wwPDB EM Validation Summary Report (i)

Nov 7, 2022 – 10:09 AM EST

PDB ID	:	6DM0
EMDB ID	:	EMD-7960
Title	:	Open state GluA2 in complex with STZ and blocked by IEM-1460, after micelle signal subtraction
Authors	:	Twomey, E.C.; Yelshanskaya, M.V.; Vassilevski, A.A.; Sobolevsky, A.I.
Deposited on	:	2018-06-04
Resolution	:	4.40 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 (1)) were used in the production of this report:

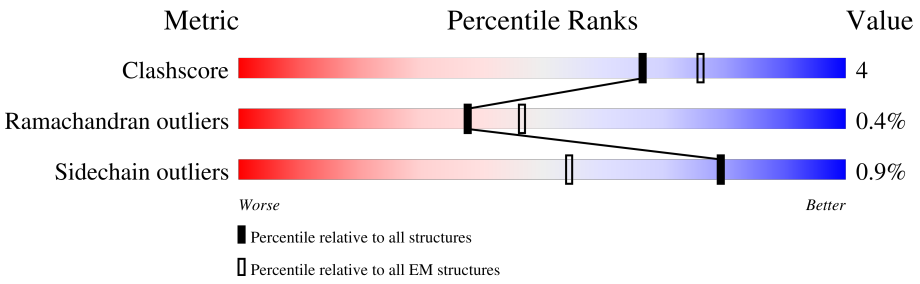
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 4.40 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	1031	23% 84% 11% 5%
1	B	1031	23% 84% 11% • •
1	C	1031	23% 84% 11% 5%
1	D	1031	23% 84% 11% • •

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 31095 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
			Total	C	N	O	S		
1	A	984	7734	4980	1278	1435	41	0	0
1	B	985	7735	4981	1279	1434	41	0	0
1	C	984	7734	4980	1278	1435	41	0	0
1	D	985	7735	4981	1279	1434	41	0	0

There are 76 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	999	GLY	-	linker	UNP P19491
A	1000	THR	-	linker	UNP P19491
A	1047	ASP	ASN	conflict	UNP Q9Y698
A	1208	THR	-	expression tag	UNP Q9Y698
A	1209	GLY	-	expression tag	UNP Q9Y698
A	1210	GLY	-	expression tag	UNP Q9Y698
A	1211	ALA	-	expression tag	UNP Q9Y698
A	1212	GLU	-	expression tag	UNP Q9Y698
B	241	GLU	ASN	conflict	UNP P19491
B	382	LEU	VAL	conflict	UNP P19491

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Chain	Residue	Modelled	Actual	Comment	Reference
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	conflict	UNP P19491
B	385	ASP	ASN	conflict	UNP P19491
B	392	GLN	ASN	conflict	UNP P19491
B	999	GLY	-	linker	UNP P19491
B	1000	THR	-	linker	UNP P19491
B	1047	ASP	ASN	conflict	UNP Q9Y698
B	1208	THR	-	expression tag	UNP Q9Y698
B	1209	GLY	-	expression tag	UNP Q9Y698
B	1210	GLY	-	expression tag	UNP Q9Y698
B	1211	ALA	-	expression tag	UNP Q9Y698
B	1212	GLU	-	expression tag	UNP Q9Y698
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	999	GLY	-	linker	UNP P19491
C	1000	THR	-	linker	UNP P19491
C	1047	ASP	ASN	conflict	UNP Q9Y698
C	1208	THR	-	expression tag	UNP Q9Y698
C	1209	GLY	-	expression tag	UNP Q9Y698
C	1210	GLY	-	expression tag	UNP Q9Y698
C	1211	ALA	-	expression tag	UNP Q9Y698
C	1212	GLU	-	expression tag	UNP Q9Y698
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

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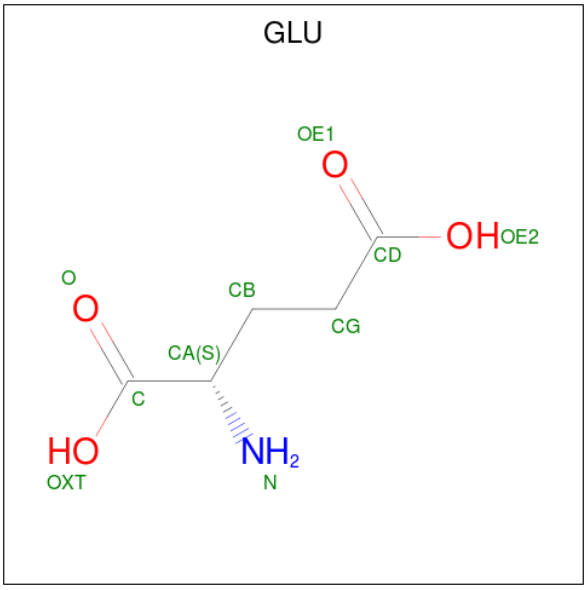
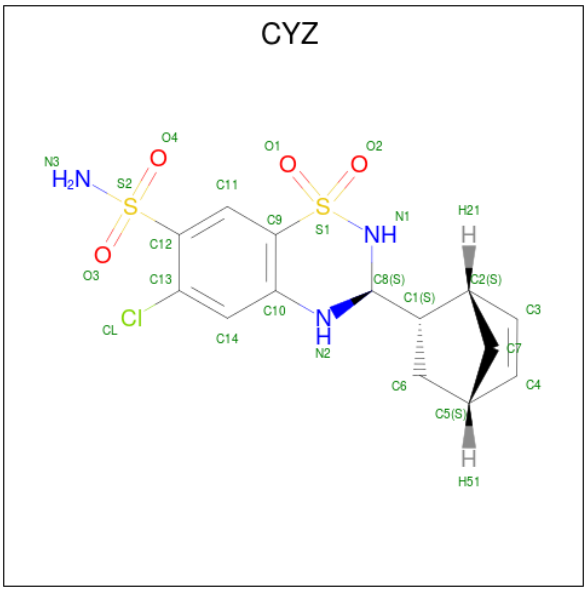
Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	PRO	deletion	UNP P19491
D	?	-	SER	deletion	UNP P19491
D	384	GLU	GLY	conflict	UNP P19491
D	385	ASP	ASN	conflict	UNP P19491
D	392	GLN	ASN	conflict	UNP P19491
D	999	GLY	-	linker	UNP P19491
D	1000	THR	-	linker	UNP P19491
D	1047	ASP	ASN	conflict	UNP Q9Y698
D	1208	THR	-	expression tag	UNP Q9Y698
D	1209	GLY	-	expression tag	UNP Q9Y698
D	1210	GLY	-	expression tag	UNP Q9Y698
D	1211	ALA	-	expression tag	UNP Q9Y698
D	1212	GLU	-	expression tag	UNP Q9Y698

- Molecule 2 is GLUTAMIC ACID (three-letter code: GLU) (formula: $C_5H_9NO_4$).



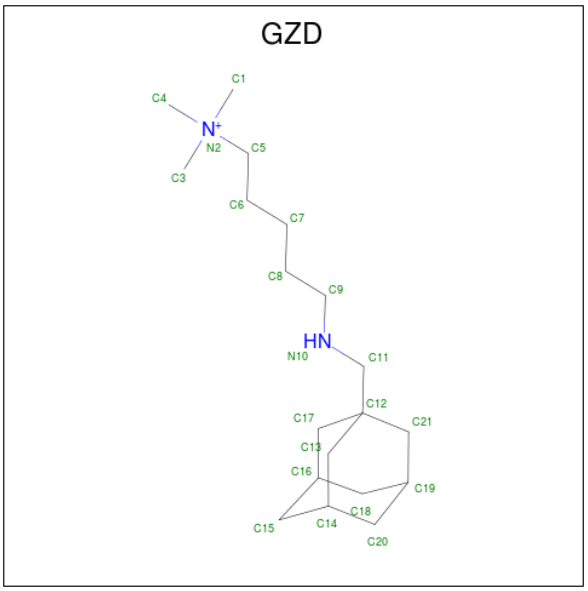
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
2	A	1	10	5	1	4	0
2	B	1	10	5	1	4	0
2	C	1	10	5	1	4	0
2	D	1	10	5	1	4	0

- Molecule 3 is CYCLOTHIAZIDE (three-letter code: CYZ) (formula: $C_{14}H_{16}ClN_3O_4S_2$).



Mol	Chain	Residues	Atoms						AltConf
3	A	1	Total	C	Cl	N	O	S	0
			24	14	1	3	4	2	
3	B	1	Total	C	Cl	N	O	S	0
			24	14	1	3	4	2	
3	C	1	Total	C	Cl	N	O	S	0
			24	14	1	3	4	2	
3	D	1	Total	C	Cl	N	O	S	0
			24	14	1	3	4	2	

- Molecule 4 is N,N,N-trimethyl-5-({[(3s,5s,7s)-tricyclo[3.3.1.1 3,7]decan-1-yl]methyl}amino) pentan-1-aminium (three-letter code: GZD) (formula: $C_{19}H_{37}N_2$).



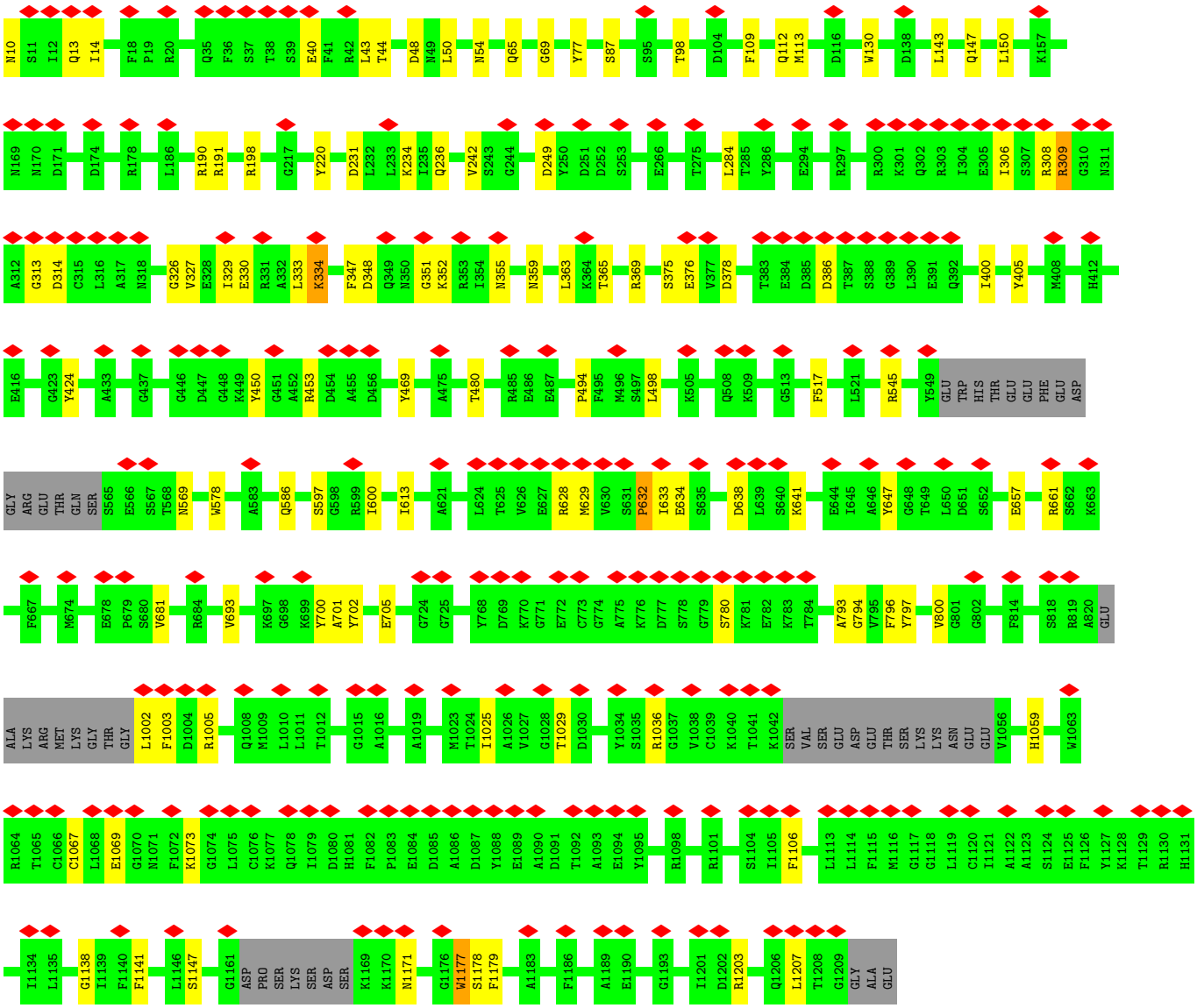
Mol	Chain	Residues	Atoms			AltConf
			Total	C	N	
4	B	1	21	19	2	0

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,Voltage-dependent calcium channel gamma-2 subunit

Chain A: 23% 84% 11% 5%

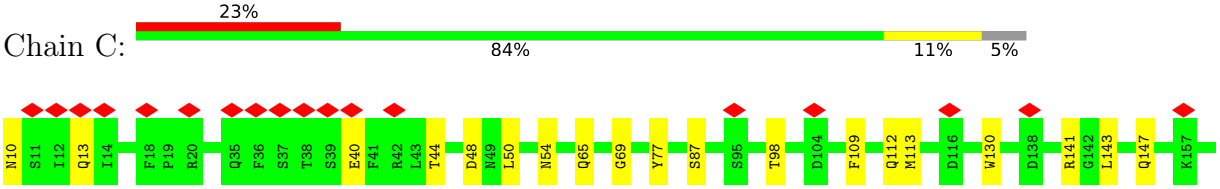


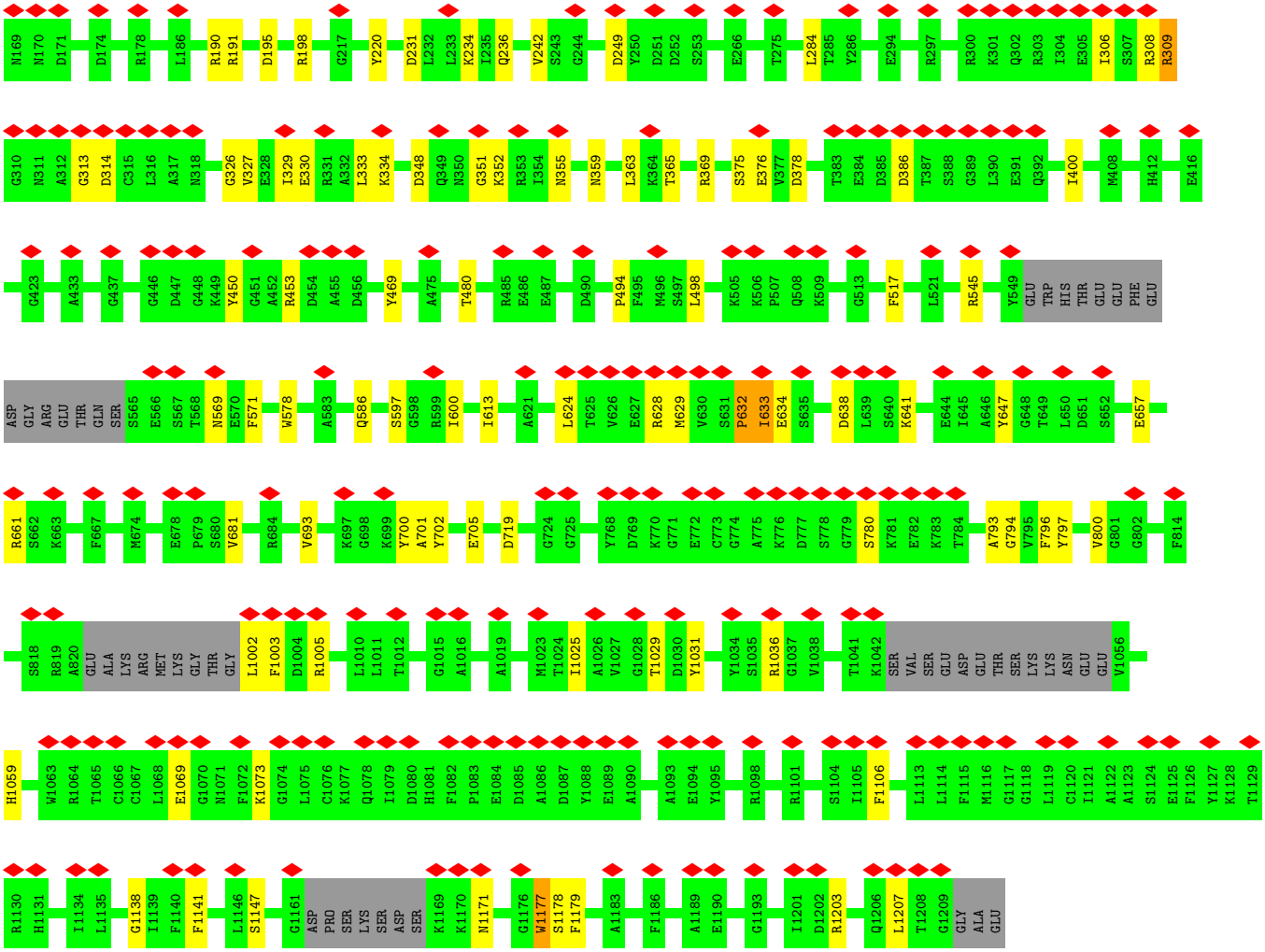
• Molecule 1: Glutamate receptor 2,Voltage-dependent calcium channel gamma-2 subunit

Chain B:

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

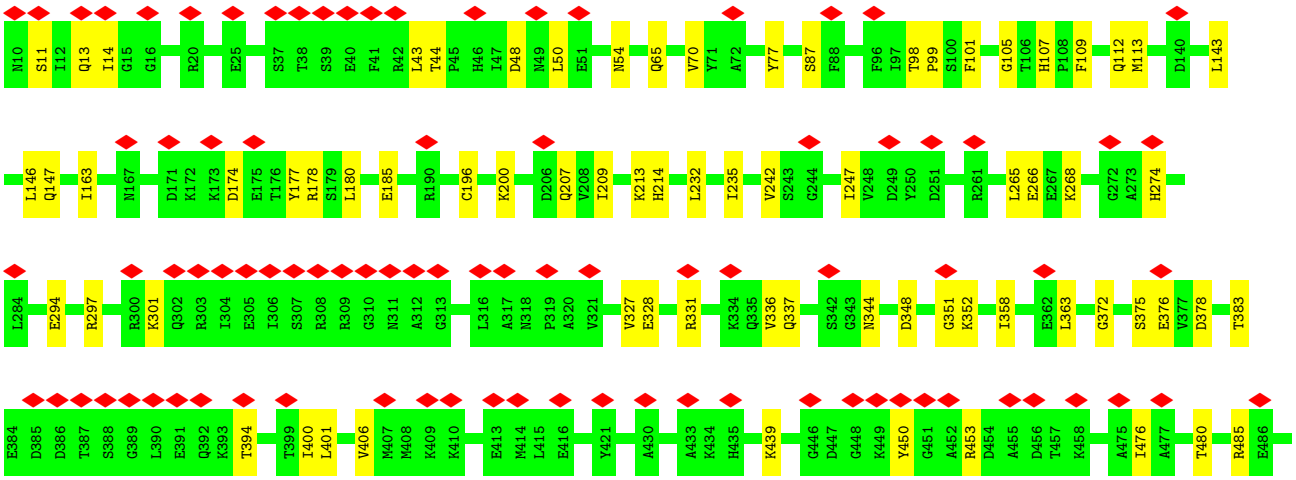
Chain C:

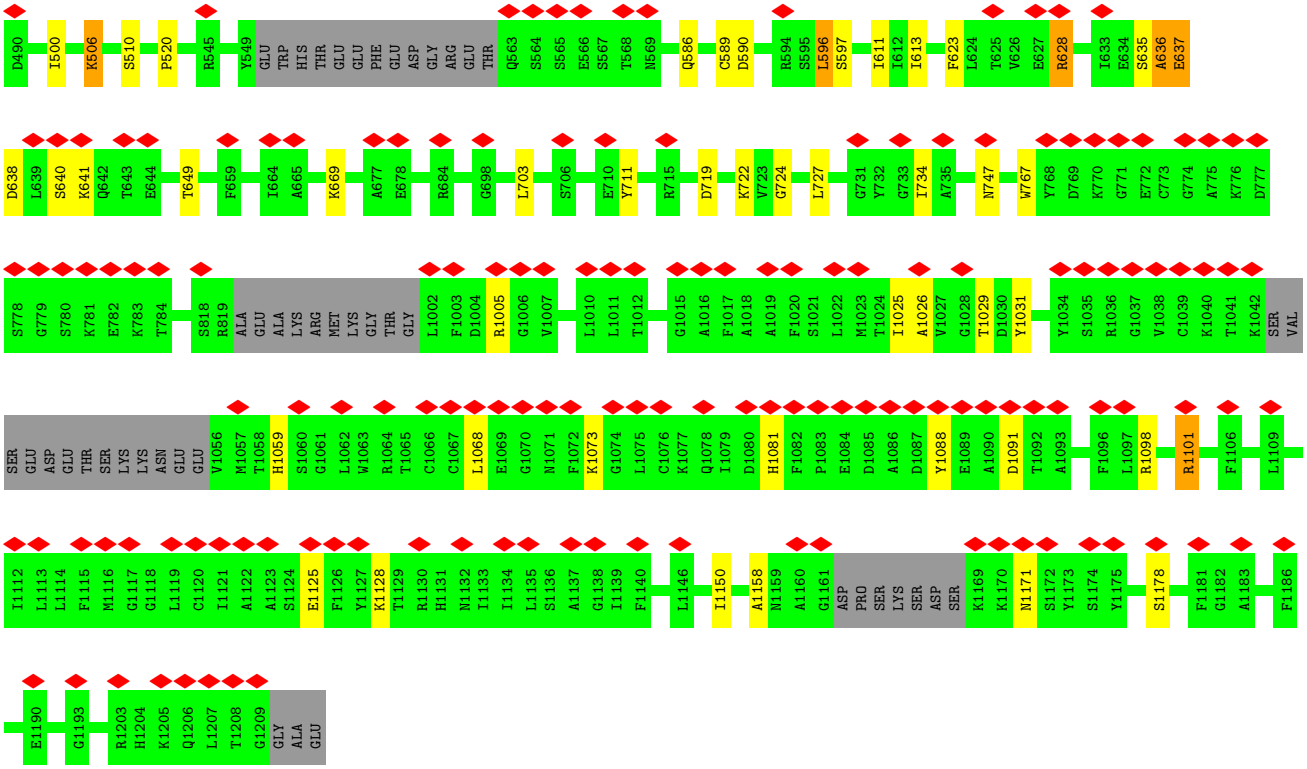




- Molecule 1: Glutamate receptor 2,Voltage-dependent calcium channel gamma-2 subunit

Chain D:




D490 I500 K506 S510 P520 R545 Y549 GLU TRP HIS THR GLU GLU PHE GLU ASP GLY ARG GLU THR Q563 S564 S565 E566 S567 T568 N569 Q586 C589 D590 R594 S595 L596 S597 I611 I612 I613 F623 L624 T625 V626 E627 R628 I633 E634 S635 A636 E637
D638 L639 S640 K641 Q642 T643 E644 T649 F659 I664 A665 K669 A677 E678 R684 G698 L703 S706 E710 Y711 R715 D719 K722 V723 G724 L727 G731 Y732 G733 I734 A735 N747 W767 Y768 D769 K770 G771 E772 C773 G774 A775 K776 D777
S778 G779 S780 K781 E782 K783 T784 S818 R819 ALA GLU ALA LYS ARG MET LYS GLY THR GLY L1002 F1003 D1004 R1005 G1006 V1007 L1010 L1011 T1012 G1015 A1016 F1017 A1018 A1019 F1020 S1021 L1022 M1023 T1024 I1025 A1026 V1027 G1028 T1029 D1030 Y1031 Y1034 S1035 R1036 G1037 V1038 C1039 K1040 T1041 K1042 SER VAL
SER GLU ASP GLU THR SER LYS LYS ASN GLU GLU V1056 M1057 T1058 H1059 S1060 G1061 L1062 W1063 R1064 T1065 C1066 C1067 L1068 E1069 G1070 N1071 F1072 K1073 G1074 L1075 C1076 K1077 Q1078 I1079 D1080 H1081 F1082 P1083 E1084 D1085 A1086 D1087 Y1088 E1089 A1090 D1091 T1092 A1093 F1096 L1097 R1098 R1101 F1106 L1109
I1112 L1113 L1114 F1115 M1116 G1117 G1118 L1119 C1120 I1121 A1122 A1123 S1124 E1125 F1126 Y1127 K1128 T1129 R1130 H1131 N1132 I1133 I1134 L1135 S1136 A1137 G1138 I1139 F1140 L1146 I1150 A1158 N1159 A1160 G1161 ASP PRO SER LYS SER ASP SER K1169 K1170 N1171 S1172 Y1173 S1174 Y1175 S1178 F1181 G1182 A1183 F1186
E1190 G1193 R1203 H1204 K1205 Q1206 L1207 T1208 G1209 GLY ALA GLU

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	30849	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 ($e^-/Å^2$)	55	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	0.141	Depositor
Minimum map value	-0.070	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	324.0, 324.0, 324.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	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: GZD, CYZ

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	0.38	0/7900	0.57	1/10670 (0.0%)
1	B	0.37	0/7901	0.55	1/10672 (0.0%)
1	C	0.38	0/7900	0.57	1/10670 (0.0%)
1	D	0.37	0/7901	0.55	1/10672 (0.0%)
All	All	0.38	0/31602	0.56	4/42684 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	2
1	C	0	3
1	D	0	2
All	All	0	10

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1207	LEU	CA-CB-CG	6.12	129.38	115.30
1	C	1207	LEU	CA-CB-CG	6.08	129.28	115.30
1	B	596	LEU	CA-CB-CG	5.37	127.64	115.30
1	D	596	LEU	CA-CB-CG	5.36	127.62	115.30

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1177	TRP	Peptide
1	A	313	GLY	Peptide
1	A	632	PRO	Peptide
1	B	1005	ARG	Peptide
1	B	635	SER	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	7734	0	7713	58	0
1	B	7735	0	7708	70	0
1	C	7734	0	7713	60	0
1	D	7735	0	7708	72	0
2	A	10	0	5	1	0
2	B	10	0	5	1	0
2	C	10	0	5	1	0
2	D	10	0	5	1	0
3	A	24	0	11	1	0
3	B	24	0	11	0	0
3	C	24	0	11	1	0
3	D	24	0	11	0	0
4	B	21	0	0	2	0
All	All	31095	0	30906	248	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

The worst 5 of 248 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:D:480:THR:HG1	2:D:1301:GLU:N	1.67	0.91
1:B:480:THR:HG1	2:B:1301:GLU:N	1.70	0.88
1:B:586:GLN:HE21	1:B:613:ILE:HD11	1.49	0.77
1:B:586:GLN:NE2	1:B:613:ILE:HD11	2.02	0.74
1:A:480:THR:HG1	2:A:1301:GLU:N	1.87	0.70

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	974/1031 (94%)	888 (91%)	81 (8%)	5 (0%)	29	68
1	B	975/1031 (95%)	889 (91%)	83 (8%)	3 (0%)	41	76
1	C	974/1031 (94%)	888 (91%)	81 (8%)	5 (0%)	29	68
1	D	975/1031 (95%)	890 (91%)	82 (8%)	3 (0%)	41	76
All	All	3898/4124 (94%)	3555 (91%)	327 (8%)	16 (0%)	38	72

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	633	ILE
1	A	1178	SER
1	B	1171	ASN
1	C	633	ILE
1	C	1178	SER

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	832/873 (95%)	822 (99%)	10 (1%)	71	84
1	B	831/873 (95%)	826 (99%)	5 (1%)	86	92
1	C	832/873 (95%)	822 (99%)	10 (1%)	71	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	831/873 (95%)	826 (99%)	5 (1%)	86	92
All	All	3326/3492 (95%)	3296 (99%)	30 (1%)	79	88

5 of 30 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1101	ARG
1	D	628	ARG
1	C	309	ARG
1	D	1101	ARG
1	C	1203	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	586	GLN
1	D	791	ASN
1	B	747	ASN
1	B	791	ASN
1	C	147	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)

9 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	CYZ	B	1302	-	26,27,27	7.10	19 (73%)	38,44,44	4.58	20 (52%)
4	GZD	B	1303	-	23,23,23	0.92	0	34,34,34	1.98	7 (20%)
2	GLU	B	1301	-	8,9,9	1.12	1 (12%)	10,11,11	1.24	1 (10%)
3	CYZ	A	1302	-	26,27,27	7.08	20 (76%)	38,44,44	4.53	18 (47%)
2	GLU	A	1301	-	8,9,9	1.09	1 (12%)	10,11,11	1.33	2 (20%)
3	CYZ	D	1302	-	26,27,27	7.09	19 (73%)	38,44,44	4.58	20 (52%)
3	CYZ	C	1302	-	26,27,27	7.07	20 (76%)	38,44,44	4.53	18 (47%)
2	GLU	D	1301	-	8,9,9	1.13	1 (12%)	10,11,11	1.25	1 (10%)
2	GLU	C	1301	-	8,9,9	1.09	1 (12%)	10,11,11	1.34	2 (20%)

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	CYZ	B	1302	-	-	0/6/42/42	0/5/4/4
4	GZD	B	1303	-	-	7/12/39/39	0/4/3/3
2	GLU	B	1301	-	-	1/9/9/9	-
3	CYZ	A	1302	-	-	0/6/42/42	0/5/4/4
2	GLU	A	1301	-	-	0/9/9/9	-
3	CYZ	D	1302	-	-	0/6/42/42	0/5/4/4
3	CYZ	C	1302	-	-	0/6/42/42	0/5/4/4
2	GLU	D	1301	-	-	1/9/9/9	-
2	GLU	C	1301	-	-	0/9/9/9	-

The worst 5 of 82 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1302	CYZ	C2-C1	-19.42	1.13	1.55
3	D	1302	CYZ	C2-C1	-19.40	1.13	1.55
3	C	1302	CYZ	C2-C1	-19.40	1.13	1.55
3	A	1302	CYZ	C2-C1	-19.38	1.13	1.55
3	B	1302	CYZ	C9-S1	-14.21	1.63	1.75

The worst 5 of 89 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1302	CYZ	C1-C2-C3	18.83	137.39	106.92
3	D	1302	CYZ	C1-C2-C3	18.81	137.36	106.92
3	B	1302	CYZ	C1-C2-C3	18.80	137.34	106.92
3	C	1302	CYZ	C1-C2-C3	18.80	137.34	106.92
3	B	1302	CYZ	O4-S2-O3	-10.74	101.10	118.76

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1303	GZD	N2-C5-C6-C7
4	B	1303	GZD	C8-C9-N10-C11
4	B	1303	GZD	C6-C7-C8-C9
4	B	1303	GZD	C5-C6-C7-C8
4	B	1303	GZD	C7-C8-C9-N10

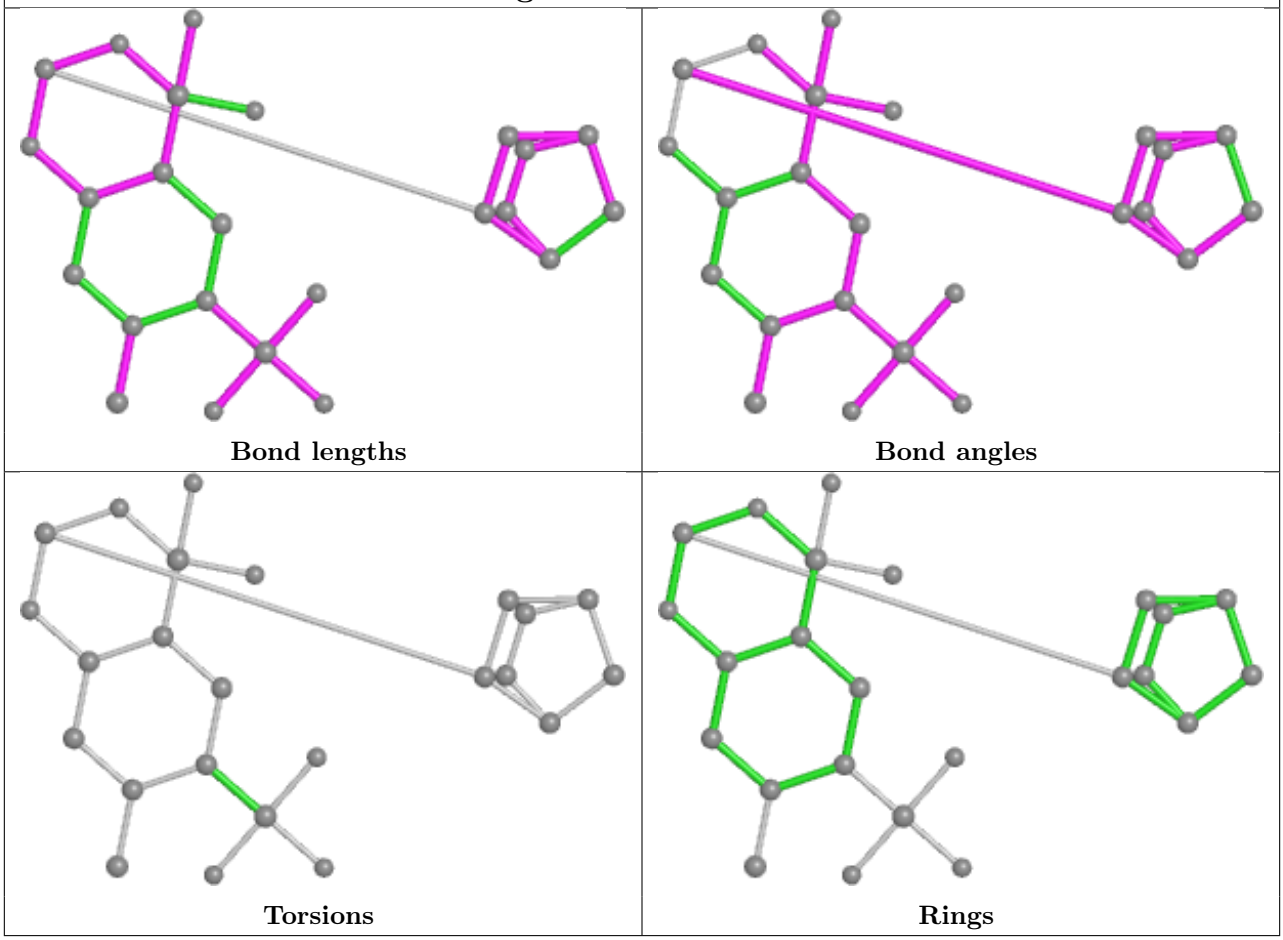
There are no ring outliers.

7 monomers are involved in 8 short contacts:

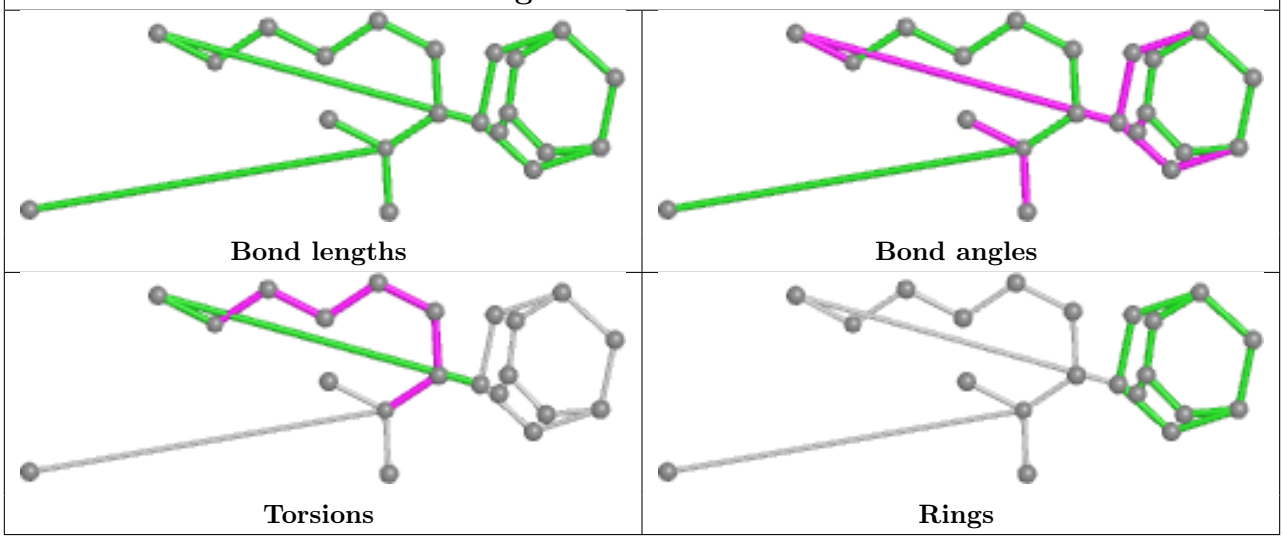
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1303	GZD	2	0
2	B	1301	GLU	1	0
3	A	1302	CYZ	1	0
2	A	1301	GLU	1	0
3	C	1302	CYZ	1	0
2	D	1301	GLU	1	0
2	C	1301	GLU	1	0

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.

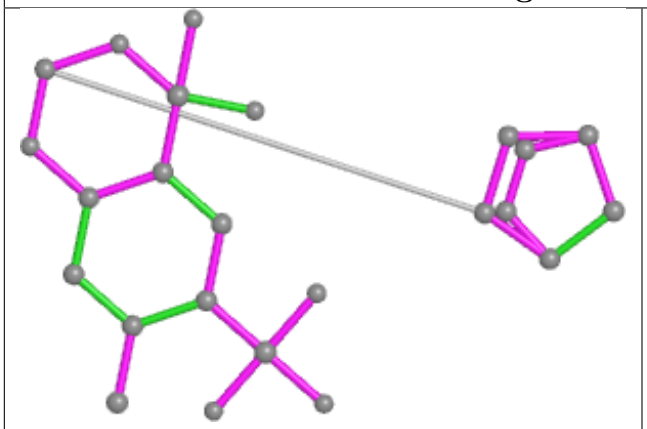
Ligand CYZ B 1302



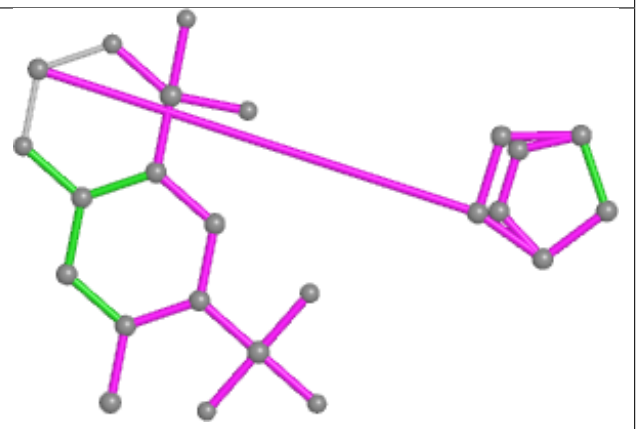
Ligand GZD B 1303



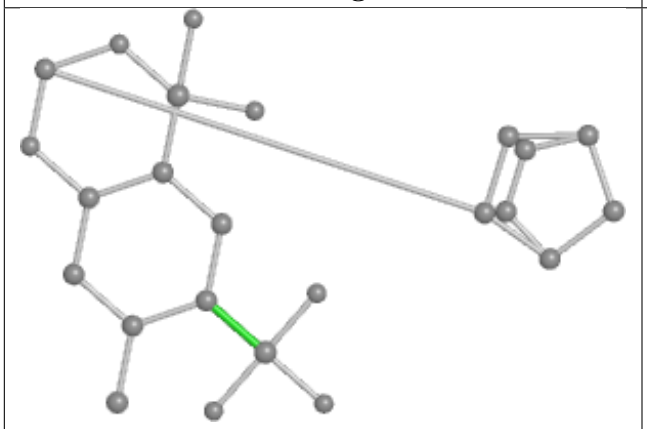
Ligand CYZ A 1302



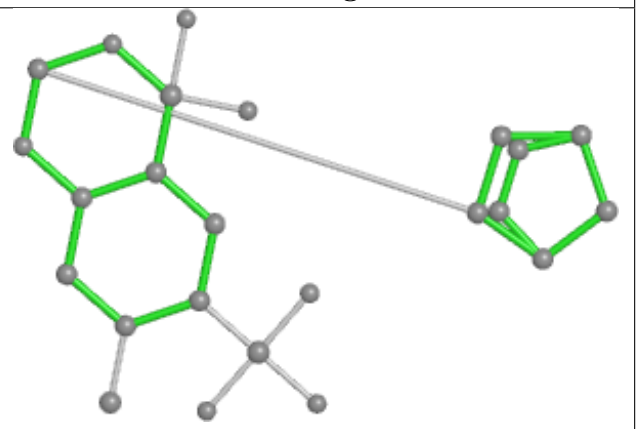
Bond lengths



Bond angles

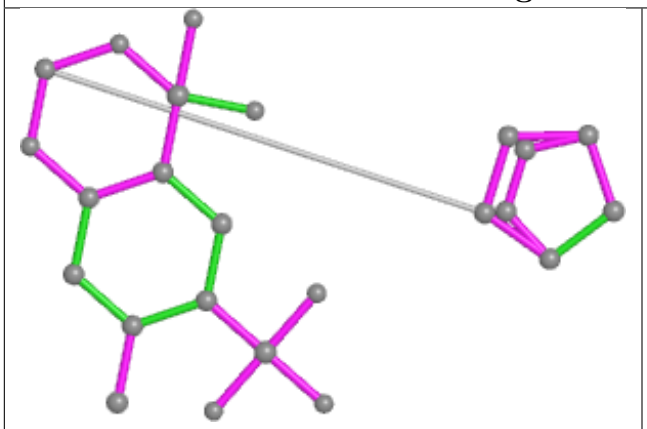


Torsions

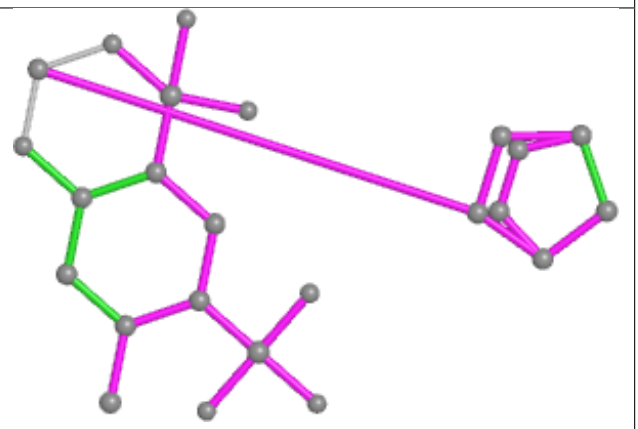


Rings

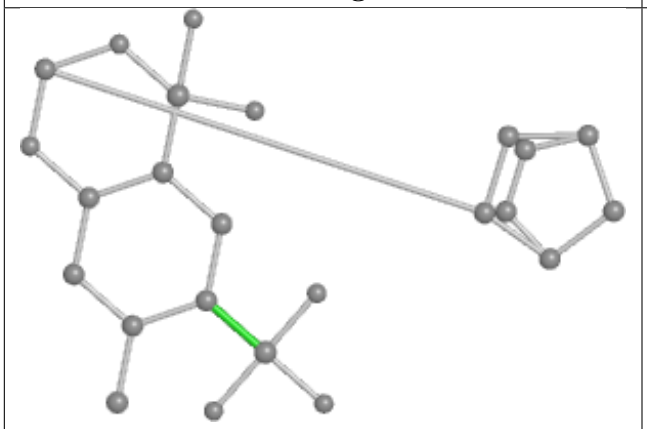
Ligand CYZ D 1302



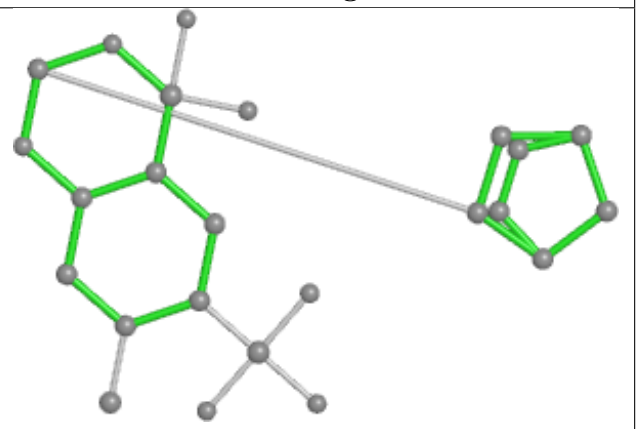
Bond lengths



Bond angles

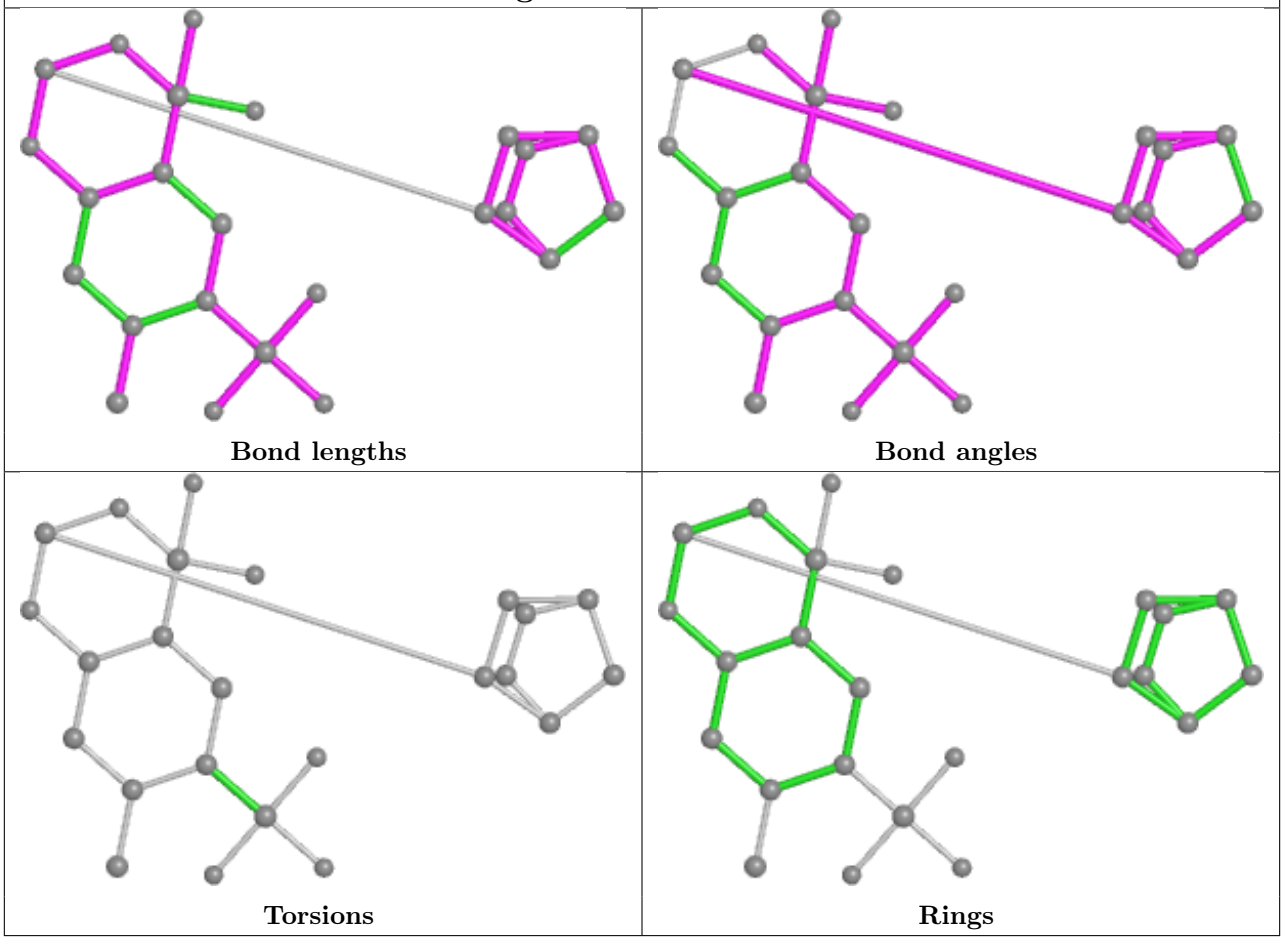


Torsions



Rings

Ligand CYZ C 1302



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.

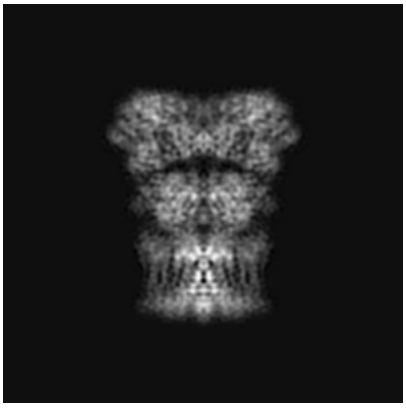
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-7960. These allow visual inspection of the internal detail of the map and identification of artifacts.

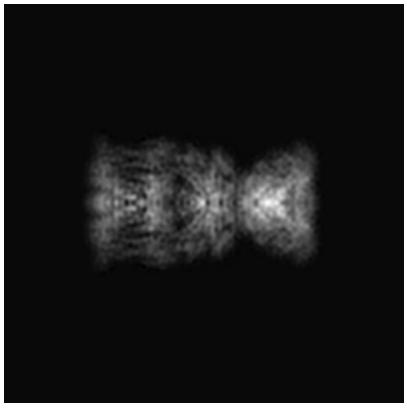
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

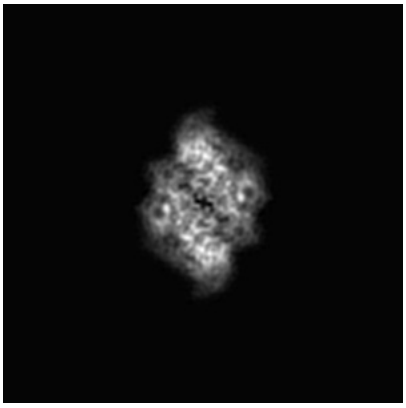
6.1.1 Primary map



X



Y



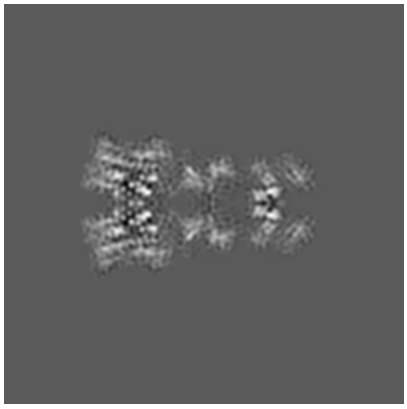
Z

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

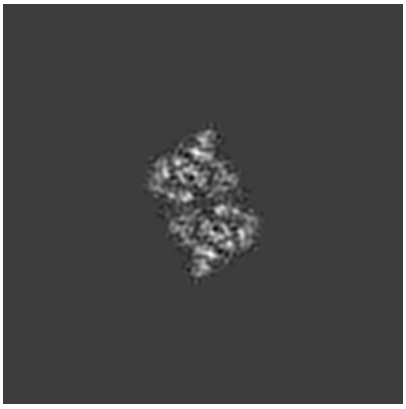
6.2 Central slices (i)

6.2.1 Primary map

X Index: 150



Y Index: 150



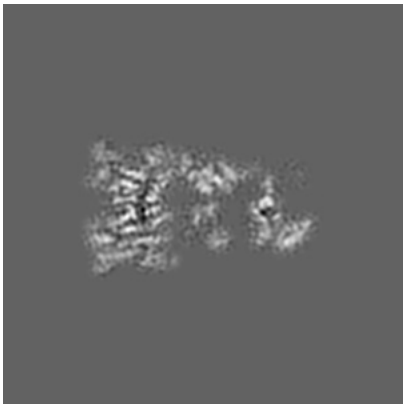
Z Index: 150

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

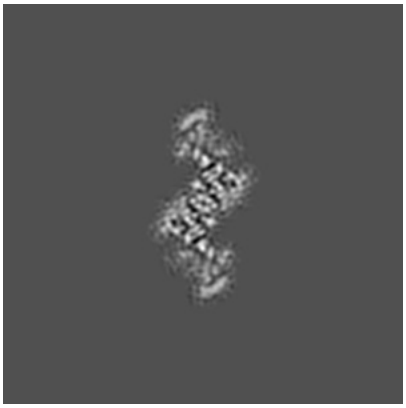
6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 154



Y Index: 145

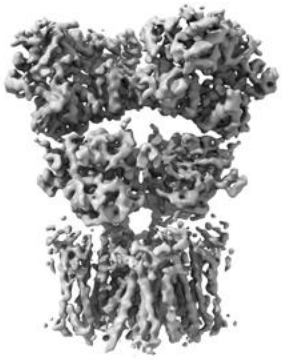


Z Index: 196

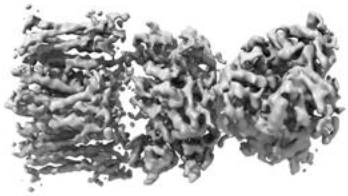
The images above show the largest variance slices of the map in three orthogonal directions.

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

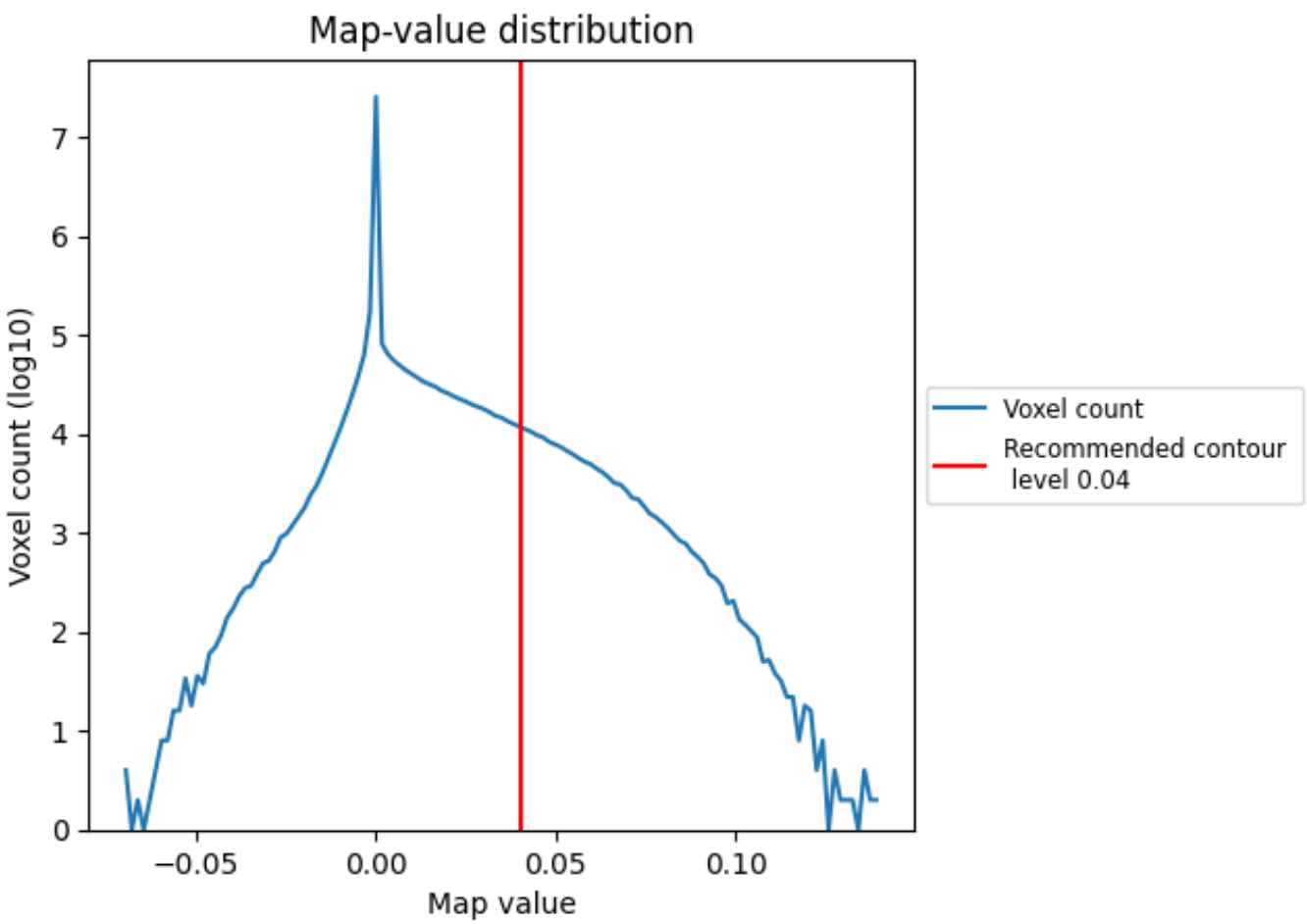
6.5 Mask visualisation (i)

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

7 Map analysis (i)

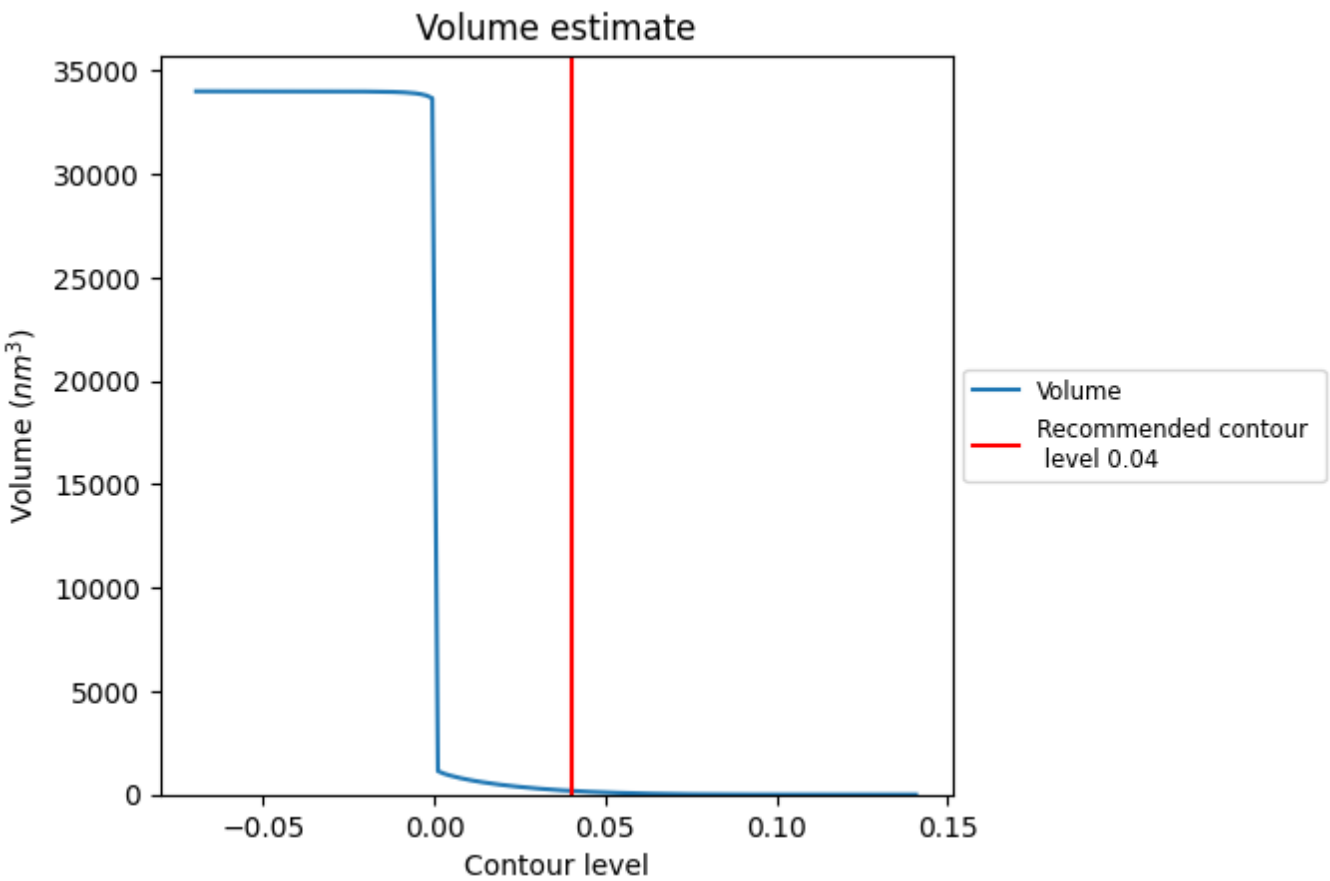
This section contains the results of statistical analysis of the map.

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.

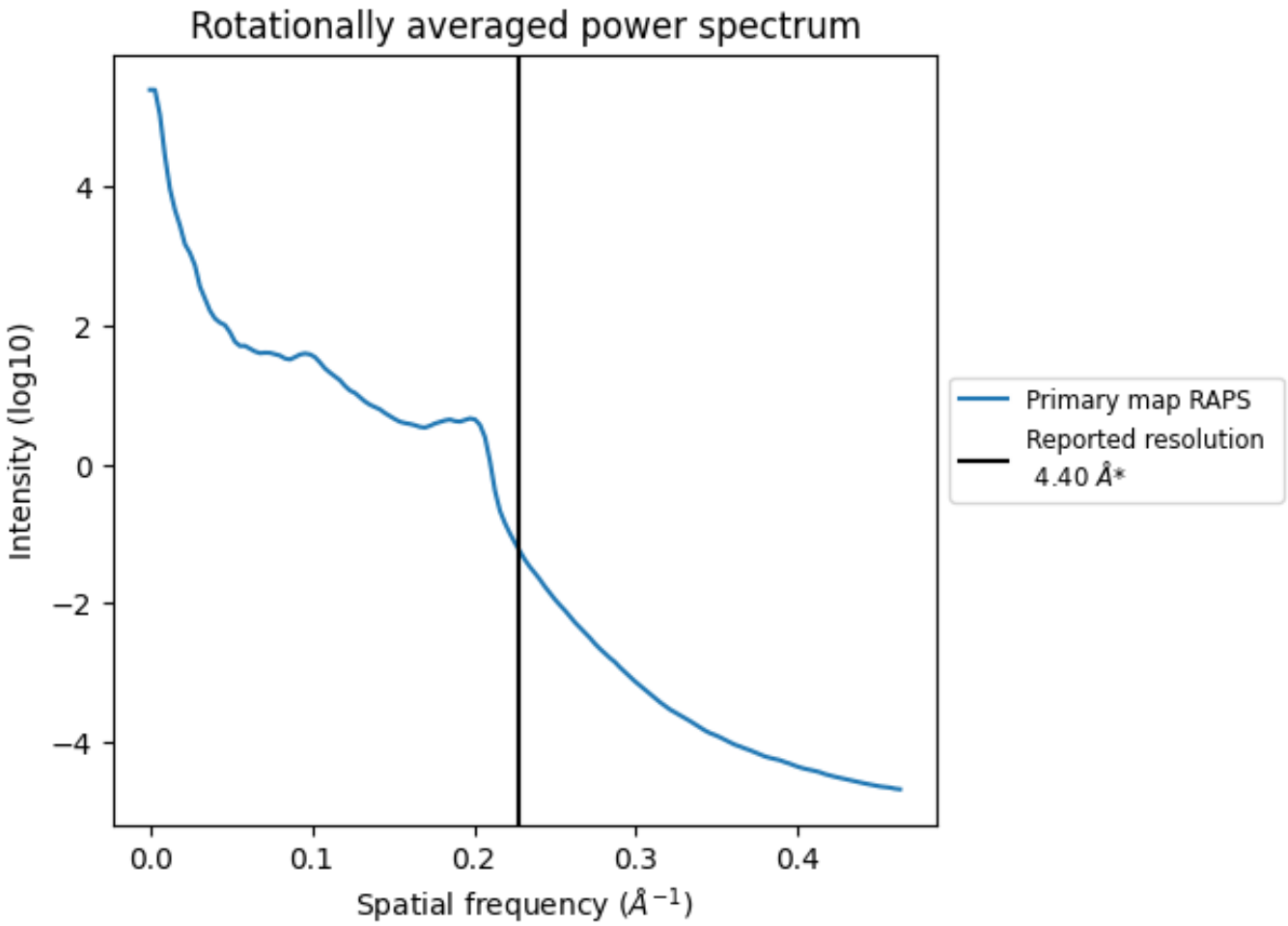
7.2 Volume estimate (i)



The volume at the recommended contour level is 180 nm^3; this corresponds to an approximate mass of 163 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 0.227 Å^{-1}

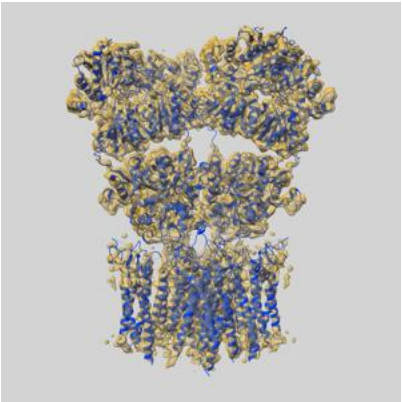
8 Fourier-Shell correlation (i)

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

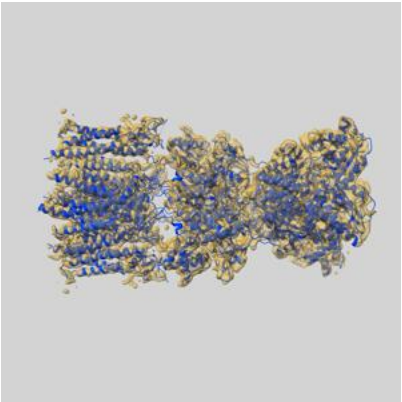
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-7960 and PDB model 6DM0. Per-residue inclusion information can be found in section 3 on page 8.

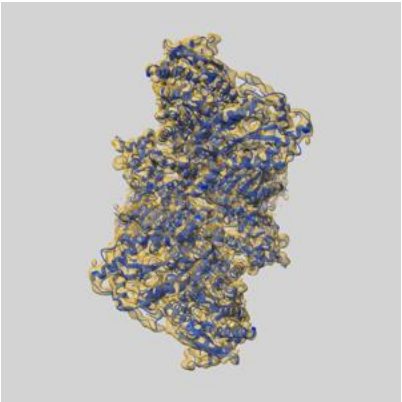
9.1 Map-model overlay (i)



X



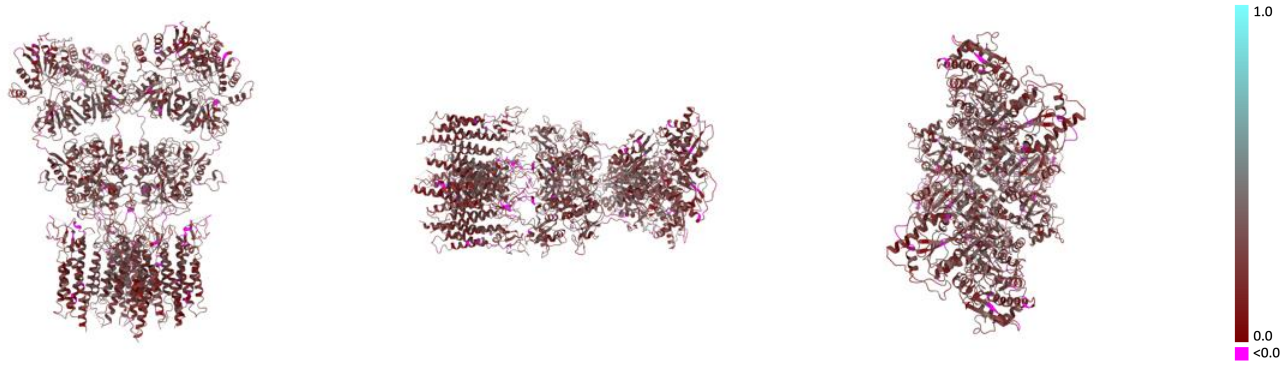
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.04 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.

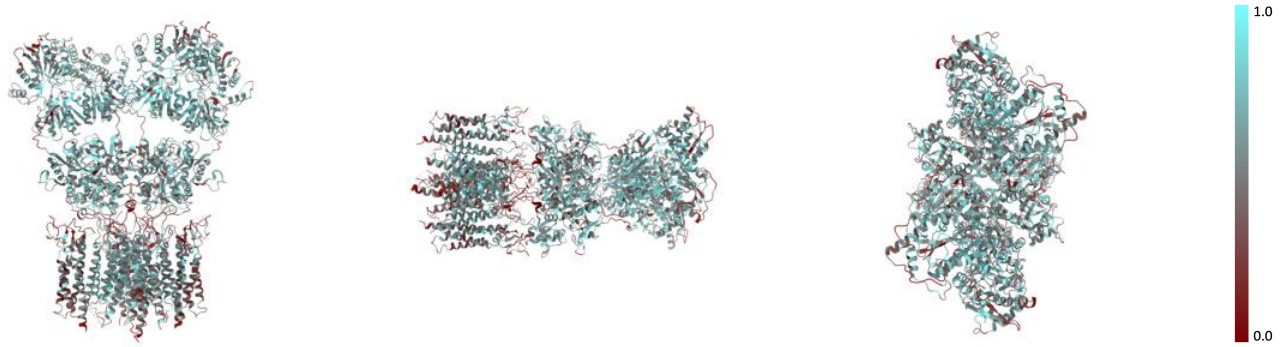
9.2 Q-score mapped to coordinate model (i)



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.

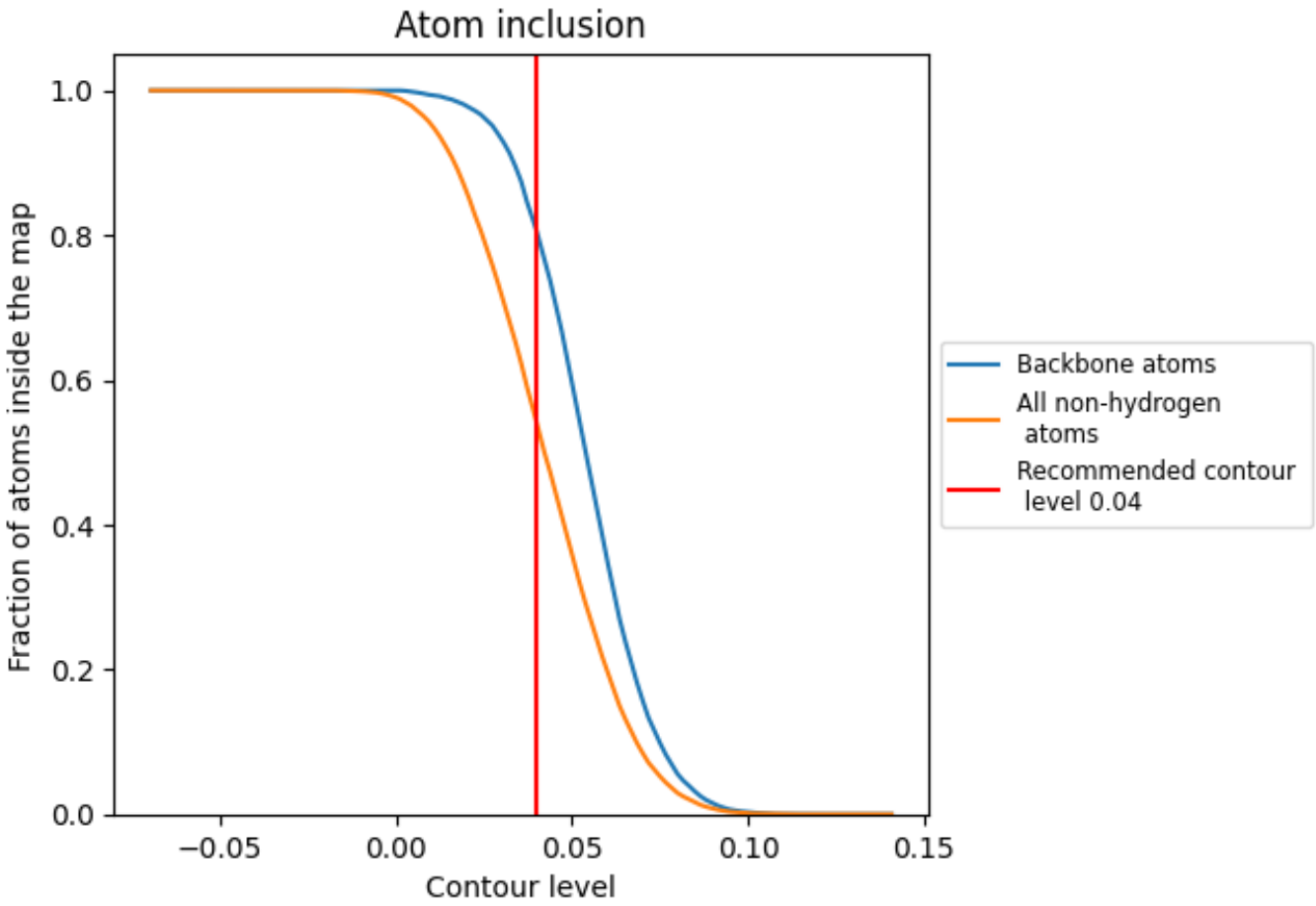
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.04).

9.4 Atom inclusion (i)



At the recommended contour level, 81% of all backbone atoms, 54% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5405	0.2680
A	0.5392	0.2690
B	0.5405	0.2660
C	0.5410	0.2690
D	0.5414	0.2660