Full wwPDB EM Validation Report (i)

Feb 25, 2024 – 10:18 AM EST

PDB ID	:	5IOV
EMDB ID	:	EMD-8098
Title	:	Cryo-EM structure of GluN1/GluN2B NMDA receptor in the glutamate/glycine/Ro25-6981-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	:	7.50 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 (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 (1)) were used in the production of this report:

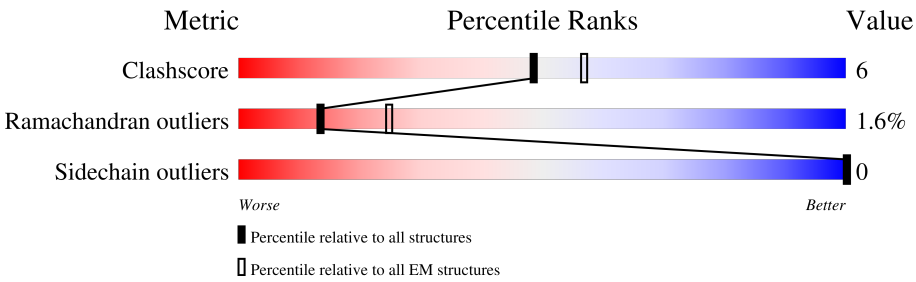
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 7.50 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
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	822	15% 91% 6% •
1	C	822	21% 92% 5% • •
2	B	825	24% 88% 8% • •
2	D	825	28% 88% 8% • •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	QEM	B	901	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	QEM	D	901	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 15879 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
			Total	C	N	O		
1	A	803	3963	2358	803	802	0	0
1	C	803	3963	2358	803	802	0	0

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
			Total	C	N	O		
2	B	798	3939	2344	798	797	0	0
2	D	797	3934	2341	797	796	0	0

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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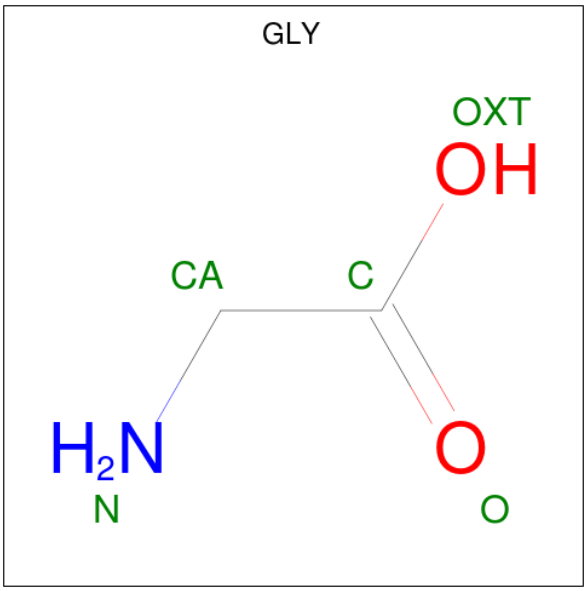
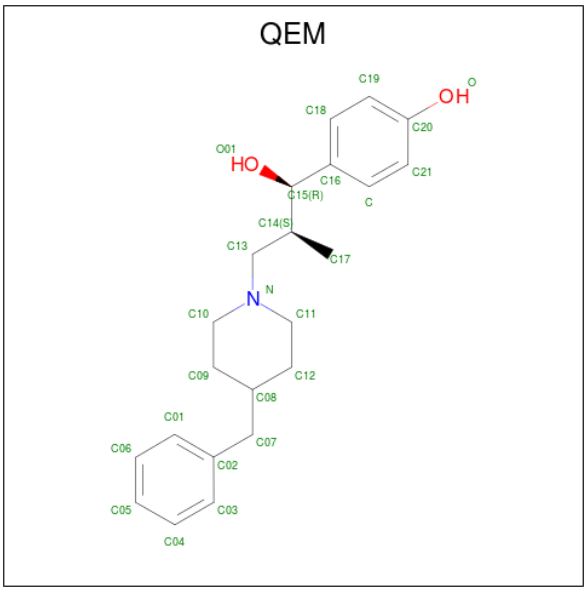
Chain	Residue	Modelled	Actual	Comment	Reference
B	640	ARG	GLU	engineered mutation	UNP A7XY94
B	641	ARG	GLU	engineered mutation	UNP A7XY94
D	20	SER	MET	engineered mutation	UNP A7XY94
D	21	ARG	GLY	engineered mutation	UNP A7XY94
D	22	ALA	CYS	engineered mutation	UNP A7XY94
D	64	GLU	ALA	engineered mutation	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 (three-letter code: GLY) (formula: $C_2H_5NO_2$).



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

- Molecule 4 is 4-[(1R,2S)-3-(4-benzylpiperidin-1-yl)-1-hydroxy-2-methylpropyl]phenol (three-letter code: QEM) (formula: $C_{22}H_{29}NO_2$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
4	B	1	25	22	1	2	0

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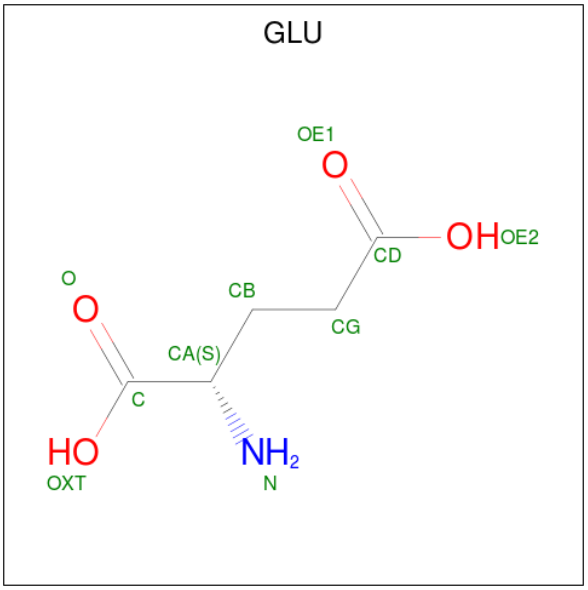
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
4	D	1	25	22	1	2	0

- Molecule 5 is GLUTAMIC ACID (three-letter code: GLU) (formula: $C_5H_9NO_4$).



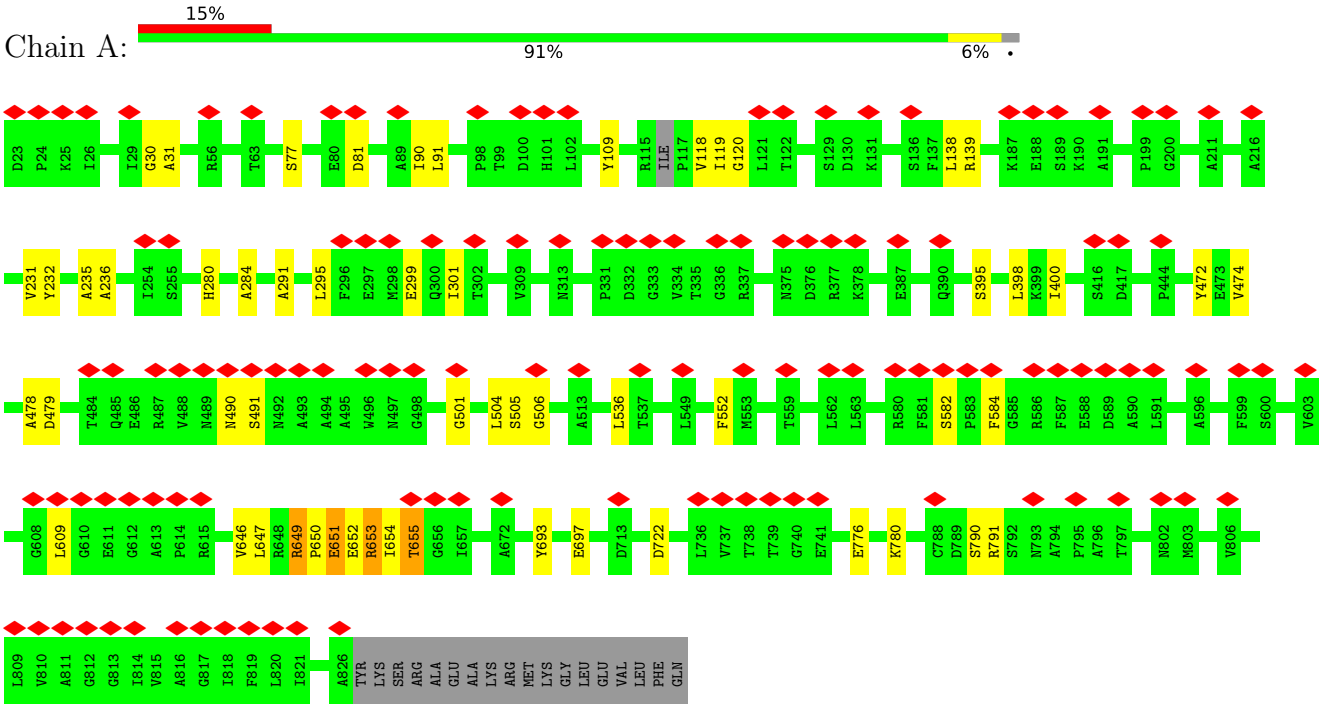
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
5	B	1	10	5	1	4	0
			Total	C	N	O	
5	D	1	10	5	1	4	0

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.

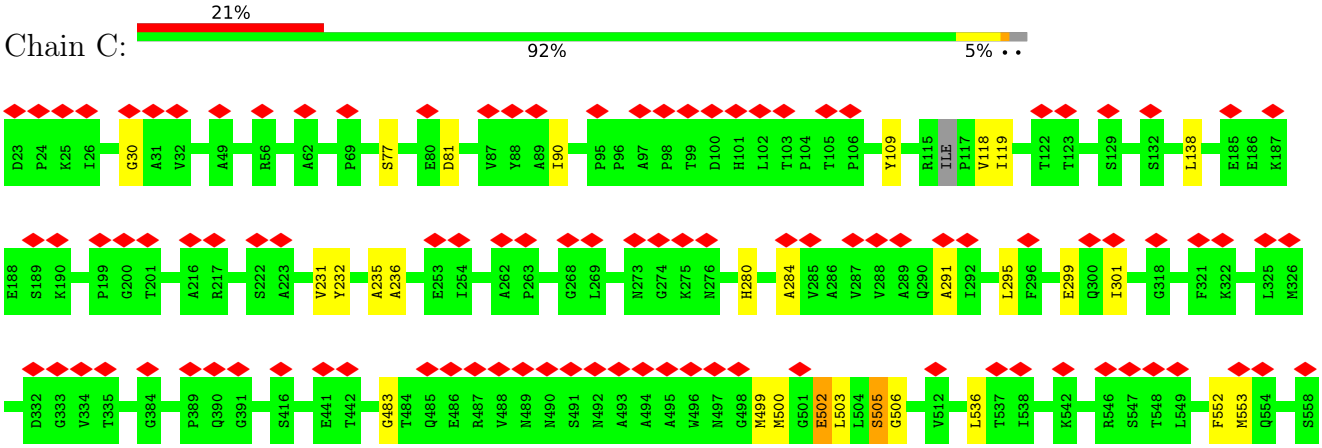
• Molecule 1: N-methyl-D-aspartate receptor subunit NR1-8a

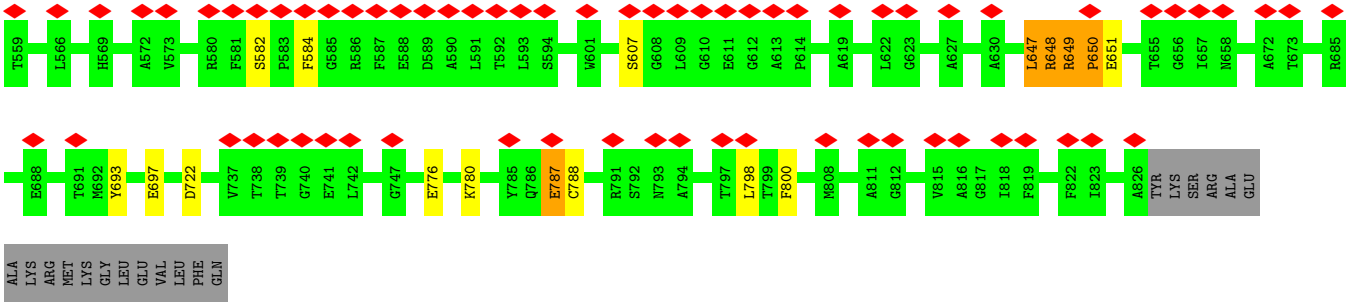
Chain A:



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

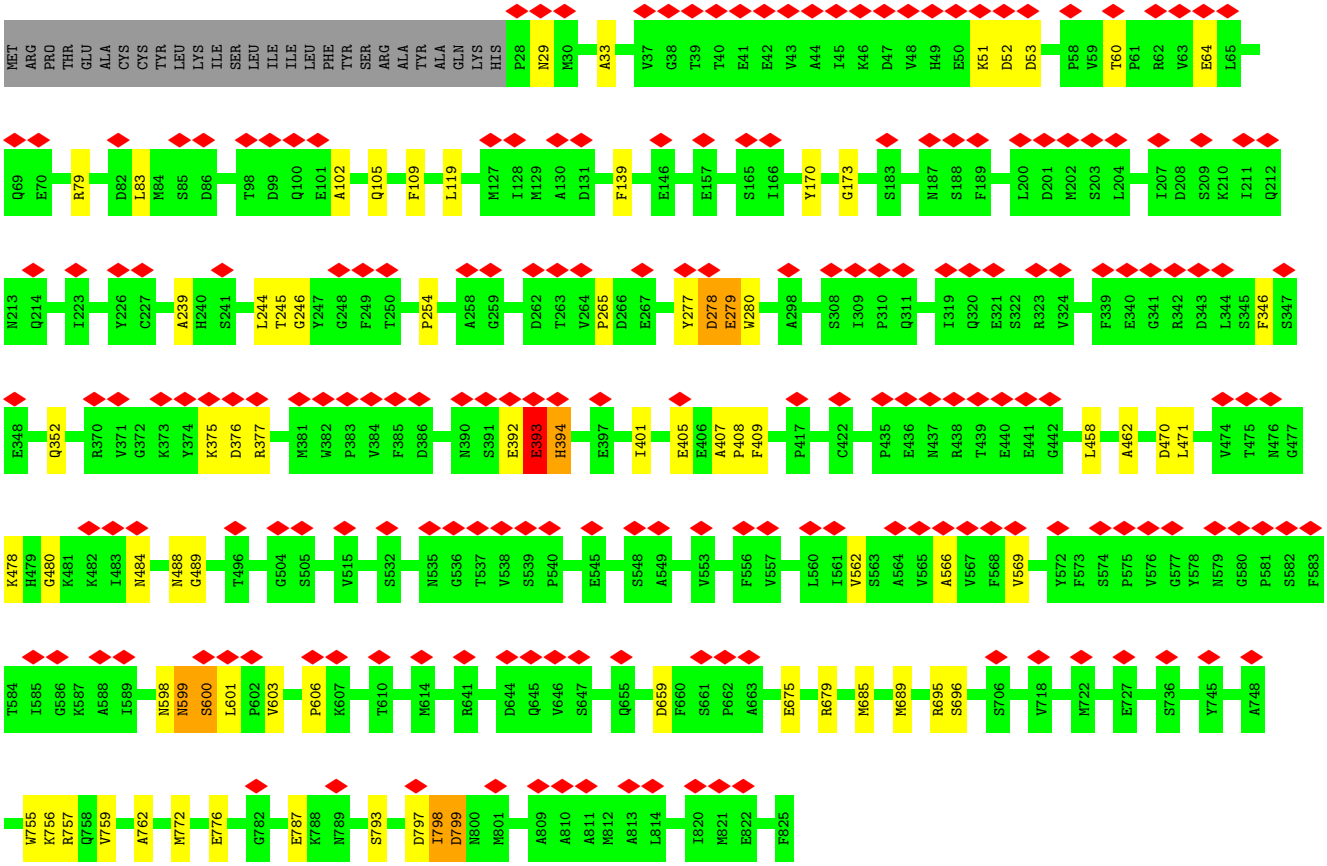
Chain C:





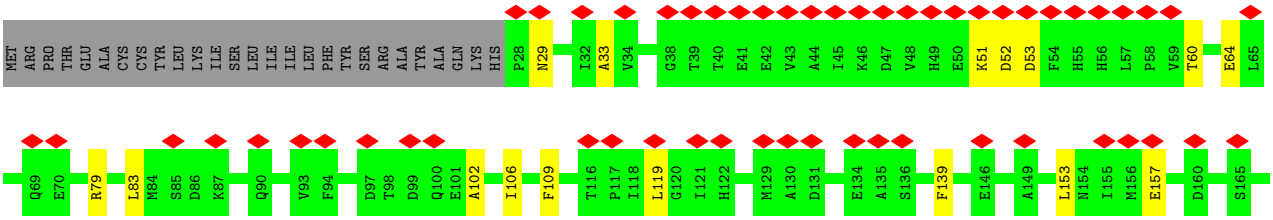
• Molecule 2: Ionotropic glutamate receptor subunit NR2B

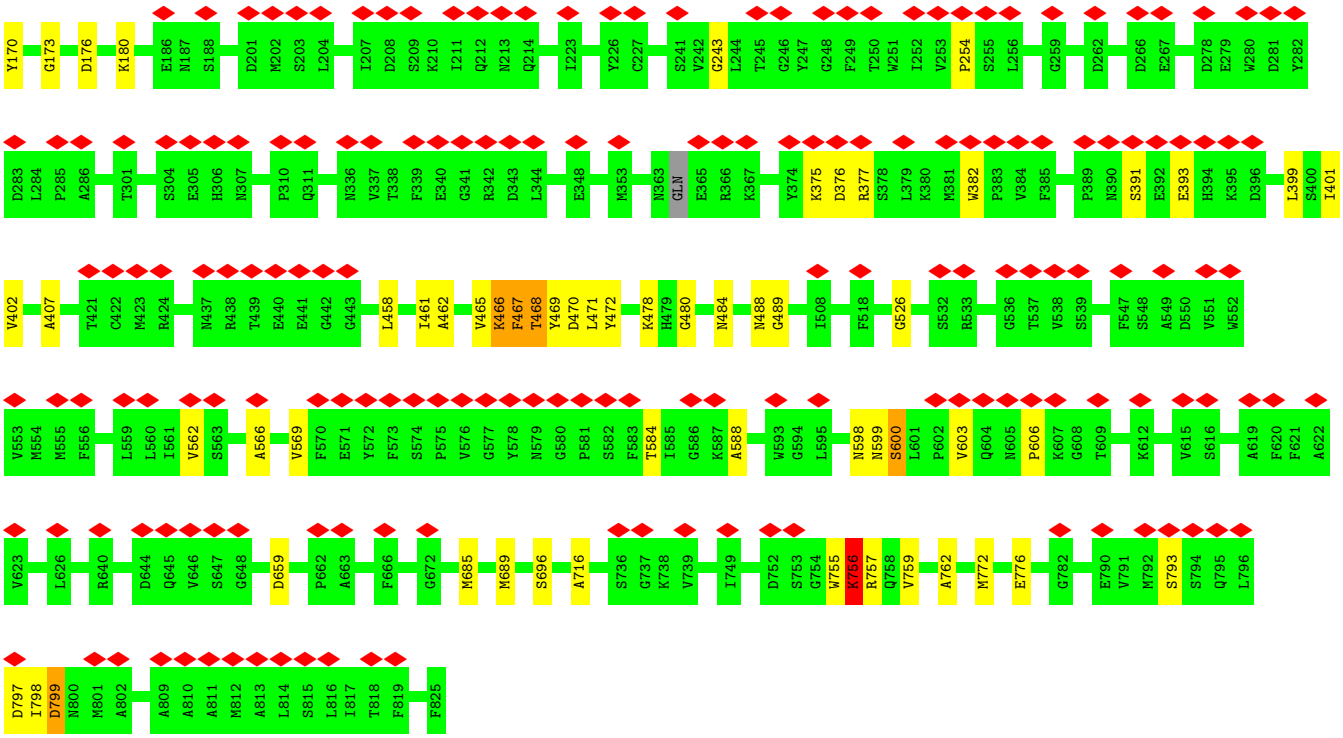
Chain B:



• Molecule 2: Ionotropic glutamate receptor subunit NR2B

Chain D:




Y170 G173 D176 K180 E186 N187 S188 D201 M202 S203 L204 I207 D208 S209 K210 I211 Q212 N213 Q214 I223 Y226 C227 S241 V242 G243 L244 T245 G246 Y247 G248 F249 T250 W251 I252 V253 P254 S255 L256 G259 D262 D266 E267 D278 E279 W280 D281 Y282
D283 L284 P285 A286 T301 S304 E305 H306 N307 P310 Q311 N336 V337 T338 F339 E340 G341 R342 D343 L344 E348 M353 N363 GLN E365 R366 K367 Y374 K375 D376 R377 S378 L379 K380 M381 W382 P383 V384 F385 P389 N390 S391 E392 E393 H394 K395 D396 L399 S400 I401
V402 A407 T421 C422 M423 R424 M437 R438 T439 E440 E441 G442 G443 L458 I461 A462 V465 K466 F467 T468 Y469 D470 L471 Y472 K478 H479 G480 N484 N488 G489 I508 F518 G526 S532 R533 G536 T537 V538 S539 F547 S548 A549 D550 V551 W552
V553 M554 M555 F556 L559 L560 I561 V562 S563 A566 V569 F570 E571 Y572 F573 S574 P575 V576 G577 Y578 N579 G580 P581 S582 F583 T584 I585 G586 K587 A588 W593 G594 L595 N598 N599 S600 L601 P602 V603 Q604 N605 P606 K607 G608 T609 K612 V615 S616 A619 F620 F621 A622
V623 L626 R640 D644 Q645 V646 S647 G648 D659 P662 A663 F666 G672 M685 M689 S696 A716 S736 G737 K738 V739 I749 D752 S753 G754 W755 K756 R757 Q758 V759 A762 M772 E776 G782 E790 V791 M792 S793 S794 Q795 L796
D797 T798 D799 N800 M801 A802 A809 A810 A811 M812 A813 L814 S815 L816 I817 T818 F819 F825

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	87851	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	10.2	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.120	Depositor
Minimum map value	-0.042	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.035	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)

Bond lengths and bond angles in the following residue types are not validated in this section: QEM

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	0.24	0/3961	0.78	16/5512 (0.3%)
1	C	0.24	0/3961	0.71	12/5512 (0.2%)
2	B	0.26	1/3938 (0.0%)	0.63	12/5482 (0.2%)
2	D	0.24	0/3932	0.62	13/5472 (0.2%)
All	All	0.24	1/15792 (0.0%)	0.69	53/21978 (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
2	B	0	2
2	D	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	393	GLU	C-N	-5.53	1.21	1.34

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	490	ASN	CB-CA-C	-18.72	72.96	110.40
1	A	584	PHE	CB-CA-C	-16.49	77.42	110.40
1	C	584	PHE	CB-CA-C	-16.31	77.78	110.40
1	A	790	SER	CB-CA-C	-15.48	80.69	110.10
1	A	504	LEU	CB-CA-C	-15.04	81.62	110.20
1	C	787	GLU	N-CA-C	14.97	151.41	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	393	GLU	C-N-CA	14.24	157.30	121.70
1	C	788	CYS	N-CA-CB	-13.72	85.90	110.60
1	A	505	SER	N-CA-CB	-12.55	91.68	110.50
1	C	502	GLU	N-CA-CB	-12.39	88.30	110.60
1	C	648	ARG	N-CA-CB	11.86	131.94	110.60
1	C	584	PHE	N-CA-C	11.12	141.02	111.00
1	A	584	PHE	N-CA-C	10.90	140.44	111.00
1	C	647	LEU	N-CA-C	10.36	138.98	111.00
1	A	478	ALA	N-CA-C	9.96	137.89	111.00
2	B	393	GLU	N-CA-C	-9.89	84.31	111.00
1	A	479	ASP	N-CA-CB	9.80	128.23	110.60
2	D	756	LYS	N-CA-C	-9.08	86.49	111.00
2	B	798	ILE	N-CA-C	-8.89	86.99	111.00
2	D	466	LYS	N-CA-C	8.86	134.91	111.00
1	C	787	GLU	CB-CA-C	-8.78	92.85	110.40
2	D	467	PHE	N-CA-CB	-8.60	95.12	110.60
1	A	791	ARG	N-CA-CB	8.37	125.67	110.60
1	A	478	ALA	CB-CA-C	-8.37	97.55	110.10
2	D	756	LYS	C-N-CA	7.91	141.47	121.70
1	C	607	SER	CB-CA-C	-7.57	95.72	110.10
2	B	393	GLU	CB-CA-C	7.39	125.18	110.40
2	D	799	ASP	N-CA-C	-7.37	91.10	111.00
2	B	799	ASP	N-CA-C	-7.32	91.25	111.00
1	A	582	SER	N-CA-CB	-7.24	99.63	110.50
2	D	659	ASP	CB-CA-C	7.12	124.64	110.40
1	C	582	SER	N-CA-CB	-7.11	99.84	110.50
1	A	479	ASP	N-CA-C	-6.94	92.25	111.00
2	D	798	ILE	N-CA-C	-6.93	92.28	111.00
2	B	393	GLU	O-C-N	-6.91	111.64	122.70
2	B	695	ARG	CB-CA-C	6.79	123.98	110.40
2	B	696	SER	N-CA-CB	-6.71	100.44	110.50
1	A	504	LEU	N-CA-C	6.65	128.96	111.00
1	A	299	GLU	N-CA-CB	-6.64	98.64	110.60
2	B	394	HIS	N-CA-CB	6.61	122.50	110.60
1	A	609	LEU	N-CA-C	-6.54	93.34	111.00
2	D	569	VAL	CB-CA-C	6.49	123.73	111.40
2	D	798	ILE	CB-CA-C	-6.41	98.77	111.60
2	B	394	HIS	N-CA-C	-5.89	95.09	111.00
2	D	600	SER	N-CA-C	-5.81	95.31	111.00
2	B	484	ASN	N-CA-C	-5.78	95.39	111.00
1	C	505	SER	N-CA-CB	5.74	119.11	110.50
2	D	756	LYS	CB-CA-C	5.59	121.59	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	299	GLU	N-CA-CB	5.51	120.52	110.60
2	D	391	SER	N-CA-CB	-5.42	102.38	110.50
1	A	491	SER	N-CA-C	5.38	125.54	111.00
2	B	659	ASP	CB-CA-C	5.25	120.91	110.40
2	D	484	ASN	N-CA-C	-5.14	97.11	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	393	GLU	Mainchain,Peptide
2	D	756	LYS	Peptide

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	29	0
1	C	3963	0	1808	23	0
2	B	3939	0	1750	41	0
2	D	3934	0	1746	50	0
3	A	5	0	2	0	0
3	C	5	0	2	0	0
4	B	25	0	29	11	0
4	D	25	0	29	11	0
5	B	10	0	5	0	0
5	D	10	0	5	0	0
All	All	15879	0	7185	143	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 6.

All (143) 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:A:109:TYR:CB	4:B:901:QEM:C01	2.14	1.25

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:649:ARG:O	1:C:651:GLU:N	1.72	1.23
2:B:109:PHE:CB	4:B:901:QEM:H04	1.76	1.14
2:D:102:ALA:HB1	4:D:901:QEM:H09A	1.32	1.10
2:D:462:ALA:HA	2:D:465:VAL:CB	1.81	1.10
2:B:239:ALA:HB1	2:B:244:LEU:CB	1.90	1.02
1:A:109:TYR:CB	4:B:901:QEM:H01	1.93	0.96
2:B:375:LYS:O	2:B:377:ARG:N	1.99	0.94
2:D:102:ALA:HB1	4:D:901:QEM:C09	1.98	0.92
1:C:648:ARG:O	1:C:650:PRO:N	2.03	0.92
1:A:400:ILE:O	1:A:474:VAL:HA	1.71	0.91
2:D:467:PHE:O	2:D:468:THR:O	1.89	0.91
2:B:29:ASN:HA	2:B:60:THR:O	1.71	0.90
2:D:106:ILE:HA	4:D:901:QEM:C06	2.01	0.90
2:D:29:ASN:HA	2:D:60:THR:O	1.72	0.89
2:D:461:ILE:C	2:D:465:VAL:CB	2.23	0.89
2:D:170:TYR:O	4:D:901:QEM:H19	1.72	0.89
1:C:119:ILE:HA	1:C:138:LEU:O	1.72	0.88
2:D:462:ALA:CA	2:D:465:VAL:CB	2.52	0.88
1:A:119:ILE:HA	1:A:138:LEU:O	1.73	0.87
1:C:90:ILE:O	1:C:118:VAL:HA	1.79	0.83
1:A:650:PRO:O	1:A:652:GLU:N	2.14	0.81
2:D:375:LYS:O	2:D:377:ARG:N	2.16	0.79
1:A:654:ILE:O	1:A:655:THR:CB	2.32	0.77
2:B:170:TYR:O	4:B:901:QEM:H21	1.85	0.77
2:D:462:ALA:O	2:D:466:LYS:N	2.17	0.75
2:B:797:ASP:O	2:B:799:ASP:N	2.19	0.75
2:D:797:ASP:O	2:D:799:ASP:N	2.20	0.75
2:D:467:PHE:O	2:D:468:THR:C	2.26	0.72
2:D:106:ILE:HA	4:D:901:QEM:H06	1.72	0.71
2:B:109:PHE:CB	4:B:901:QEM:C04	2.65	0.69
1:A:90:ILE:O	1:A:118:VAL:HA	1.93	0.68
2:D:102:ALA:CB	4:D:901:QEM:H09A	2.16	0.68
2:B:102:ALA:HB1	4:B:901:QEM:H11	1.76	0.67
1:A:398:LEU:O	1:A:472:TYR:HA	1.95	0.67
2:D:462:ALA:N	2:D:465:VAL:CB	2.58	0.67
2:D:399:LEU:O	2:D:469:TYR:HA	1.96	0.65
2:D:480:GLY:HA2	2:D:488:ASN:O	1.97	0.64
1:A:650:PRO:O	1:A:651:GLU:C	2.36	0.64
2:B:480:GLY:HA2	2:B:488:ASN:O	1.97	0.64
2:D:756:LYS:O	2:D:759:VAL:N	2.21	0.62
2:B:239:ALA:CB	2:B:244:LEU:CB	2.75	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:401:ILE:O	2:D:471:LEU:HA	2.00	0.62
1:C:503:LEU:O	1:C:505:SER:N	2.33	0.62
2:B:105:GLN:CB	4:B:901:QEM:H12A	2.30	0.61
2:D:106:ILE:HA	4:D:901:QEM:C01	2.30	0.61
2:B:393:GLU:O	2:B:394:HIS:O	2.18	0.61
2:D:170:TYR:O	4:D:901:QEM:C19	2.46	0.61
1:A:109:TYR:CB	4:B:901:QEM:C06	2.75	0.60
2:B:480:GLY:HA2	2:B:489:GLY:HA3	1.83	0.60
2:D:480:GLY:HA2	2:D:489:GLY:HA3	1.84	0.58
2:B:797:ASP:O	2:B:798:ILE:C	2.42	0.58
2:B:170:TYR:O	4:B:901:QEM:C21	2.53	0.57
2:B:102:ALA:CB	4:B:901:QEM:H11	2.35	0.57
2:D:562:VAL:O	2:D:566:ALA:CB	2.53	0.56
2:B:119:LEU:HA	2:B:139:PHE:O	2.05	0.56
2:D:584:THR:O	2:D:588:ALA:HB2	2.06	0.56
1:C:536:LEU:HA	1:C:722:ASP:HA	1.88	0.55
1:A:109:TYR:CB	4:B:901:QEM:C02	2.81	0.54
2:B:562:VAL:O	2:B:566:ALA:CB	2.56	0.54
1:A:30:GLY:O	1:A:90:ILE:HA	2.07	0.54
2:D:562:VAL:O	2:D:566:ALA:HB3	2.08	0.54
2:B:239:ALA:O	2:B:244:LEU:CB	2.57	0.53
2:D:458:LEU:O	2:D:462:ALA:HB2	2.09	0.53
2:B:401:ILE:O	2:B:471:LEU:HA	2.08	0.53
2:D:755:TRP:O	2:D:756:LYS:C	2.46	0.53
1:C:648:ARG:O	1:C:649:ARG:C	2.48	0.52
2:D:462:ALA:C	2:D:466:LYS:H	2.12	0.52
1:A:291:ALA:O	1:A:295:LEU:CB	2.58	0.52
1:A:536:LEU:HA	1:A:722:ASP:HA	1.93	0.51
1:C:291:ALA:O	1:C:295:LEU:CB	2.59	0.51
2:D:119:LEU:HA	2:D:139:PHE:O	2.11	0.51
2:D:797:ASP:C	2:D:799:ASP:N	2.65	0.50
2:B:239:ALA:O	2:B:244:LEU:N	2.39	0.50
2:D:755:TRP:O	2:D:757:ARG:N	2.44	0.50
1:C:280:HIS:O	1:C:284:ALA:HB2	2.11	0.50
2:B:346:PHE:HA	2:B:352:GLN:HA	1.94	0.50
2:B:407:ALA:O	2:B:409:PHE:N	2.44	0.50
2:B:458:LEU:O	2:B:462:ALA:HB2	2.12	0.50
2:B:772:MET:O	2:B:776:GLU:CB	2.60	0.50
1:C:647:LEU:O	1:C:649:ARG:N	2.38	0.50
2:D:598:ASN:O	2:D:600:SER:N	2.45	0.50
2:B:278:ASP:O	2:B:280:TRP:N	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:598:ASN:O	2:B:600:SER:N	2.44	0.50
2:D:772:MET:O	2:D:776:GLU:CB	2.59	0.50
1:A:646:VAL:O	1:A:647:LEU:C	2.50	0.49
2:B:562:VAL:O	2:B:566:ALA:HB3	2.13	0.49
2:D:685:MET:O	2:D:689:MET:CB	2.61	0.49
1:A:652:GLU:O	1:A:653:ARG:CB	2.60	0.48
2:B:685:MET:O	2:B:689:MET:CB	2.61	0.48
1:A:280:HIS:O	1:A:284:ALA:HB2	2.12	0.48
1:C:30:GLY:O	1:C:90:ILE:HA	2.13	0.48
1:C:77:SER:O	1:C:81:ASP:CB	2.62	0.48
1:C:231:VAL:O	1:C:235:ALA:HB3	2.14	0.47
1:A:649:ARG:C	1:A:651:GLU:N	2.66	0.47
1:C:649:ARG:C	1:C:651:GLU:N	2.58	0.47
2:D:33:ALA:HA	2:D:64:GLU:O	2.13	0.47
2:B:33:ALA:HA	2:B:64:GLU:O	2.15	0.47
1:C:649:ARG:O	1:C:650:PRO:C	2.42	0.47
2:B:392:GLU:O	2:B:393:GLU:C	2.51	0.47
1:A:77:SER:O	1:A:81:ASP:CB	2.63	0.47
2:D:51:LYS:O	2:D:53:ASP:N	2.48	0.46
1:A:232:TYR:O	1:A:236:ALA:HB2	2.16	0.46
2:B:79:ARG:O	2:B:83:LEU:CB	2.63	0.46
2:B:51:LYS:O	2:B:53:ASP:N	2.49	0.46
2:B:277:TYR:O	2:B:279:GLU:N	2.48	0.46
2:D:79:ARG:O	2:D:83:LEU:CB	2.64	0.46
1:C:109:TYR:CB	4:D:901:QEM:H12	2.47	0.45
2:D:458:LEU:O	2:D:462:ALA:CB	2.64	0.45
2:D:462:ALA:O	2:D:466:LYS:HA	2.16	0.45
1:C:798:LEU:O	1:C:800:PHE:N	2.45	0.45
1:A:649:ARG:O	1:A:651:GLU:N	2.49	0.45
2:D:759:VAL:O	2:D:762:ALA:HB3	2.16	0.44
1:C:648:ARG:O	1:C:650:PRO:CB	2.64	0.44
2:B:759:VAL:O	2:B:762:ALA:HB3	2.17	0.44
1:A:650:PRO:C	1:A:652:GLU:N	2.69	0.44
1:C:483:GLY:HA2	1:C:500:MET:H	1.82	0.43
1:A:231:VAL:O	1:A:235:ALA:HB3	2.18	0.43
2:D:401:ILE:CB	2:D:470:ASP:O	2.66	0.43
1:A:649:ARG:C	1:A:651:GLU:H	2.21	0.43
2:B:458:LEU:O	2:B:462:ALA:CB	2.67	0.43
2:B:755:TRP:O	2:B:757:ARG:N	2.52	0.43
2:D:106:ILE:CA	4:D:901:QEM:C01	2.95	0.43
1:C:232:TYR:O	1:C:236:ALA:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:467:PHE:C	2:D:468:THR:O	2.55	0.42
2:D:402:VAL:HA	2:D:472:TYR:O	2.19	0.42
2:D:526:GLY:O	2:D:716:ALA:N	2.53	0.42
1:A:120:GLY:H	1:A:139:ARG:HA	1.84	0.42
2:D:584:THR:O	2:D:588:ALA:CB	2.67	0.42
1:C:500:MET:O	1:C:502:GLU:N	2.52	0.42
1:C:776:GLU:O	1:C:780:LYS:CB	2.68	0.42
1:A:776:GLU:O	1:A:780:LYS:CB	2.68	0.42
2:B:392:GLU:O	2:B:394:HIS:N	2.53	0.42
2:B:675:GLU:O	2:B:679:ARG:CB	2.68	0.42
2:B:599:ASN:O	2:B:601:LEU:N	2.52	0.42
2:B:401:ILE:CB	2:B:470:ASP:O	2.67	0.41
2:D:176:ASP:O	2:D:180:LYS:CB	2.69	0.41
2:D:153:LEU:O	2:D:157:GLU:CB	2.69	0.41
1:A:31:ALA:HA	1:A:91:LEU:H	1.85	0.41
1:C:693:TYR:O	1:C:697:GLU:CB	2.69	0.41
1:A:693:TYR:O	1:A:697:GLU:CB	2.69	0.40
2:D:109:PHE:CB	4:D:901:QEM:H06	2.51	0.40
1:A:232:TYR:O	1:A:236:ALA:CB	2.69	0.40

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	799/822 (97%)	684 (86%)	106 (13%)	9 (1%)	14 52
1	C	799/822 (97%)	681 (85%)	110 (14%)	8 (1%)	15 54
2	B	796/825 (96%)	666 (84%)	110 (14%)	20 (2%)	5 32
2	D	793/825 (96%)	678 (86%)	100 (13%)	15 (2%)	8 38
All	All	3187/3294 (97%)	2709 (85%)	426 (13%)	52 (2%)	13 44

All (52) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	651	GLU
1	A	655	THR
1	C	506	GLY
1	C	649	ARG
1	C	650	PRO
2	B	278	ASP
2	B	376	ASP
2	B	408	PRO
2	D	376	ASP
2	D	468	THR
1	A	552	PHE
1	A	653	ARG
2	B	245	THR
2	B	254	PRO
2	B	265	PRO
2	B	569	VAL
2	D	254	PRO
1	A	395	SER
1	A	649	ARG
1	C	552	PHE
1	C	787	GLU
2	B	52	ASP
2	B	279	GLU
2	B	478	LYS
2	B	599	ASN
2	B	600	SER
2	B	606	PRO
2	B	756	LYS
2	D	52	ASP
2	D	478	LYS
2	D	599	ASN
2	D	696	SER
2	D	793	SER
2	B	787	GLU
2	B	793	SER
2	D	603	VAL
1	A	301	ILE
1	A	501	GLY
1	C	301	ILE
1	C	553	MET
2	B	603	VAL
2	D	393	GLU

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Mol	Chain	Res	Type
2	D	606	PRO
1	C	499	MET
2	B	173	GLY
2	B	246	GLY
2	B	405	GLU
2	D	243	GLY
2	D	407	ALA
2	D	173	GLY
2	D	382	TRP
1	A	506	GLY

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)

6 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	$\#\|Z\| > 2$
5	GLU	B	902	-	8,9,9	1.08	1 (12%)	10,11,11	1.27	2 (20%)
4	QEM	B	901	-	27,27,27	1.00	1 (3%)	35,36,36	1.28	5 (14%)
4	QEM	D	901	-	27,27,27	0.86	1 (3%)	35,36,36	1.19	4 (11%)
5	GLU	D	902	-	8,9,9	1.08	1 (12%)	10,11,11	1.27	2 (20%)
3	GLY	A	901	-	4,4,4	1.15	1 (25%)	3,4,4	1.67	1 (33%)
3	GLY	C	1001	-	4,4,4	1.13	1 (25%)	3,4,4	1.66	1 (33%)

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
5	GLU	B	902	-	-	2/9/9/9	-
4	QEM	B	901	-	-	4/16/26/26	0/3/3/3
4	QEM	D	901	-	-	5/16/26/26	0/3/3/3
5	GLU	D	902	-	-	2/9/9/9	-
3	GLY	A	901	-	-	0/2/2/2	-
3	GLY	C	1001	-	-	0/2/2/2	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	901	QEM	C06-C01	-2.52	1.33	1.38
3	A	901	GLY	OXT-C	-2.16	1.23	1.30
5	D	902	GLU	OXT-C	-2.14	1.23	1.30
5	B	902	GLU	OXT-C	-2.14	1.23	1.30
3	C	1001	GLY	OXT-C	-2.12	1.23	1.30
4	D	901	QEM	O-C20	2.08	1.41	1.37

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	901	QEM	C11-N-C10	3.56	116.84	108.83
4	D	901	QEM	C11-N-C10	3.27	116.19	108.83
4	D	901	QEM	C14-C13-N	-2.90	109.06	115.33
4	B	901	QEM	C14-C13-N	-2.82	109.23	115.33
5	D	902	GLU	OXT-C-O	-2.71	117.94	124.09
4	B	901	QEM	C09-C08-C07	-2.70	105.57	111.88
5	B	902	GLU	OXT-C-O	-2.69	117.98	124.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	901	QEM	C12-C11-N	2.45	114.92	111.11
4	D	901	QEM	C12-C11-N	2.32	114.72	111.11
5	B	902	GLU	OXT-C-CA	2.25	121.04	113.38
5	D	902	GLU	OXT-C-CA	2.25	121.04	113.38
3	A	901	GLY	OXT-C-O	-2.13	117.98	123.30
3	C	1001	GLY	OXT-C-O	-2.13	117.99	123.30
4	D	901	QEM	C16-C15-C14	-2.11	109.26	113.10
4	B	901	QEM	C18-C16-C15	-2.07	117.63	120.73

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	901	QEM	C13-C14-C15-O01
4	B	901	QEM	C01-C02-C07-C08
4	B	901	QEM	C03-C02-C07-C08
4	B	901	QEM	C14-C15-C16-C
4	B	901	QEM	C14-C15-C16-C18
4	D	901	QEM	N-C13-C14-C17
5	B	902	GLU	OE2-CD-CG-CB
5	B	902	GLU	OE1-CD-CG-CB
5	D	902	GLU	OE2-CD-CG-CB
5	D	902	GLU	OE1-CD-CG-CB
4	D	901	QEM	C14-C13-N-C11
4	D	901	QEM	C01-C02-C07-C08
4	D	901	QEM	C03-C02-C07-C08

There are no ring outliers.

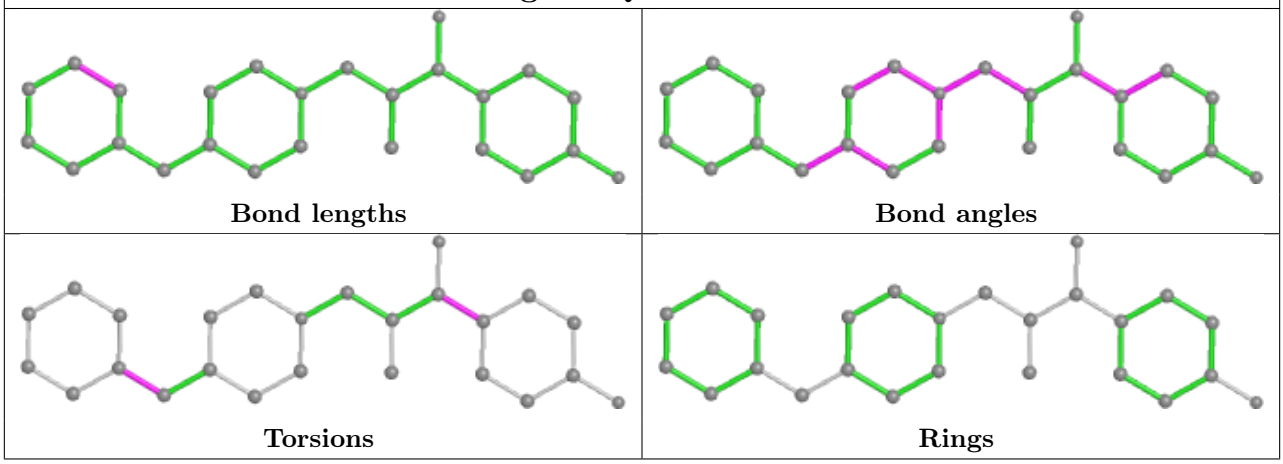
2 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	901	QEM	11	0
4	D	901	QEM	11	0

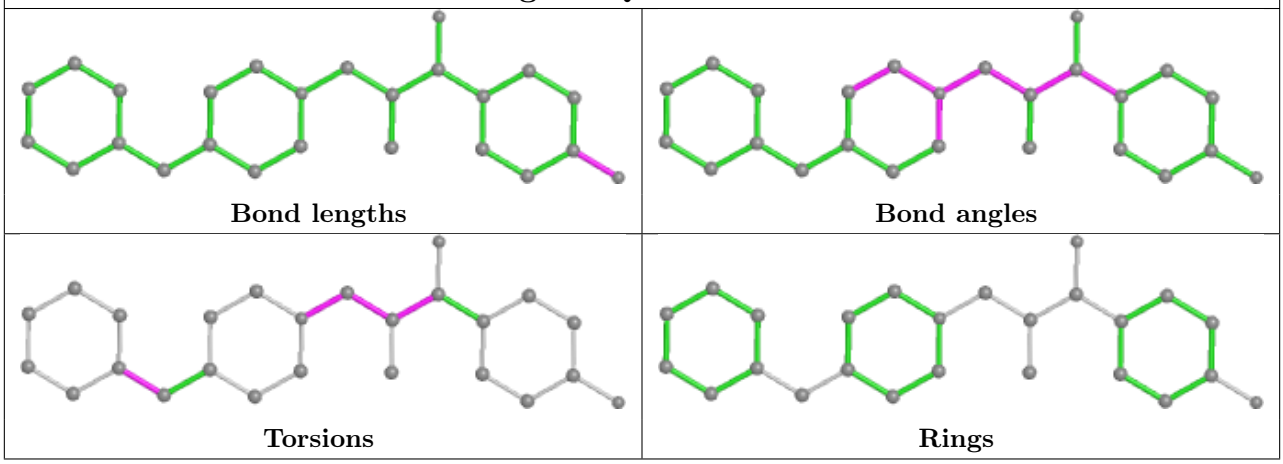
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand QEM B 901



Ligand QEM D 901



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.

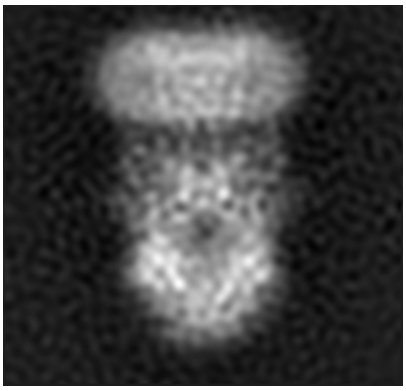
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-8098. These allow visual inspection of the internal detail of the map and identification of artifacts.

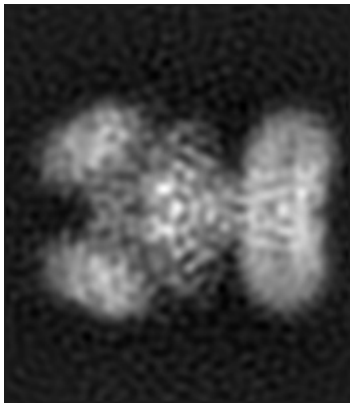
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

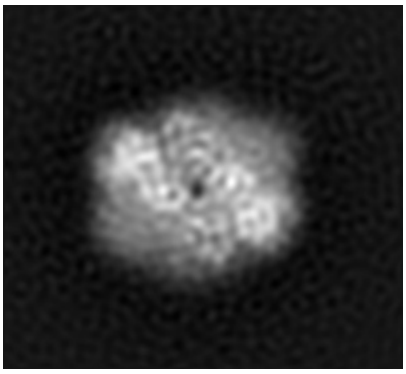
6.1.1 Primary map



X



Y

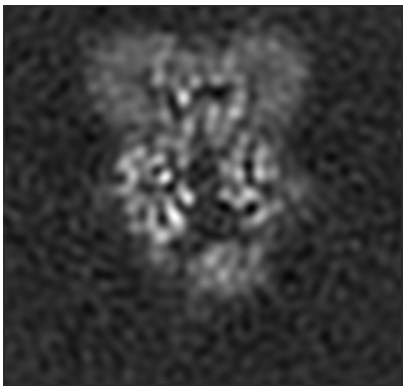


Z

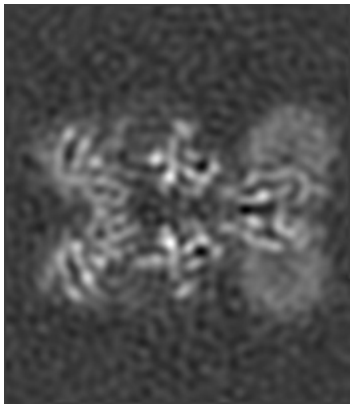
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

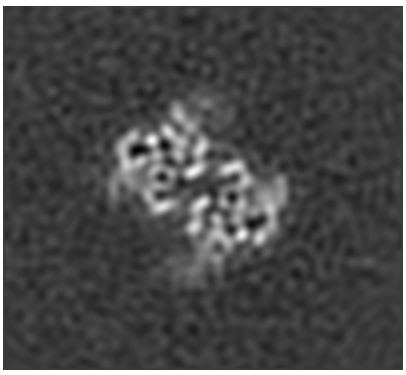
6.2.1 Primary map



X Index: 110



Y Index: 100

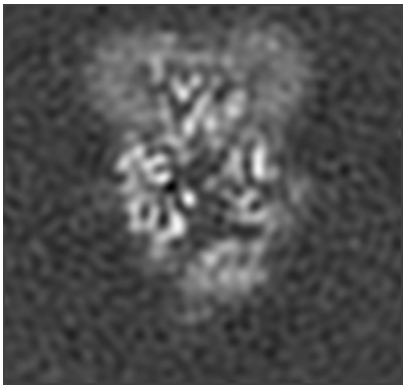


Z Index: 95

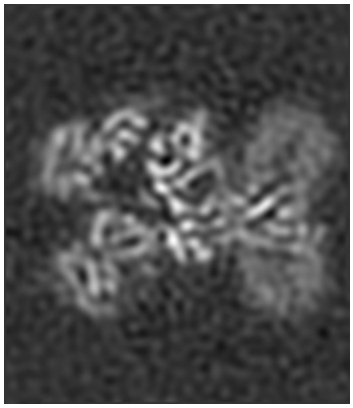
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

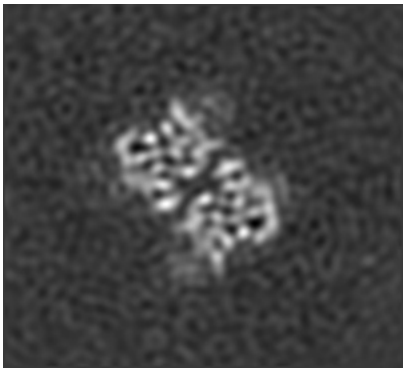
6.3.1 Primary map



X Index: 112



Y Index: 91

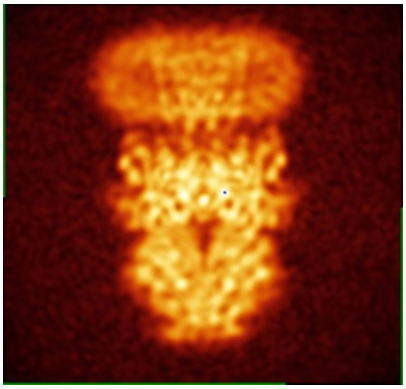


Z Index: 93

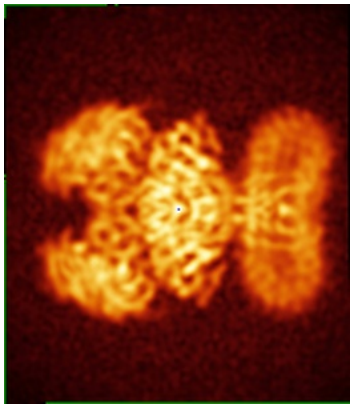
The images above show the largest variance slices of the map in three orthogonal directions.

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

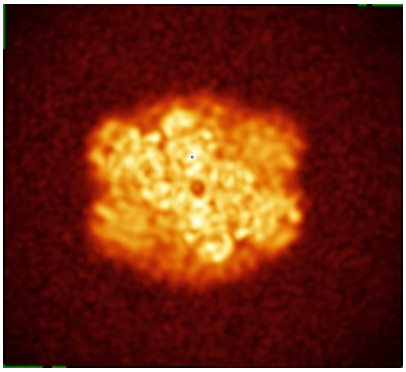
6.4.1 Primary map



X



Y

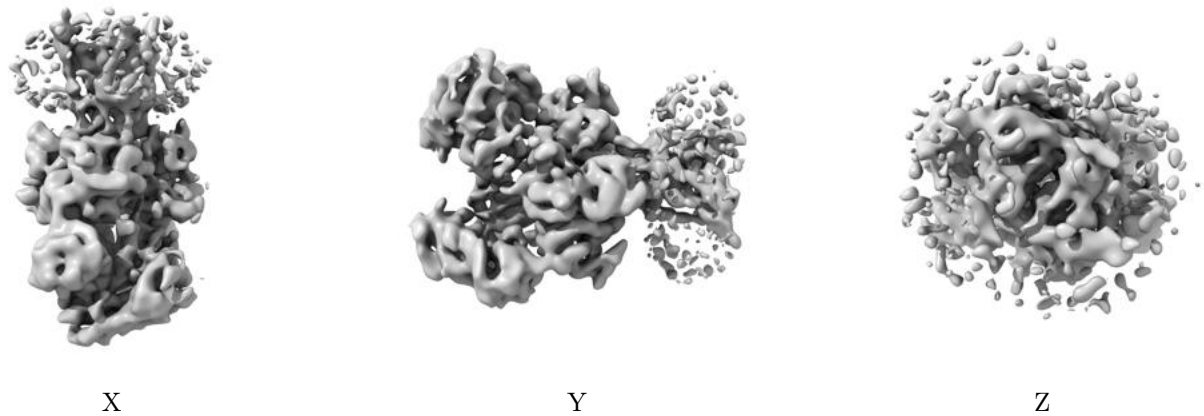


Z

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



The images above show the 3D surface view of the map at the recommended contour level 0.035. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

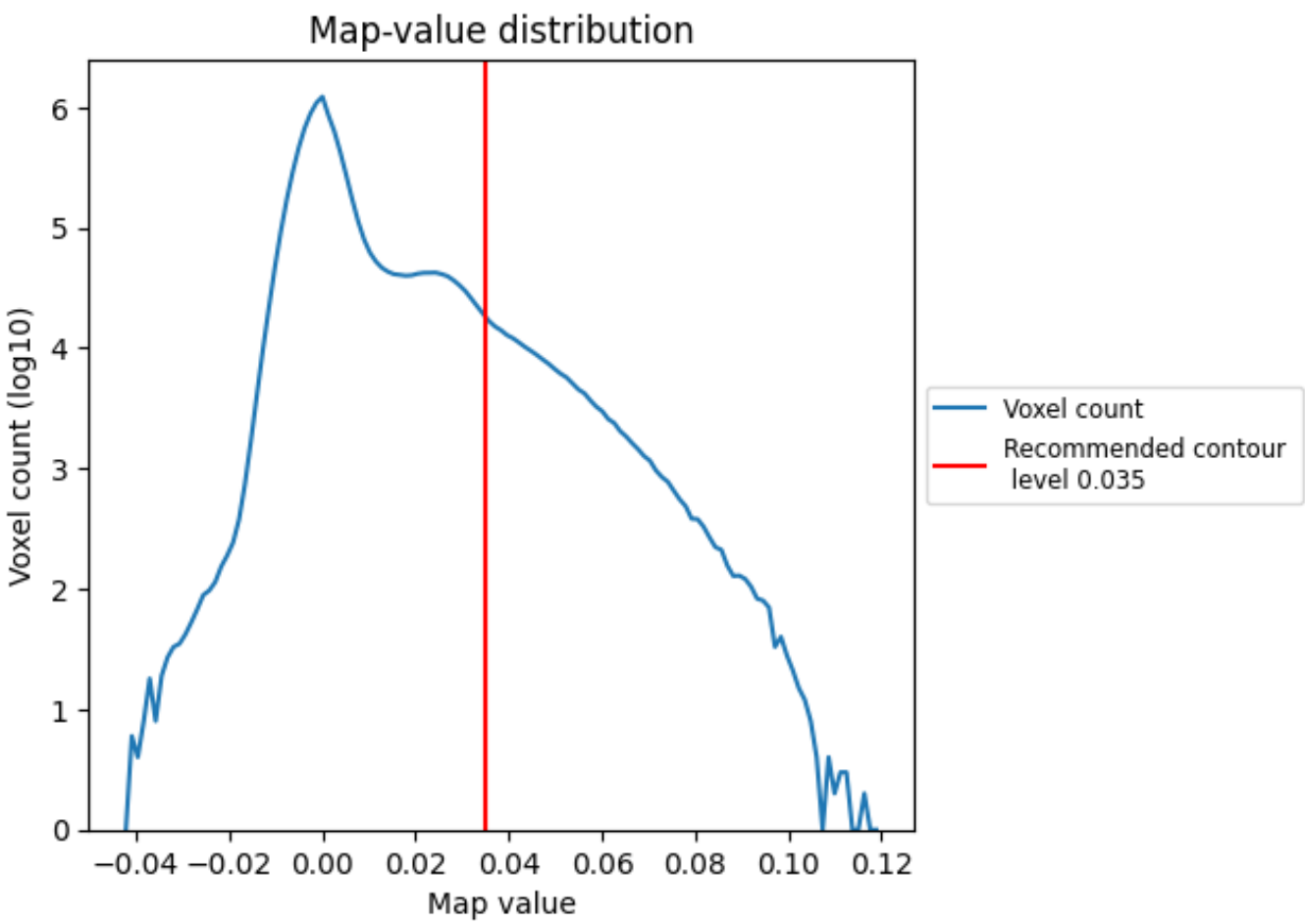
6.6 Mask visualisation (i)

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

7 Map analysis (i)

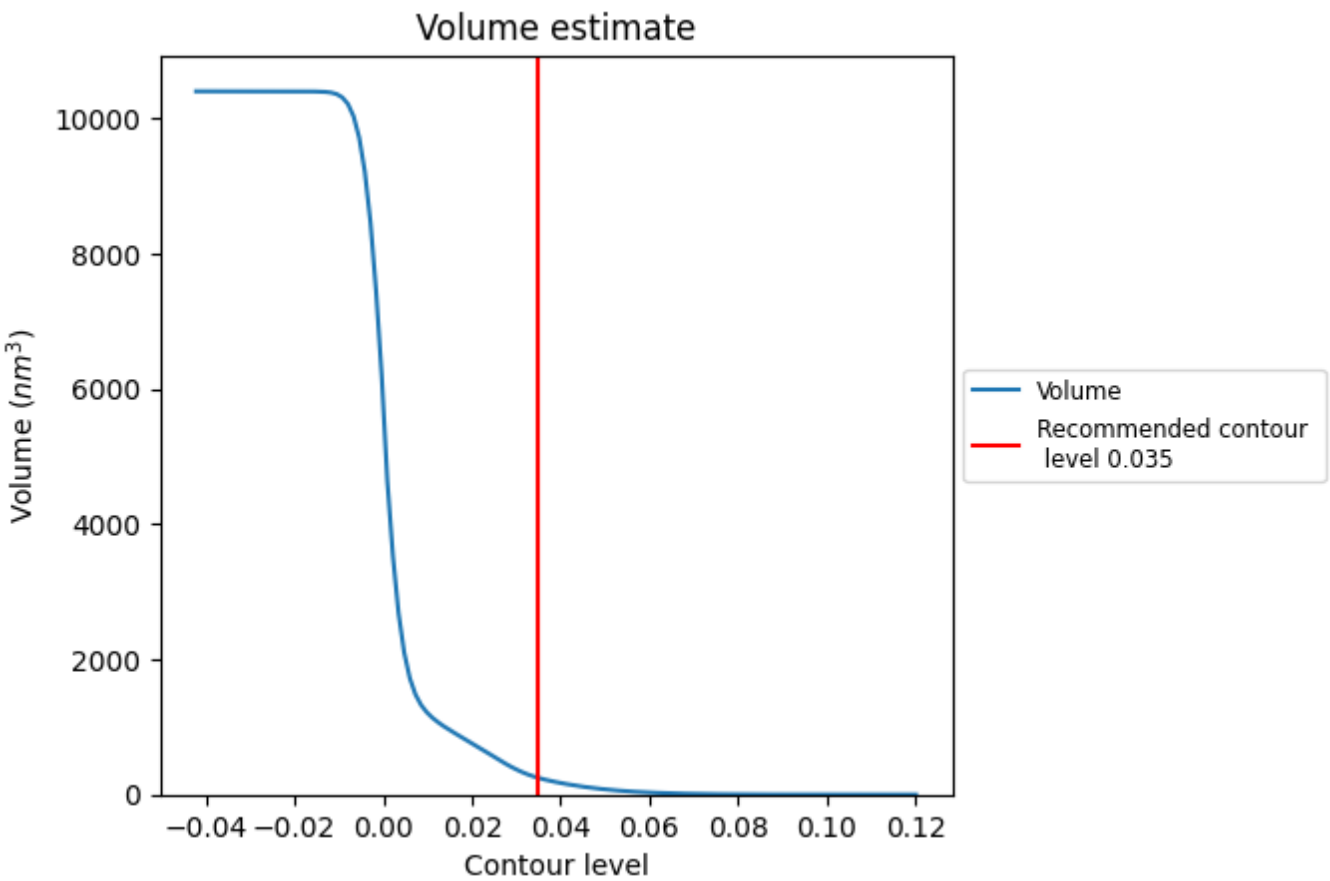
This section contains the results of statistical analysis of the map.

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 246 nm^3; this corresponds to an approximate mass of 223 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.

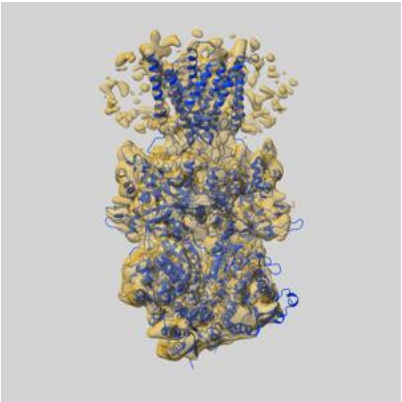
8 Fourier-Shell correlation (i)

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

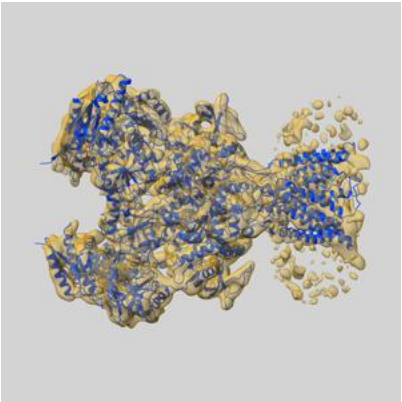
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-8098 and PDB model 5IOV. Per-residue inclusion information can be found in section 3 on page 10.

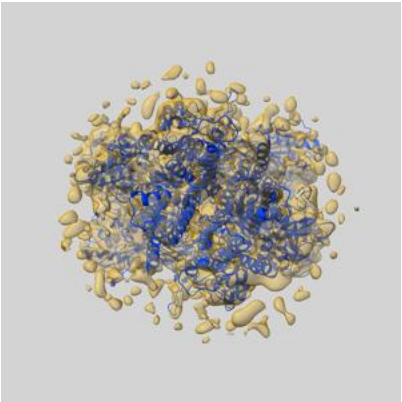
9.1 Map-model overlay (i)



X



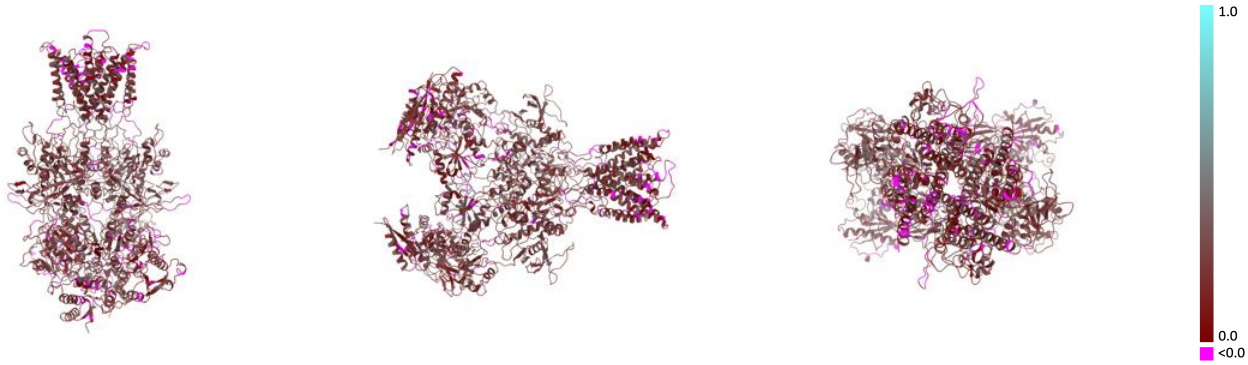
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.035 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.

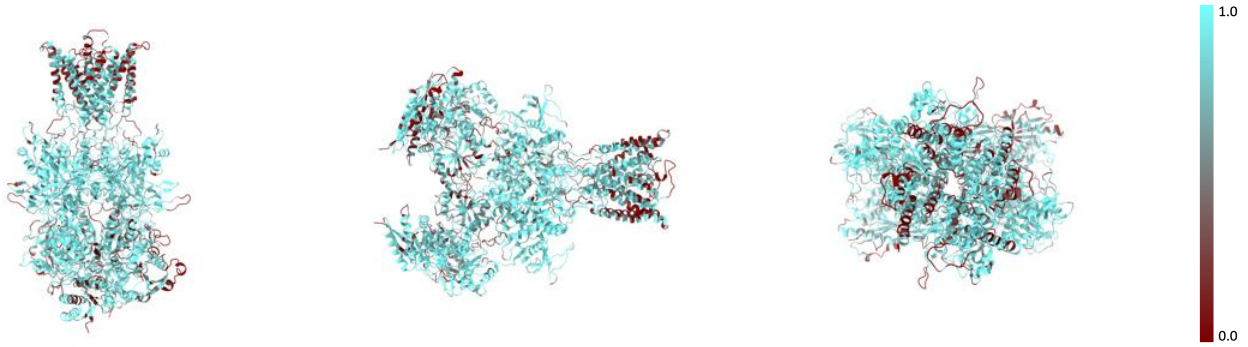
9.2 Q-score mapped to coordinate model (i)



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.

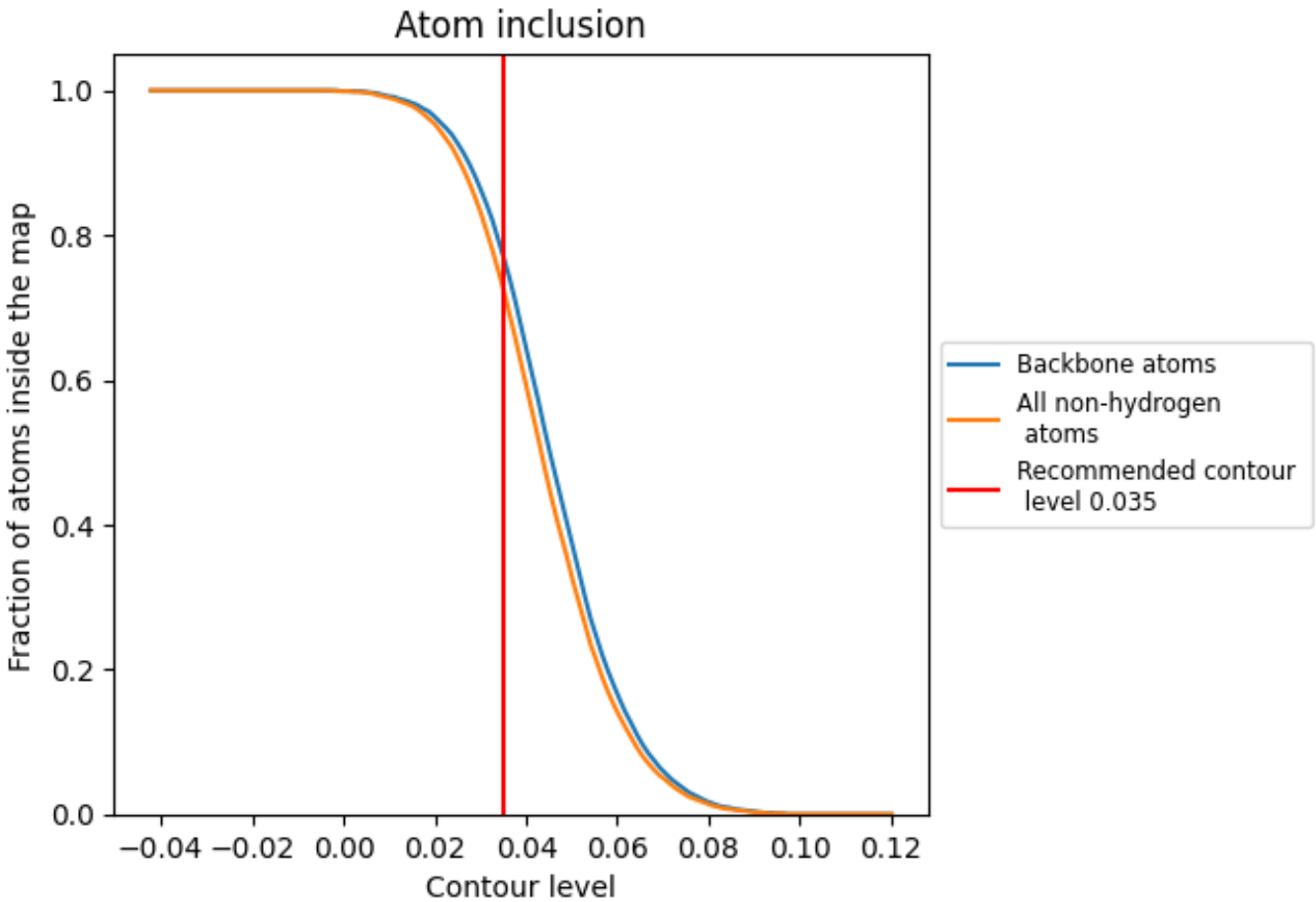
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.035).

9.4 Atom inclusion (i)



At the recommended contour level, 77% of all backbone atoms, 73% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.035) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7270	0.2030
A	0.7870	0.2180
B	0.7010	0.2020
C	0.7480	0.2050
D	0.6710	0.1880