



wwPDB EM Validation Summary Report ⓘ

Nov 10, 2024 – 06:15 PM EST

PDB ID : 7TNP
EMDB ID : EMD-26017
Title : Complex GGGG of AMPA-subtype iGluR GluA2 in complex with auxiliary subunit gamma2 (Stargazin) at low glutamate concentration (20 uM) in the presence of cyclothiazide (100 uM)
Authors : Yelshanskaya, M.V.; Sobolevsky, A.I.
Deposited on : 2022-01-21
Resolution : 3.96 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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

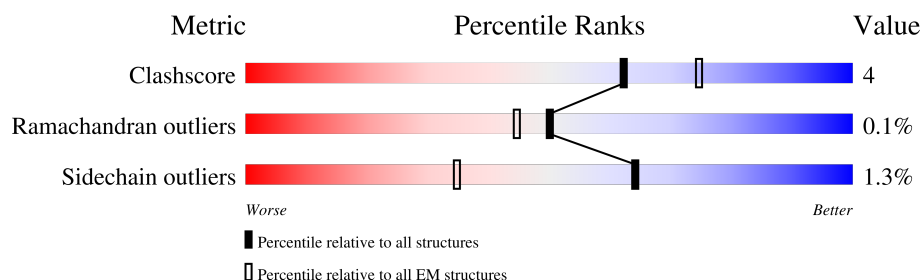
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.96 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	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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1033	<div> <div>12%</div> <div>51%</div> <div>7%</div> <div>42%</div> </div>
1	B	1033	<div> <div>13%</div> <div>52%</div> <div>6%</div> <div>42%</div> </div>
1	C	1033	<div> <div>12%</div> <div>52%</div> <div>6%</div> <div>42%</div> </div>
1	D	1033	<div> <div>12%</div> <div>53%</div> <div>5%</div> <div>42%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 18840 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 Isoform Flip of Glutamate receptor 2, Voltage-dependent calcium channel gamma-3 subunit chimera.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	601	Total	C	N	O	S	0	0
			4673	3033	757	851	32		
1	B	601	Total	C	N	O	S	0	0
			4679	3038	758	851	32		
1	C	601	Total	C	N	O	S	0	0
			4673	3033	757	851	32		
1	D	601	Total	C	N	O	S	0	0
			4679	3038	758	851	32		

There are 228 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	1001	GLY	-	linker	UNP P19491
A	1002	LEU	-	linker	UNP P19491
A	1003	PHE	-	linker	UNP P19491
A	1007	VAL	ILE	conflict	UNP Q8VHX0
A	1011	LEU	ILE	conflict	UNP Q8VHX0
A	1040	LYS	ARG	conflict	UNP Q8VHX0
A	1044	VAL	THR	conflict	UNP Q8VHX0
A	1046	GLU	ASP	conflict	UNP Q8VHX0

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1047	ASP	ASN	conflict	UNP Q8VHX0
A	1051	LYS	ARG	conflict	UNP Q8VHX0
A	1071	ASN	ALA	conflict	UNP Q8VHX0
A	1073	LYS	ARG	conflict	UNP Q8VHX0
A	1075	LEU	VAL	conflict	UNP Q8VHX0
A	1078	GLN	LYS	conflict	UNP Q8VHX0
A	1090	ALA	GLN	conflict	UNP Q8VHX0
A	1096	PHE	LEU	conflict	UNP Q8VHX0
A	1105	ILE	VAL	conflict	UNP Q8VHX0
A	1112	ILE	THR	conflict	UNP Q8VHX0
A	1116	MET	PHE	conflict	UNP Q8VHX0
A	1121	ILE	VAL	conflict	UNP Q8VHX0
A	1127	TYR	HIS	conflict	UNP Q8VHX0
A	1128	LYS	ARG	conflict	UNP Q8VHX0
A	1129	THR	SER	conflict	UNP Q8VHX0
A	1132	ASN	SER	conflict	UNP Q8VHX0
A	1133	ILE	VAL	conflict	UNP Q8VHX0
A	1164	SER	GLY	conflict	UNP Q8VHX0
A	1165	LYS	GLN	conflict	UNP Q8VHX0
A	1166	SER	ARG	conflict	UNP Q8VHX0
A	1171	ASN	-	insertion	UNP Q8VHX0
A	1184	LEU	PHE	conflict	UNP Q8VHX0
A	1191	MET	ILE	conflict	UNP Q8VHX0
A	1195	LEU	VAL	conflict	UNP Q8VHX0
A	1199	MET	ILE	conflict	UNP Q8VHX0
A	1200	PHE	TYR	conflict	UNP Q8VHX0
A	1202	ASP	GLU	conflict	UNP Q8VHX0
A	1203	ARG	LYS	conflict	UNP Q8VHX0
A	1205	LYS	GLN	conflict	UNP Q8VHX0
A	1208	THR	-	expression tag	UNP Q8VHX0
A	1209	GLY	-	expression tag	UNP Q8VHX0
A	1210	GLY	-	expression tag	UNP Q8VHX0
A	1211	LEU	-	expression tag	UNP Q8VHX0
A	1212	VAL	-	expression tag	UNP Q8VHX0
A	1213	PRO	-	expression tag	UNP Q8VHX0
A	1214	ARG	-	expression tag	UNP Q8VHX0
B	241	GLU	ASN	conflict	UNP P19491
B	382	LEU	VAL	conflict	UNP P19491
B	?	-	LEU	deletion	UNP P19491
B	?	-	THR	deletion	UNP P19491
B	?	-	GLU	deletion	UNP P19491
B	?	-	LEU	deletion	UNP P19491

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Chain	Residue	Modelled	Actual	Comment	Reference
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	1001	GLY	-	linker	UNP P19491
B	1002	LEU	-	linker	UNP P19491
B	1003	PHE	-	linker	UNP P19491
B	1007	VAL	ILE	conflict	UNP Q8VHX0
B	1011	LEU	ILE	conflict	UNP Q8VHX0
B	1040	LYS	ARG	conflict	UNP Q8VHX0
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B	1047	ASP	ASN	conflict	UNP Q8VHX0
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B	1075	LEU	VAL	conflict	UNP Q8VHX0
B	1078	GLN	LYS	conflict	UNP Q8VHX0
B	1090	ALA	GLN	conflict	UNP Q8VHX0
B	1096	PHE	LEU	conflict	UNP Q8VHX0
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B	1129	THR	SER	conflict	UNP Q8VHX0
B	1132	ASN	SER	conflict	UNP Q8VHX0
B	1133	ILE	VAL	conflict	UNP Q8VHX0
B	1164	SER	GLY	conflict	UNP Q8VHX0
B	1165	LYS	GLN	conflict	UNP Q8VHX0
B	1166	SER	ARG	conflict	UNP Q8VHX0
B	1171	ASN	-	insertion	UNP Q8VHX0
B	1184	LEU	PHE	conflict	UNP Q8VHX0
B	1191	MET	ILE	conflict	UNP Q8VHX0
B	1195	LEU	VAL	conflict	UNP Q8VHX0
B	1199	MET	ILE	conflict	UNP Q8VHX0
B	1200	PHE	TYR	conflict	UNP Q8VHX0
B	1202	ASP	GLU	conflict	UNP Q8VHX0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1203	ARG	LYS	conflict	UNP Q8VHX0
B	1205	LYS	GLN	conflict	UNP Q8VHX0
B	1208	THR	-	expression tag	UNP Q8VHX0
B	1209	GLY	-	expression tag	UNP Q8VHX0
B	1210	GLY	-	expression tag	UNP Q8VHX0
B	1211	LEU	-	expression tag	UNP Q8VHX0
B	1212	VAL	-	expression tag	UNP Q8VHX0
B	1213	PRO	-	expression tag	UNP Q8VHX0
B	1214	ARG	-	expression tag	UNP Q8VHX0
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	1001	GLY	-	linker	UNP P19491
C	1002	LEU	-	linker	UNP P19491
C	1003	PHE	-	linker	UNP P19491
C	1007	VAL	ILE	conflict	UNP Q8VHX0
C	1011	LEU	ILE	conflict	UNP Q8VHX0
C	1040	LYS	ARG	conflict	UNP Q8VHX0
C	1044	VAL	THR	conflict	UNP Q8VHX0
C	1046	GLU	ASP	conflict	UNP Q8VHX0
C	1047	ASP	ASN	conflict	UNP Q8VHX0
C	1051	LYS	ARG	conflict	UNP Q8VHX0
C	1071	ASN	ALA	conflict	UNP Q8VHX0
C	1073	LYS	ARG	conflict	UNP Q8VHX0
C	1075	LEU	VAL	conflict	UNP Q8VHX0
C	1078	GLN	LYS	conflict	UNP Q8VHX0
C	1090	ALA	GLN	conflict	UNP Q8VHX0
C	1096	PHE	LEU	conflict	UNP Q8VHX0
C	1105	ILE	VAL	conflict	UNP Q8VHX0
C	1112	ILE	THR	conflict	UNP Q8VHX0
C	1116	MET	PHE	conflict	UNP Q8VHX0
C	1121	ILE	VAL	conflict	UNP Q8VHX0

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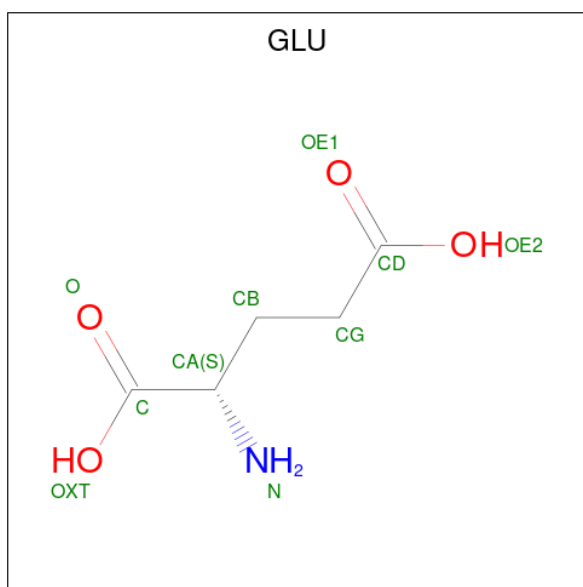
Chain	Residue	Modelled	Actual	Comment	Reference
C	1127	TYR	HIS	conflict	UNP Q8VHX0
C	1128	LYS	ARG	conflict	UNP Q8VHX0
C	1129	THR	SER	conflict	UNP Q8VHX0
C	1132	ASN	SER	conflict	UNP Q8VHX0
C	1133	ILE	VAL	conflict	UNP Q8VHX0
C	1164	SER	GLY	conflict	UNP Q8VHX0
C	1165	LYS	GLN	conflict	UNP Q8VHX0
C	1166	SER	ARG	conflict	UNP Q8VHX0
C	1171	ASN	-	insertion	UNP Q8VHX0
C	1184	LEU	PHE	conflict	UNP Q8VHX0
C	1191	MET	ILE	conflict	UNP Q8VHX0
C	1195	LEU	VAL	conflict	UNP Q8VHX0
C	1199	MET	ILE	conflict	UNP Q8VHX0
C	1200	PHE	TYR	conflict	UNP Q8VHX0
C	1202	ASP	GLU	conflict	UNP Q8VHX0
C	1203	ARG	LYS	conflict	UNP Q8VHX0
C	1205	LYS	GLN	conflict	UNP Q8VHX0
C	1208	THR	-	expression tag	UNP Q8VHX0
C	1209	GLY	-	expression tag	UNP Q8VHX0
C	1210	GLY	-	expression tag	UNP Q8VHX0
C	1211	LEU	-	expression tag	UNP Q8VHX0
C	1212	VAL	-	expression tag	UNP Q8VHX0
C	1213	PRO	-	expression tag	UNP Q8VHX0
C	1214	ARG	-	expression tag	UNP Q8VHX0
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	999	GLY	-	linker	UNP P19491
D	1000	THR	-	linker	UNP P19491
D	1001	GLY	-	linker	UNP P19491
D	1002	LEU	-	linker	UNP P19491
D	1003	PHE	-	linker	UNP P19491
D	1007	VAL	ILE	conflict	UNP Q8VHX0
D	1011	LEU	ILE	conflict	UNP Q8VHX0

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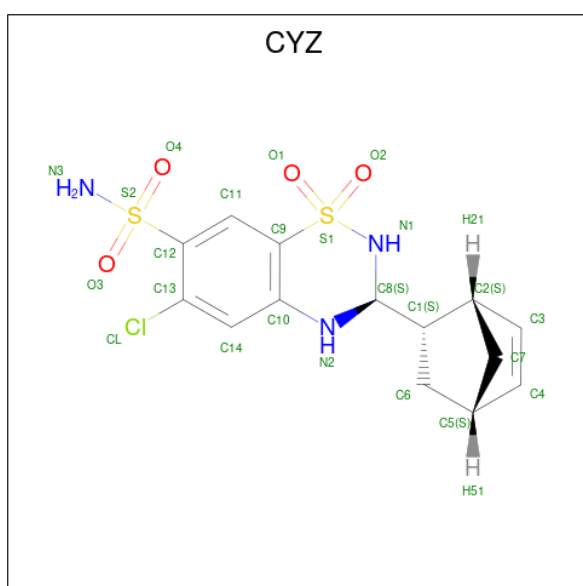
Chain	Residue	Modelled	Actual	Comment	Reference
D	1040	LYS	ARG	conflict	UNP Q8VHX0
D	1044	VAL	THR	conflict	UNP Q8VHX0
D	1046	GLU	ASP	conflict	UNP Q8VHX0
D	1047	ASP	ASN	conflict	UNP Q8VHX0
D	1051	LYS	ARG	conflict	UNP Q8VHX0
D	1071	ASN	ALA	conflict	UNP Q8VHX0
D	1073	LYS	ARG	conflict	UNP Q8VHX0
D	1075	LEU	VAL	conflict	UNP Q8VHX0
D	1078	GLN	LYS	conflict	UNP Q8VHX0
D	1090	ALA	GLN	conflict	UNP Q8VHX0
D	1096	PHE	LEU	conflict	UNP Q8VHX0
D	1105	ILE	VAL	conflict	UNP Q8VHX0
D	1112	ILE	THR	conflict	UNP Q8VHX0
D	1116	MET	PHE	conflict	UNP Q8VHX0
D	1121	ILE	VAL	conflict	UNP Q8VHX0
D	1127	TYR	HIS	conflict	UNP Q8VHX0
D	1128	LYS	ARG	conflict	UNP Q8VHX0
D	1129	THR	SER	conflict	UNP Q8VHX0
D	1132	ASN	SER	conflict	UNP Q8VHX0
D	1133	ILE	VAL	conflict	UNP Q8VHX0
D	1164	SER	GLY	conflict	UNP Q8VHX0
D	1165	LYS	GLN	conflict	UNP Q8VHX0
D	1166	SER	ARG	conflict	UNP Q8VHX0
D	1171	ASN	-	insertion	UNP Q8VHX0
D	1184	LEU	PHE	conflict	UNP Q8VHX0
D	1191	MET	ILE	conflict	UNP Q8VHX0
D	1195	LEU	VAL	conflict	UNP Q8VHX0
D	1199	MET	ILE	conflict	UNP Q8VHX0
D	1200	PHE	TYR	conflict	UNP Q8VHX0
D	1202	ASP	GLU	conflict	UNP Q8VHX0
D	1203	ARG	LYS	conflict	UNP Q8VHX0
D	1205	LYS	GLN	conflict	UNP Q8VHX0
D	1208	THR	-	expression tag	UNP Q8VHX0
D	1209	GLY	-	expression tag	UNP Q8VHX0
D	1210	GLY	-	expression tag	UNP Q8VHX0
D	1211	LEU	-	expression tag	UNP Q8VHX0
D	1212	VAL	-	expression tag	UNP Q8VHX0
D	1213	PRO	-	expression tag	UNP Q8VHX0
D	1214	ARG	-	expression tag	UNP Q8VHX0

- Molecule 2 is GLUTAMIC ACID (three-letter code: GLU) (formula: C₅H₉NO₄) (labeled as "Ligand of Interest" by depositor).



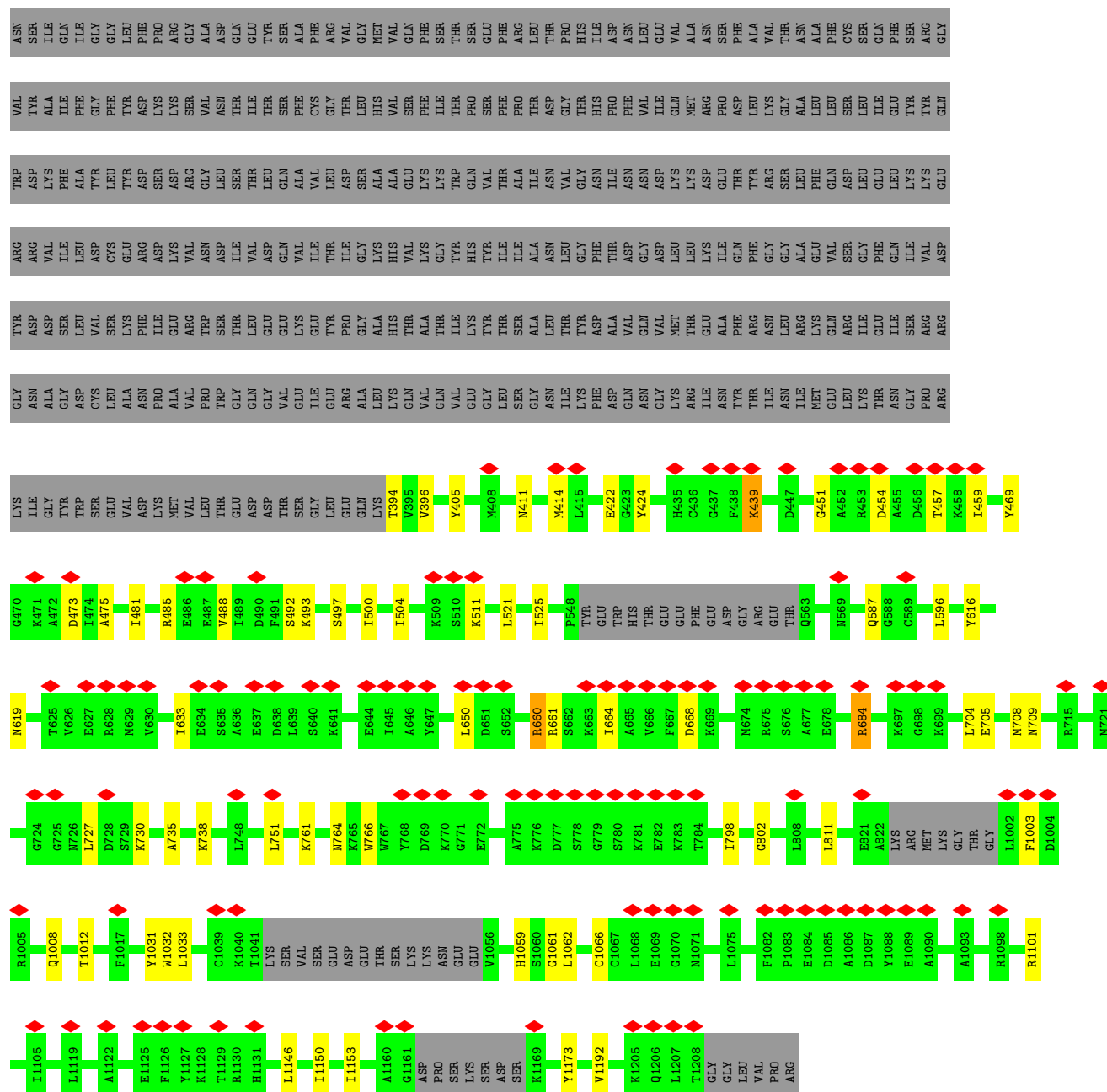
Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	N	O	0
			10	5	1	4	
2	B	1	Total	C	N	O	0
			10	5	1	4	
2	C	1	Total	C	N	O	0
			10	5	1	4	
2	D	1	Total	C	N	O	0
			10	5	1	4	

- Molecule 3 is CYCLOTHIAZIDE (three-letter code: CYZ) (formula: $C_{14}H_{16}ClN_3O_4S_2$) (labeled as "Ligand of Interest" by depositor).

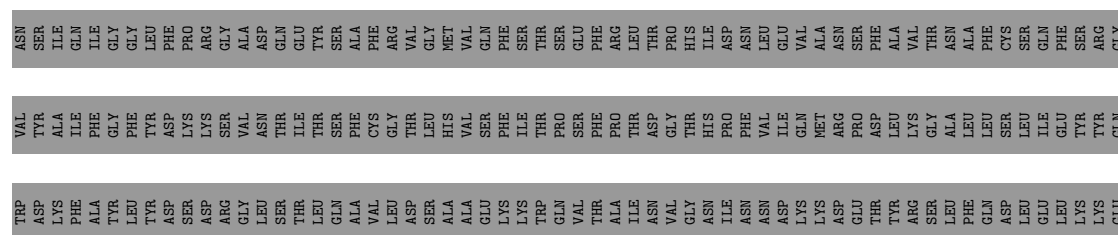


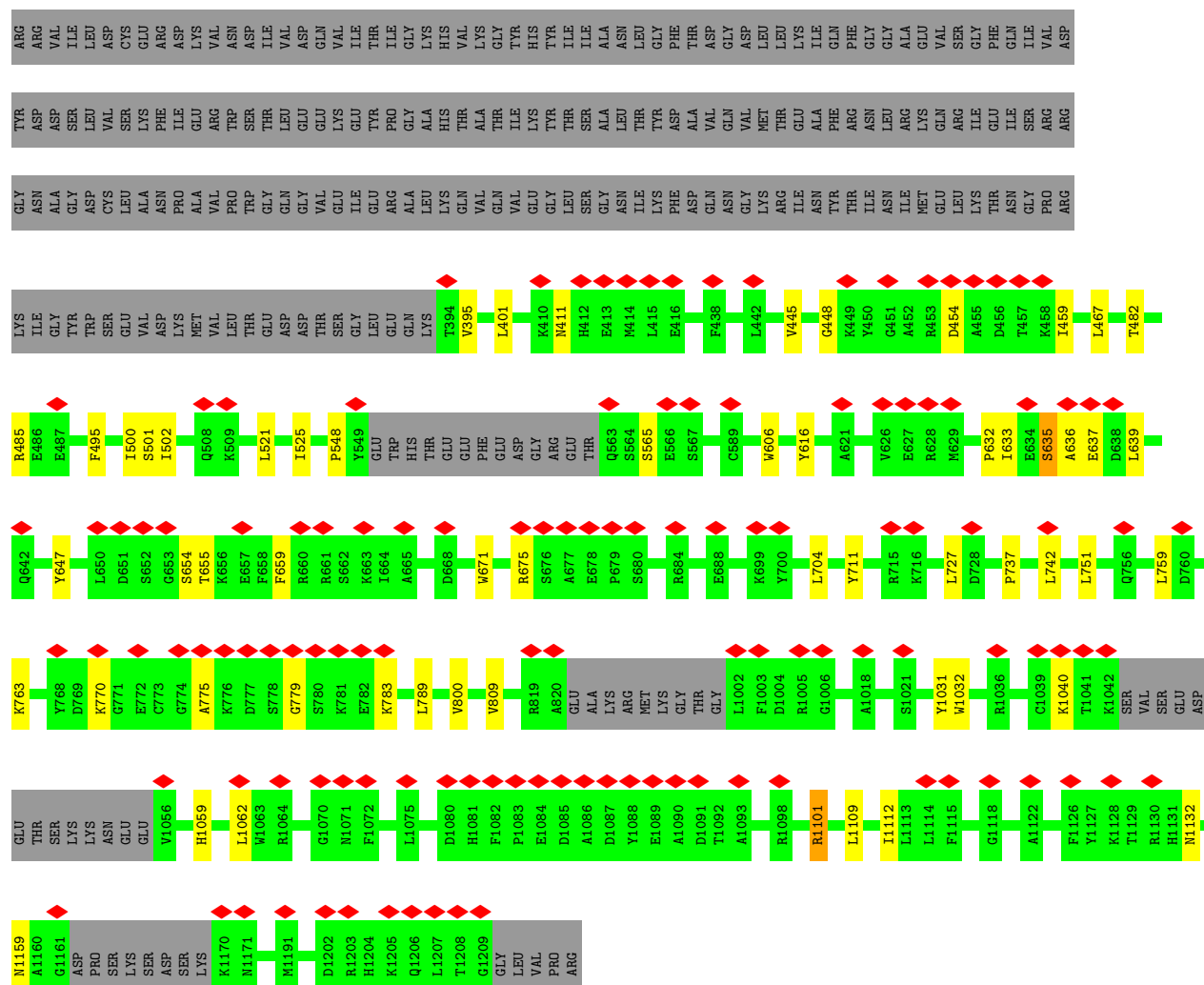
Mol	Chain	Residues	Atoms						AltConf
3	A	1	Total 24	C 14	Cl 1	N 3	O 4	S 2	0
3	B	1	Total 24	C 14	Cl 1	N 3	O 4	S 2	0
3	C	1	Total 24	C 14	Cl 1	N 3	O 4	S 2	0
3	D	1	Total 24	C 14	Cl 1	N 3	O 4	S 2	0





- Molecule 1: Isoform Flip of Glutamate receptor 2, Voltage-dependent calcium channel gamma-3 subunit chimera





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	53197	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	58.5	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.073	Depositor
Minimum map value	-0.039	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.015	Depositor
Map size (\AA)	265.6, 265.6, 265.6	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.83000004, 0.83000004, 0.83000004	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.44	0/4775	0.59	0/6445
1	B	0.42	0/4782	0.59	1/6454 (0.0%)
1	C	0.44	0/4775	0.59	0/6445
1	D	0.42	0/4782	0.59	1/6454 (0.0%)
All	All	0.43	0/19114	0.59	2/25798 (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	B	0	1
1	D	0	1
All	All	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	401	LEU	CA-CB-CG	5.63	128.25	115.30
1	B	401	LEU	CA-CB-CG	5.62	128.23	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	635	SER	Peptide
1	D	635	SER	Peptide

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	4673	0	4699	46	0
1	B	4679	0	4706	41	0
1	C	4673	0	4699	41	0
1	D	4679	0	4706	35	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	16	2	0
3	B	24	0	16	5	0
3	C	24	0	16	3	0
3	D	24	0	16	4	0
All	All	18840	0	18894	153	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 153 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:B:751:LEU:HG	3:B:1302:CYZ:H71	1.61	0.79
1:B:751:LEU:HD21	1:C:481:ILE:HG22	1.72	0.72
1:D:751:LEU:HG	3:D:1302:CYZ:H71	1.80	0.61
1:C:704:LEU:HD12	1:C:708:MET:HG3	1.83	0.60
1:A:500:ILE:HB	1:A:727:LEU:HB2	1.84	0.60

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	591/1033 (57%)	556 (94%)	35 (6%)	0	100	100
1	B	591/1033 (57%)	562 (95%)	28 (5%)	1 (0%)	44	76
1	C	591/1033 (57%)	556 (94%)	35 (6%)	0	100	100
1	D	591/1033 (57%)	561 (95%)	29 (5%)	1 (0%)	44	76
All	All	2364/4132 (57%)	2235 (94%)	127 (5%)	2 (0%)	50	81

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	636	ALA
1	D	636	ALA

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	500/876 (57%)	495 (99%)	5 (1%)	73	81
1	B	501/876 (57%)	493 (98%)	8 (2%)	58	73
1	C	500/876 (57%)	495 (99%)	5 (1%)	73	81
1	D	501/876 (57%)	493 (98%)	8 (2%)	58	73
All	All	2002/3504 (57%)	1976 (99%)	26 (1%)	64	76

5 of 26 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	511	LYS
1	C	684	ARG
1	D	1132	ASN
1	C	660	ARG
1	D	411	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	435	HIS
1	C	642	GLN
1	D	791	ASN
1	C	619	ASN
1	C	764	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [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	$\# Z > 2$
2	GLU	A	1301	-	8,9,9	1.05	1 (12%)	8,11,11	1.67	1 (12%)
3	CYZ	A	1302	-	26,27,27	0.49	0	38,44,44	0.51	1 (2%)
2	GLU	C	1301	-	8,9,9	1.05	1 (12%)	8,11,11	1.67	1 (12%)
3	CYZ	C	1302	-	26,27,27	0.49	0	38,44,44	0.51	1 (2%)
2	GLU	D	1301	-	8,9,9	1.10	1 (12%)	8,11,11	1.54	1 (12%)
3	CYZ	B	1302	-	26,27,27	0.47	0	38,44,44	0.51	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	CYZ	D	1302	-	26,27,27	0.47	0	38,44,44	0.55	1 (2%)
2	GLU	B	1301	-	8,9,9	1.08	1 (12%)	8,11,11	1.54	1 (12%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLU	A	1301	-	-	0/9/9/9	-
3	CYZ	A	1302	-	-	7/7/42/42	0/5/4/4
2	GLU	C	1301	-	-	0/9/9/9	-
3	CYZ	C	1302	-	-	7/7/42/42	0/5/4/4
2	GLU	D	1301	-	-	0/9/9/9	-
3	CYZ	B	1302	-	-	1/7/42/42	0/5/4/4
3	CYZ	D	1302	-	-	1/7/42/42	0/5/4/4
2	GLU	B	1301	-	-	0/9/9/9	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1301	GLU	OXT-C	-2.29	1.23	1.30
2	B	1301	GLU	OXT-C	-2.26	1.23	1.30
2	A	1301	GLU	OXT-C	-2.21	1.23	1.30
2	C	1301	GLU	OXT-C	-2.20	1.23	1.30

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1301	GLU	OXT-C-O	-3.97	115.07	124.08
2	A	1301	GLU	OXT-C-O	-3.96	115.10	124.08
2	B	1301	GLU	OXT-C-O	-3.53	116.07	124.08
2	D	1301	GLU	OXT-C-O	-3.53	116.07	124.08
3	D	1302	CYZ	C2-C1-C8	2.26	118.11	114.88

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1302	CYZ	C6-C1-C8-N2

Continued on next page...

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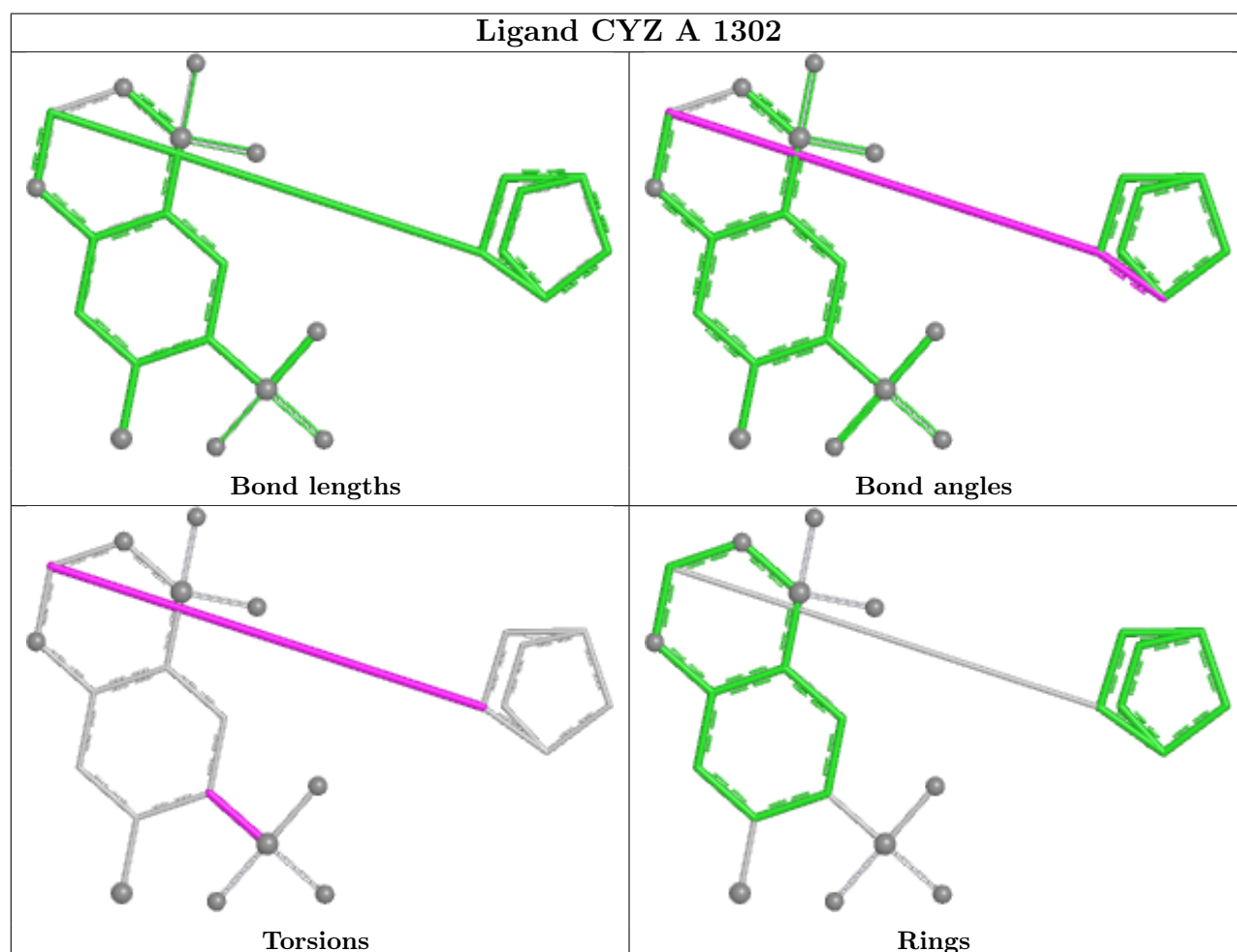
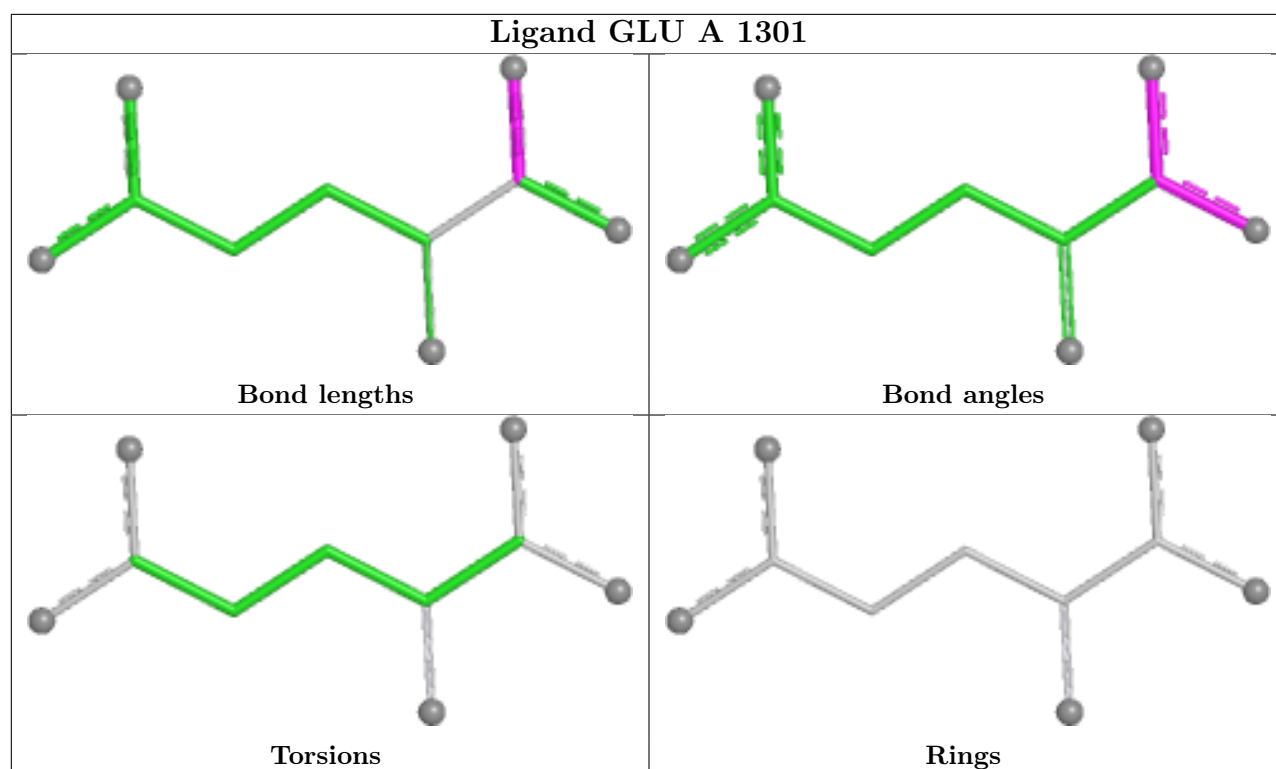
Mol	Chain	Res	Type	Atoms
3	A	1302	CYZ	C11-C12-S2-N3
3	A	1302	CYZ	C13-C12-S2-O3
3	A	1302	CYZ	C13-C12-S2-N3
3	B	1302	CYZ	C6-C1-C8-N2

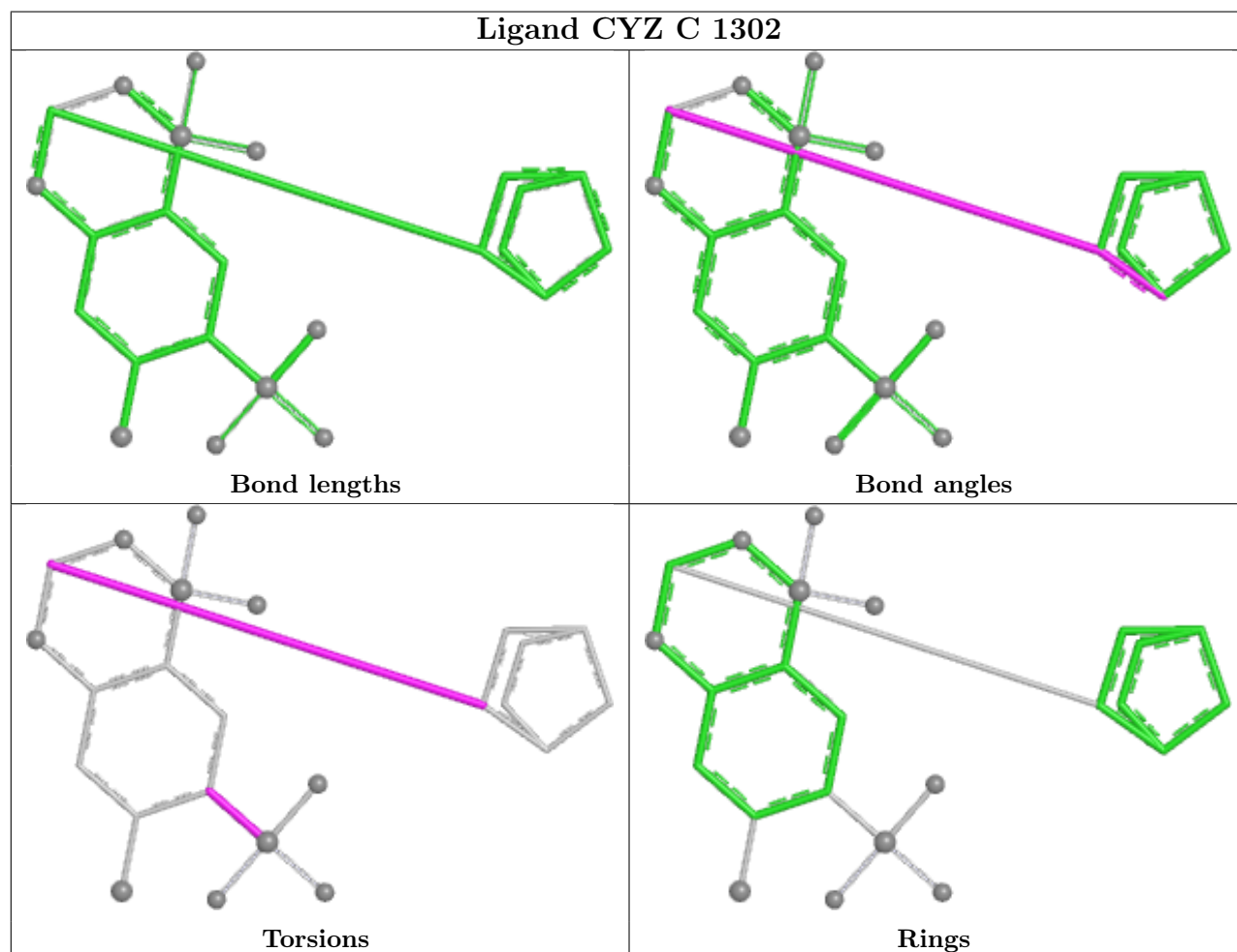
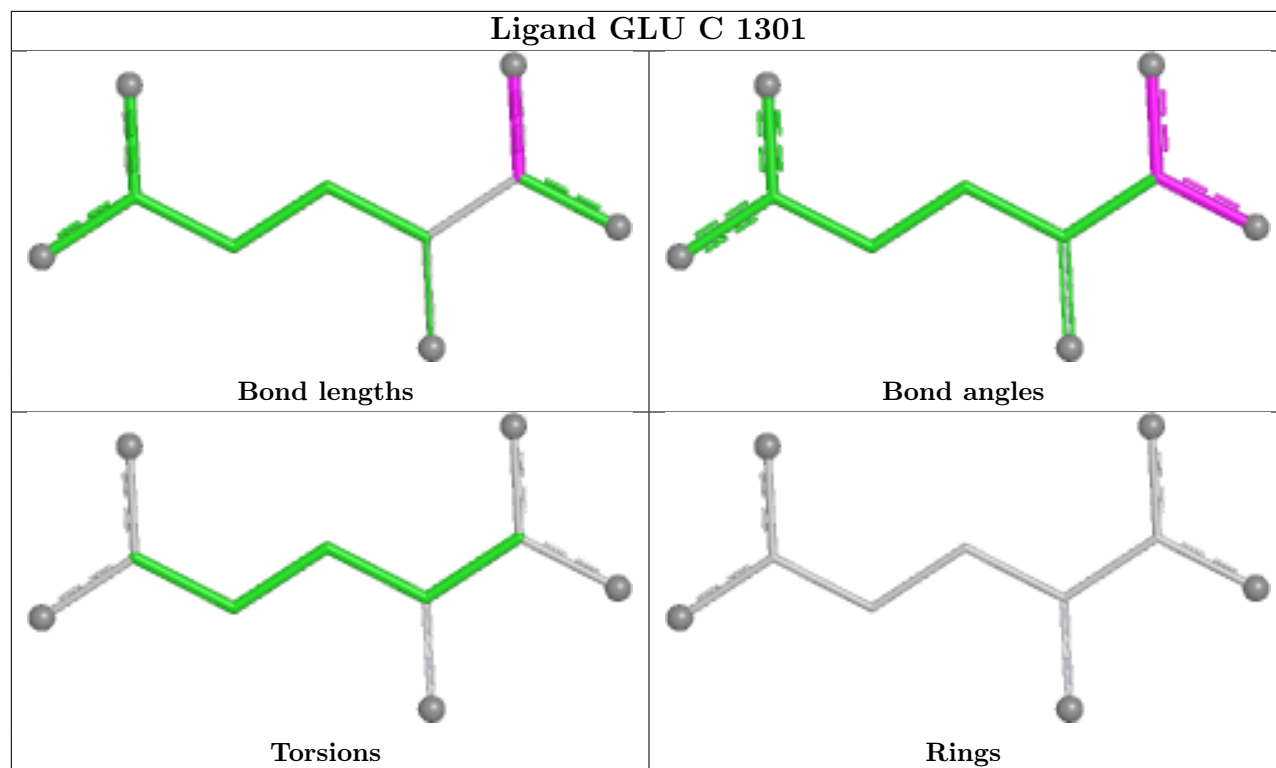
There are no ring outliers.

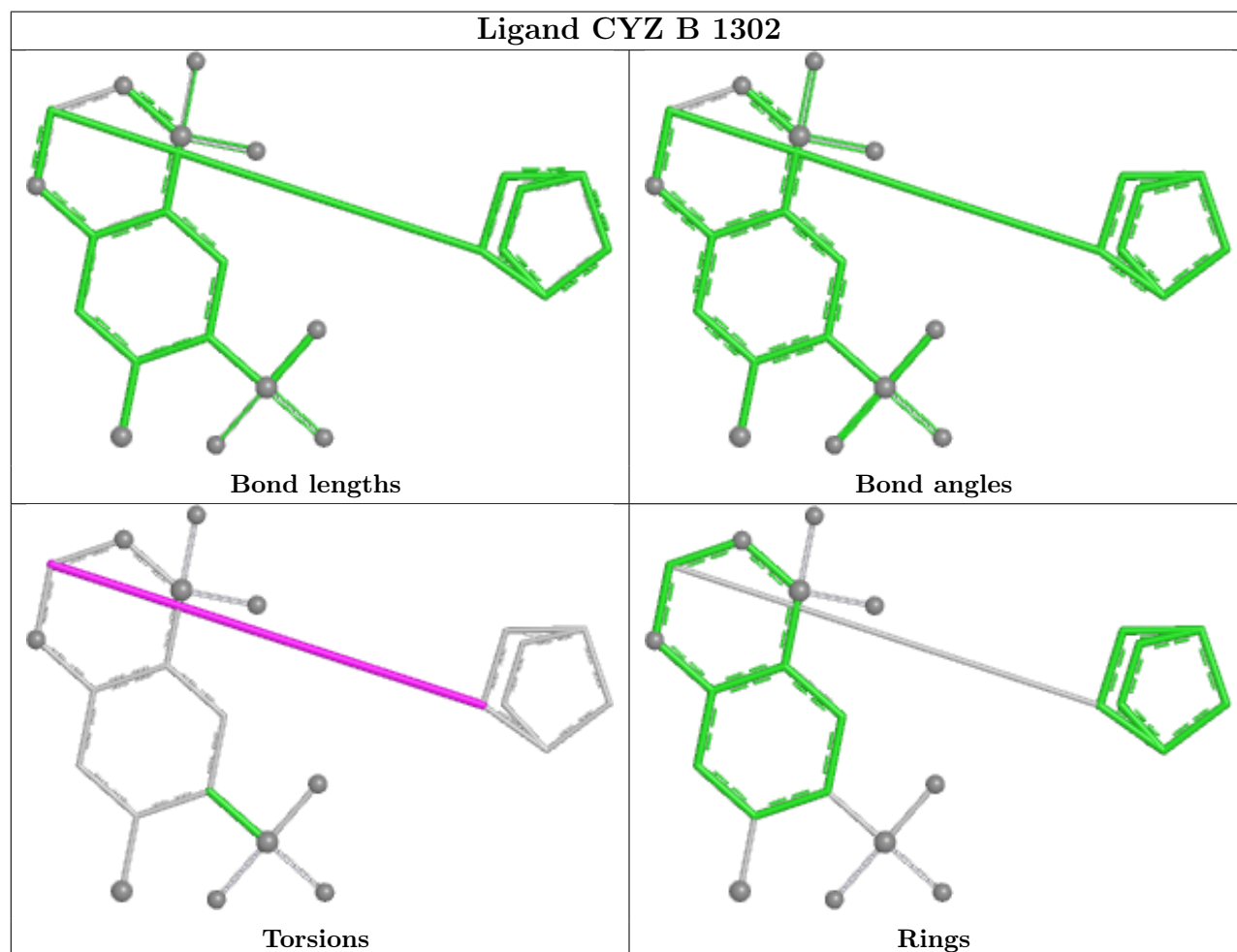
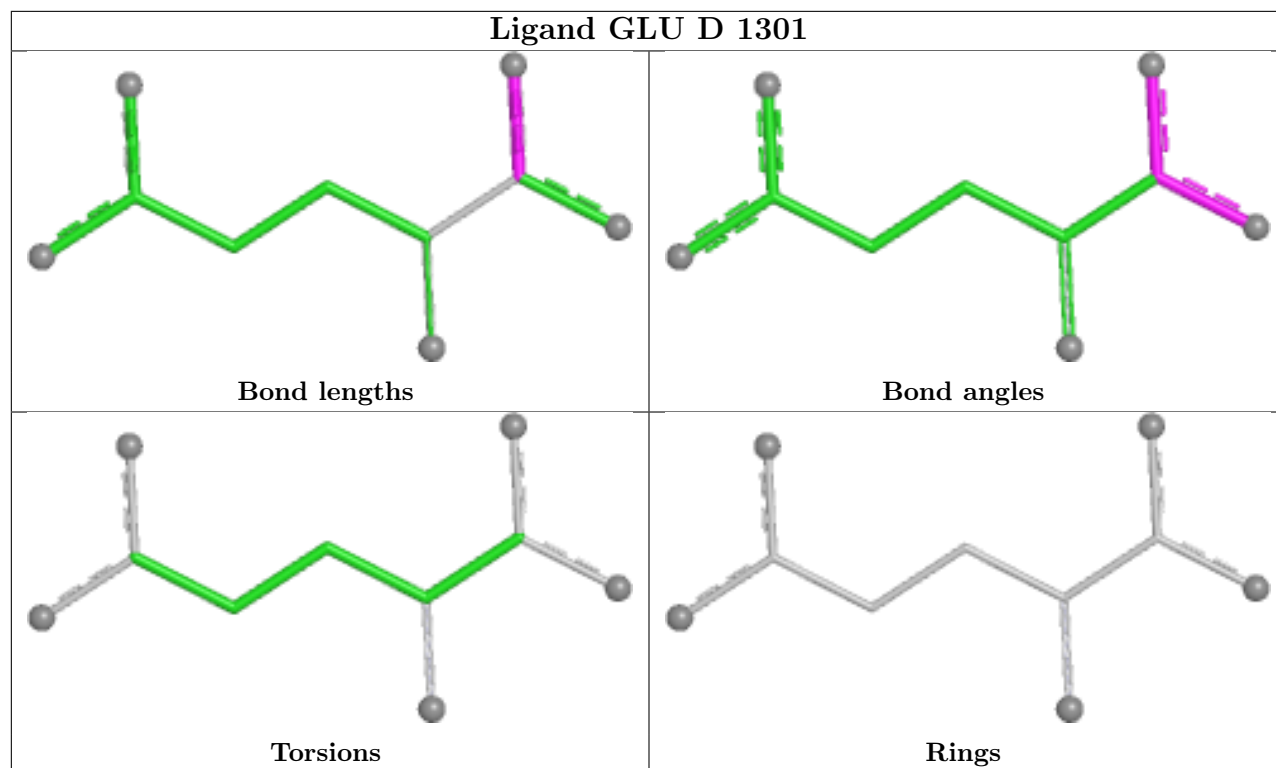
8 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1301	GLU	1	0
3	A	1302	CYZ	2	0
2	C	1301	GLU	1	0
3	C	1302	CYZ	3	0
2	D	1301	GLU	1	0
3	B	1302	CYZ	5	0
3	D	1302	CYZ	4	0
2	B	1301	GLU	1	0

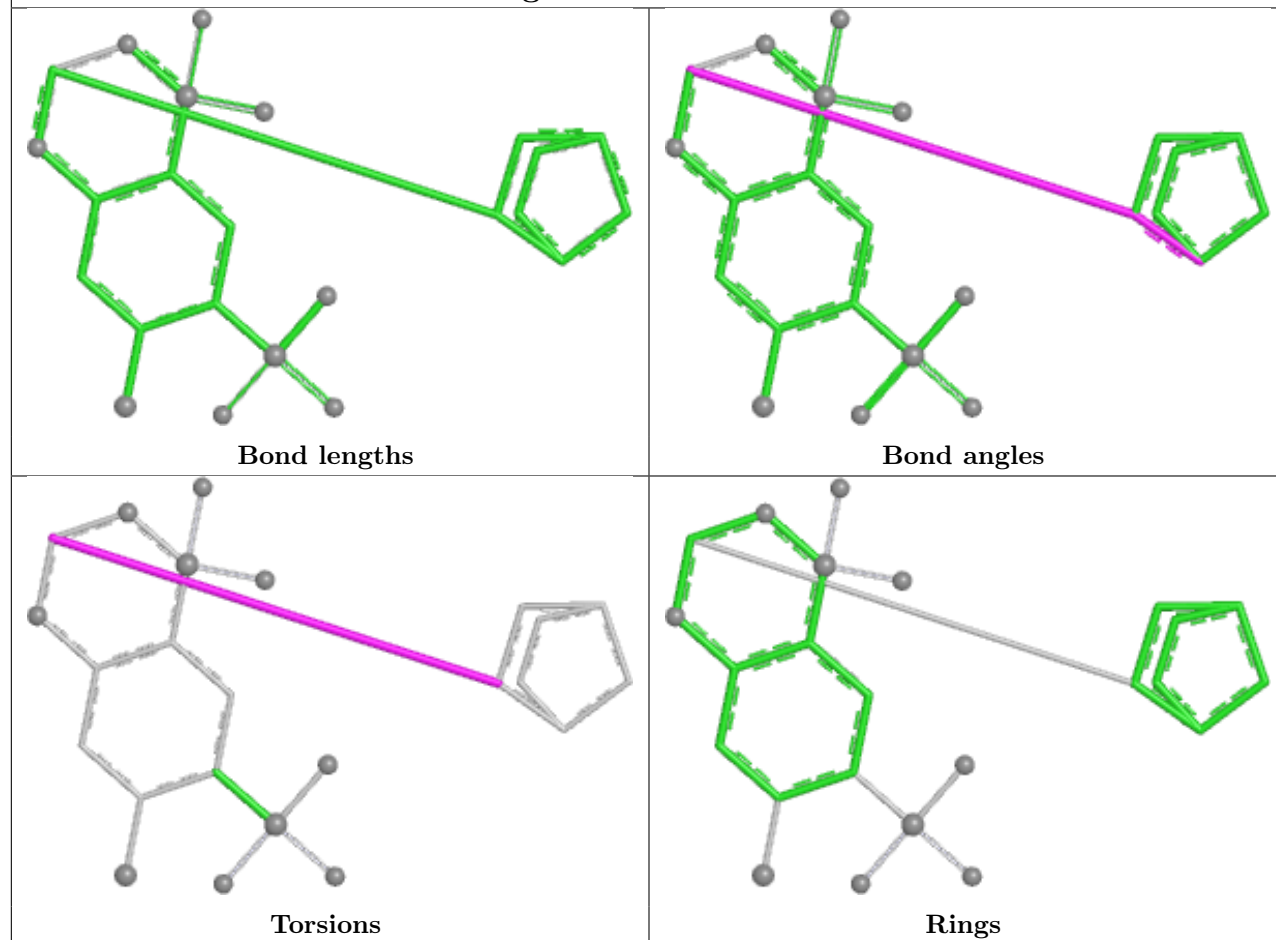
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 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.



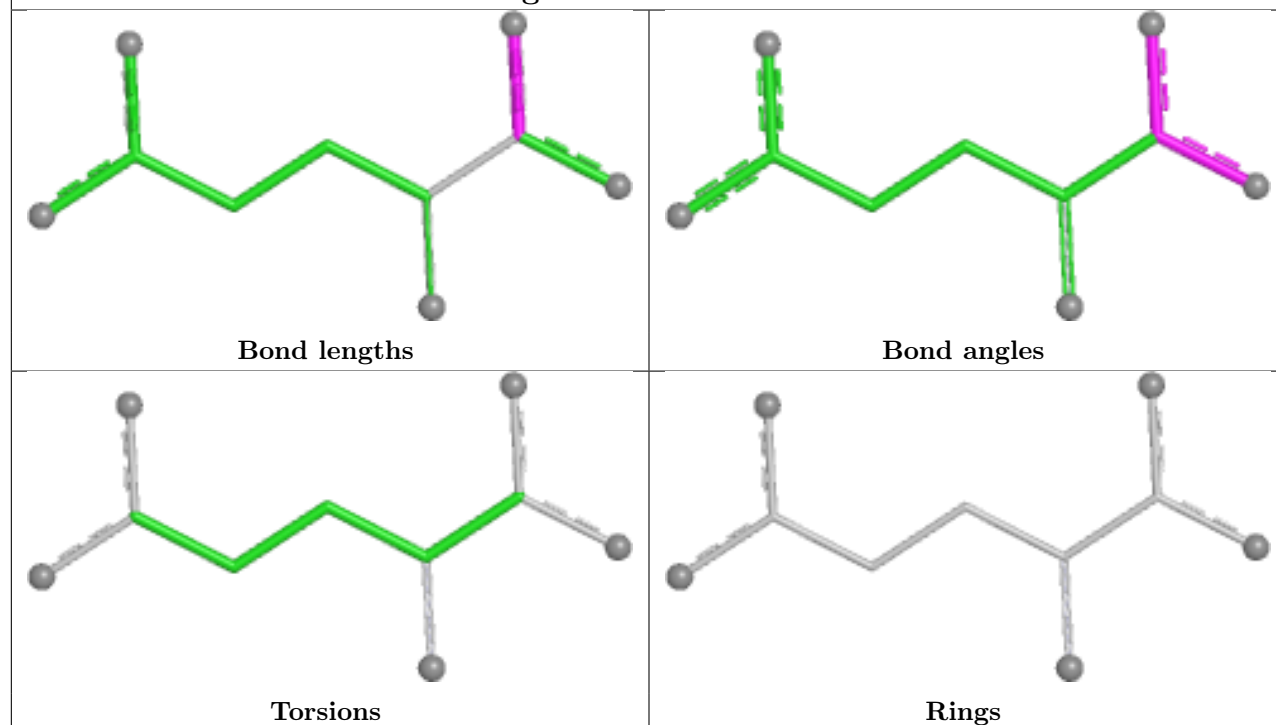




Ligand CYZ D 1302



Ligand GLU B 1301



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

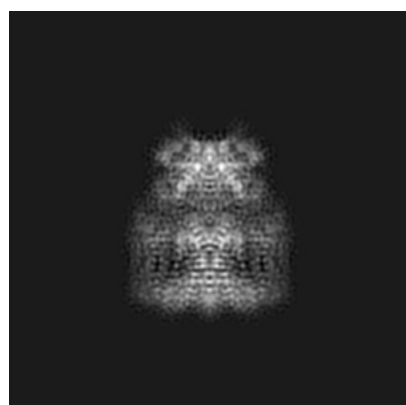
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26017. These allow visual inspection of the internal detail of the map and identification of artifacts.

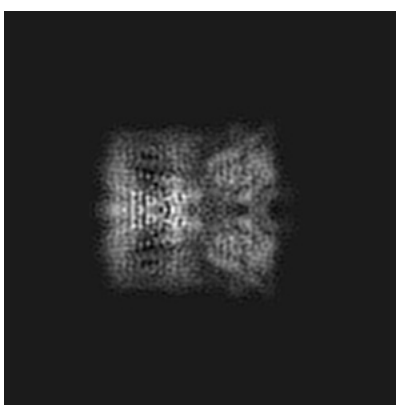
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

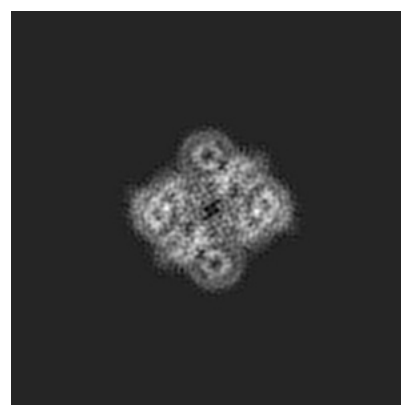
6.1.1 Primary map



X



Y

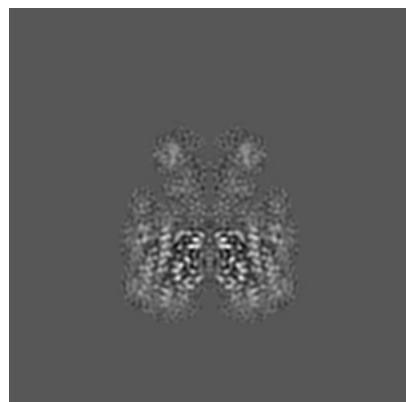


Z

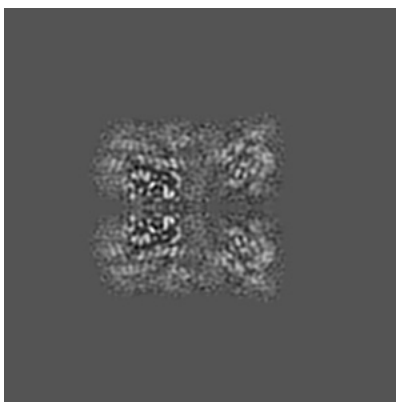
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

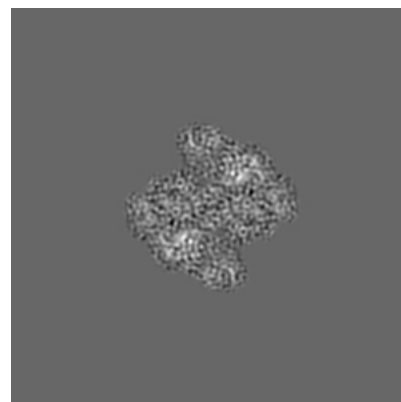
6.2.1 Primary map



X Index: 160



Y Index: 160

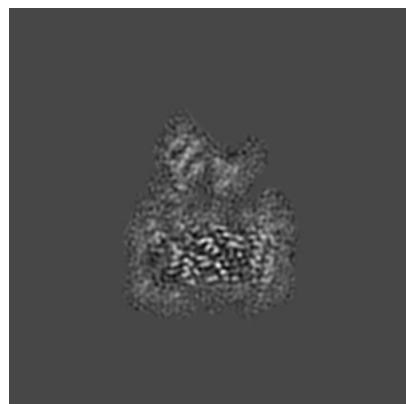


Z Index: 160

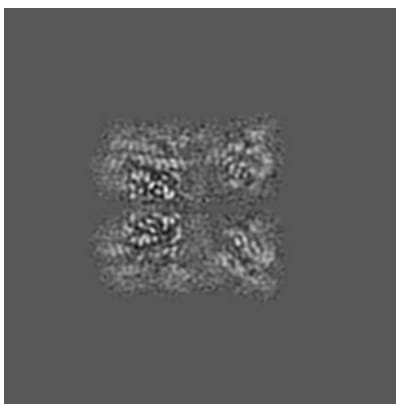
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

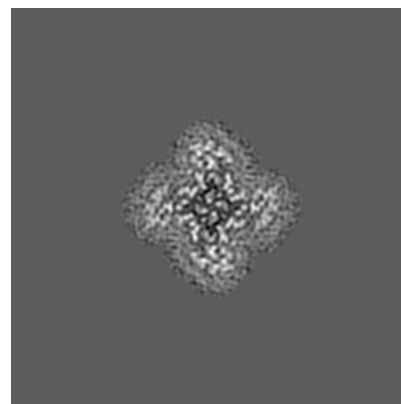
6.3.1 Primary map



X Index: 150



Y Index: 159

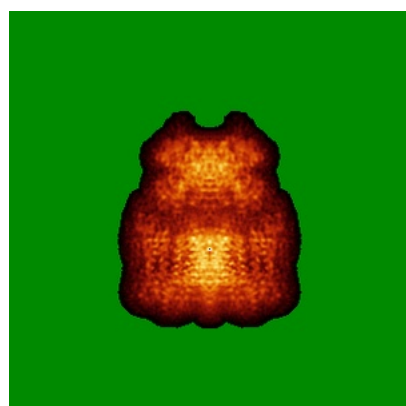


Z Index: 136

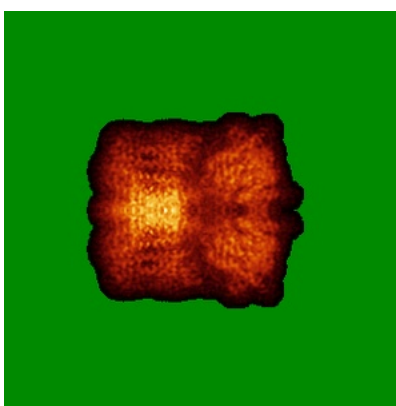
The images above show the largest variance slices of the map in three orthogonal directions.

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

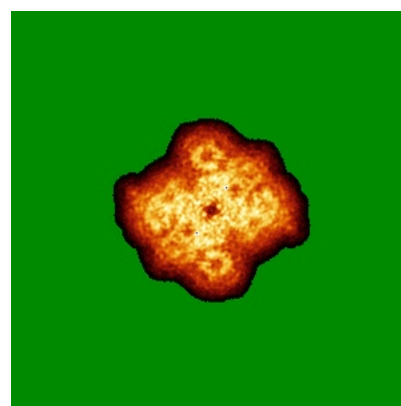
6.4.1 Primary map



X



Y

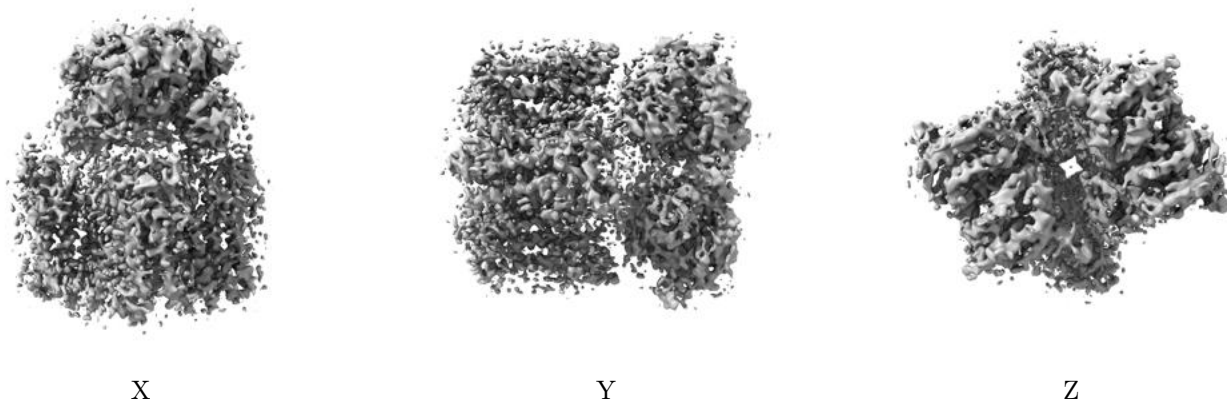


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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

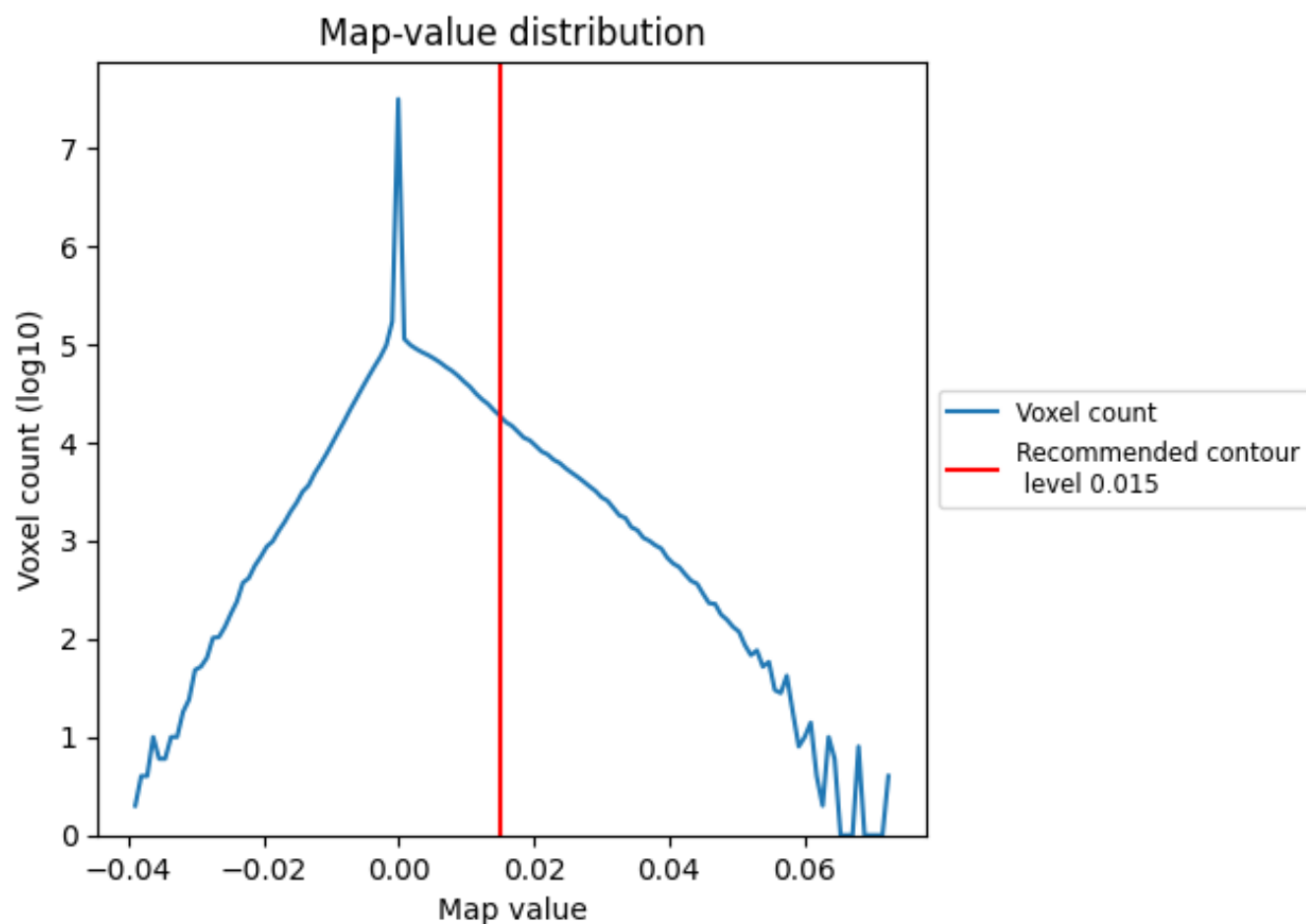
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

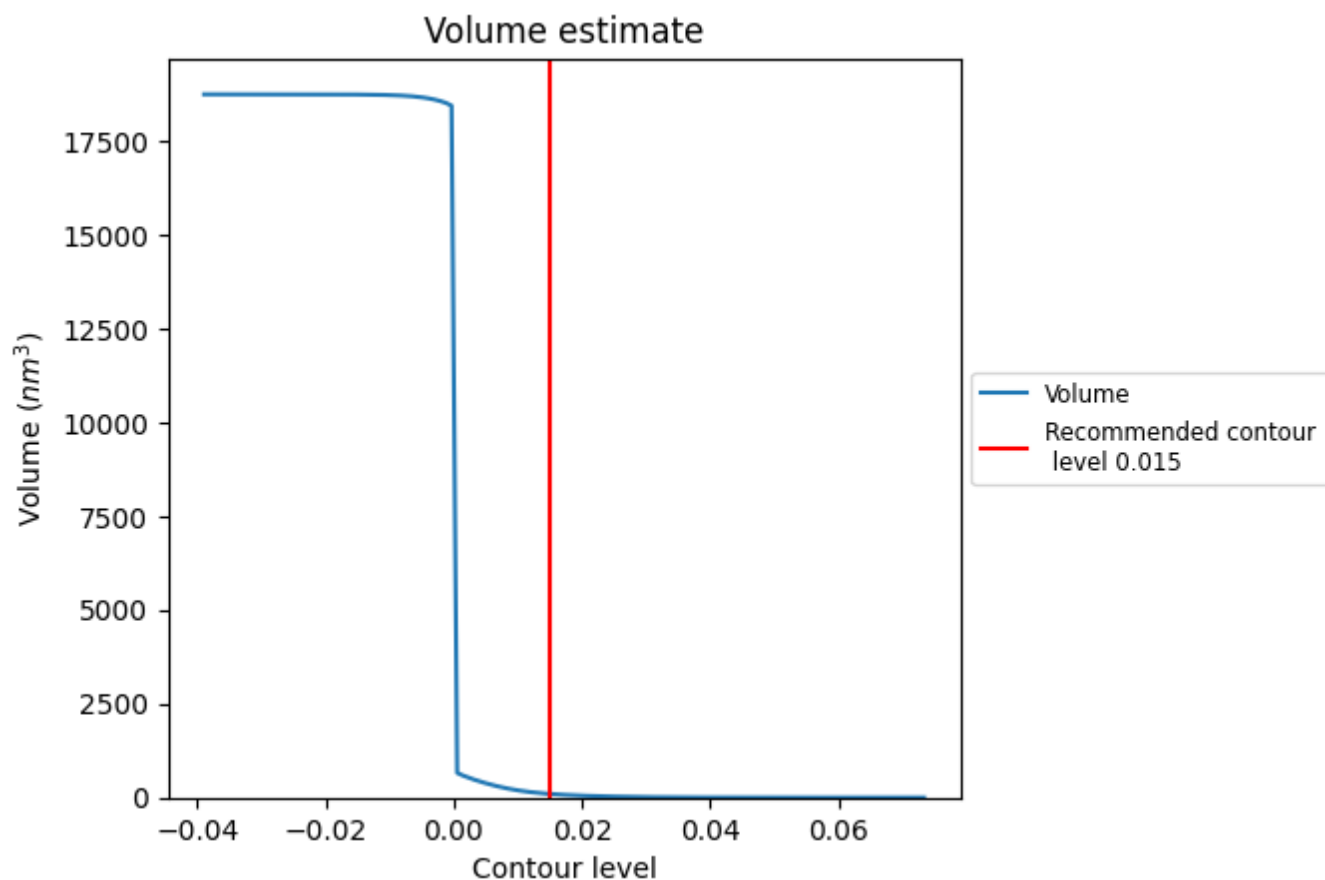
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

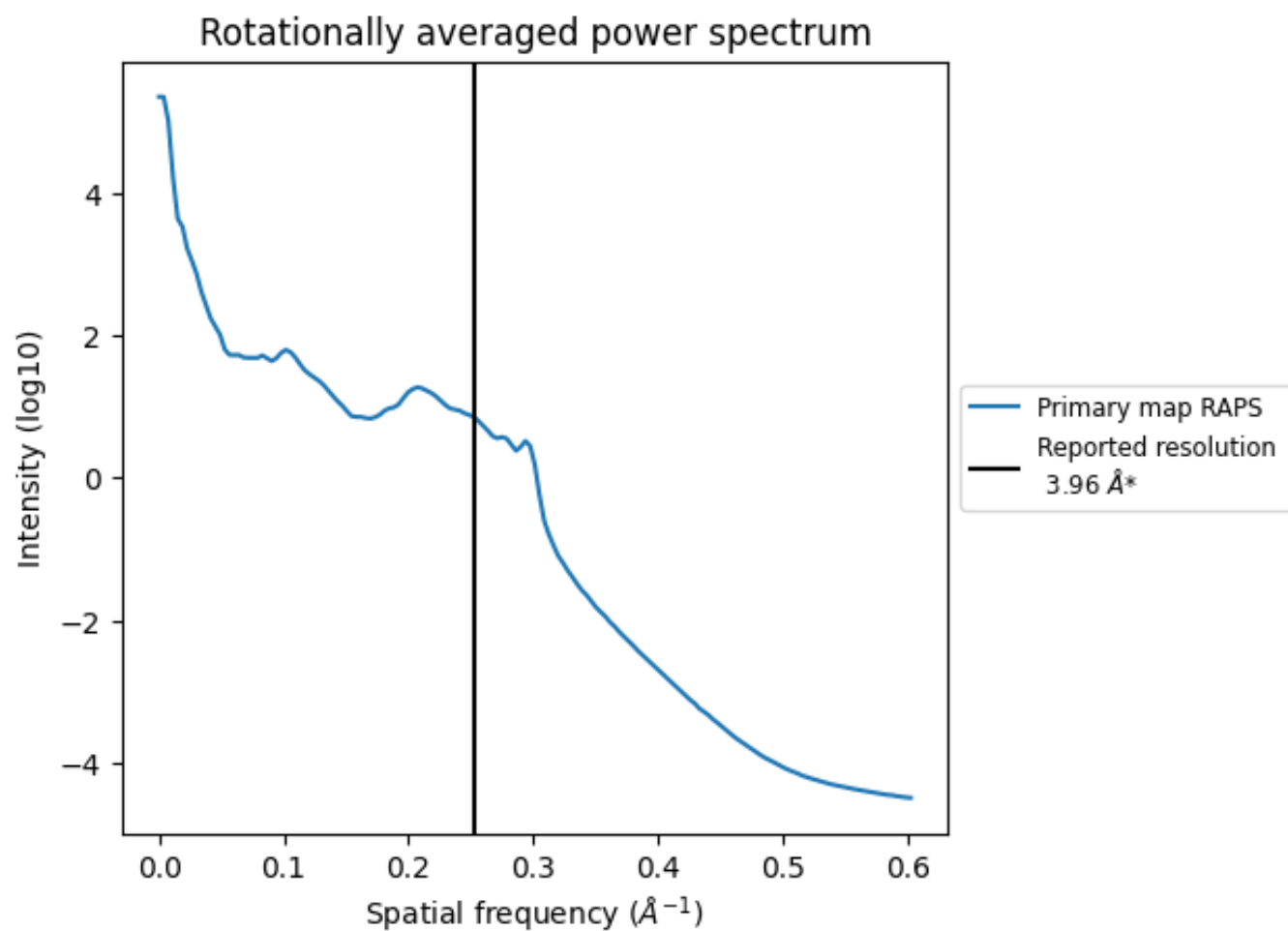
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 97 nm³; this corresponds to an approximate mass of 87 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 ⓘ

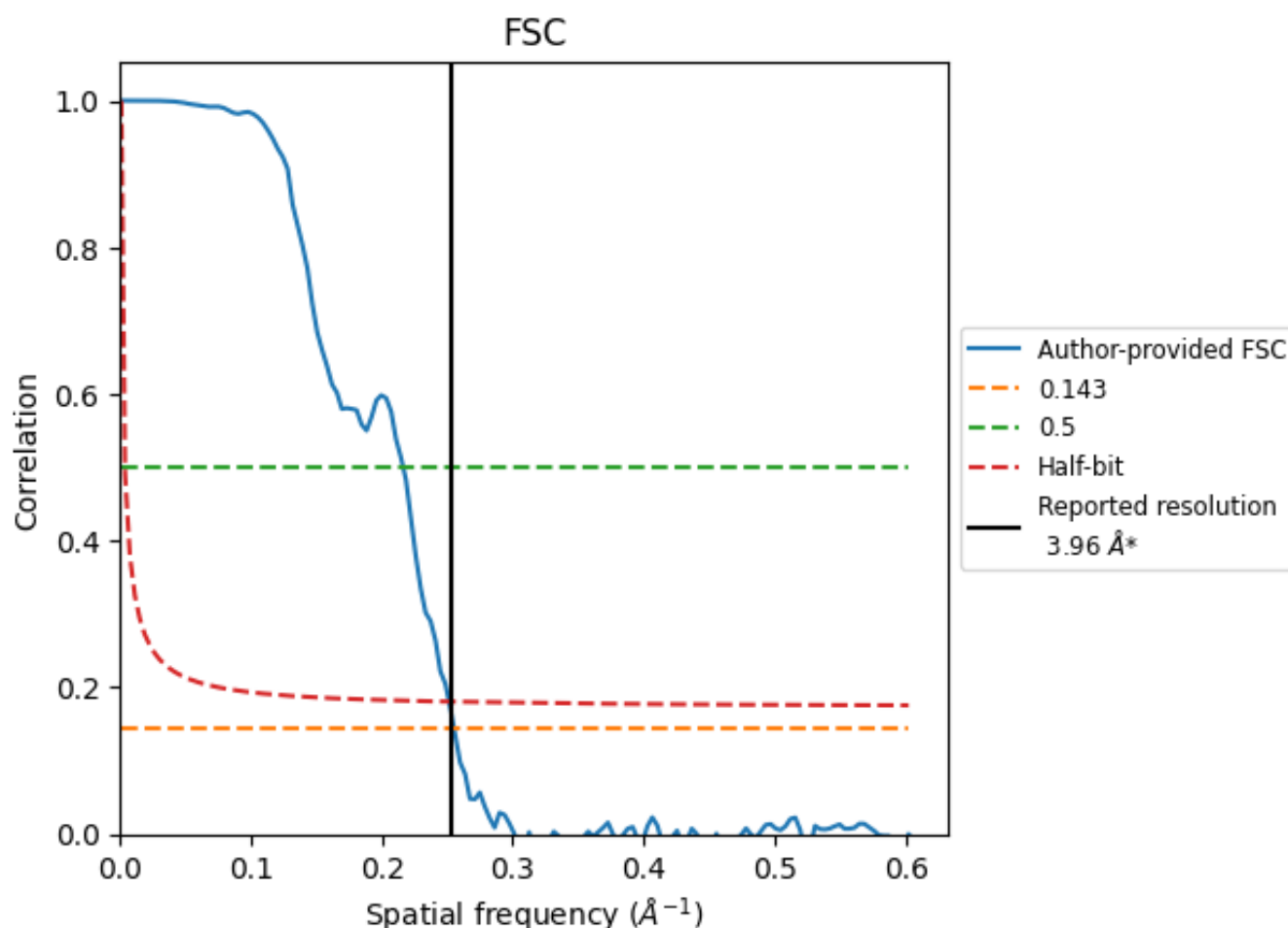


*Reported resolution corresponds to spatial frequency of 0.253 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.253 Å⁻¹

8.2 Resolution estimates [i](#)

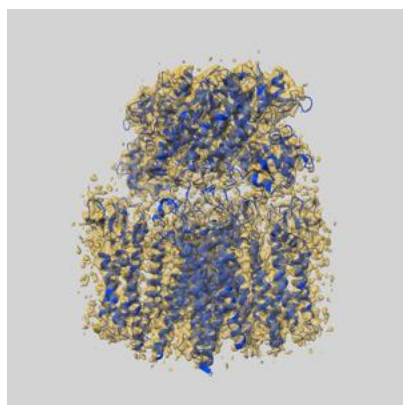
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.96	-	-
Author-provided FSC curve	3.92	4.63	3.98
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

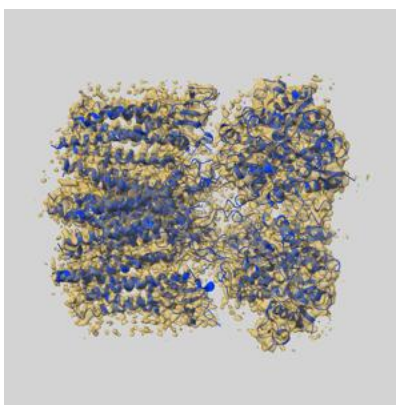
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-26017 and PDB model 7TNP. Per-residue inclusion information can be found in section [3](#) on page [11](#).

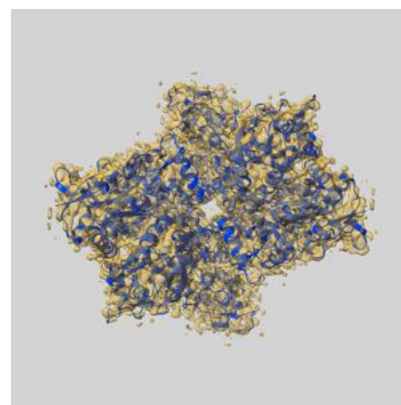
9.1 Map-model overlay [i](#)



X



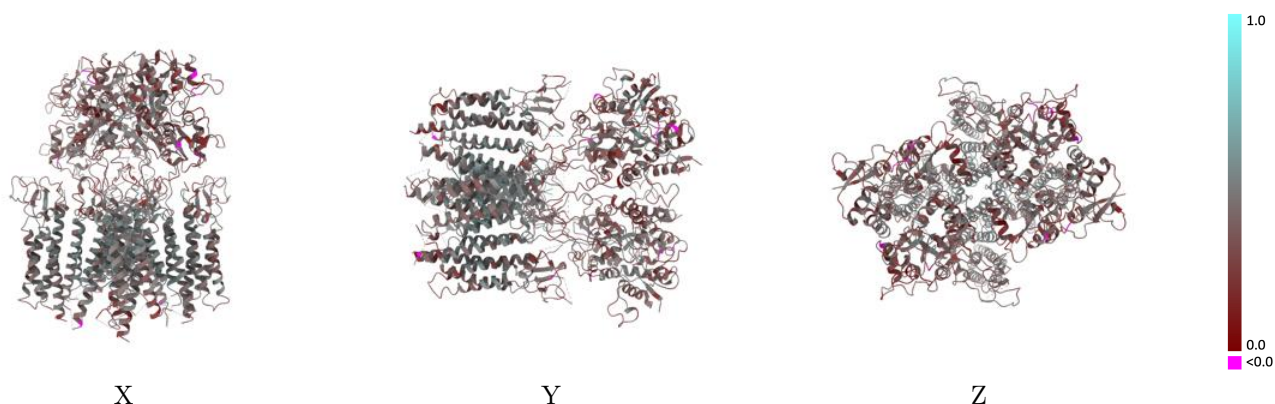
Y



Z

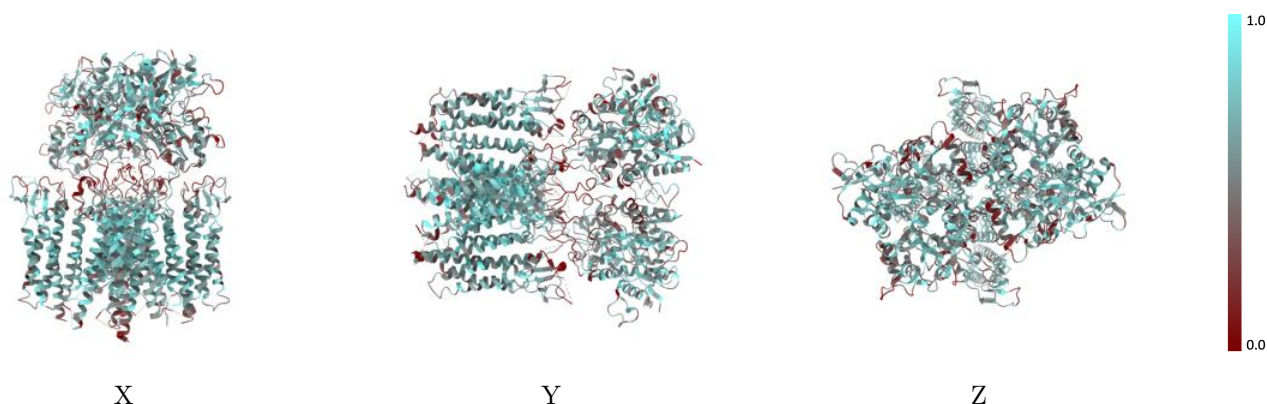
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



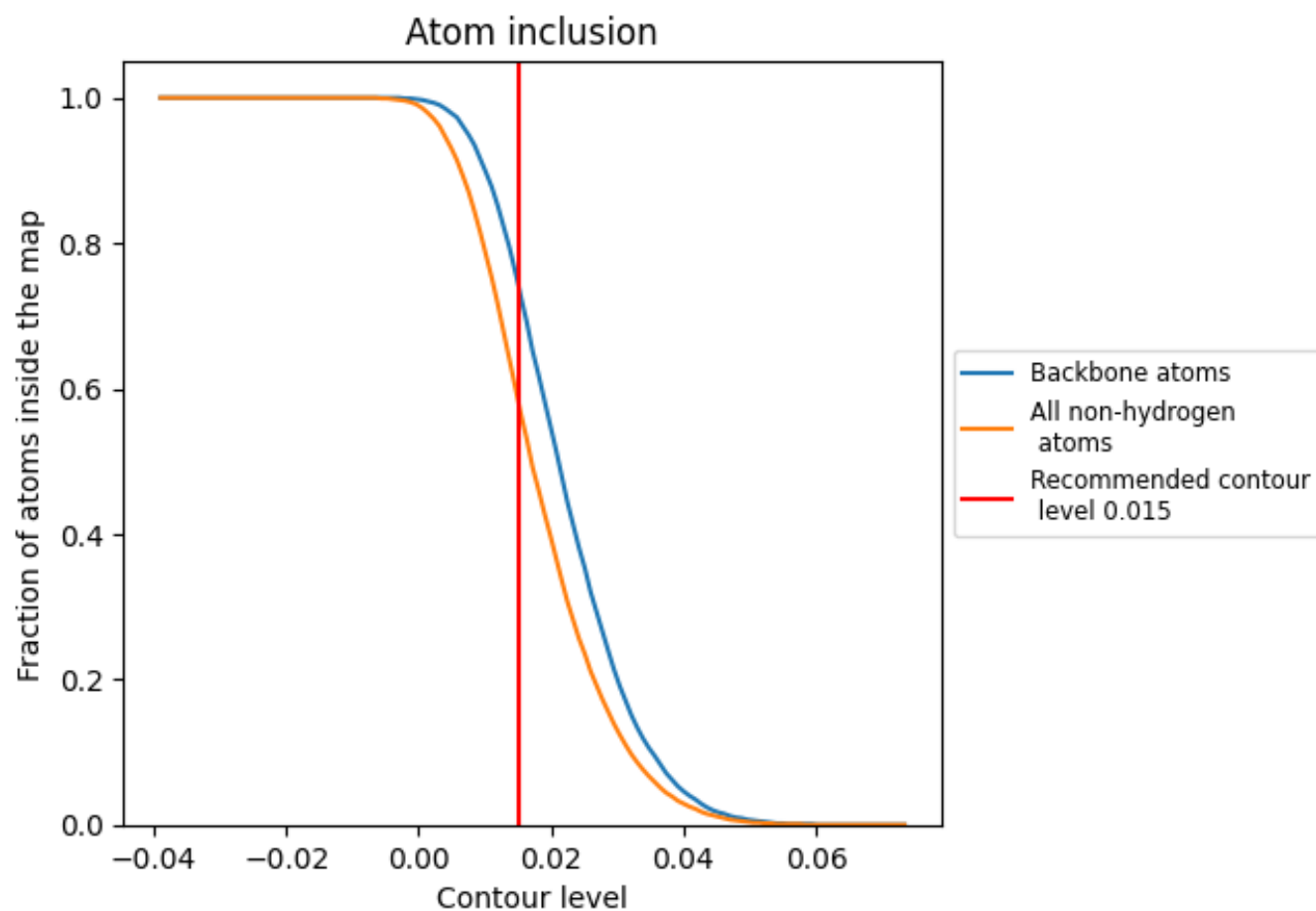
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



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, 74% of all backbone atoms, 58% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.5840	<div></div> 0.3930
A	<div></div> 0.5910	<div></div> 0.4010
B	<div></div> 0.5720	<div></div> 0.3860
C	<div></div> 0.5990	<div></div> 0.4020
D	<div></div> 0.5750	<div></div> 0.3840

