W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

wwPDB EM Validation Summary Report (i)

Nov 9, 2024 – 11:41 AM EST

|		
PDB ID	:	5KBU
EMDB ID	:	EMD-8231
Title	:	Cryo-EM structure of GluA2-2xSTZ complex at 7.8 Angstrom resolution
Authors	:	Twomey, E.C.; Yelshanskaya, M.V.; Grassucci, R.A.; Frank, J.; Sobolevsky, A.I.
Deposited on	:	2016-06-03
Resolution	:	7.80 Å(reported)

---

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 7.80 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	Percentile Ranks	Value
Clashscore		50
Ramachandran outliers		3.4%
Sidechain outliers		1.8%

Worse ← → Better

■ Percentile relative to all structures
▯ Percentile relative to all EM structures
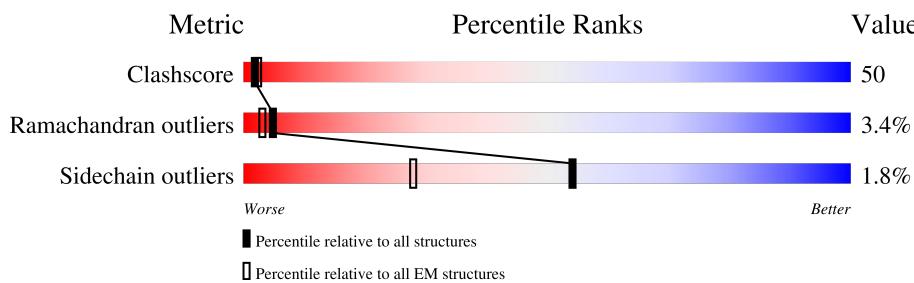
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	1034	22% / 60% 29% ·· 6%
1	B	1034	11% / 56% 18% · 25%
1	C	1034	24% / 60% 29% ·· 6%
1	D	1034	13% / 56% 18% · 25%

2   Entity composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 25678 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,Voltage-dependent calcium channel gamma-2 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	973	Total	C	N	O	S	0	0
			7110	4589	1138	1346	37		
1	B	779	Total	C	N	O	S	0	0
			5647	3635	902	1083	27		
1	C	973	Total	C	N	O	S	0	0
			7110	4589	1138	1346	37		
1	D	779	Total	C	N	O	S	0	0
			5647	3635	902	1083	27		

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	241	GLU	ASN	engineered mutation	UNP P19491
A	382	LEU	VAL	engineered mutation	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	engineered mutation	UNP P19491
A	385	ASP	ASN	engineered mutation	UNP P19491
A	392	GLN	ASN	conflict	UNP P19491
A	758	LEU	VAL	engineered mutation	UNP P19491
A	827	GLY	-	linker	UNP P19491
A	828	THR	-	linker	UNP P19491
A	1047	ASP	ASN	conflict	UNP O88602
A	1208	THR	-	expression tag	UNP O88602
A	1209	GLY	-	expression tag	UNP O88602
A	1210	GLY	-	expression tag	UNP O88602
A	1211	LEU	-	expression tag	UNP O88602
A	1212	VAL	-	expression tag	UNP O88602
A	1213	PRO	-	expression tag	UNP O88602

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	1214	ARG	-	expression tag	UNP O88602
A	1215	GLY	-	expression tag	UNP O88602
B	241	GLU	ASN	engineered mutation	UNP P19491
B	382	LEU	VAL	engineered mutation	UNP P19491
B	?	-	LEU	deletion	UNP P19491
B	?	-	THR	deletion	UNP P19491
B	?	-	GLU	deletion	UNP P19491
B	?	-	LEU	deletion	UNP P19491
B	?	-	PRO	deletion	UNP P19491
B	?	-	SER	deletion	UNP P19491
B	384	GLU	GLY	engineered mutation	UNP P19491
B	385	ASP	ASN	engineered mutation	UNP P19491
B	392	GLN	ASN	conflict	UNP P19491
B	758	LEU	VAL	engineered mutation	UNP P19491
B	827	GLY	-	linker	UNP P19491
B	828	THR	-	linker	UNP P19491
B	1047	ASP	ASN	conflict	UNP O88602
B	1208	THR	-	expression tag	UNP O88602
B	1209	GLY	-	expression tag	UNP O88602
B	1210	GLY	-	expression tag	UNP O88602
B	1211	LEU	-	expression tag	UNP O88602
B	1212	VAL	-	expression tag	UNP O88602
B	1213	PRO	-	expression tag	UNP O88602
B	1214	ARG	-	expression tag	UNP O88602
B	1215	GLY	-	expression tag	UNP O88602
C	241	GLU	ASN	engineered mutation	UNP P19491
C	382	LEU	VAL	engineered mutation	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	engineered mutation	UNP P19491
C	385	ASP	ASN	engineered mutation	UNP P19491
C	392	GLN	ASN	conflict	UNP P19491
C	758	LEU	VAL	engineered mutation	UNP P19491
C	827	GLY	-	linker	UNP P19491
C	828	THR	-	linker	UNP P19491
C	1047	ASP	ASN	conflict	UNP O88602
C	1208	THR	-	expression tag	UNP O88602
C	1209	GLY	-	expression tag	UNP O88602

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	1210	GLY	-	expression tag	UNP O88602
C	1211	LEU	-	expression tag	UNP O88602
C	1212	VAL	-	expression tag	UNP O88602
C	1213	PRO	-	expression tag	UNP O88602
C	1214	ARG	-	expression tag	UNP O88602
C	1215	GLY	-	expression tag	UNP O88602
D	241	GLU	ASN	engineered mutation	UNP P19491
D	382	LEU	VAL	engineered mutation	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	engineered mutation	UNP P19491
D	385	ASP	ASN	engineered mutation	UNP P19491
D	392	GLN	ASN	conflict	UNP P19491
D	758	LEU	VAL	engineered mutation	UNP P19491
D	827	GLY	-	linker	UNP P19491
D	828	THR	-	linker	UNP P19491
D	1047	ASP	ASN	conflict	UNP O88602
D	1208	THR	-	expression tag	UNP O88602
D	1209	GLY	-	expression tag	UNP O88602
D	1210	GLY	-	expression tag	UNP O88602
D	1211	LEU	-	expression tag	UNP O88602
D	1212	VAL	-	expression tag	UNP O88602
D	1213	PRO	-	expression tag	UNP O88602
D	1214	ARG	-	expression tag	UNP O88602
D	1215	GLY	-	expression tag	UNP O88602

- Molecule 2 is {[7-morpholin-4-yl-2,3-dioxo-6-(trifluoromethyl)-3,4-dihydroquinoxalin-1(2H)-yl]methyl}phosphonic acid (three-letter code: ZK1) (formula: $C_{14}H_{15}F_3N_3O_6P$).
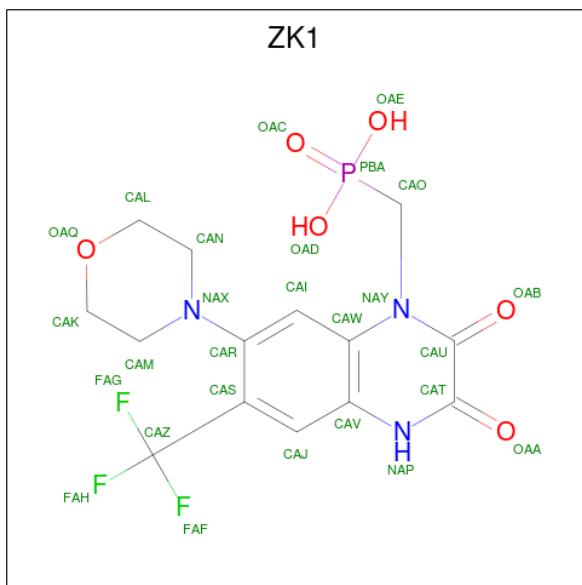
Mol	Chain	Residues	Atoms							AltConf
2	A	1	Total	C	F	N	O	P		0
			27	14	3	3	6	1		
2	B	1	Total	C	F	N	O	P		0
			27	14	3	3	6	1		
2	C	1	Total	C	F	N	O	P		0
			27	14	3	3	6	1		
2	D	1	Total	C	F	N	O	P		0
			27	14	3	3	6	1		

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).
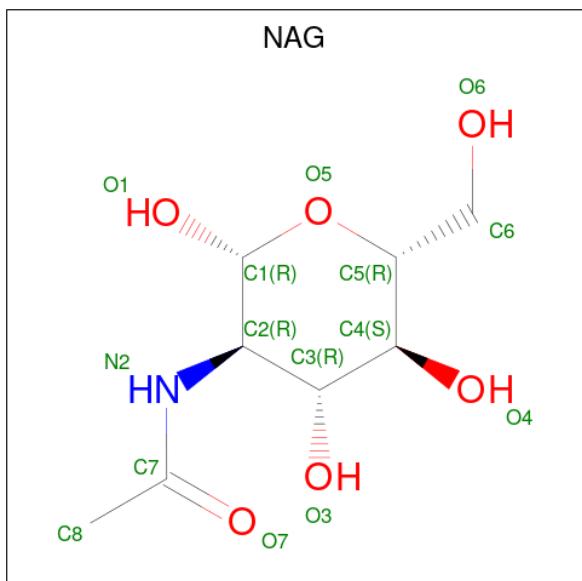
Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total 14	C 8	N 1	O 5	0
3	B	1	Total 14	C 8	N 1	O 5	0
3	C	1	Total 14	C 8	N 1	O 5	0
3	D	1	Total 14	C 8	N 1	O 5	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Glutamate receptor 2,Voltage-dependent calcium channel gamma-2 subunit
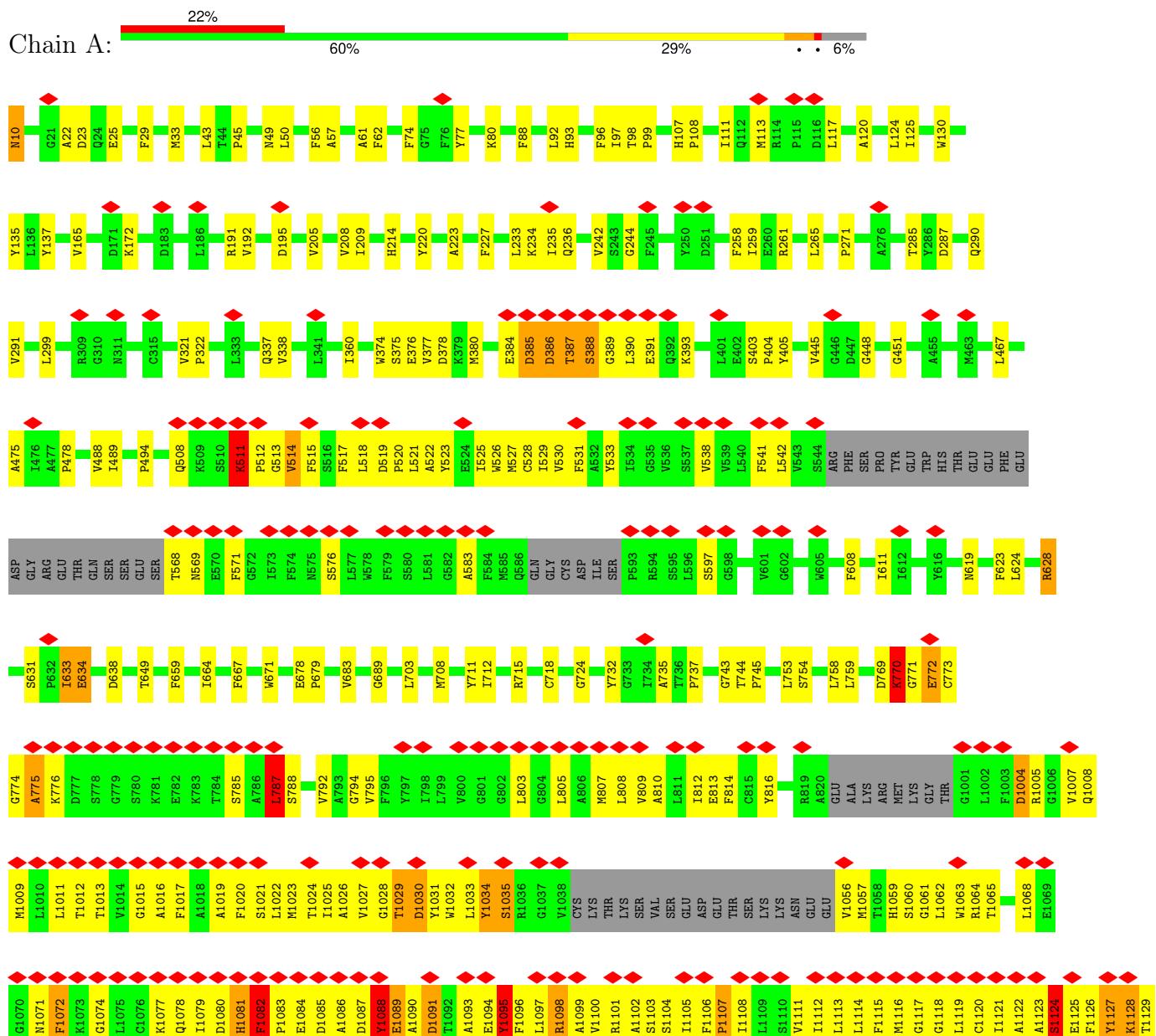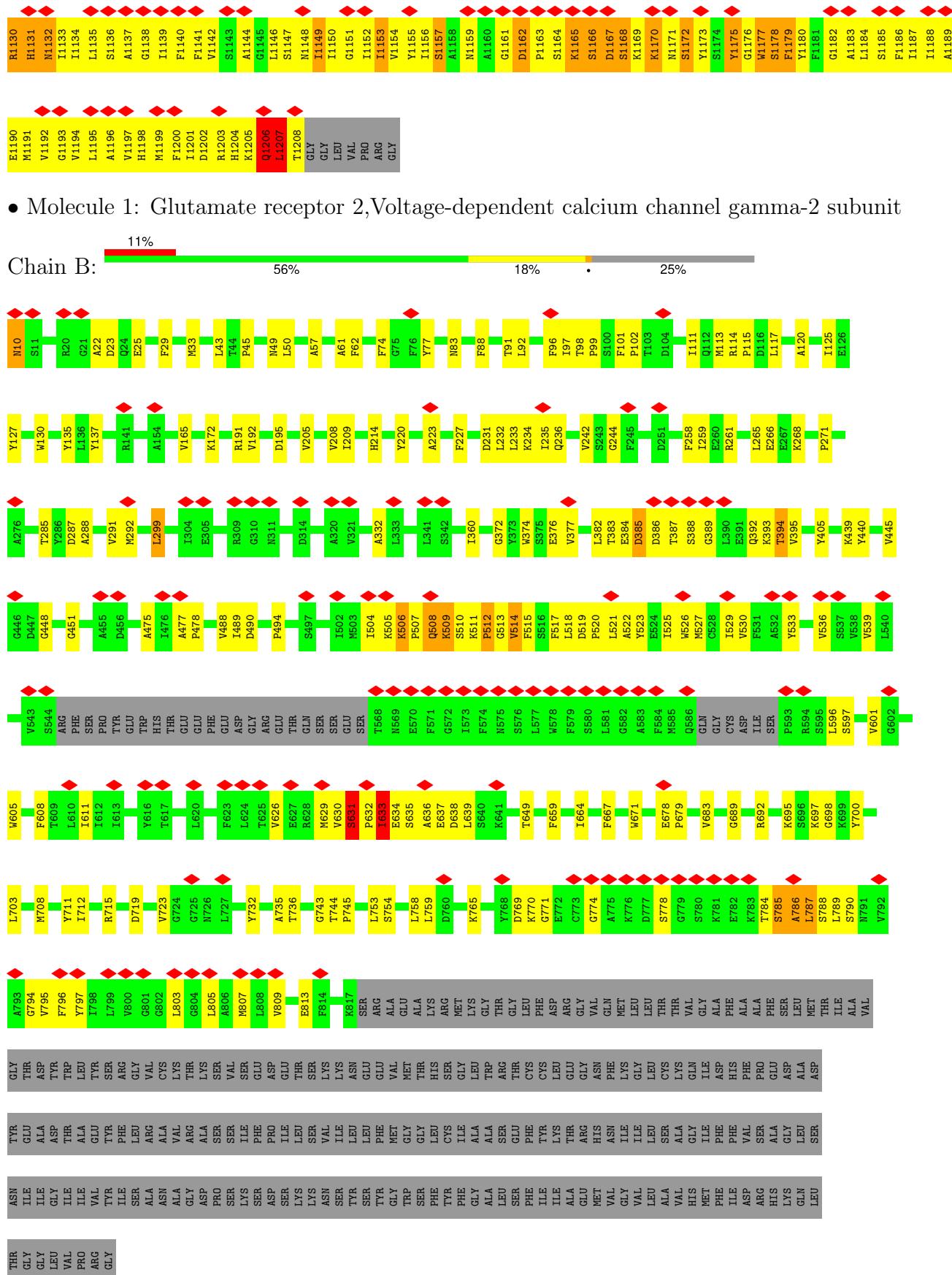
• Molecule 1: Glutamate receptor 2,Voltage-dependent calcium channel gamma-2 subunit

Chain B:

• Molecule 1: Glutamate receptor 2,Voltage-dependent calcium channel gamma-2 subunit

Chain C:

• Molecule 1: Glutamate receptor 2,Voltage-dependent calcium channel gamma-2 subunit

Chain D:
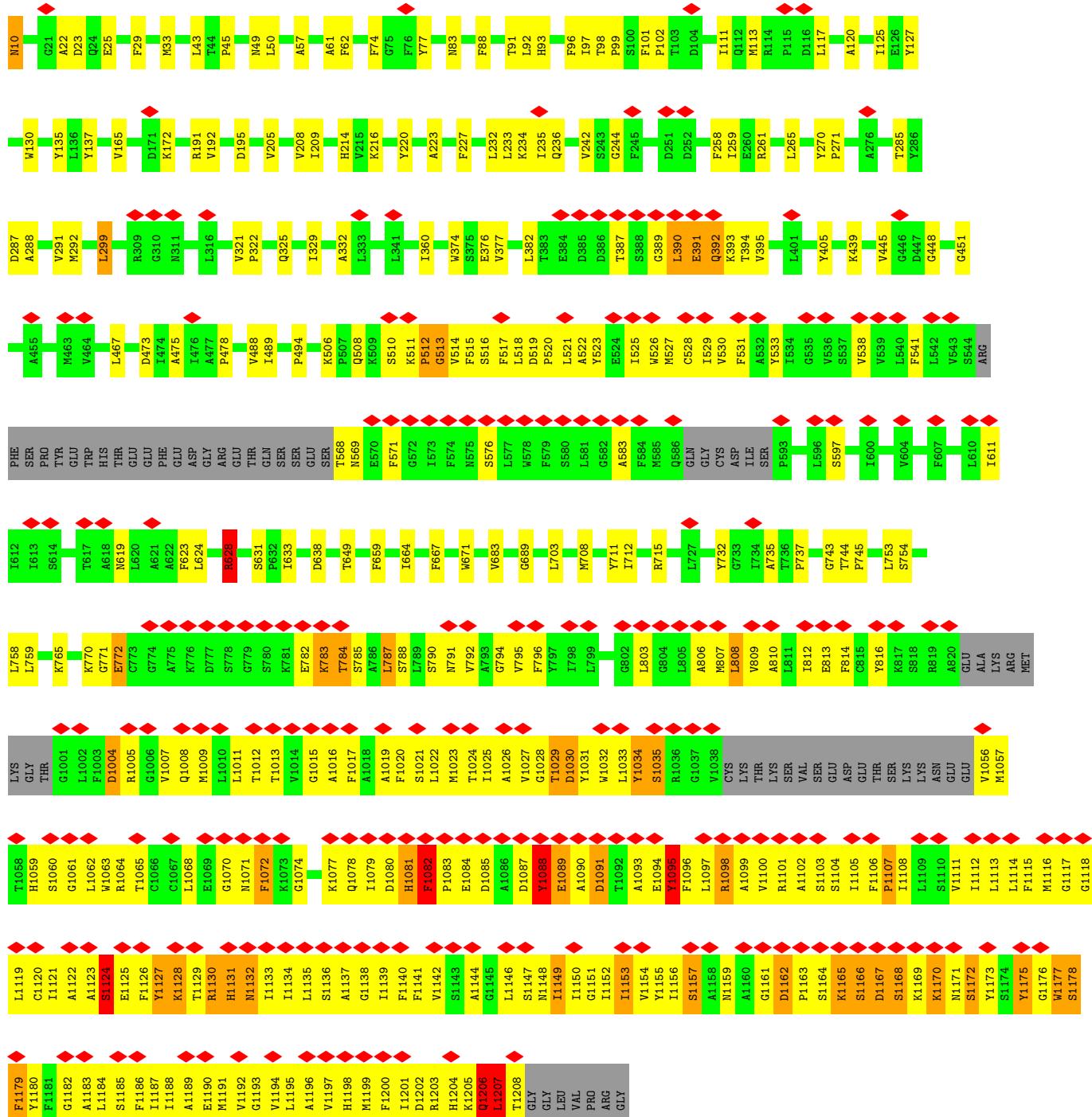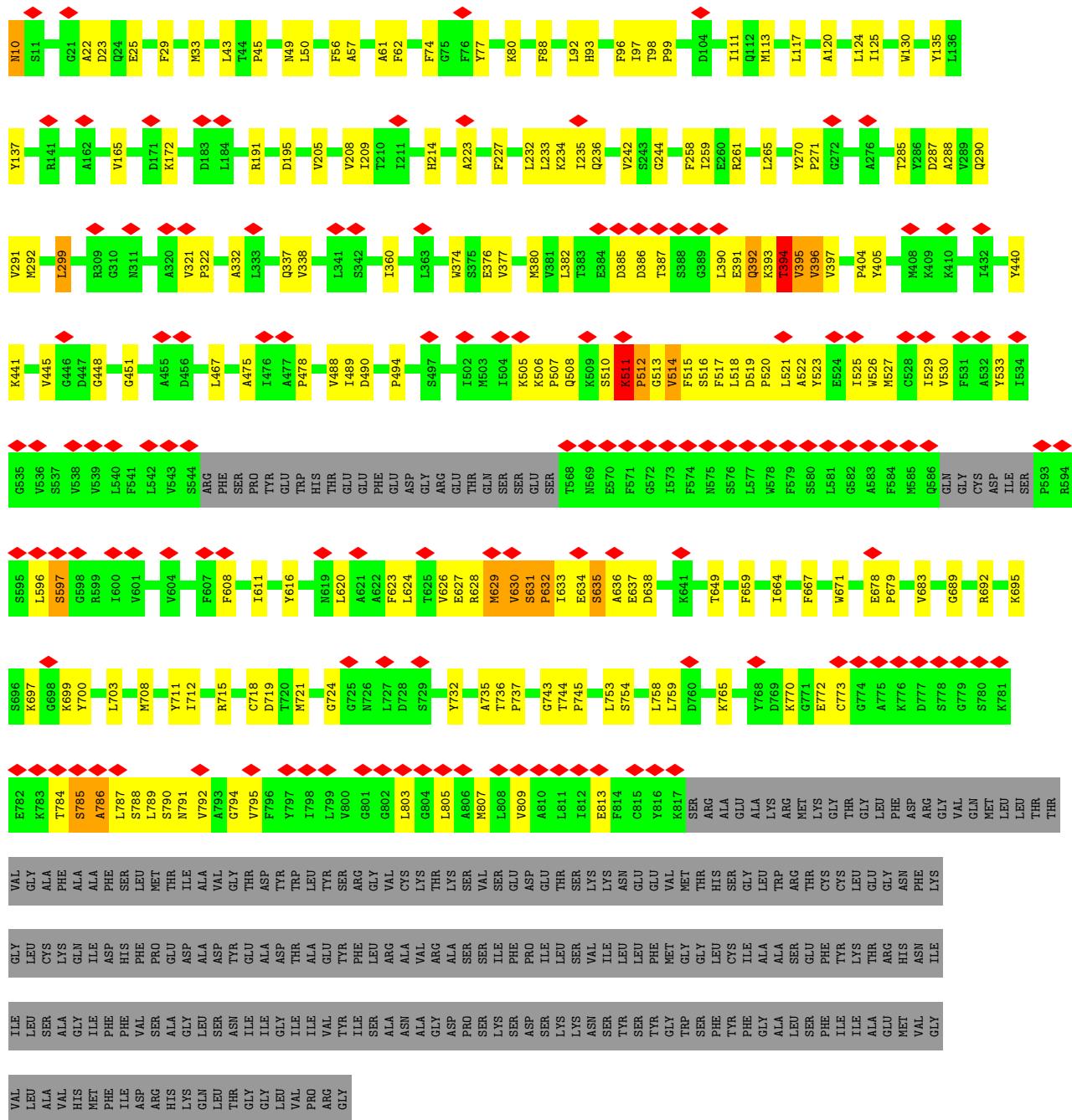
4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	10293	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 $(e^-/\text{Å}^2)$	80	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	0.055	Depositor
Minimum map value	-0.022	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.019	Depositor
Map size (Å)	367.19998, 367.19998, 367.19998	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.02, 1.02, 1.02	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: NAG, ZK1

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	0.33	2/7267 (0.0%)	0.60	15/9925 (0.2%)
1	B	0.24	0/5768	0.37	2/7888 (0.0%)
1	C	0.34	2/7267 (0.0%)	0.54	16/9925 (0.2%)
1	D	0.23	0/5768	0.36	1/7888 (0.0%)
All	All	0.30	4/26070 (0.0%)	0.49	34/35626 (0.1%)

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	3
1	C	0	2
All	All	0	5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	1157	SER	C-N	-10.31	1.10	1.34
1	A	1157	SER	C-N	-10.30	1.10	1.34
1	C	808	LEU	C-N	8.81	1.54	1.34
1	A	787	LEU	C-N	-5.18	1.22	1.34

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	787	LEU	O-C-N	-28.18	77.62	122.70
1	C	628	ARG	NE-CZ-NH1	-13.77	113.42	120.30
1	A	628	ARG	NE-CZ-NH2	-12.47	114.06	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	628	ARG	NE-CZ-NH2	11.86	126.23	120.30
1	A	628	ARG	NE-CZ-NH1	11.01	125.80	120.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1206	GLN	Mainchain
1	A	1207	LEU	Mainchain
1	A	787	LEU	Mainchain
1	C	1206	GLN	Mainchain
1	C	1207	LEU	Mainchain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7110	0	6571	1036	0
1	B	5647	0	5177	227	0
1	C	7110	0	6573	1039	0
1	D	5647	0	5177	238	0
2	A	27	0	13	0	0
2	B	27	0	13	1	0
2	C	27	0	13	0	0
2	D	27	0	13	0	0
3	A	14	0	13	2	0
3	B	14	0	13	0	0
3	C	14	0	13	0	0
3	D	14	0	13	2	0
All	All	25678	0	23602	2456	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 50.

The worst 5 of 2456 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:1114:LEU:CD1	1:C:1141:PHE:CZ	1.75	1.69
1:A:1114:LEU:CD1	1:A:1141:PHE:CZ	1.75	1.68
1:C:1134:ILE:CG2	1:C:1200:PHE:HB3	1.21	1.66
1:A:1083:PRO:HG2	1:A:1098:ARG:CG	1.16	1.62
1:A:1114:LEU:HD13	1:A:1141:PHE:CZ	1.31	1.60

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	963/1034 (93%)	844 (88%)	78 (8%)	41 (4%)	2	17
1	B	773/1034 (75%)	699 (90%)	56 (7%)	18 (2%)	5	28
1	C	963/1034 (93%)	845 (88%)	82 (8%)	36 (4%)	2	20
1	D	773/1034 (75%)	693 (90%)	57 (7%)	23 (3%)	3	23
All	All	3472/4136 (84%)	3081 (89%)	273 (8%)	118 (3%)	5	21

5 of 118 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	172	LYS
1	A	385	ASP
1	A	387	THR
1	A	389	GLY
1	A	511	LYS

5.3.2 Protein sidechains ⓘ

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	693/876 (79%)	676 (98%)	17 (2%)	42	61
1	B	546/876 (62%)	540 (99%)	6 (1%)	70	80
1	C	693/876 (79%)	676 (98%)	17 (2%)	42	61
1	D	546/876 (62%)	541 (99%)	5 (1%)	75	83
All	All	2478/3504 (71%)	2433 (98%)	45 (2%)	54	71

5 of 45 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	1035	SER
1	C	1149	ILE
1	C	1088	TYR
1	C	1127	TYR
1	C	1167	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	83	ASN
1	C	1059	HIS
1	D	344	ASN
1	C	1198	HIS
1	D	337	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

8 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	NAG	B	1302	1	14,14,15	0.49	0	17,19,21	0.69	0
2	ZK1	C	1301	-	29,29,29	3.63	12 (41%)	45,45,45	1.57	7 (15%)
2	ZK1	B	1301	-	29,29,29	3.63	11 (37%)	45,45,45	1.55	7 (15%)
3	NAG	C	1302	1	14,14,15	0.47	0	17,19,21	0.93	1 (5%)
3	NAG	D	1302	1	14,14,15	0.50	0	17,19,21	0.67	0
2	ZK1	D	1301	-	29,29,29	3.64	12 (41%)	45,45,45	1.57	8 (17%)
2	ZK1	A	1301	-	29,29,29	3.64	12 (41%)	45,45,45	1.57	7 (15%)
3	NAG	A	1302	1	14,14,15	0.48	0	17,19,21	0.70	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
3	NAG	B	1302	1	-	0/6/23/26	0/1/1/1
2	ZK1	C	1301	-	-	5/13/23/23	0/3/3/3
2	ZK1	B	1301	-	-	5/13/23/23	0/3/3/3
3	NAG	C	1302	1	-	2/6/23/26	0/1/1/1
3	NAG	D	1302	1	-	2/6/23/26	0/1/1/1
2	ZK1	D	1301	-	-	5/13/23/23	0/3/3/3
2	ZK1	A	1301	-	-	5/13/23/23	0/3/3/3
3	NAG	A	1302	1	-	2/6/23/26	0/1/1/1

The worst 5 of 47 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1301	ZK1	OAA-CAT	9.38	1.41	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1301	ZK1	OAA-CAT	9.36	1.41	1.23
2	B	1301	ZK1	OAA-CAT	9.31	1.41	1.23
2	C	1301	ZK1	OAA-CAT	9.28	1.41	1.23
2	C	1301	ZK1	OAB-CAU	8.77	1.41	1.23

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	1301	ZK1	CAN-NAX-CAM	4.46	121.61	111.57
2	A	1301	ZK1	CAN-NAX-CAM	4.42	121.51	111.57
2	D	1301	ZK1	CAN-NAX-CAM	4.39	121.45	111.57
2	B	1301	ZK1	CAN-NAX-CAM	4.39	121.44	111.57
2	A	1301	ZK1	CAO-NAY-CAU	3.74	120.35	116.55

There are no chirality outliers.

5 of 26 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1301	ZK1	NAY-CAO-PBA-OAC
2	A	1301	ZK1	NAY-CAO-PBA-OAE
2	B	1301	ZK1	NAY-CAO-PBA-OAC
2	B	1301	ZK1	NAY-CAO-PBA-OAE
2	C	1301	ZK1	NAY-CAO-PBA-OAC

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1301	ZK1	1	0
3	D	1302	NAG	2	0
3	A	1302	NAG	2	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 ZK1 C 1301

Bond lengths

Bond angles

Torsions

Rings

Ligand ZK1 B 1301

Bond lengths

Bond angles

Torsions

Rings

Ligand ZK1 D 1301

Bond lengths

Bond angles

Torsions

Rings

Ligand ZK1 A 1301

Bond lengths

Bond angles

Torsions

Rings
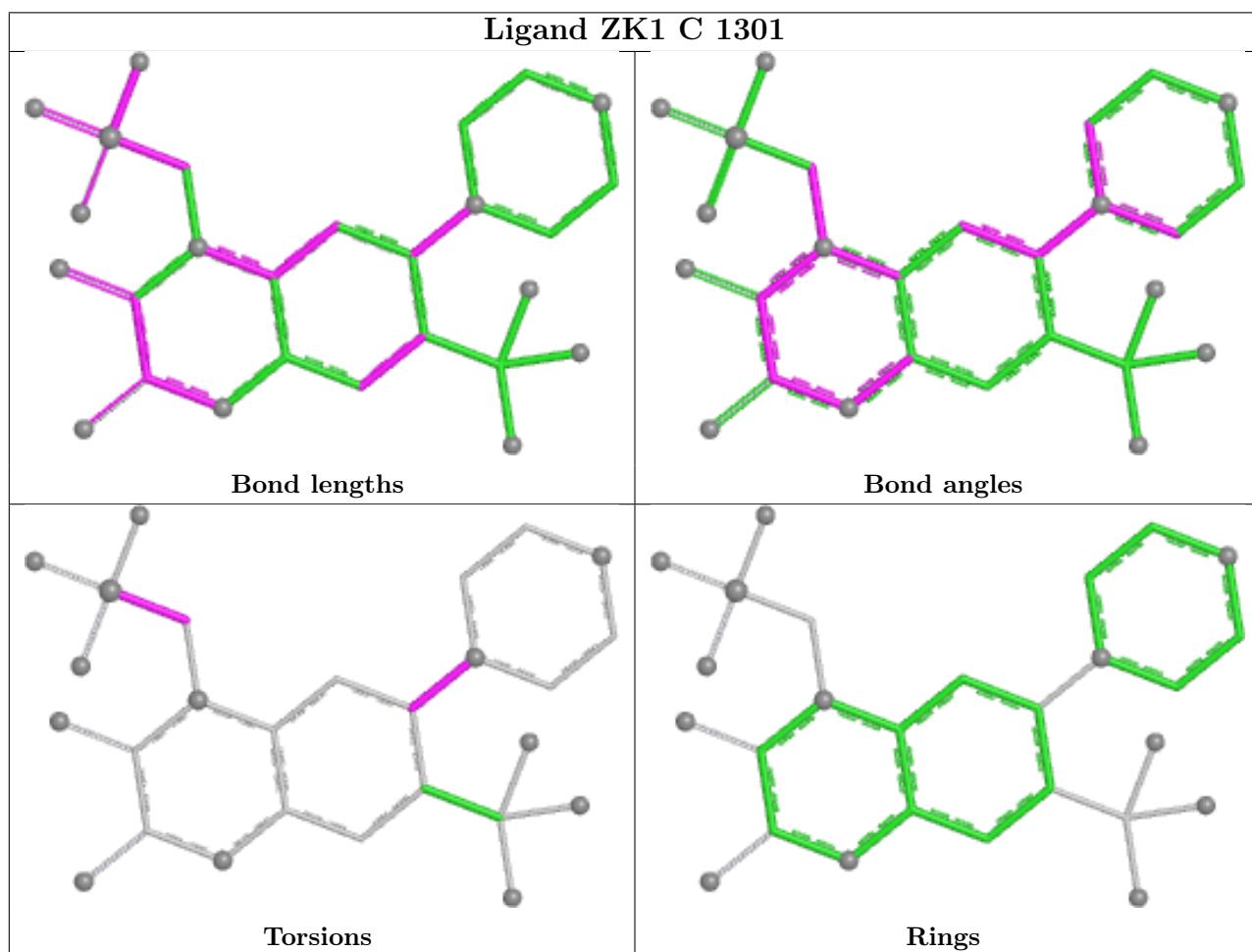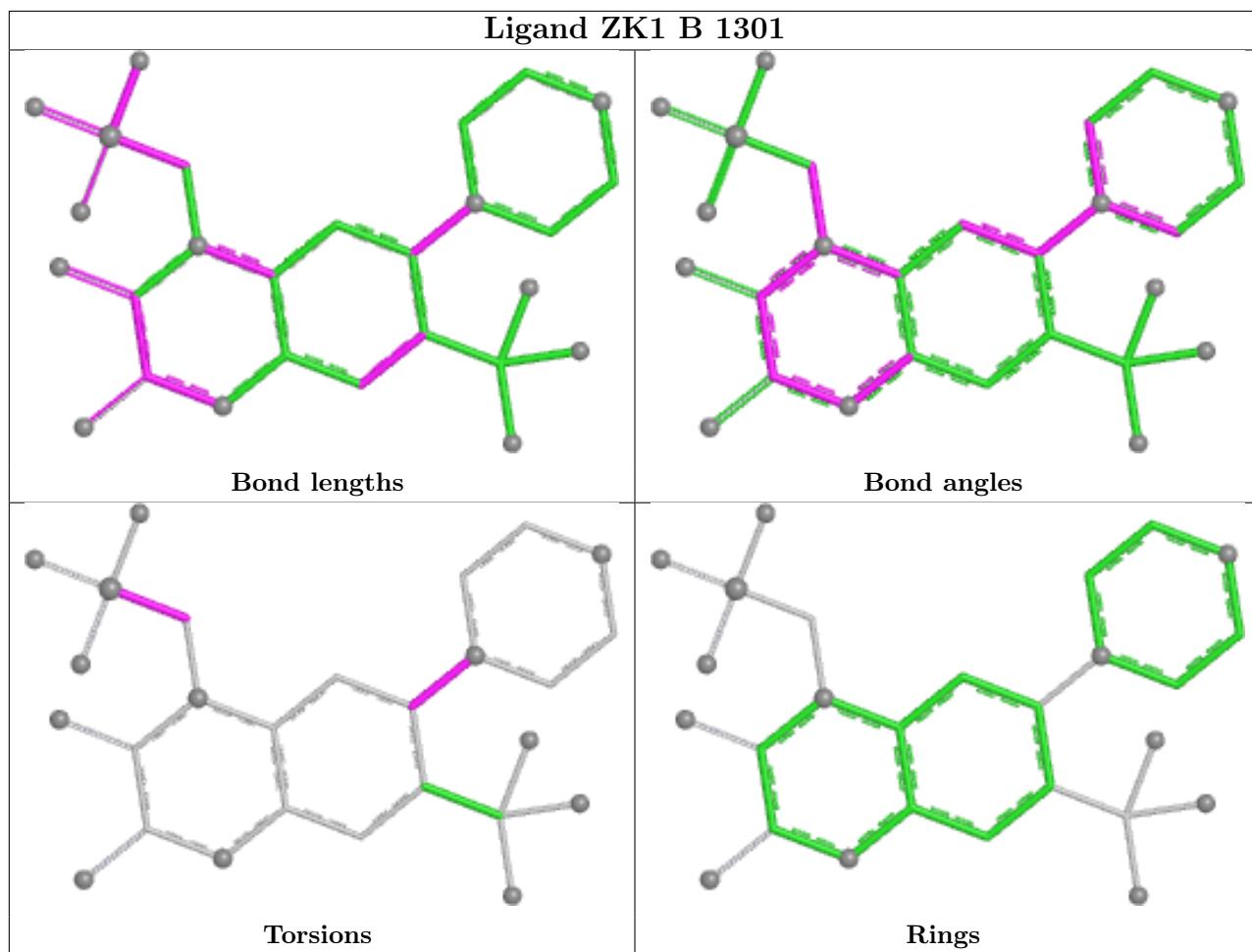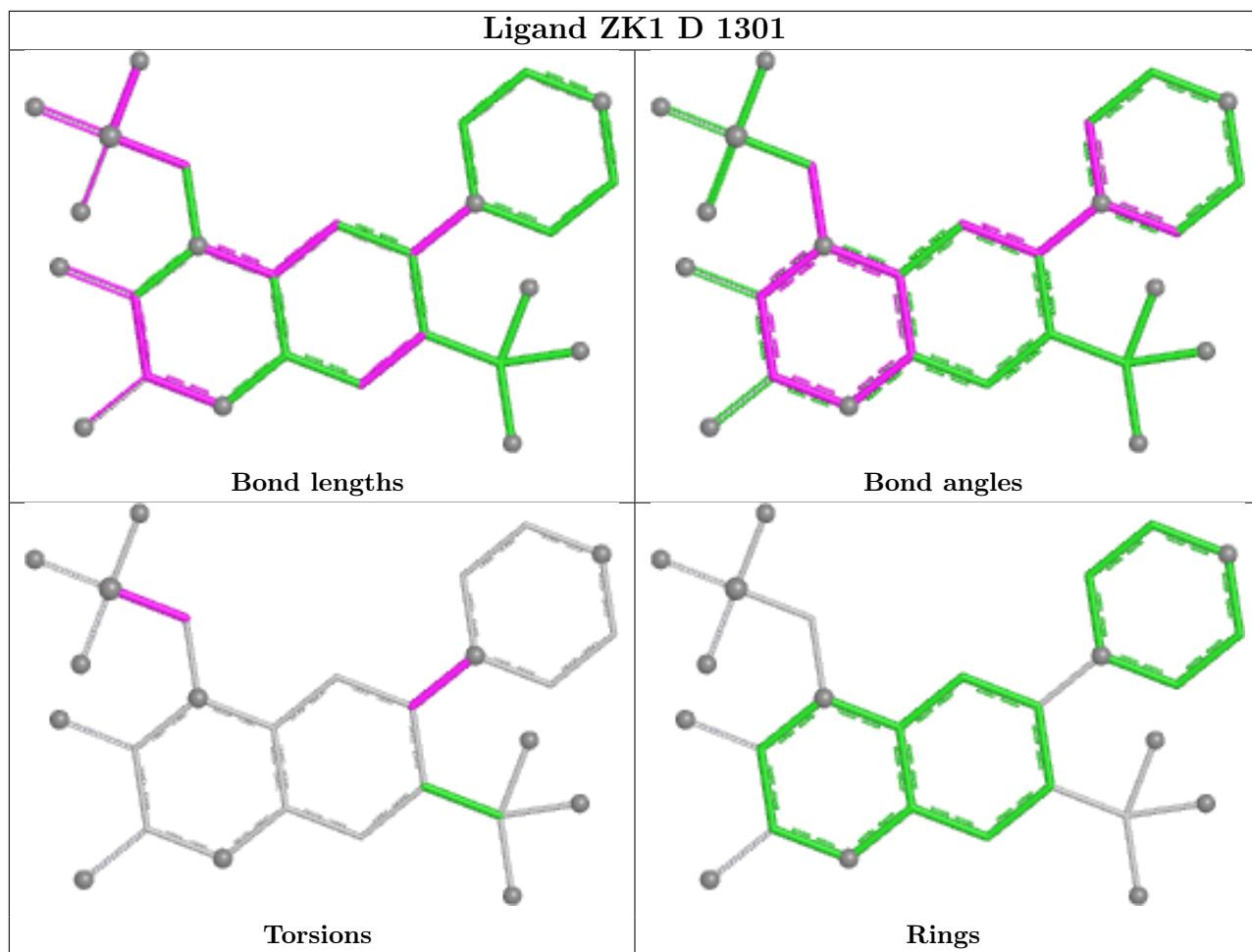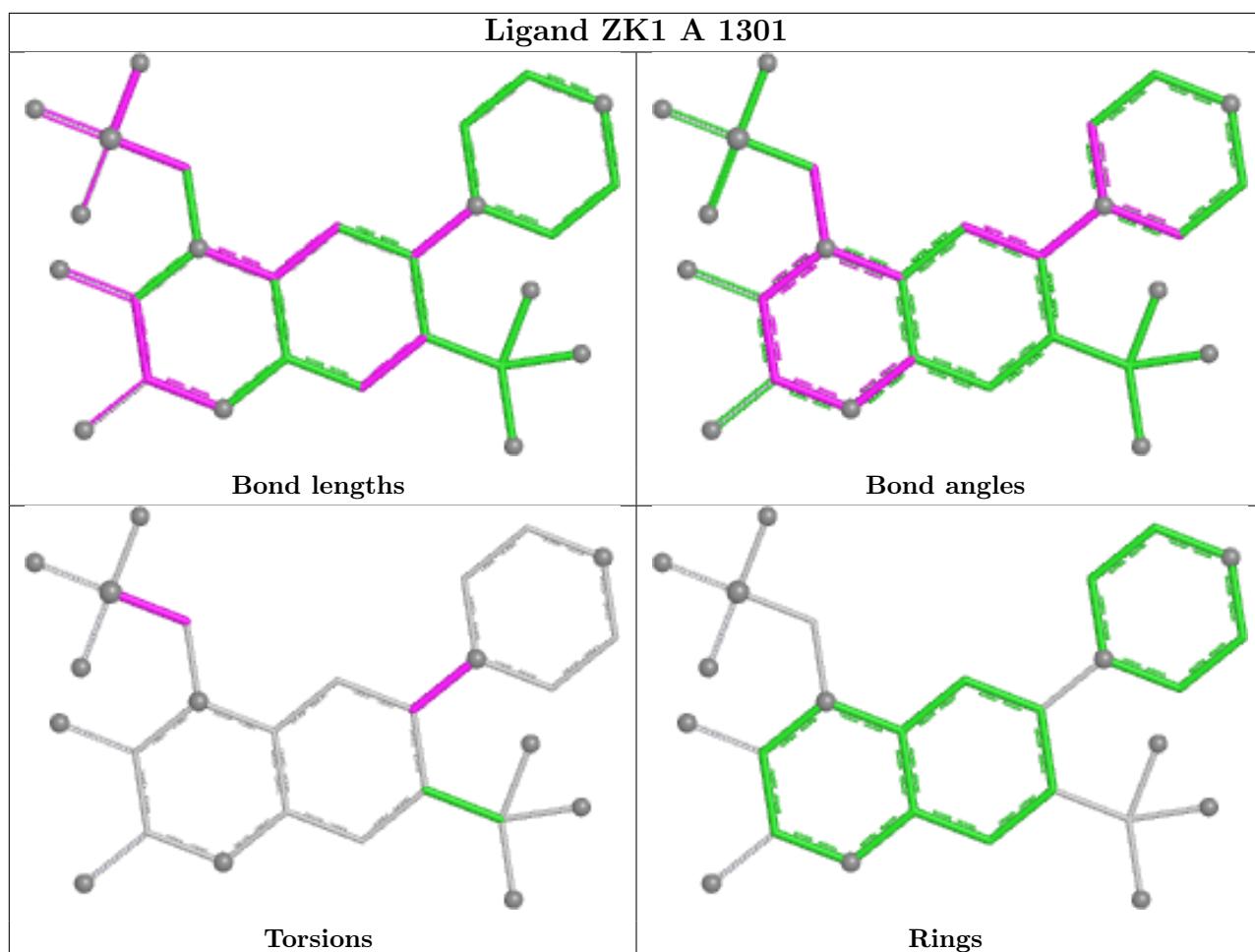
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1
1	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1157:SER	C	1158:ALA	N	1.10
1	C	1157:SER	C	1158:ALA	N	1.10

6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-8231. 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 ⓘ

6.1.1 Primary map

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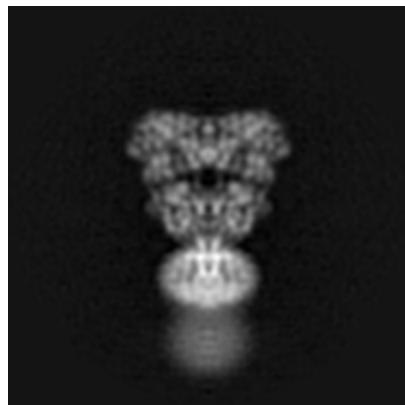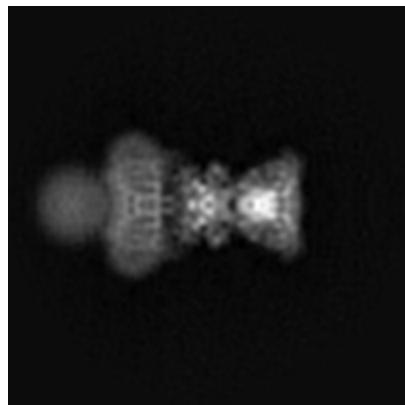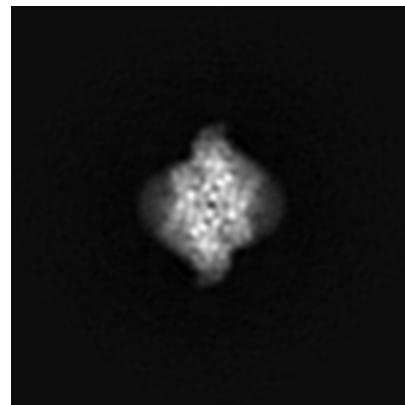
The images above show the map projected in three orthogonal directions.

6.2 Central slices ⓘ

6.2.1 Primary map
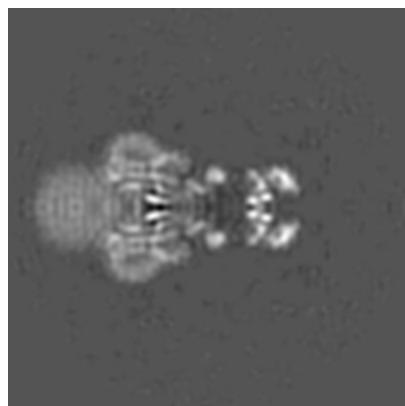
X Index: 180	Y Index: 180	Z Index: 180
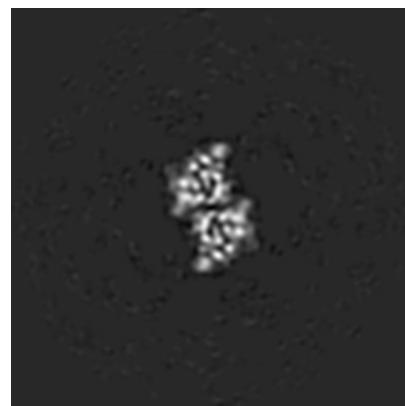
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices ⓘ
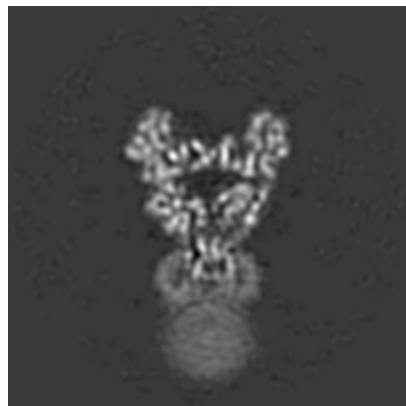
6.3.1 Primary map
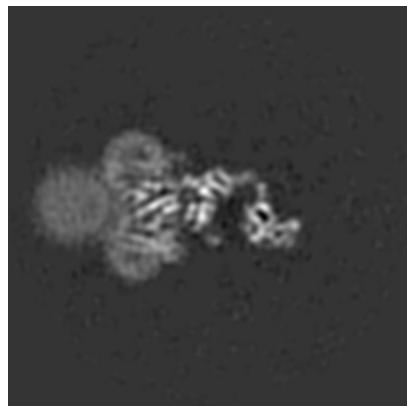
| X Index: 176 | Y Index: 173 | Z Index: 250 |

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

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

6.4.1 Primary map

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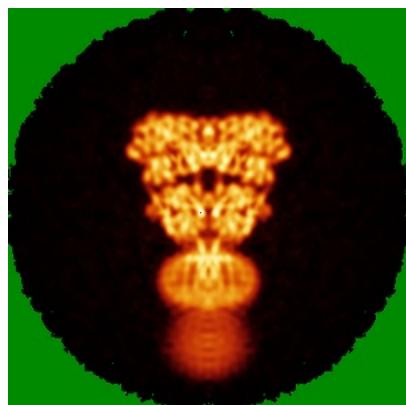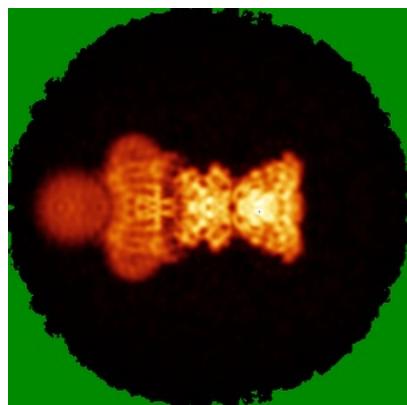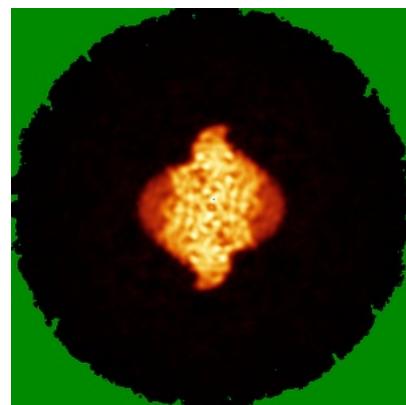
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z
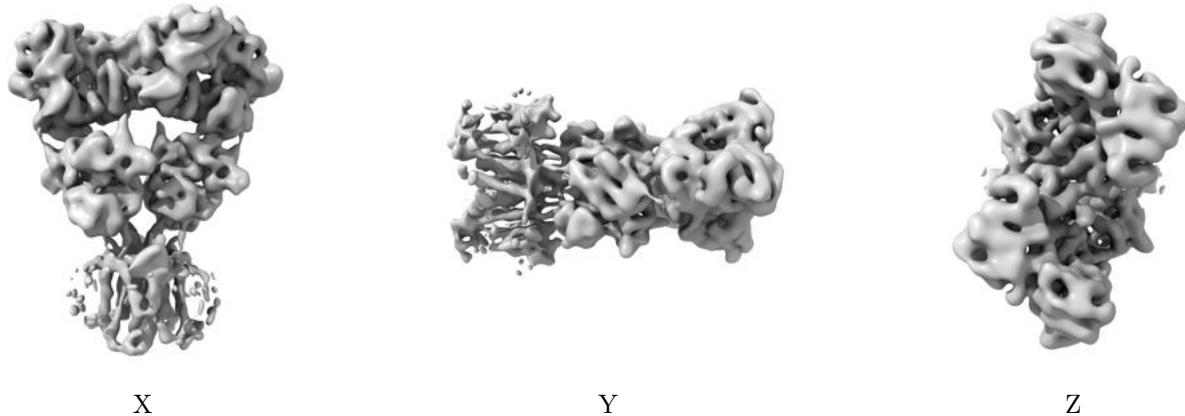
The images above show the 3D surface view of the map at the recommended contour level 0.019. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.6 Mask visualisation (i)

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

7 Map analysis ⓘ

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

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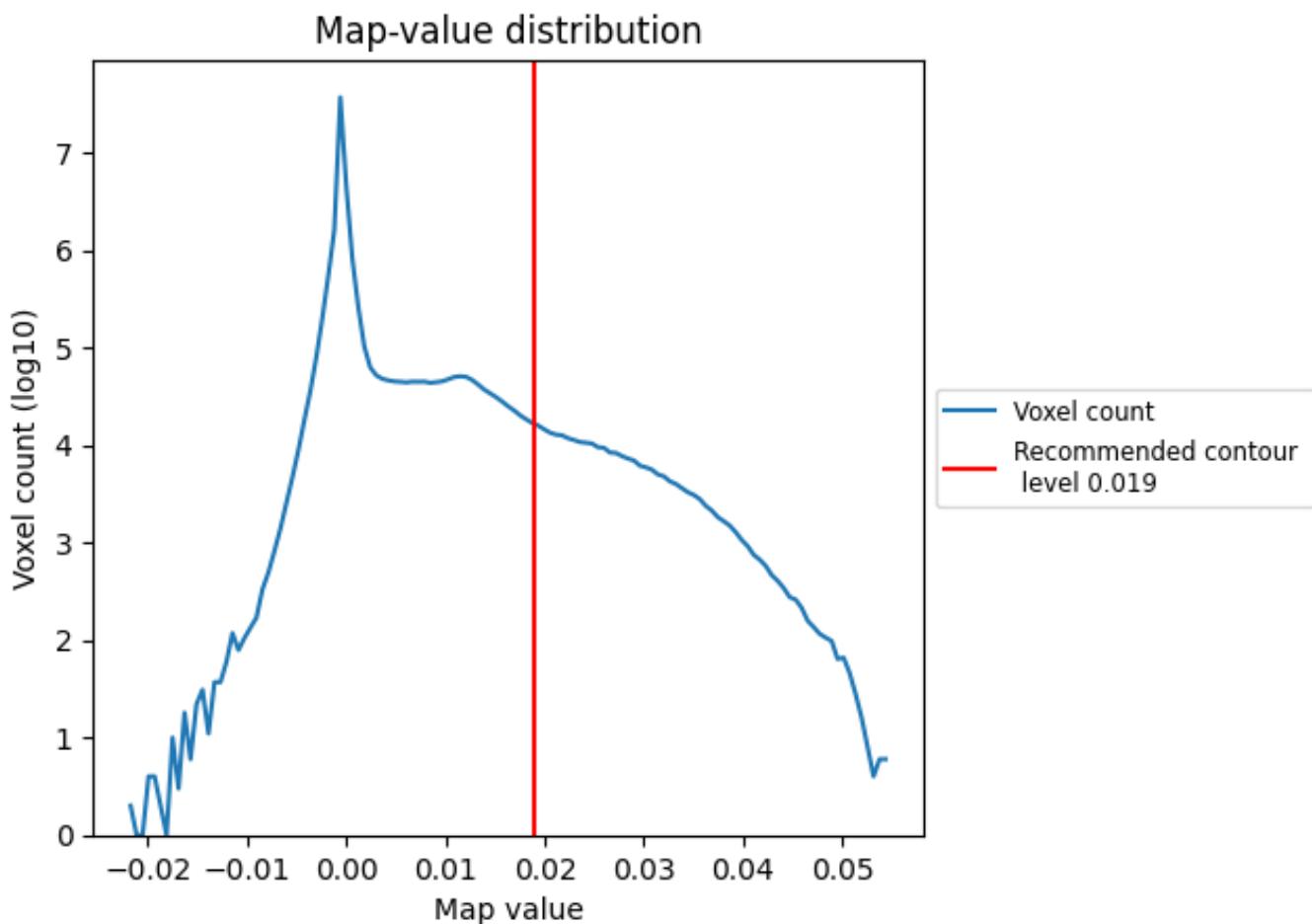
The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2   Volume estimate ⓘ
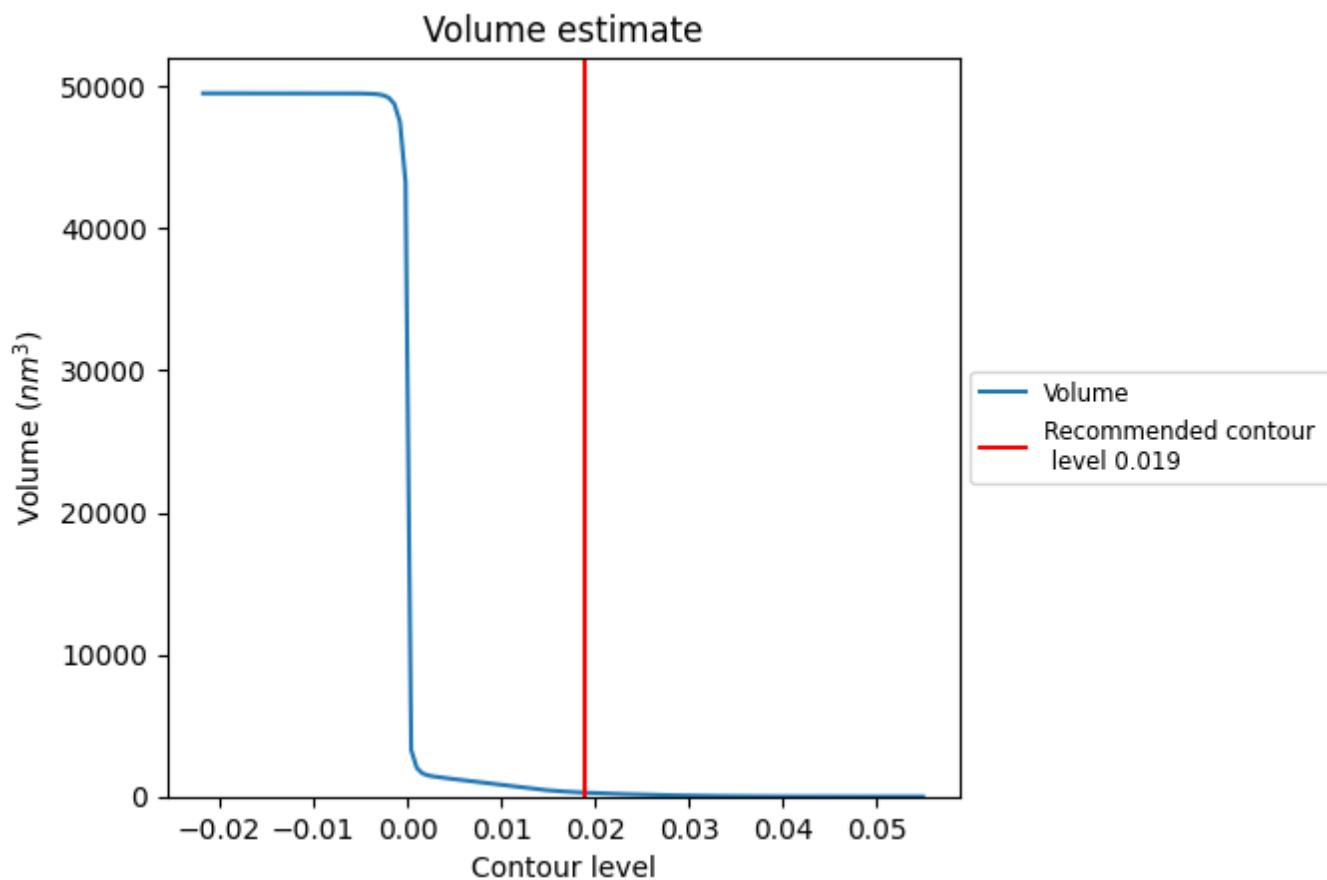
The volume at the recommended contour level is 273 nm^3; this corresponds to an approximate mass of 246 kDa.

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 ⓘ
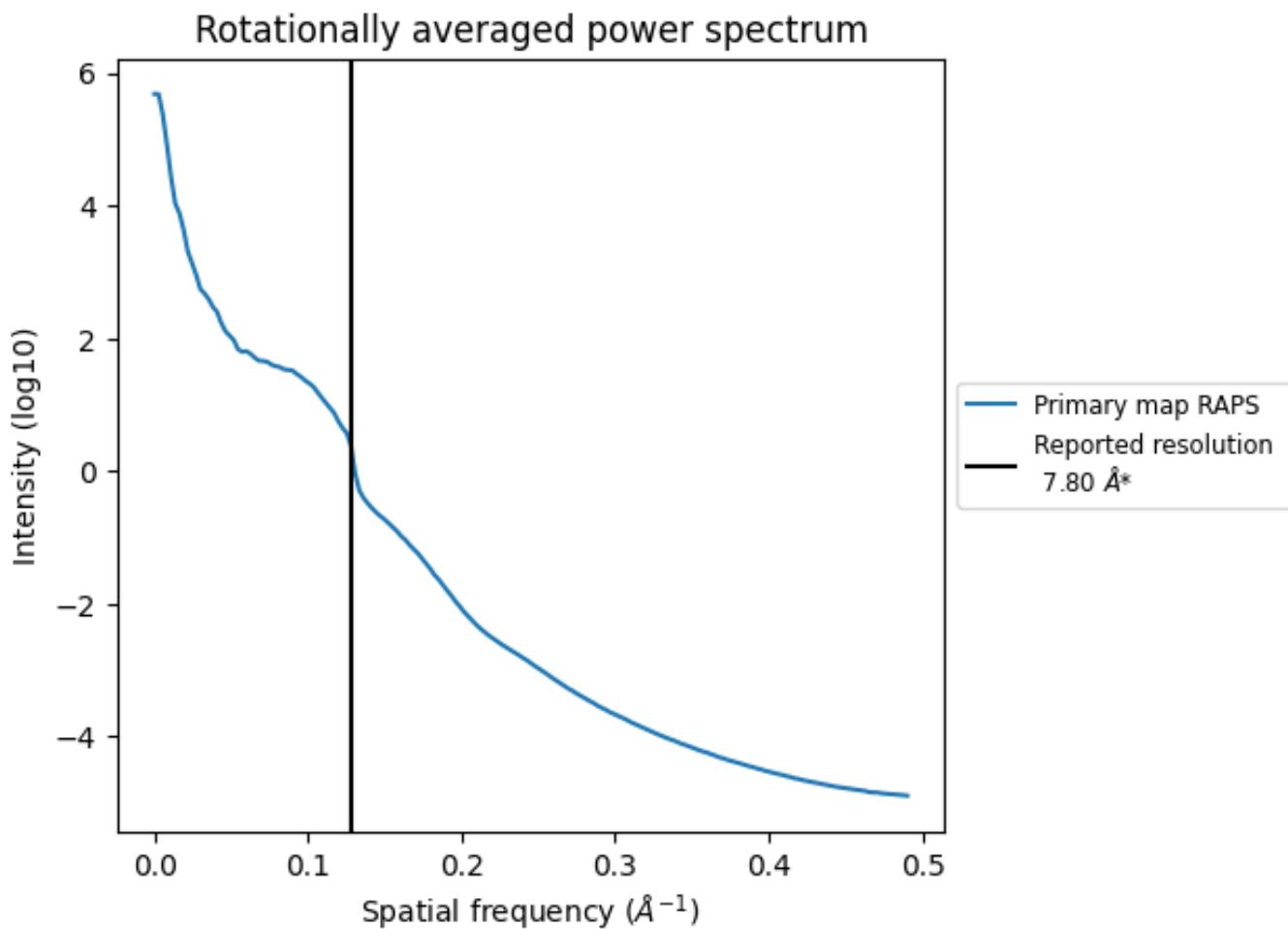
*Reported resolution corresponds to spatial frequency of 0.128 Å^{-1}

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-8231 and PDB model 5KBU. Per-residue inclusion information can be found in section 3 on page 8.

9.1   Map-model overlay (i)
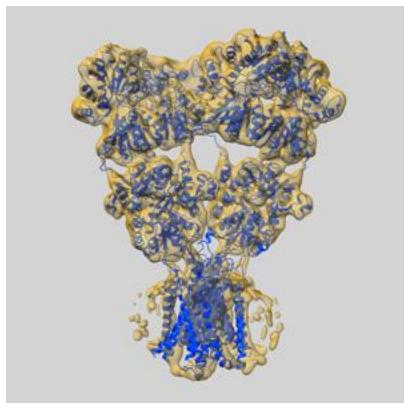
| X | Y | Z |
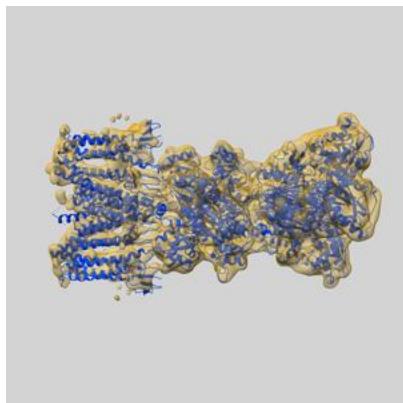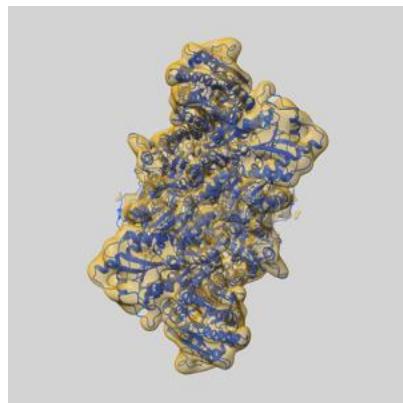
The images above show the 3D surface view of the map at the recommended contour level 0.019 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Q-score mapped to coordinate model ⓘ

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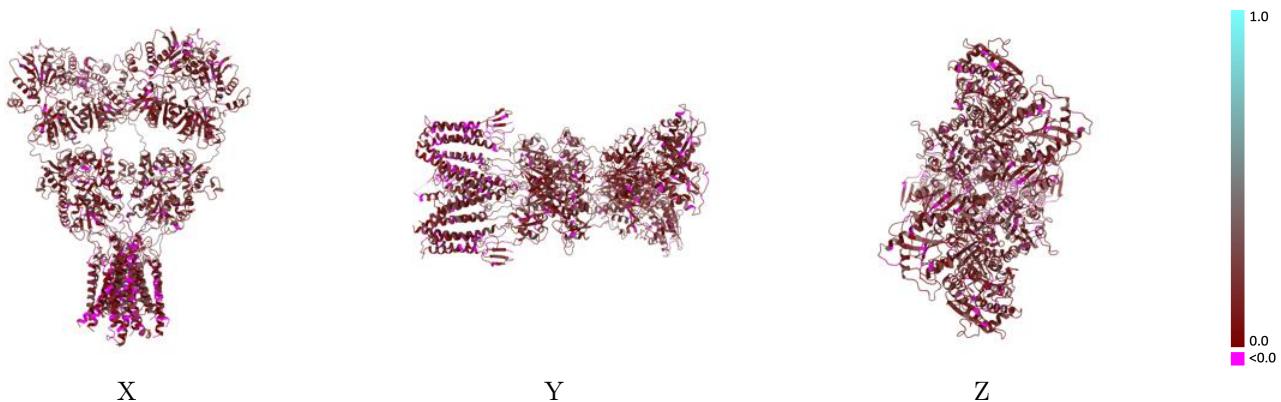
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

X   Y   Z
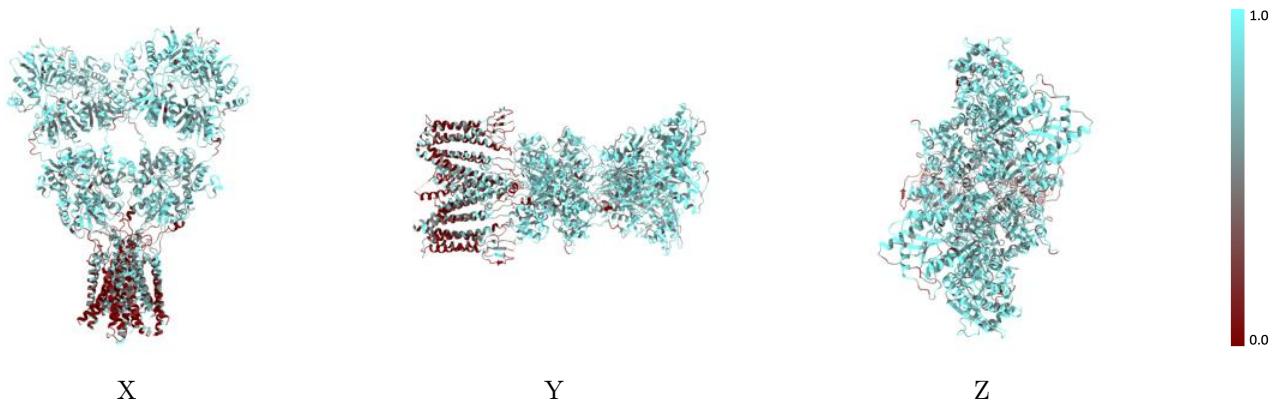
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.019).

9.4   Atom inclusion ⓘ
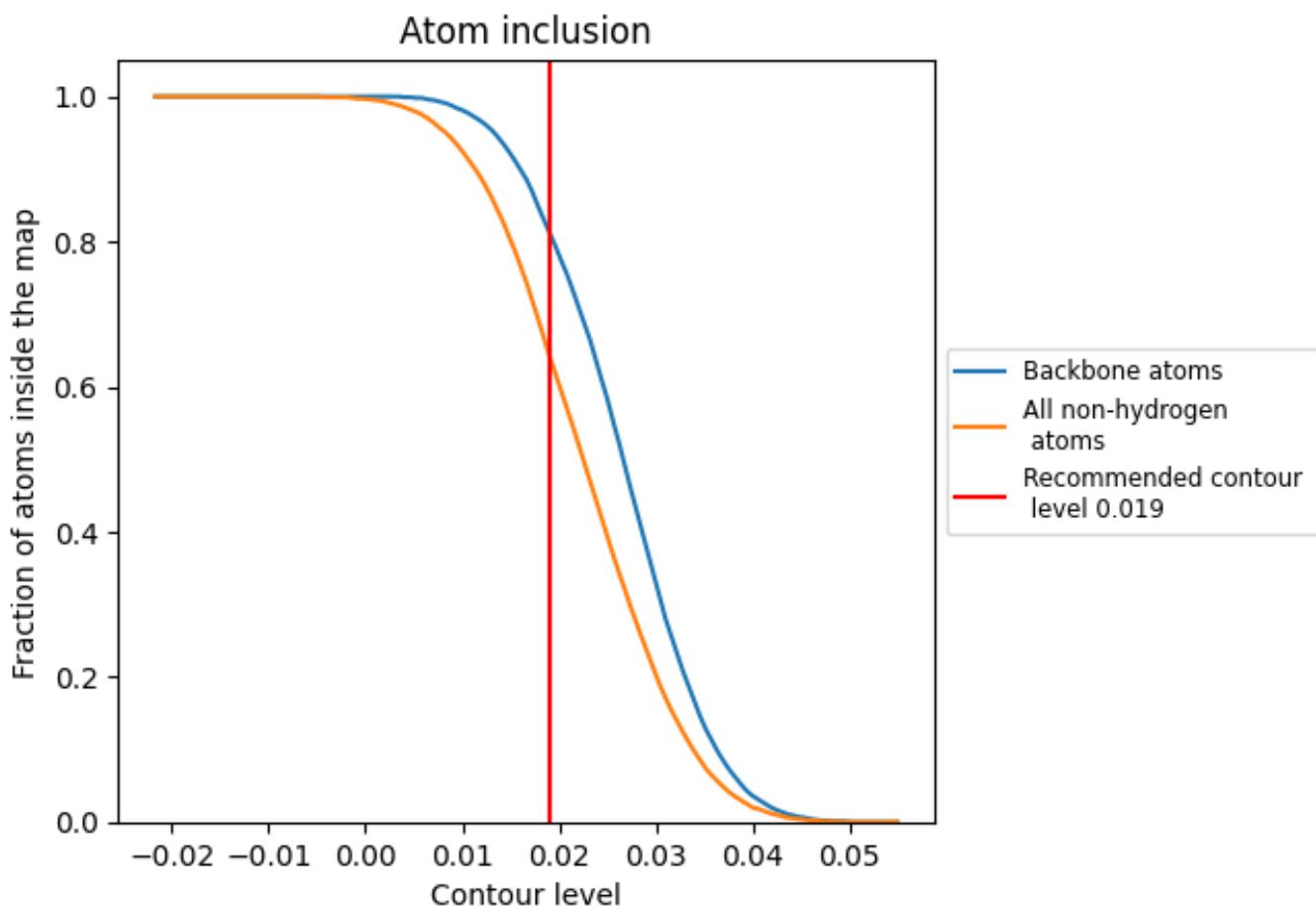
At the recommended contour level, 81% of all backbone atoms, 64% of all non-hydrogen atoms, are inside the map.

9.5   Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.019) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6430	0.1530
A	0.6180	0.1570
B	0.6920	0.1610
C	0.6040	0.1420
D	0.6750	0.1530