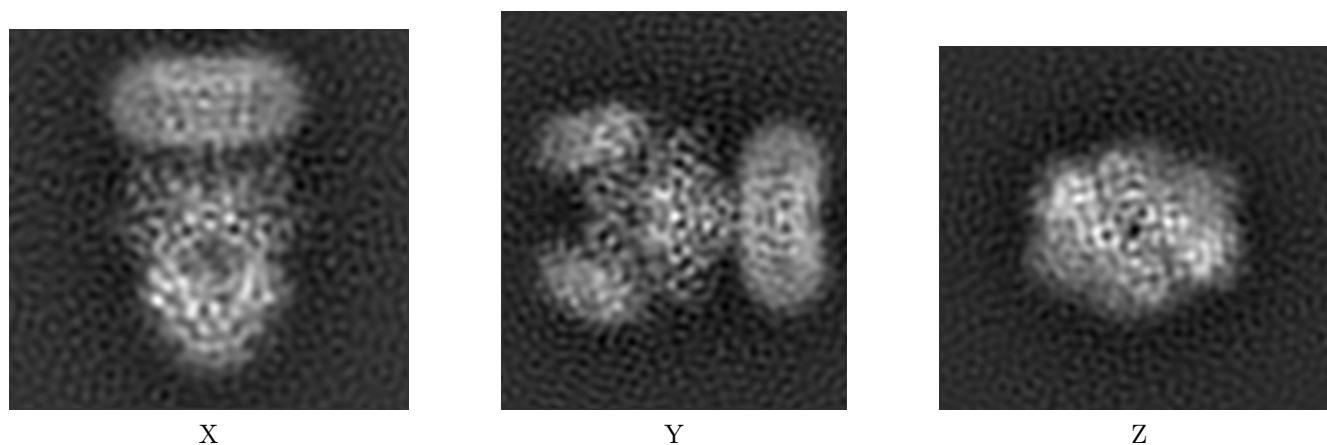
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8097. 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](#)

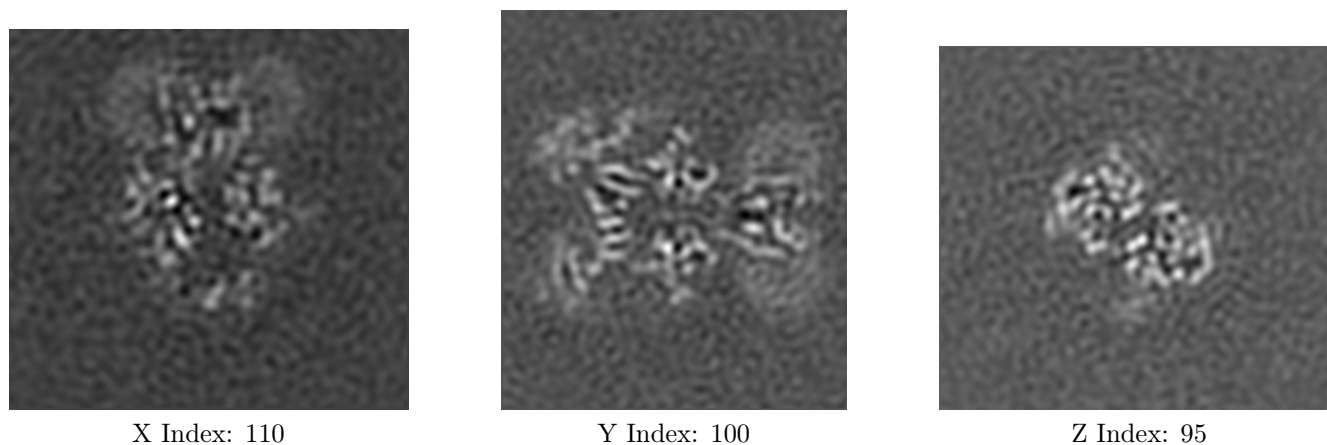
6.1.1 Primary map



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

6.2 Central slices [i](#)

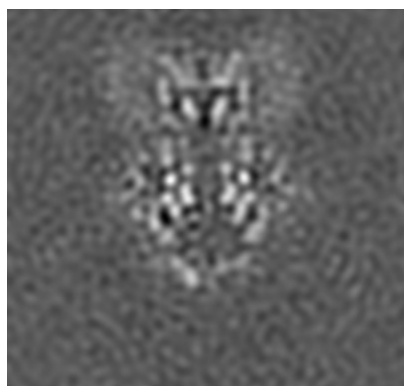
6.2.1 Primary map



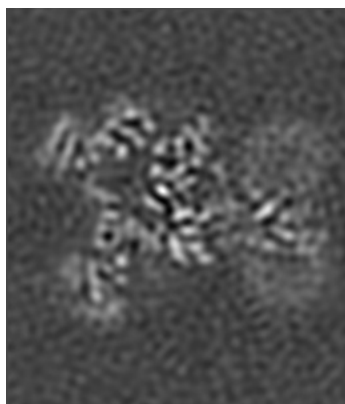
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

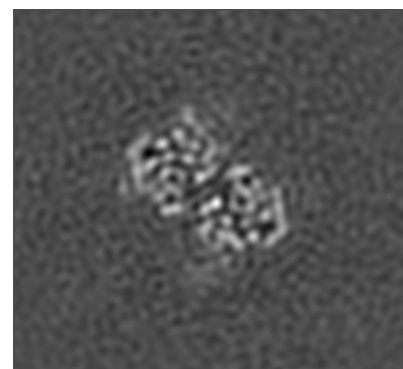
6.3.1 Primary map



X Index: 107



Y Index: 90

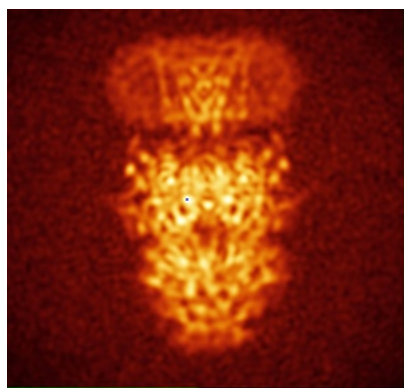


Z Index: 94

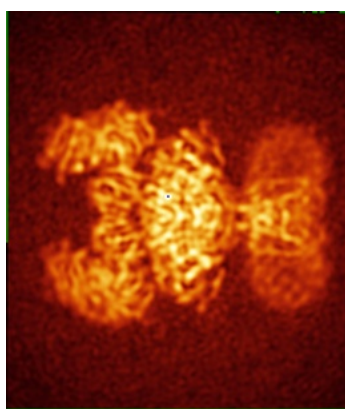
The images above show the largest variance slices of the map in three orthogonal directions.

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

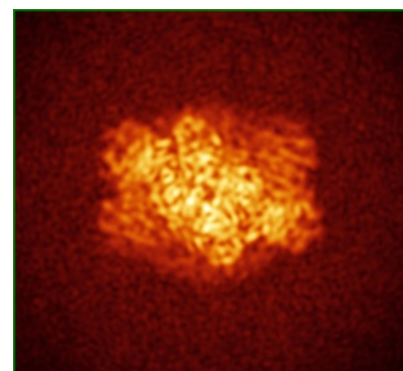
6.4.1 Primary map



X



Y



Z

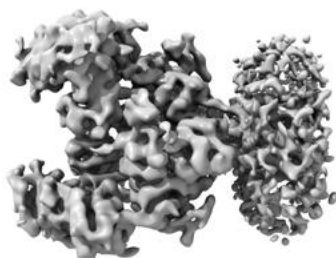
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

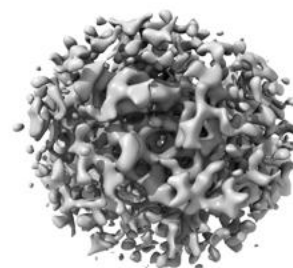
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.022. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

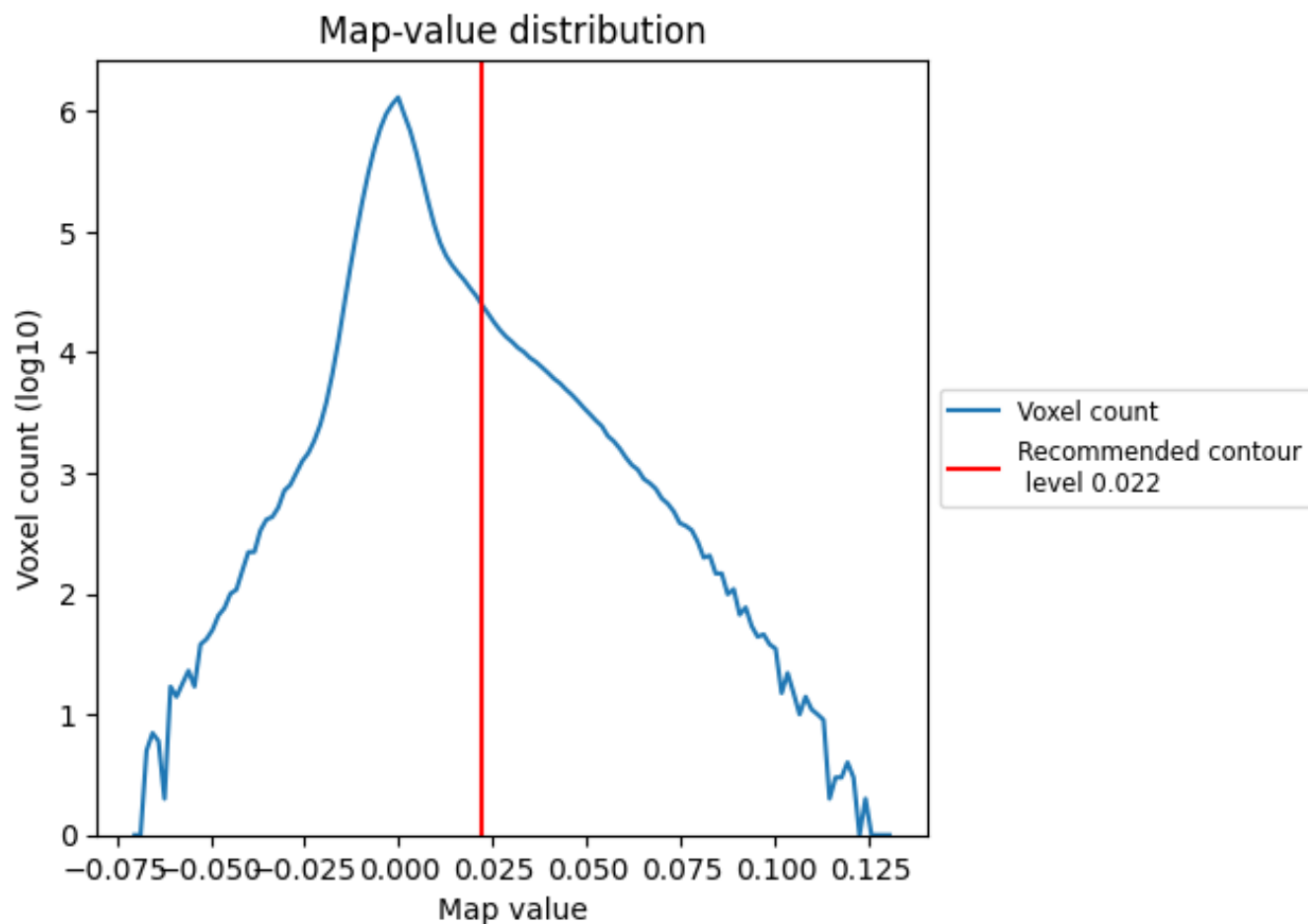
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

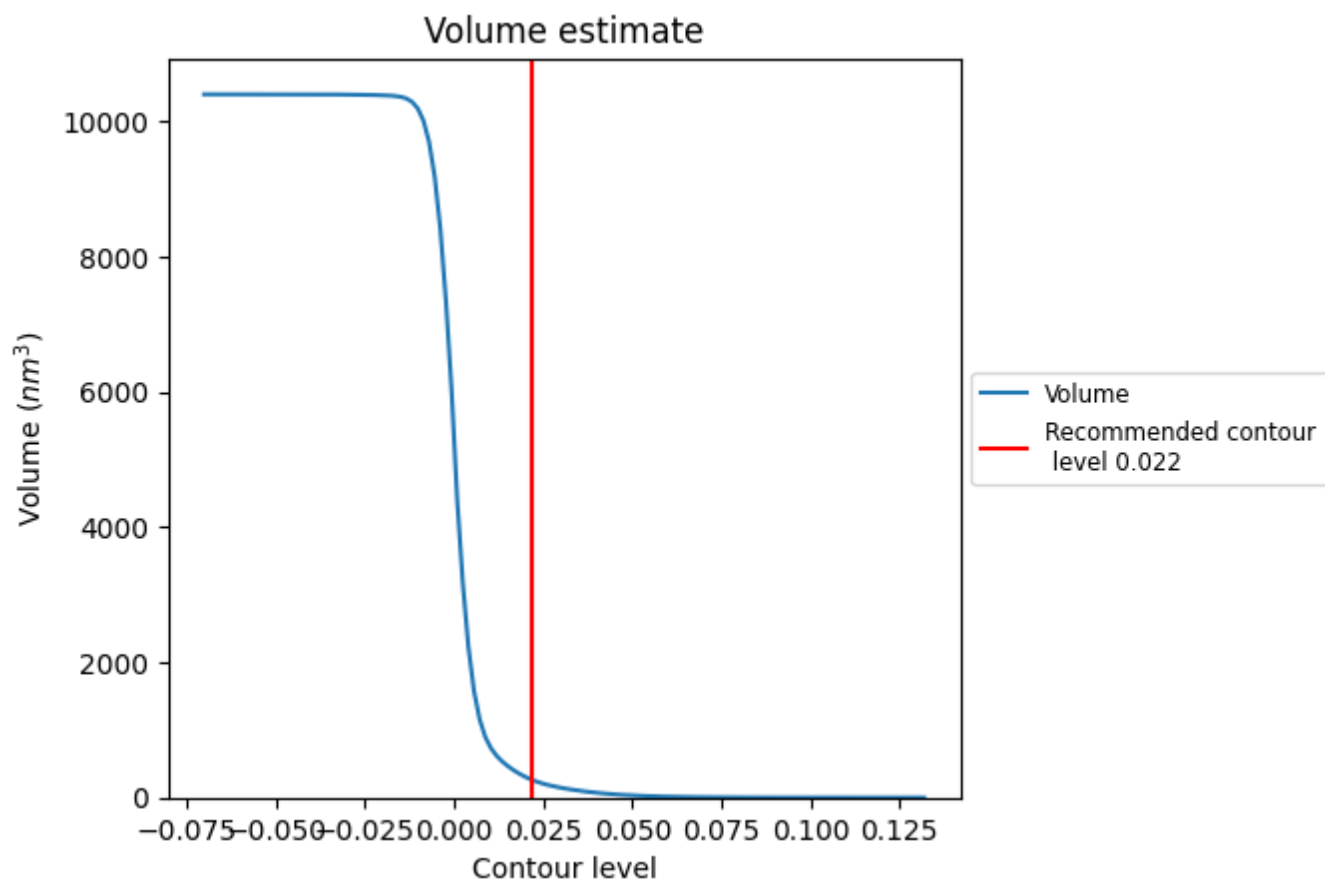
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

7.2 Volume estimate [i](#)



The volume at the recommended contour level is 259 nm³; this corresponds to an approximate mass of 234 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.

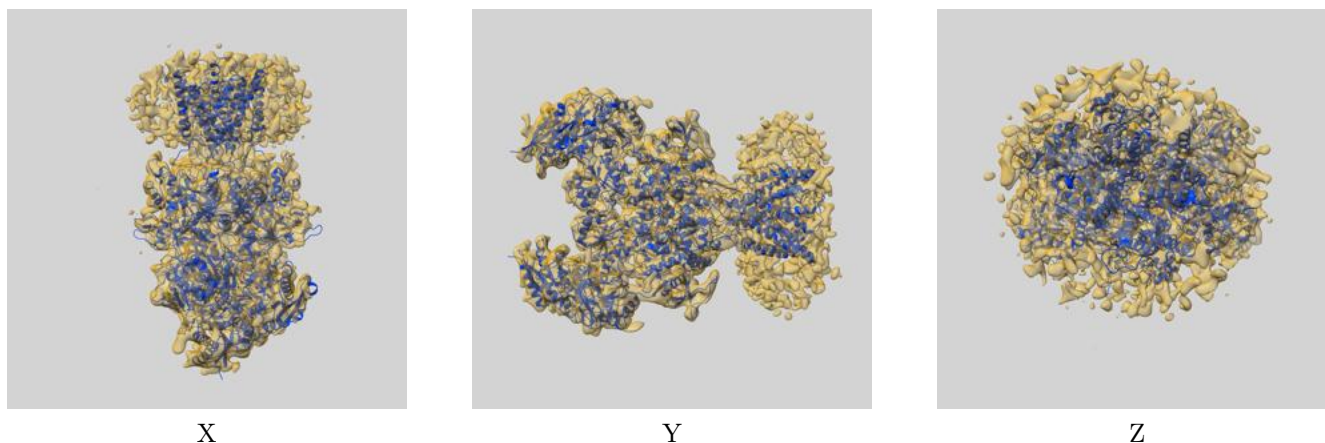
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

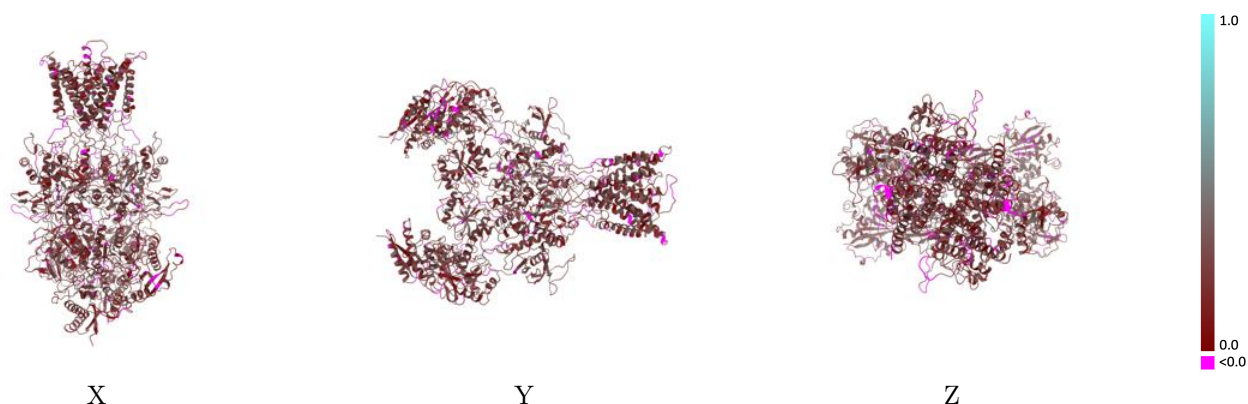
This section contains information regarding the fit between EMDB map EMD-8097 and PDB model 5IOU. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.022 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](#)

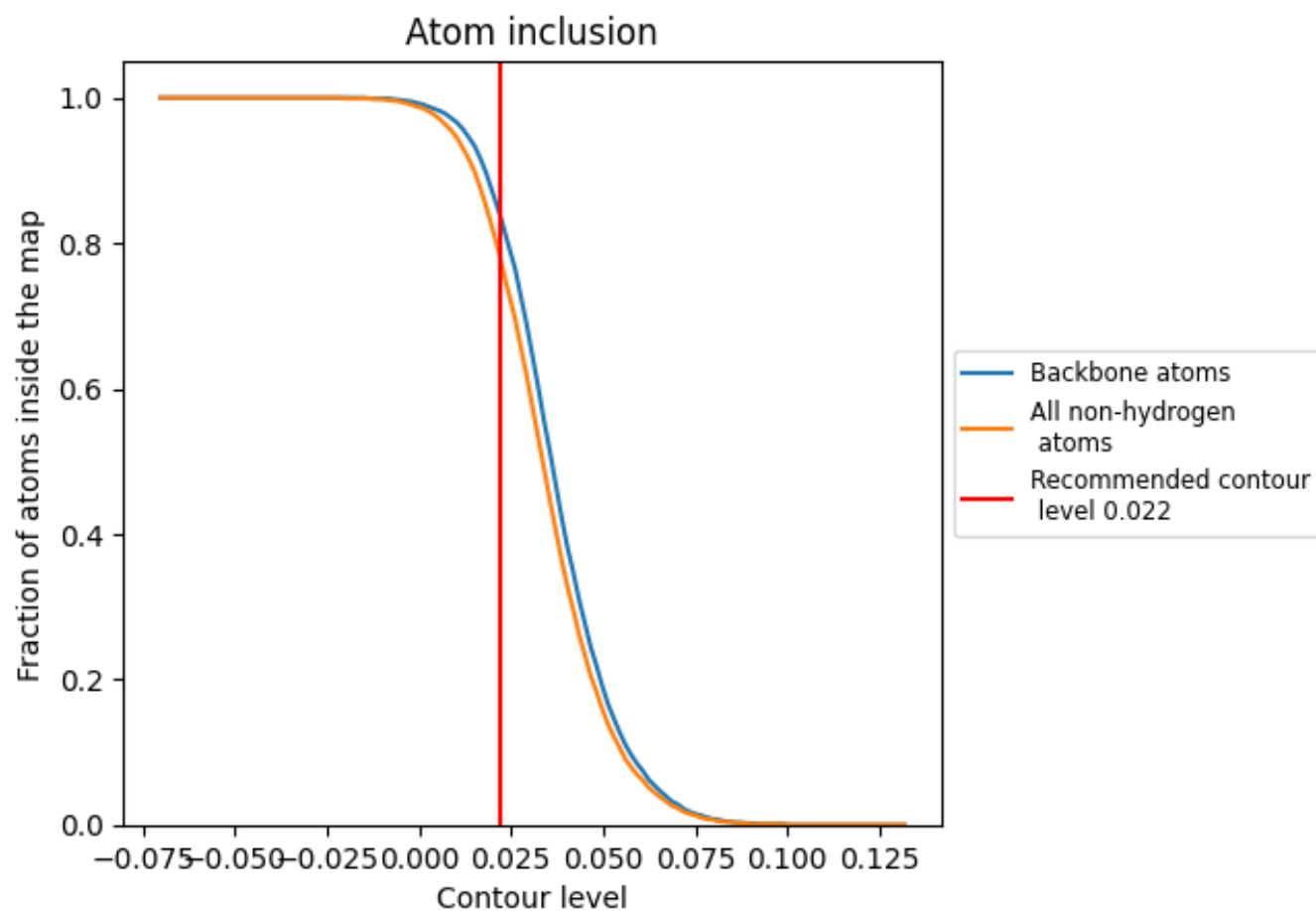


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion ⓘ



At the recommended contour level, 84% of all backbone atoms, 78% 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 (0.022) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7820	0.2230
A	0.7880	0.2260
B	0.7740	0.2210
C	0.8000	0.2260
D	0.7660	0.2180

