wwPDB EM Validation Summary Report (i)

Nov 5, 2022 – 10:52 AM EDT

PDB ID	:	5VHZ
EMDB ID	:	EMD-8688
Title	:	GluA2-2xGSG1L bound to L-Quisqualate
Authors	:	Twomey, E.C.; Yelshanskaya, M.V.; Grassucci, R.A.; Frank, J.; Sobolevsky, A.I.
Deposited on	:	2017-04-13
Resolution	:	8.40 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 (i) symbol.

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

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

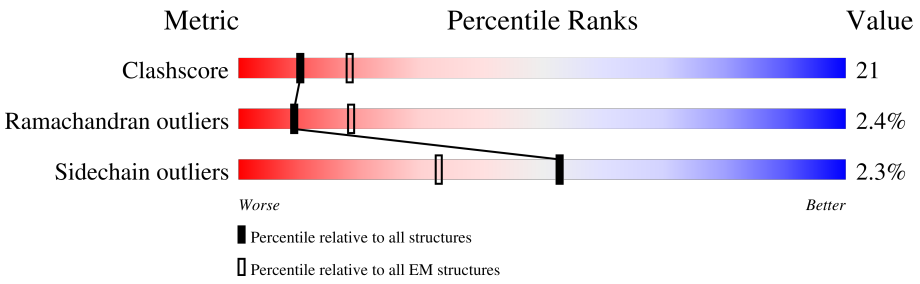
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 8.40 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
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	1057	9% 47% 24% • 26%
1	B	1057	13% 47% 24% • 26%
1	C	1057	10% 48% 24% • 26%
1	D	1057	13% 48% 23% • 26%
1	E	1057	7% 9% 7% • 83%
1	F	1057	7% 9% 8% 83%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 27460 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 Glutamate receptor 2,Germ cell-specific gene 1-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	783	6159	3950	1023	1156	30	0	0
1	B	780	6137	3938	1017	1152	30	0	0
1	C	783	6159	3950	1023	1156	30	0	0
1	D	780	6137	3938	1017	1152	30	0	0
1	E	179	1408	920	231	245	12	0	0
1	F	179	1408	920	231	245	12	0	0

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	241	GLU	ASN	conflict	UNP P19491
A	382	LEU	VAL	conflict	UNP P19491
A	?	-	LEU	deletion	UNP P19491
A	?	-	THR	deletion	UNP P19491
A	?	-	GLU	deletion	UNP P19491
A	?	-	LEU	deletion	UNP P19491
A	?	-	PRO	deletion	UNP P19491
A	?	-	SER	deletion	UNP P19491
A	384	GLU	GLY	conflict	UNP P19491
A	385	ASP	ASN	conflict	UNP P19491
A	392	GLN	ASN	conflict	UNP P19491
A	827	GLY	-	linker	UNP P19491
A	828	THR	-	linker	UNP P19491
A	829	GLY	-	linker	UNP P19491
B	241	GLU	ASN	conflict	UNP P19491
B	382	LEU	VAL	conflict	UNP P19491
B	?	-	LEU	deletion	UNP P19491
B	?	-	THR	deletion	UNP P19491

Continued on next page...

Continued from previous page...

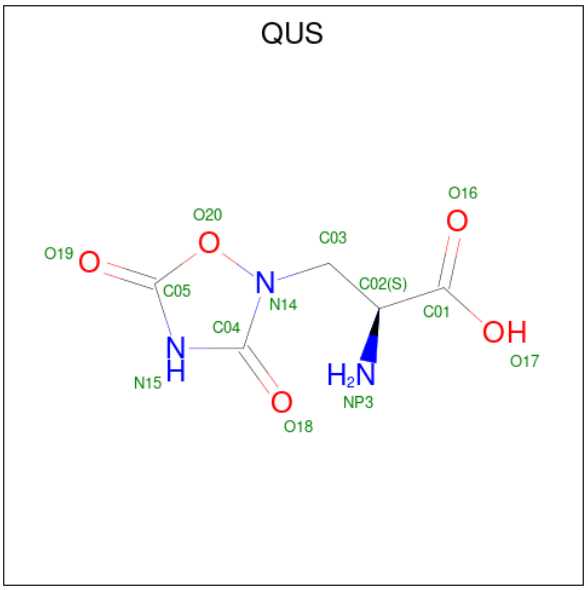
Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	GLU	deletion	UNP P19491
B	?	-	LEU	deletion	UNP P19491
B	?	-	PRO	deletion	UNP P19491
B	?	-	SER	deletion	UNP P19491
B	384	GLU	GLY	conflict	UNP P19491
B	385	ASP	ASN	conflict	UNP P19491
B	392	GLN	ASN	conflict	UNP P19491
B	827	GLY	-	linker	UNP P19491
B	828	THR	-	linker	UNP P19491
B	829	GLY	-	linker	UNP P19491
C	241	GLU	ASN	conflict	UNP P19491
C	382	LEU	VAL	conflict	UNP P19491
C	?	-	LEU	deletion	UNP P19491
C	?	-	THR	deletion	UNP P19491
C	?	-	GLU	deletion	UNP P19491
C	?	-	LEU	deletion	UNP P19491
C	?	-	PRO	deletion	UNP P19491
C	?	-	SER	deletion	UNP P19491
C	384	GLU	GLY	conflict	UNP P19491
C	385	ASP	ASN	conflict	UNP P19491
C	392	GLN	ASN	conflict	UNP P19491
C	827	GLY	-	linker	UNP P19491
C	828	THR	-	linker	UNP P19491
C	829	GLY	-	linker	UNP P19491
D	241	GLU	ASN	conflict	UNP P19491
D	382	LEU	VAL	conflict	UNP P19491
D	?	-	LEU	deletion	UNP P19491
D	?	-	THR	deletion	UNP P19491
D	?	-	GLU	deletion	UNP P19491
D	?	-	LEU	deletion	UNP P19491
D	?	-	PRO	deletion	UNP P19491
D	?	-	SER	deletion	UNP P19491
D	384	GLU	GLY	conflict	UNP P19491
D	385	ASP	ASN	conflict	UNP P19491
D	392	GLN	ASN	conflict	UNP P19491
D	827	GLY	-	linker	UNP P19491
D	828	THR	-	linker	UNP P19491
D	829	GLY	-	linker	UNP P19491
E	-588	GLU	ASN	conflict	UNP P19491
E	-447	LEU	VAL	conflict	UNP P19491
E	?	-	LEU	deletion	UNP P19491
E	?	-	THR	deletion	UNP P19491

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	?	-	GLU	deletion	UNP P19491
E	?	-	LEU	deletion	UNP P19491
E	?	-	PRO	deletion	UNP P19491
E	?	-	SER	deletion	UNP P19491
E	-445	GLU	GLY	conflict	UNP P19491
E	-444	ASP	ASN	conflict	UNP P19491
E	-437	GLN	ASN	conflict	UNP P19491
E	-2	GLY	-	linker	UNP P19491
E	-1	THR	-	linker	UNP P19491
E	0	GLY	-	linker	UNP P19491
F	-588	GLU	ASN	conflict	UNP P19491
F	-447	LEU	VAL	conflict	UNP P19491
F	?	-	LEU	deletion	UNP P19491
F	?	-	THR	deletion	UNP P19491
F	?	-	GLU	deletion	UNP P19491
F	?	-	LEU	deletion	UNP P19491
F	?	-	PRO	deletion	UNP P19491
F	?	-	SER	deletion	UNP P19491
F	-445	GLU	GLY	conflict	UNP P19491
F	-444	ASP	ASN	conflict	UNP P19491
F	-437	GLN	ASN	conflict	UNP P19491
F	-2	GLY	-	linker	UNP P19491
F	-1	THR	-	linker	UNP P19491
F	0	GLY	-	linker	UNP P19491

- Molecule 2 is (S)-2-AMINO-3-(3,5-DIOXO-[1,2,4]OXADIAZOLIDIN-2-YL)-PROPIONIC ACID (three-letter code: QUS) (formula: $C_5H_7N_3O_5$).



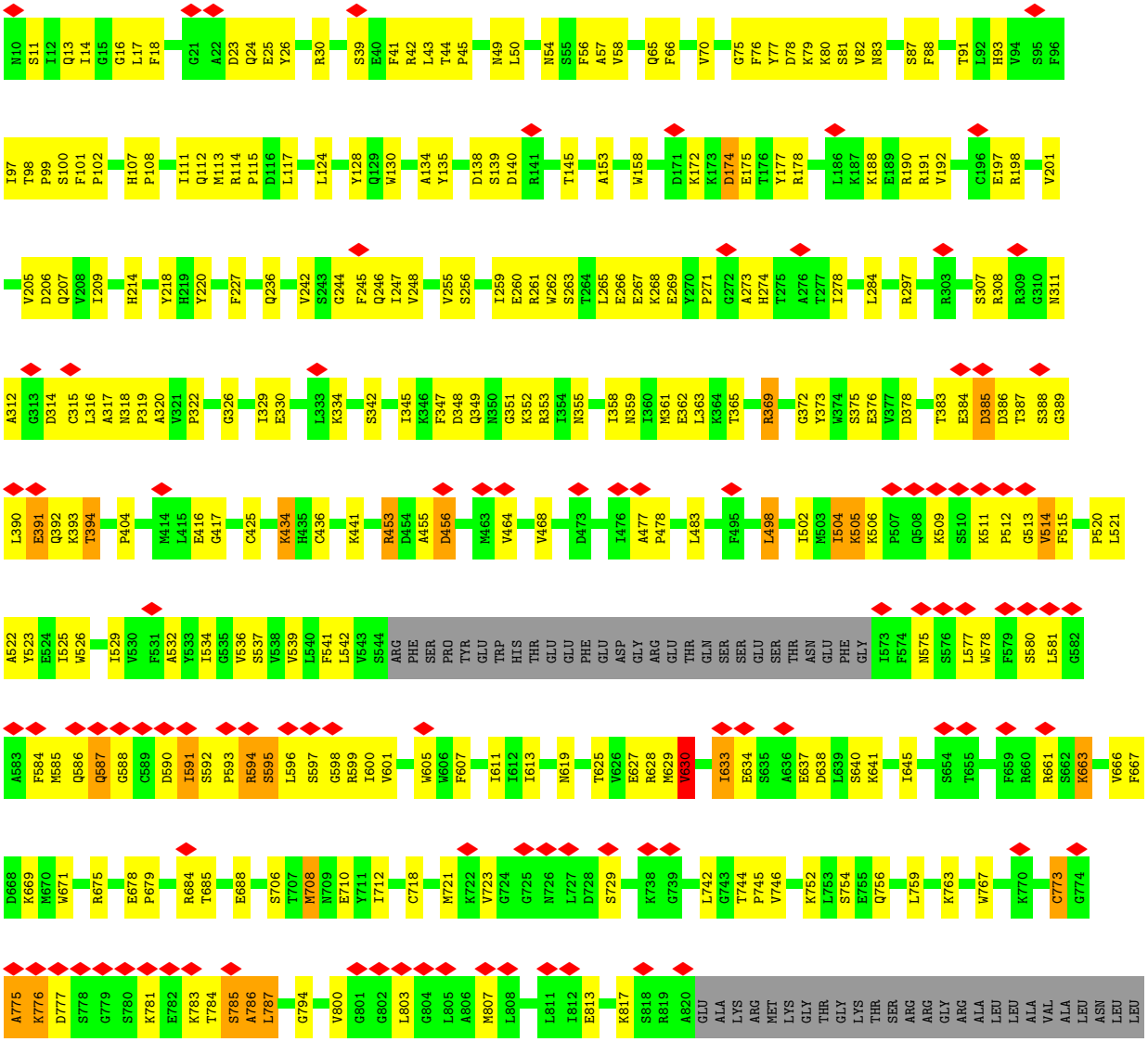
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
2	A	1	13	5	3	5	0
2	B	1	13	5	3	5	0
2	C	1	13	5	3	5	0
2	D	1	13	5	3	5	0

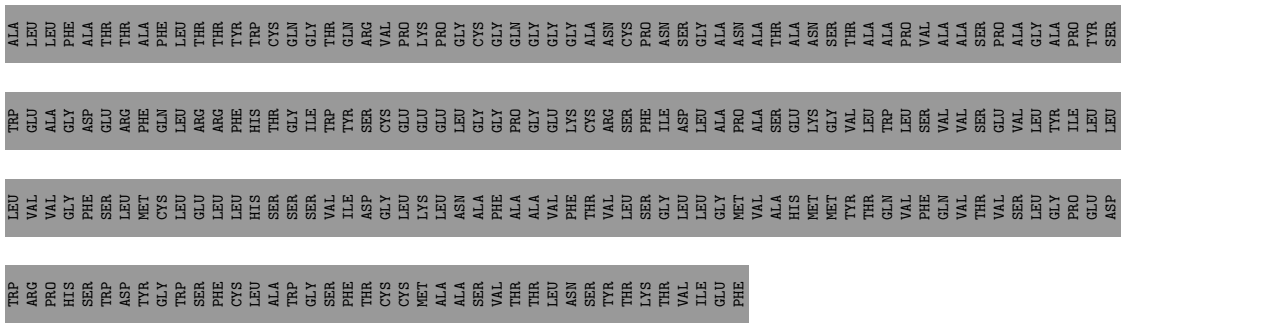
3 Residue-property plots (i)

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: Glutamate receptor 2,Germ cell-specific gene 1-like protein

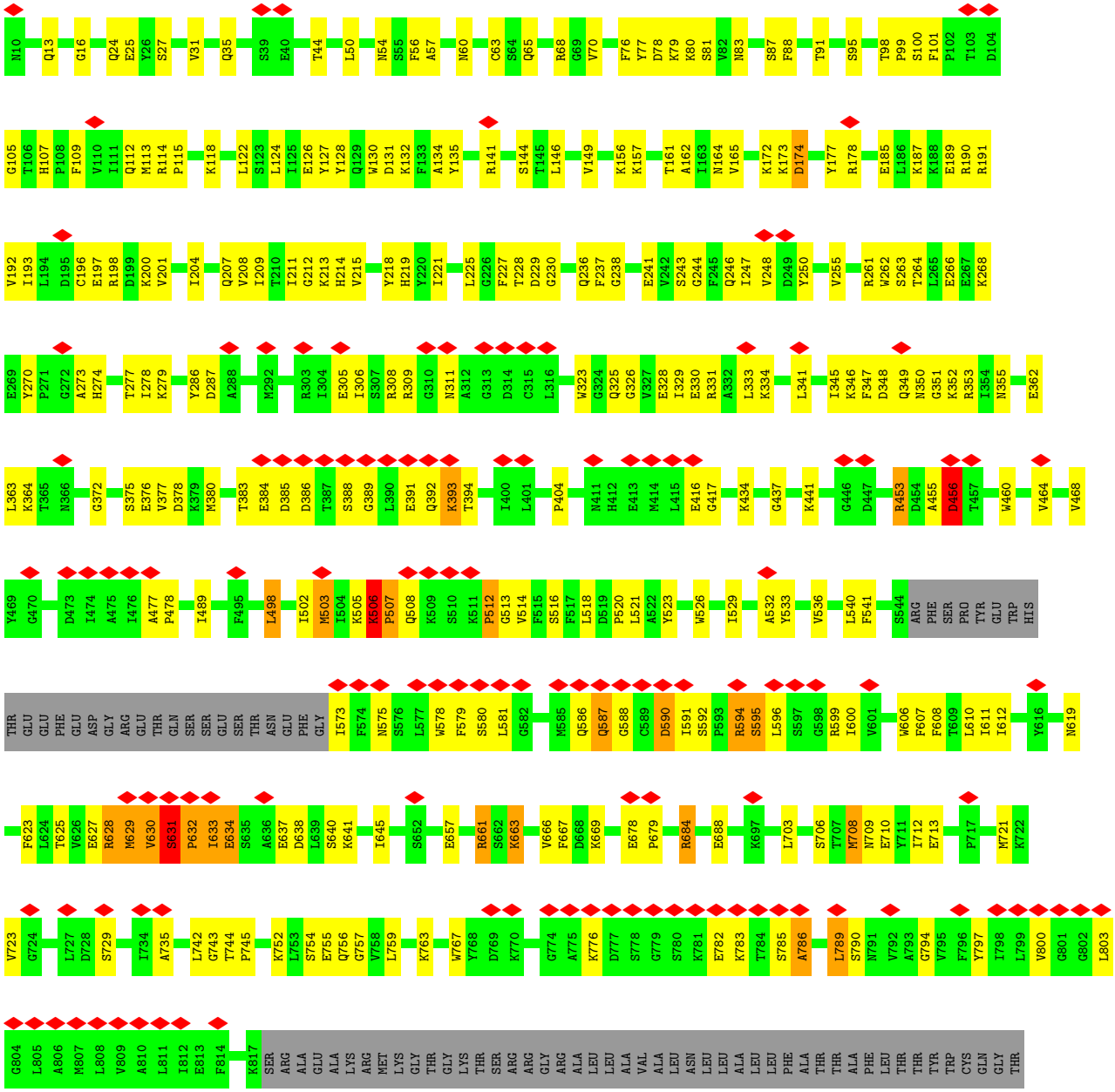
Chain A:

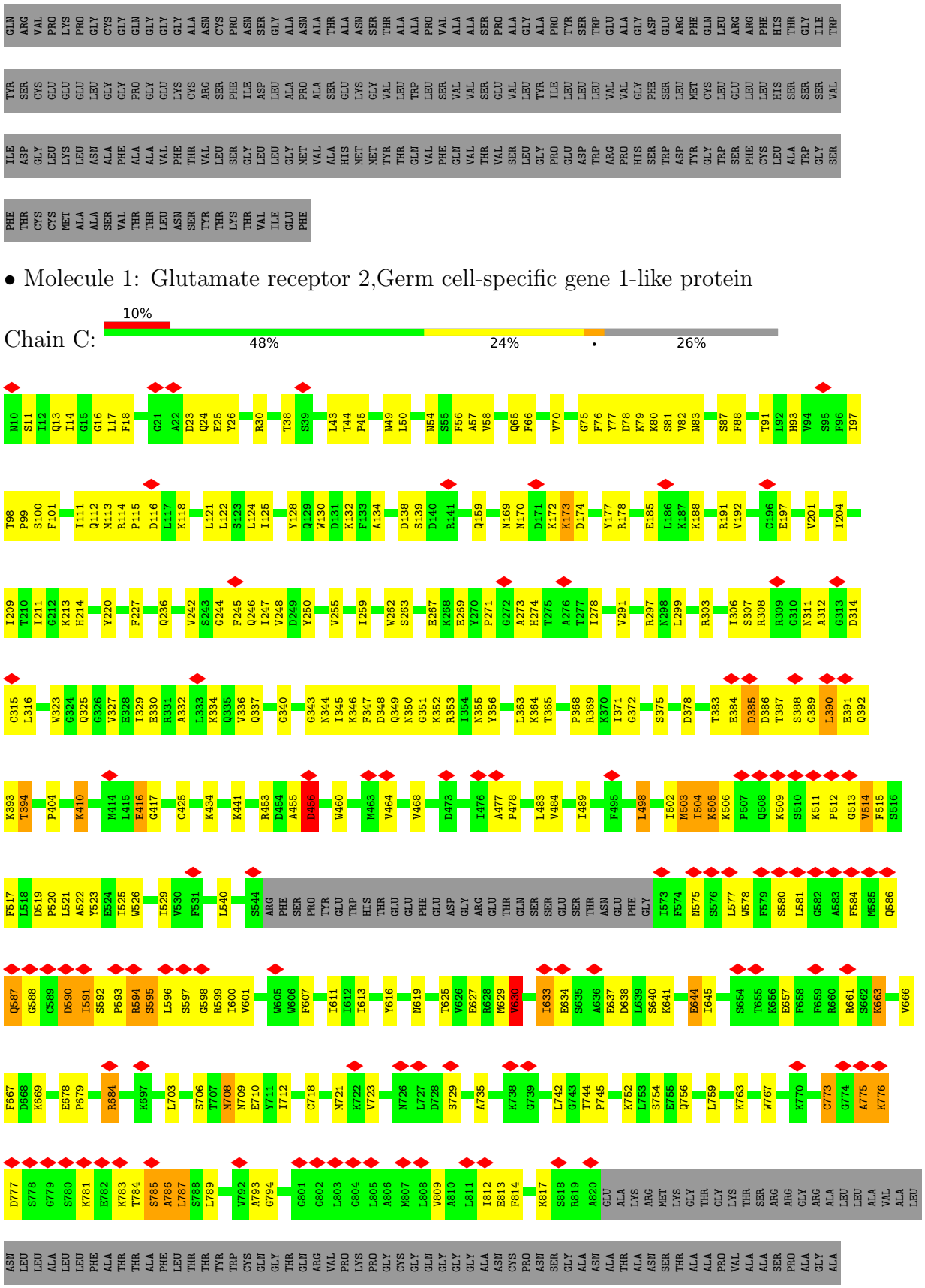




- Molecule 1: Glutamate receptor 2,Germ cell-specific gene 1-like protein

Chain B:





• Molecule 1: Glutamate receptor 2,Germ cell-specific gene 1-like protein

PRO TYR SER TRP GLU ALA GLY ASP GLU ARG PHE GLN LEU ARG ARG PHE HIS THR GLY ILE TRP TYR SER CYS GLU GLU GLU LEU GLY GLY PRO GLY GLU LYS CYS ARG SER PHE ILE ASP LEU ALA PRO ALA SER GLU LYS GLY VAL LEU TRP LEU SER VAL VAL SER GLU VAL LEU TYR

ILE LEU LEU LEU VAL VAL GLY PHE SER LEU MET CYS LEU GLU LEU LEU HIS SER SER SER VAL ILE ASP GLY LEU LYS LEU ASN ALA PHE ALA ALA VAL PHE THR VAL LEU SER GLY LEU LEU GLY MET VAL ALA HIS MET MET TYR THR GLN VAL PHE GLN VAL VAL THR VAL SER LEU GLY

PRO GLU ASP TRP ARG PRO HIS SER TRP ASP TYR GLY TRP SER PHE CYS LEU ALA TRP GLY SER PHE THR CYS CYS MET ALA ALA SER VAL THR THR LEU ASN SER TYR THR LYS THR VAL ILE GLU PHE

- Molecule 1: Glutamate receptor 2,Germ cell-specific gene 1-like protein

Chain D:

N10 S11 I12 Q13 G16 Q24 E25 Y26 S27 V31 Q35 F36 S37 T38 S39 E40 F41 T44 L50 E51 V52 A53 N54 S55 F56 A57 N60 A61 F62 C63 S64 Q65 F76 Y77 D78 K79 K80 N83 S87 F88 T91 S95 T98 P99 S100 F101 P102

T103 D104 F109 V110 M113 R114 P115 D116 L117 K118 L122 S123 L124 I125 E126 Y127 Y128 Q129 W130 D131 K132 F133 A134 Y135 L136 Y137 R141 L146 V149 T161 A162 I163 N164 D174 Y177 R178 K187 R190 R191 V192 I193 E197 V201 I204 V205 D206

Q207 V208 I209 G212 K213 H214 V215 Y218 H219 Y220 I221 L225 G226 F227 D231 K234 I235 Q236 F237 G238 E241 V242 S243 G244 F245 Q246 I247 V248 D249 Y250 V255 R261 W262 S263 T264 G272 A273 H274 T277 I278 K279 Y286 D287 A288 M292 L299

R303 T304 E305 I306 S307 R308 R309 G310 N311 A312 G313 D314 G315 L316 W323 G324 Q325 G326 I329 E330 R331 A332 L333 K334 Q335 V336 Q337 I341 I345 K346 F347 D348 Q349 N350 G351 K352 R353 I354 N355 E362 L363 K364 T365 N366 I371 G372 Y373 W374 S375 E376 V377 D378 T383

E384 D385 D386 T387 S388 G389 L390 E391 Q392 K393 T394 I400 L401 P404 N411 H412 E413 M414 L415 E416 G417 C425 K434 G437 K441 G446 D447 G448 A455 D456 T457 V464 V468 Y469 G470 K471 A472 D473 I474 A475 I476 A477 P478 I489 F495 L498

M503 I504 K505 K506 P507 Q508 K509 S510 K511 P512 G513 V514 F515 S516 P520 L521 A522 Y523 W526 I529 A532 Y533 I534 G535 V536 S537 L540 F541 S544 ARG PHE SER PRO TYR GLU TRP HIS THR GLU GLU PHE GLU ASP GLY ARG GLU THR GLN SER SER GLU SER THR

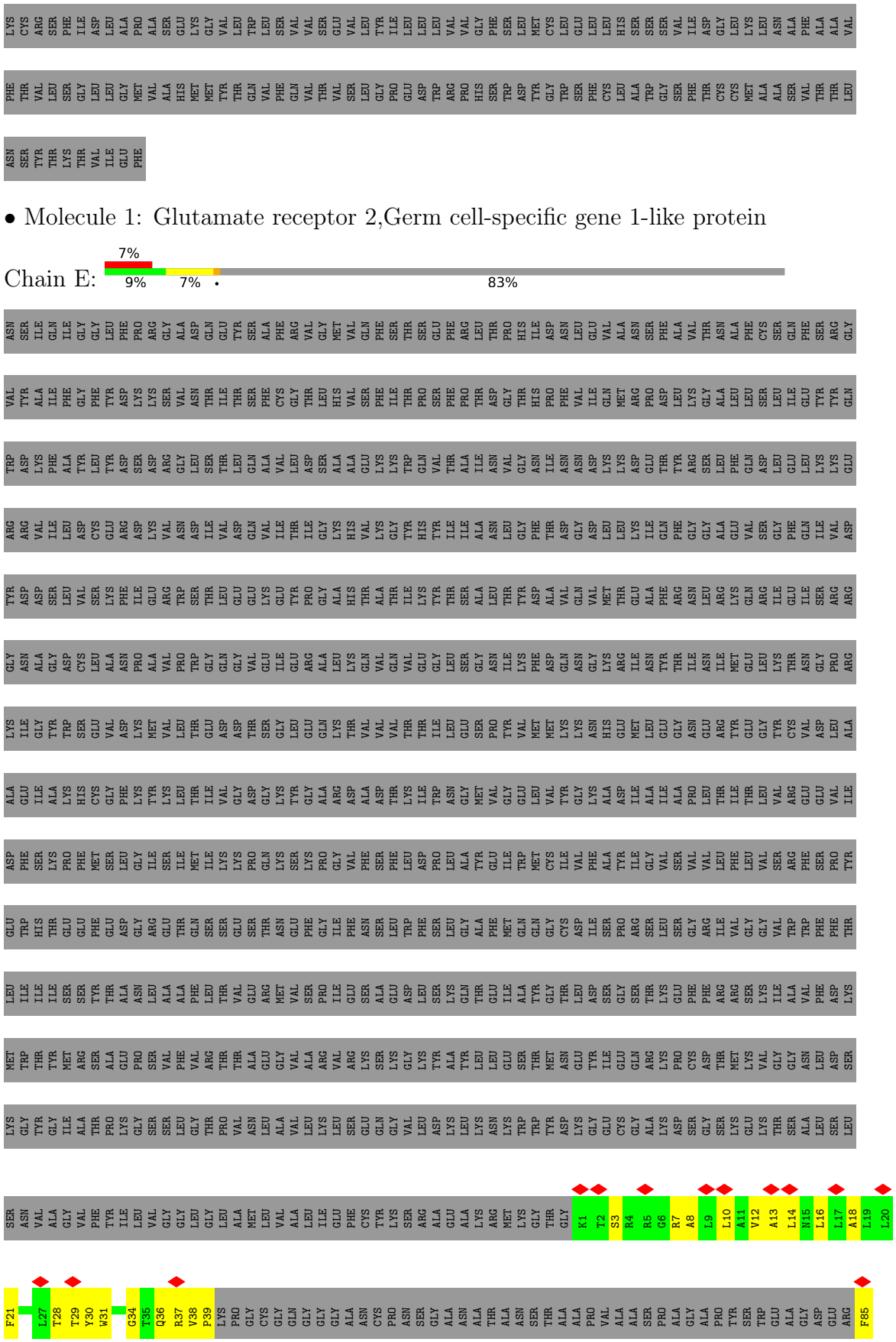
ASN GLU PHE GLY I573 F574 N575 S576 L577 W578 F579 S580 L581 G582 A583 F584 M585 Q586 Q587 G588 C589 D590 I591 S592 P593 R594 S595 L596 S597 G598 R599 I600 V601 G602 G603 W606 F607 F608 T609 L610 I611 I612 Y616 N619 A622 F623 L624 T625 V626 E627 R628 M629 V630 S631 P632 I633

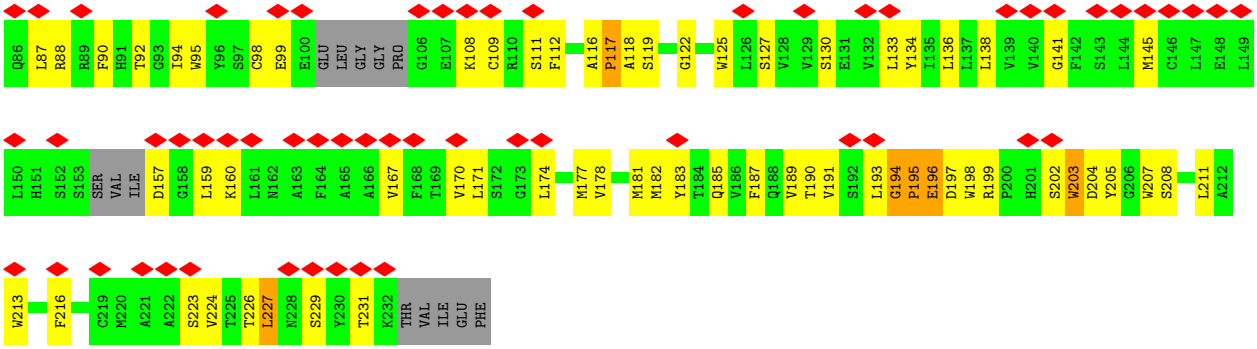
E634 S635 A636 E637 D638 L639 S640 K641 E644 I645 S652 E657 R661 S662 K663 V666 F667 D668 K669 E678 P679 R684 E688 K695 S696 K697 S706 T707 M708 N709 E710 Y711 I712 E713 P717 M721 K722 V723 G724 S729 I734 A735 L742 G743 T744

P745 V746 K752 L753 S754 E755 Q756 L759 K763 W767 Y768 D769 K770 G774 A775 K776 D777 S778 G779 S780 K781 E782 K783 T784 S785 A786 L787 S788 L789 S790 N791 V792 A793 G794 V795 F796 Y797 T798 L799 V800 G801 G802 L803 G804 L805 A806 M807 L808 V809 A810 L811 I812 E813 F814

K817 SER ARG ALA GLU ALA LYS ARG MET LYS GLY THR GLY LYS THR SER ARG ARG GLY ARG ALA ALA LEU LEU ALA VAL ALA LEU ASN LEU LEU LEU ALA LEU LEU PHE ALA THR THR ALA PHE LEU THR THR TYR TRP CYS GLN GLY THR GLN ARG VAL PRO LYS PRO GLY CYS GLY GLN GLN GLY GLY

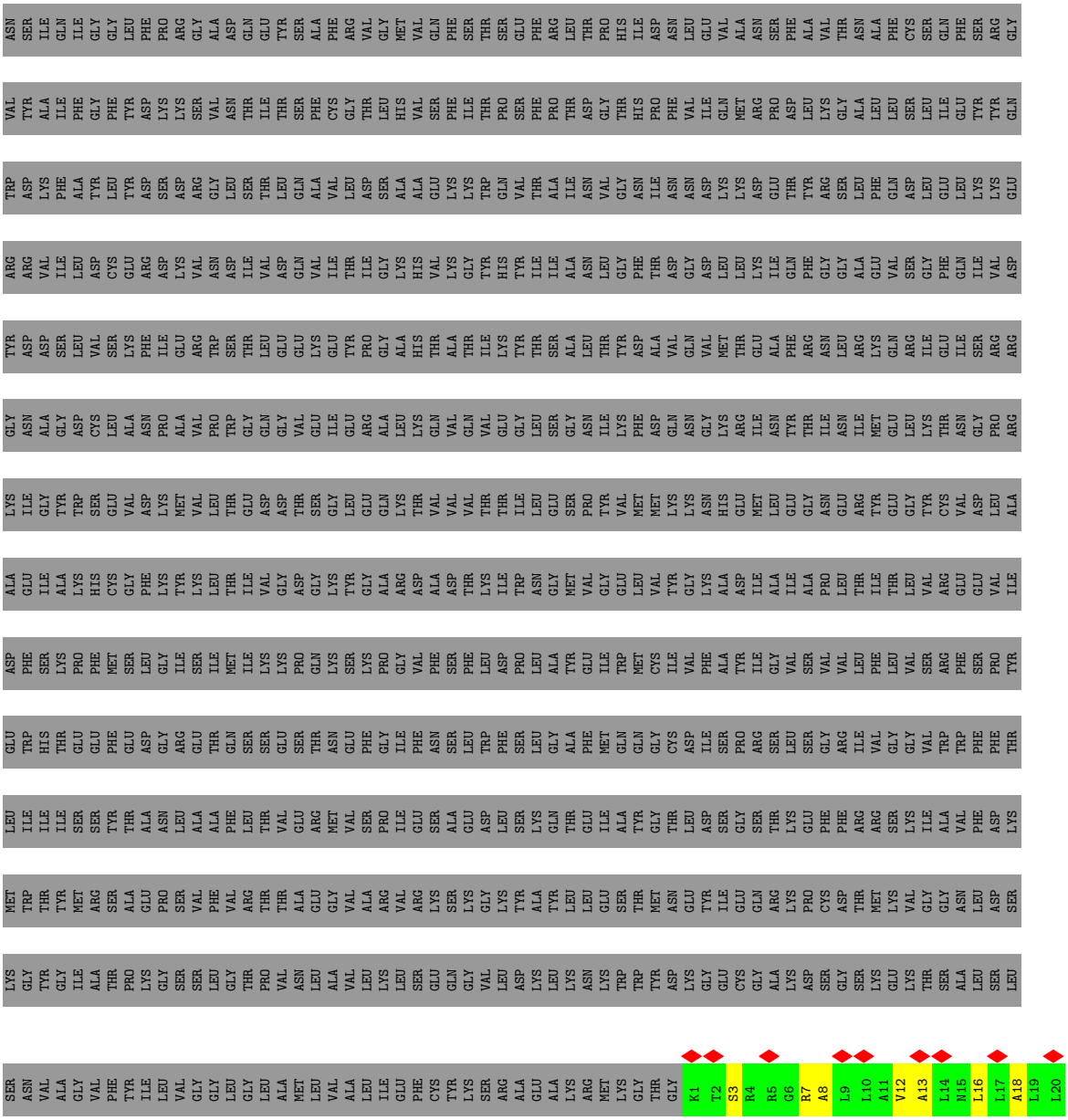
GLY ALA ASN CYS PRO ASN SER GLY ALA ASN ALA THR ALA ASN SER THR ALA ALA PRO VAL ALA ALA SER PRO ALA GLY ALA PRO TYR SER TRP GLU ALA GLY ASP GLU ARG PHE GLN LEU ARG ARG PHE HIS THR GLY ILE TRP TYR SER CYS GLU GLU GLU LEU GLY GLY PRO GLY GLU

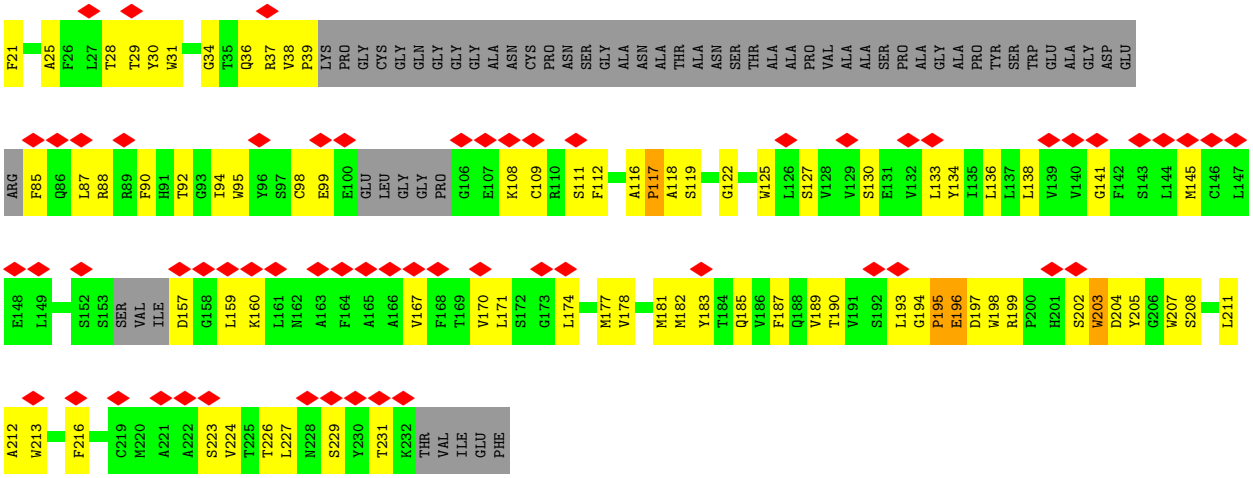

• Molecule 1: Glutamate receptor 2,Germ cell-specific gene 1-like protein
Chain E:
7%
9%
7%
83%



- Molecule 1: Glutamate receptor 2,Germ cell-specific gene 1-like protein

Chain F: 7% 9% 8% 83%




F21 A25 F26 L27 T28 T29 Y30 W31 G34 T35 Q36 R37 V38 P39 LYS PRO GLY CYS GLY GLN GLY GLY GLY ALA ASN CYS PRO ASN SER GLY ALA ASN ALA THR ALA ASN SER THR ALA ALA PRO VAL ALA ALA SER PRO ALA GLY ALA PRO TYR SER TRP GLU ALA GLY ASP GLU
ARG F85 Q86 L87 R88 R89 F90 H91 T92 G93 I94 W95 Y96 S97 C98 E99 E100 GLU LEU GLY GLY PRO G106 E107 K108 C109 R110 S111 F112 A116 P117 A118 S119 G122 W125 L126 S127 V128 V129 S130 E131 V132 L133 Y134 I135 L136 L137 L138 V139 V140 G141 F142 S143 L144 M145 C146 L147
E148 L149 S152 S153 SER VAL ILE D157 G158 L159 K160 L161 N162 A163 F164 A165 A166 V167 F168 T169 V170 L171 S172 G173 L174 M177 V178 M181 M182 Y183 T184 Q185 V186 F187 Q188 V189 T190 V191 S192 L193 G194 P195 E196 D197 W198 R199 P200 H201 S202 W203 D204 Y205 G206 W207 S208 L211
A212 W213 F216 C219 M220 A221 A222 S223 V224 T225 T226 L227 N228 S229 Y230 T231 K232 THR VAL ILE GLU PHE

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	51130	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	67	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.053	Depositor
Minimum map value	-0.026	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	352.80002, 352.80002, 352.80002	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.9800001, 0.9800001, 0.9800001	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: QUS

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	0.32	0/6287	0.50	0/8493
1	B	0.33	0/6265	0.56	4/8464 (0.0%)
1	C	0.32	0/6287	0.50	1/8493 (0.0%)
1	D	0.35	1/6265 (0.0%)	0.57	5/8464 (0.1%)
1	E	0.29	0/1443	0.49	0/1959
1	F	0.29	0/1443	0.48	0/1959
All	All	0.33	1/27990 (0.0%)	0.53	10/37832 (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	D	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	786	ALA	C-N	-11.69	1.07	1.34

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	506	LYS	C-N-CD	-17.67	81.72	120.60
1	D	506	LYS	C-N-CD	-17.65	81.76	120.60
1	B	631	SER	C-N-CD	-16.78	83.69	120.60
1	D	631	SER	C-N-CD	-16.76	83.72	120.60
1	D	786	ALA	O-C-N	-8.83	108.58	122.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	786	ALA	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	6159	0	6157	283	0
1	B	6137	0	6132	321	0
1	C	6159	0	6157	309	0
1	D	6137	0	6131	291	0
1	E	1408	0	1406	61	0
1	F	1408	0	1406	54	0
2	A	13	0	6	0	0
2	B	13	0	6	0	0
2	C	13	0	6	0	0
2	D	13	0	6	0	0
All	All	27460	0	27413	1177	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 21.

The worst 5 of 1177 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:506:LYS:CE	1:C:721:MET:HB2	1.20	1.65
1:A:506:LYS:CE	1:A:721:MET:HB2	1.16	1.58
1:A:506:LYS:HE3	1:A:721:MET:CB	1.33	1.57
1:C:506:LYS:HE3	1:C:721:MET:CB	1.35	1.56
1:A:506:LYS:CE	1:A:721:MET:CB	1.86	1.53

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	779/1057 (74%)	716 (92%)	47 (6%)	16 (2%)	7	36
1	B	776/1057 (73%)	723 (93%)	39 (5%)	14 (2%)	8	40
1	C	779/1057 (74%)	716 (92%)	45 (6%)	18 (2%)	6	34
1	D	776/1057 (73%)	723 (93%)	35 (4%)	18 (2%)	6	34
1	E	171/1057 (16%)	156 (91%)	7 (4%)	8 (5%)	2	21
1	F	171/1057 (16%)	156 (91%)	7 (4%)	8 (5%)	2	21
All	All	3452/6342 (54%)	3190 (92%)	180 (5%)	82 (2%)	9	33

5 of 82 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	385	ASP
1	A	456	ASP
1	A	514	VAL
1	A	630	VAL
1	A	776	LYS

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	666/888 (75%)	648 (97%)	18 (3%)	44	65
1	B	664/888 (75%)	645 (97%)	19 (3%)	42	64
1	C	666/888 (75%)	648 (97%)	18 (3%)	44	65

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	664/888 (75%)	652 (98%)	12 (2%)	59	77
1	E	152/888 (17%)	151 (99%)	1 (1%)	84	90
1	F	152/888 (17%)	152 (100%)	0	100	100
All	All	2964/5328 (56%)	2896 (98%)	68 (2%)	53	70

5 of 68 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	393	LYS
1	D	416	GLU
1	D	663	LYS
1	B	453	ARG
1	B	434	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 49 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	325	GLN
1	C	619	ASN
1	C	337	GLN
1	C	412	HIS
1	D	65	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	$\#\|Z\| > 2$
2	QUS	B	1101	-	6,13,13	1.25	0	4,18,18	1.40	0
2	QUS	A	1101	-	6,13,13	1.26	0	4,18,18	1.39	0
2	QUS	D	1101	-	6,13,13	1.26	0	4,18,18	1.40	0
2	QUS	C	1101	-	6,13,13	1.25	0	4,18,18	1.40	0

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
2	QUS	B	1101	-	-	2/6/8/8	0/1/1/1
2	QUS	A	1101	-	-	2/6/8/8	0/1/1/1
2	QUS	D	1101	-	-	2/6/8/8	0/1/1/1
2	QUS	C	1101	-	-	2/6/8/8	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1101	QUS	C01-C02-C03-N14
2	B	1101	QUS	C01-C02-C03-N14
2	C	1101	QUS	C01-C02-C03-N14
2	D	1101	QUS	C01-C02-C03-N14
2	A	1101	QUS	NP3-C02-C03-N14

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)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	786:ALA	C	787:LEU	N	1.07

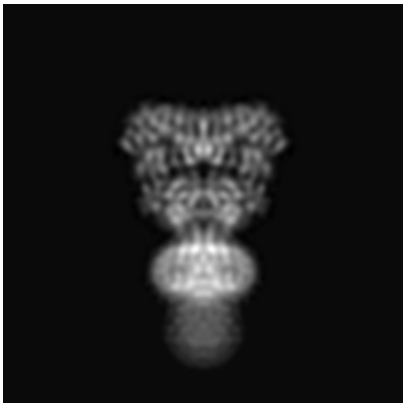
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-8688. 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.

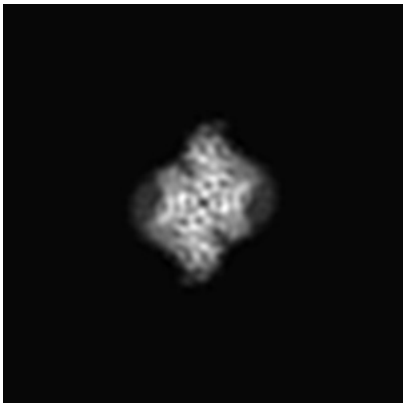
6.1 Orthogonal projections (i)

6.1.1 Primary map



X

Y



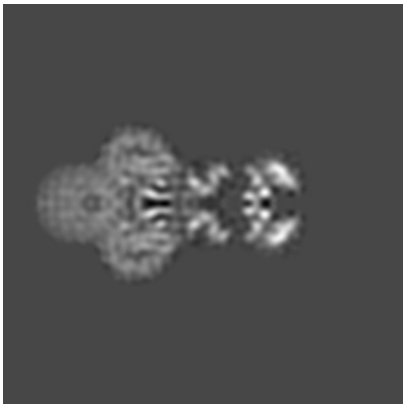
Z

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

6.2 Central slices (i)

6.2.1 Primary map

X Index: 180



Y Index: 180

Z Index: 180

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: 180

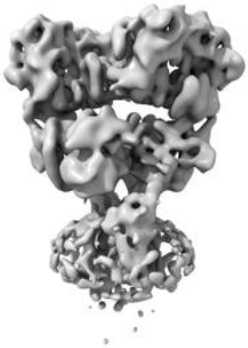
Y Index: 189

Z Index: 227

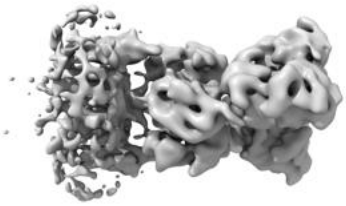
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

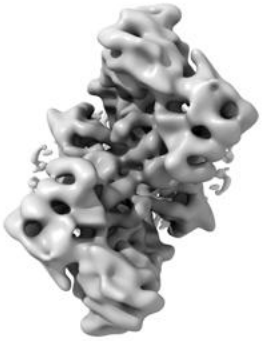
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.015. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

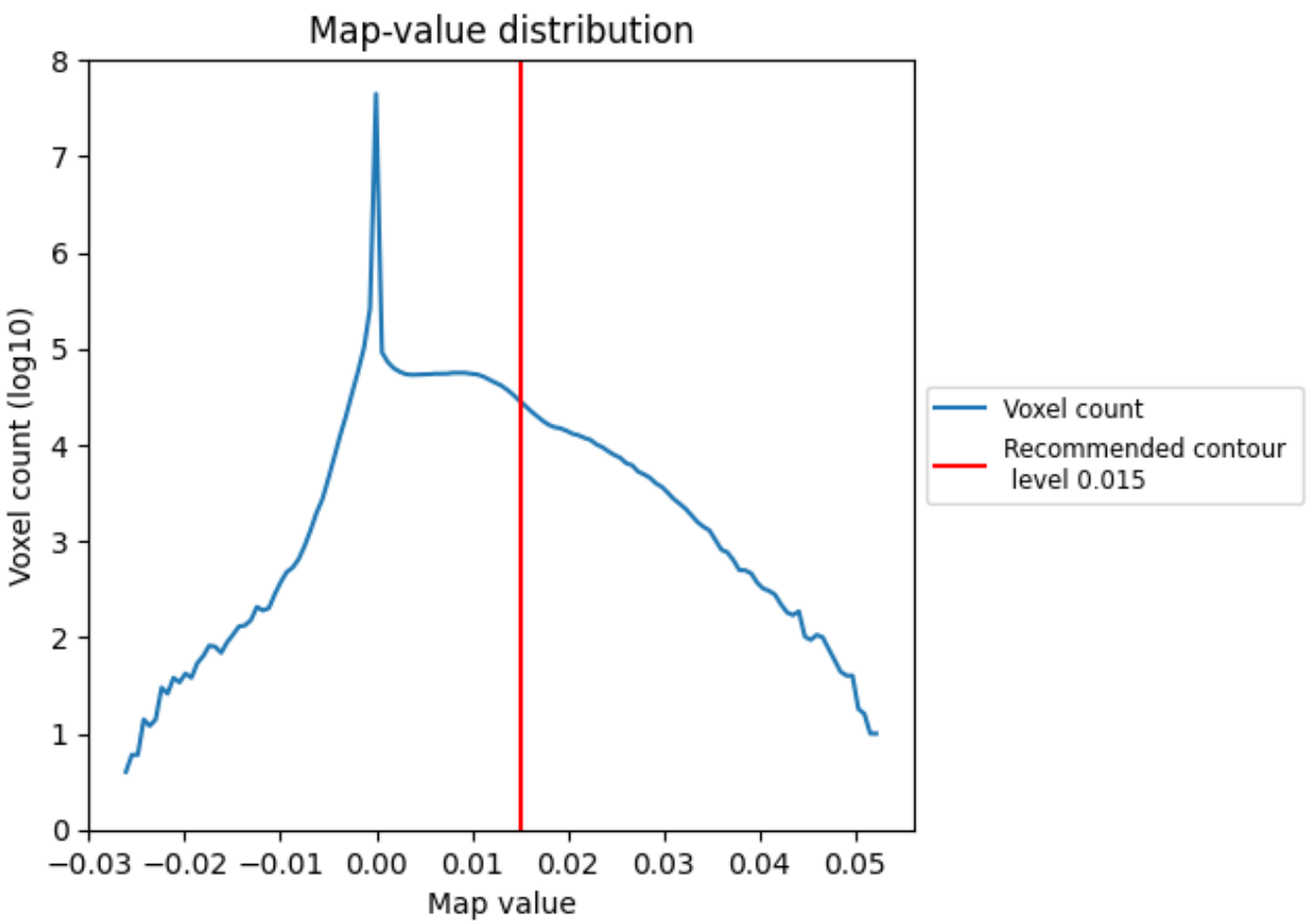
6.5 Mask visualisation (i)

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

7 Map analysis (i)

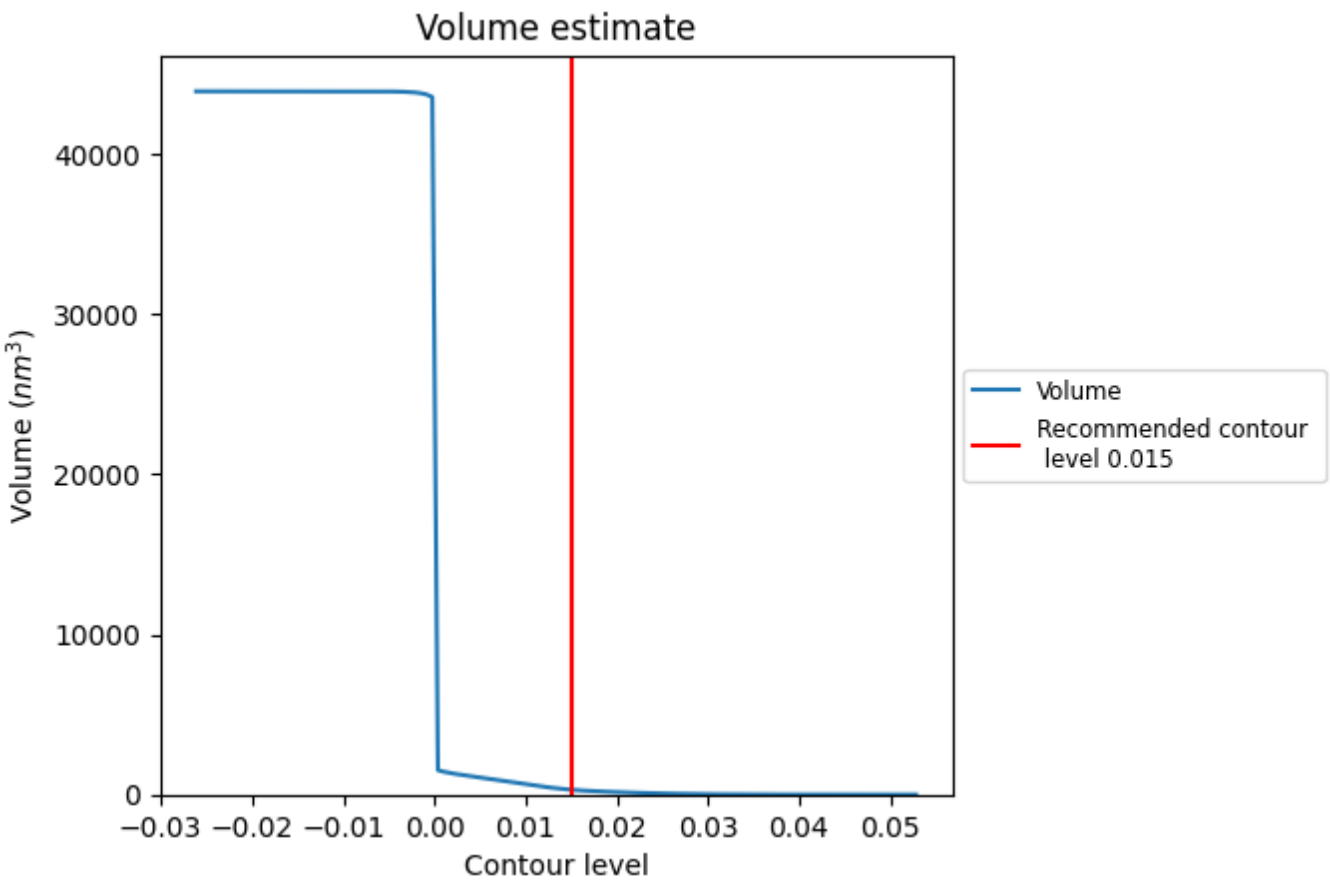
This section contains the results of statistical analysis of the map.

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.

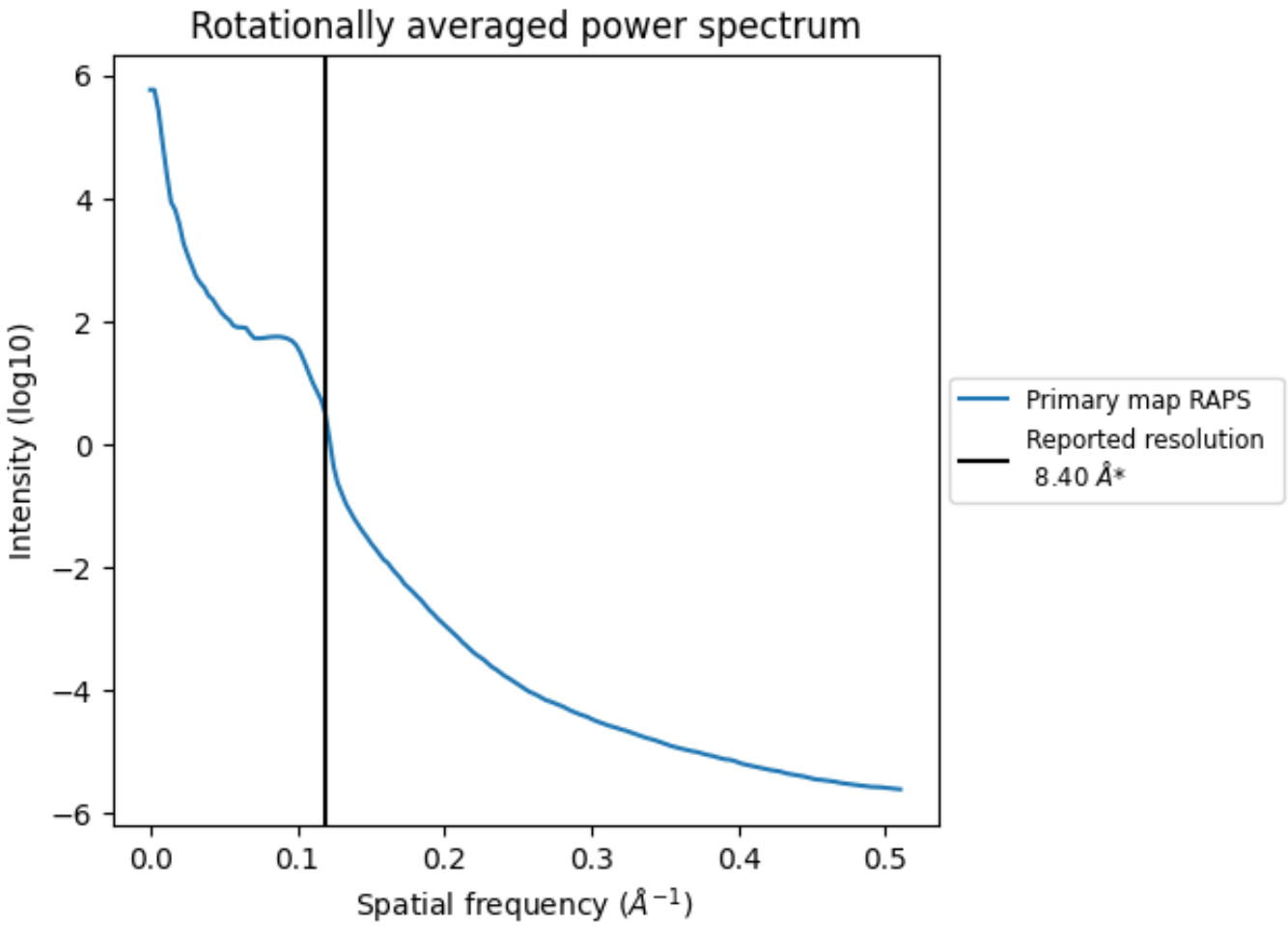
7.2 Volume estimate (i)



The volume at the recommended contour level is 303 nm^3; this corresponds to an approximate mass of 274 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)



*Reported resolution corresponds to spatial frequency of 0.119 Å^{-1}

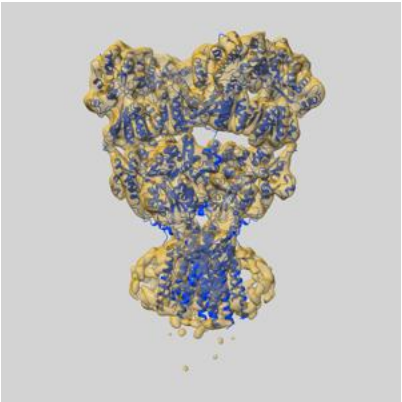
8 Fourier-Shell correlation (i)

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

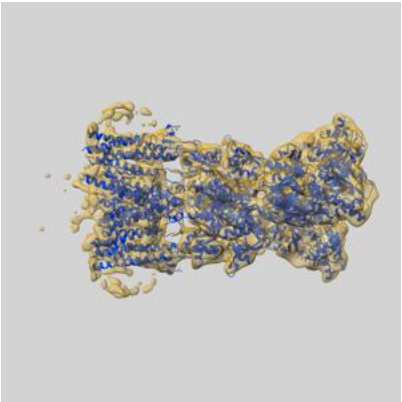
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-8688 and PDB model 5VHZ. Per-residue inclusion information can be found in section 3 on page 7.

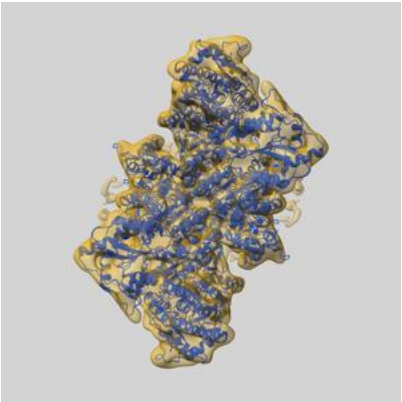
9.1 Map-model overlay (i)



X



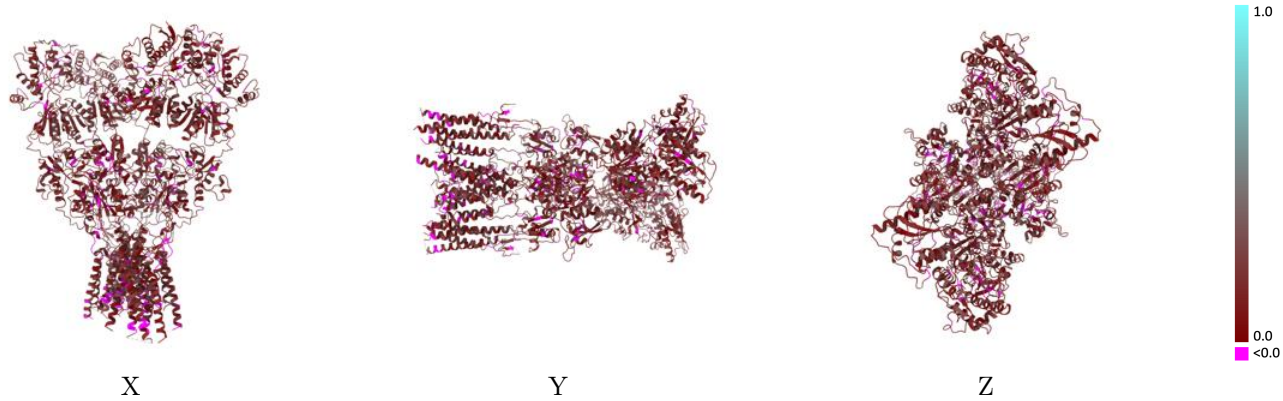
Y



Z

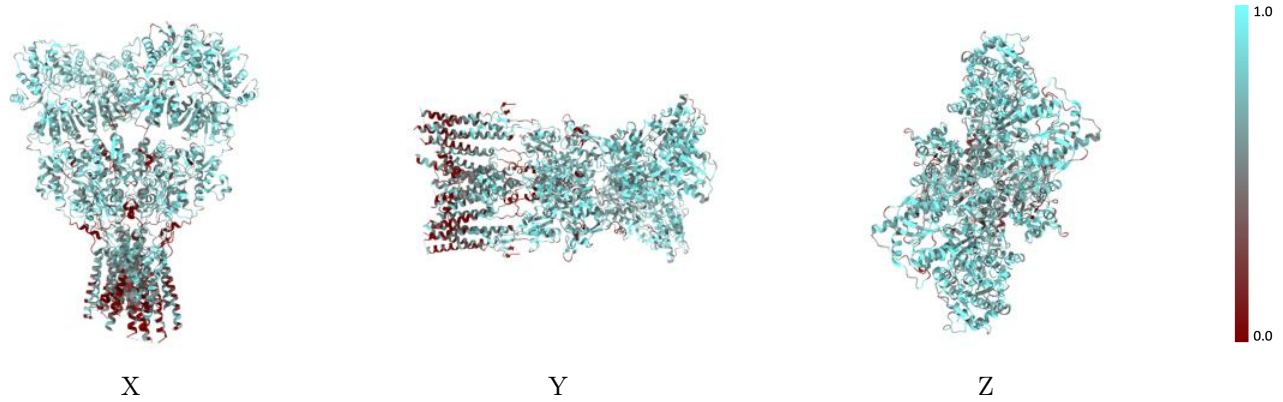
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



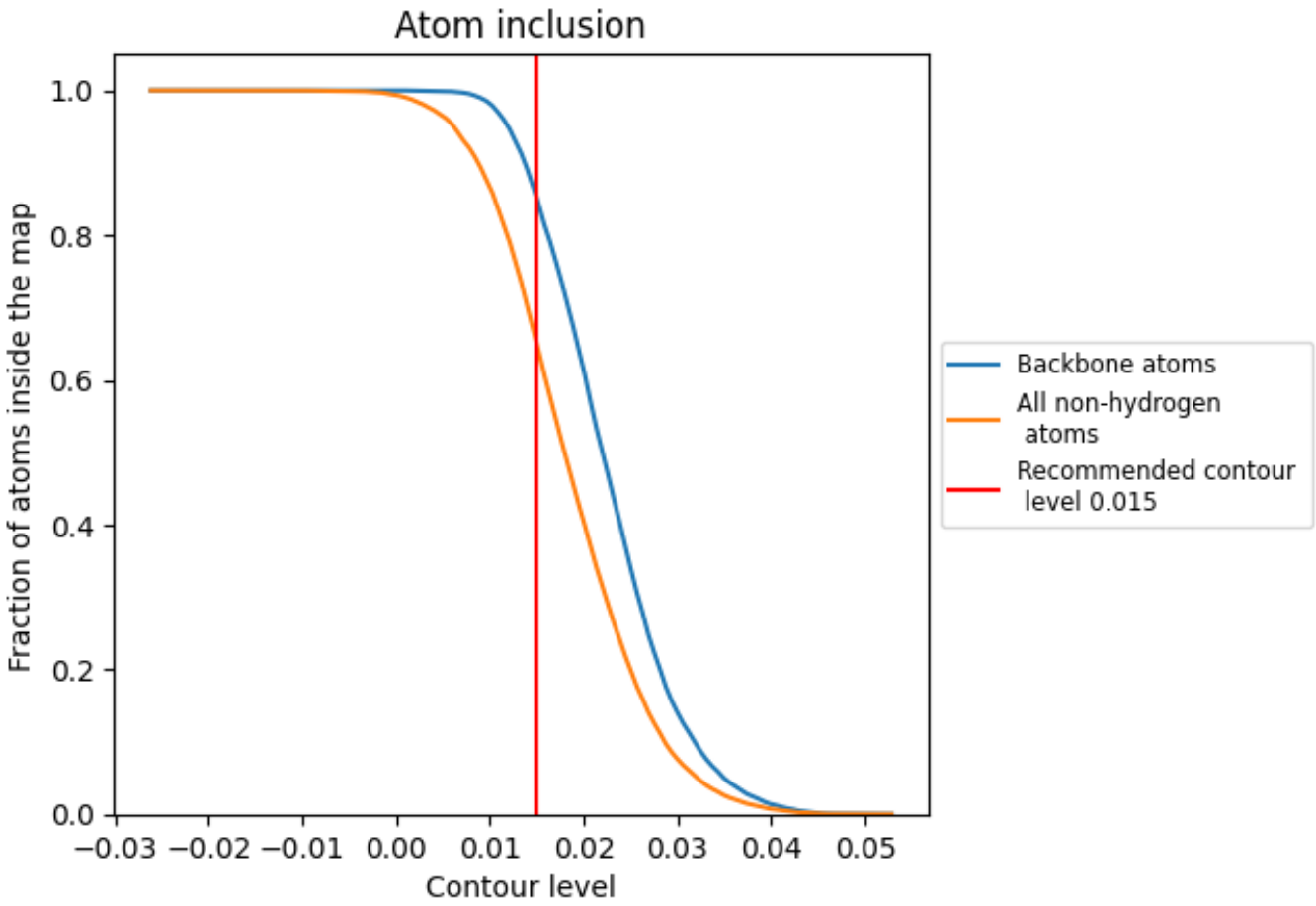
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.015).

9.4 Atom inclusion (i)



At the recommended contour level, 85% of all backbone atoms, 65% 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 (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6504	0.1510
A	0.6834	0.1530
B	0.6577	0.1530
C	0.6806	0.1530
D	0.6534	0.1500
E	0.4866	0.1390
F	0.4917	0.1400