



Full wwPDB EM Validation Report ⓘ

Feb 21, 2022 – 03:34 am GMT

PDB ID : 7QHB
EMDB ID : EMD-13969
Title : Active state of GluA1/2 in complex with TARP gamma 8, L-glutamate and CTZ
Authors : Herguedas, B.; Kohegyi, B.; Zhang, D.; Greger, I.H.
Deposited on : 2021-12-11
Resolution : 3.50 Å (reported)
Based on initial models : 3TKD, 6QKC

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

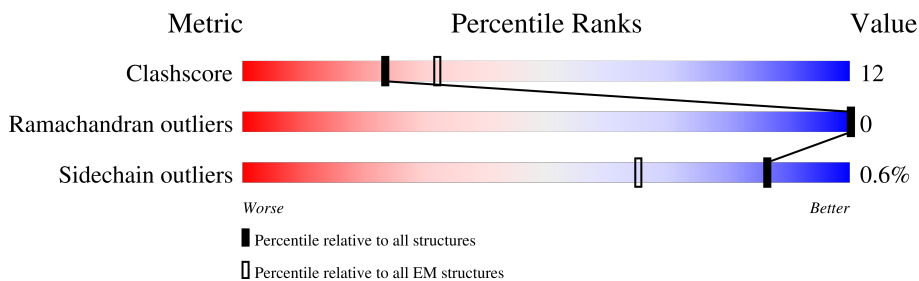
EMDB validation analysis : 0.0.0.dev97
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.26

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 3.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	915	
1	C	915	
2	B	860	
2	D	860	
3	I	423	
3	J	423	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	GLU	A	1202	-	-	X	-
5	GLU	C	1202	-	-	X	-

2 Entry composition i

There are 8 unique types of molecules in this entry. The entry contains 15052 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 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	398	2934	1912	475	530	17	0	0
1	C	398	2934	1912	475	530	17	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	ASP	-	insertion	UNP P19490
A	-5	TYR	-	insertion	UNP P19490
A	-4	LYS	-	insertion	UNP P19490
A	-3	ASP	-	insertion	UNP P19490
A	-2	ASP	-	insertion	UNP P19490
A	-1	ASP	-	insertion	UNP P19490
A	0	ASP	-	insertion	UNP P19490
A	1	LYS	-	insertion	UNP P19490
C	-6	ASP	-	insertion	UNP P19490
C	-5	TYR	-	insertion	UNP P19490
C	-4	LYS	-	insertion	UNP P19490
C	-3	ASP	-	insertion	UNP P19490
C	-2	ASP	-	insertion	UNP P19490
C	-1	ASP	-	insertion	UNP P19490
C	0	ASP	-	insertion	UNP P19490
C	1	LYS	-	insertion	UNP P19490

- Molecule 2 is a protein called Isoform Flip of Glutamate receptor 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	398	2999	1953	485	542	19	0	0
2	D	398	2999	1953	485	542	19	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	586	ARG	GLN	variant	UNP P19491
D	586	ARG	GLN	variant	UNP P19491

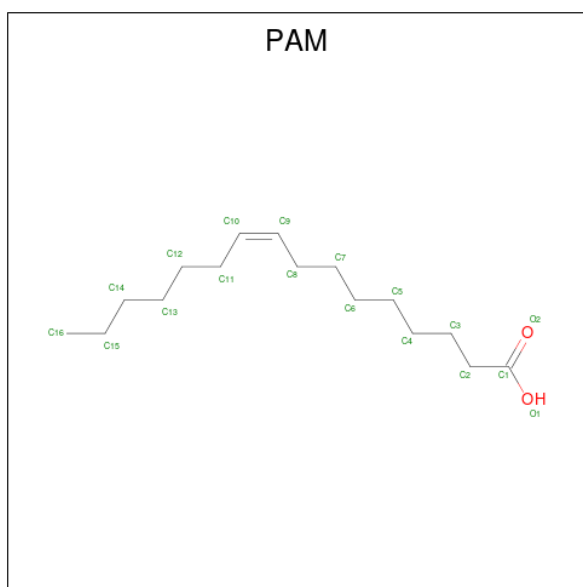
- Molecule 3 is a protein called Voltage-dependent calcium channel gamma-8 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	I	185	1328	869	219	233	7	0	0
3	J	185	1328	869	219	233	7	0	0

There are 14 discrepancies between the modelled and reference sequences:

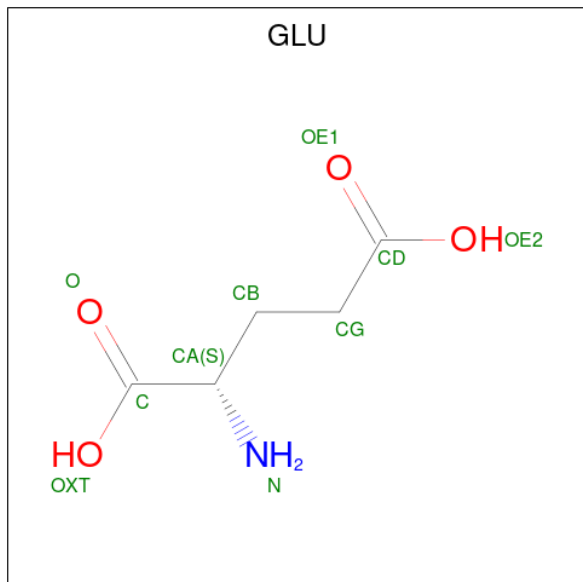
Chain	Residue	Modelled	Actual	Comment	Reference
I	1	GLY	-	expression tag	UNP Q8VHW5
I	418	LEU	-	expression tag	UNP Q8VHW5
I	419	GLU	-	expression tag	UNP Q8VHW5
I	420	VAL	-	expression tag	UNP Q8VHW5
I	421	LEU	-	expression tag	UNP Q8VHW5
I	422	PHE	-	expression tag	UNP Q8VHW5
I	423	GLN	-	expression tag	UNP Q8VHW5
J	1	GLY	-	expression tag	UNP Q8VHW5
J	418	LEU	-	expression tag	UNP Q8VHW5
J	419	GLU	-	expression tag	UNP Q8VHW5
J	420	VAL	-	expression tag	UNP Q8VHW5
J	421	LEU	-	expression tag	UNP Q8VHW5
J	422	PHE	-	expression tag	UNP Q8VHW5
J	423	GLN	-	expression tag	UNP Q8VHW5

- Molecule 4 is PALMITOLEIC ACID (three-letter code: PAM) (formula: C₁₆H₃₀O₂).



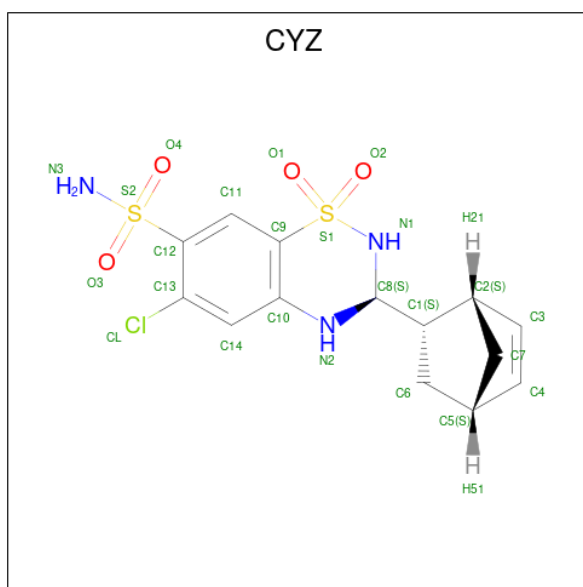
Mol	Chain	Residues	Atoms			AltConf
4	A	1	Total	C	O	0
			36	32	4	
4	A	1	Total	C	O	0
			36	32	4	
4	B	1	Total	C	O	0
			18	16	2	
4	C	1	Total	C	O	0
			36	32	4	
4	C	1	Total	C	O	0
			36	32	4	
4	D	1	Total	C	O	0
			18	16	2	
4	I	1	Total	C	O	0
			72	64	8	
4	I	1	Total	C	O	0
			72	64	8	
4	I	1	Total	C	O	0
			72	64	8	
4	I	1	Total	C	O	0
			72	64	8	
4	J	1	Total	C	O	0
			72	64	8	
4	J	1	Total	C	O	0
			72	64	8	
4	J	1	Total	C	O	0
			72	64	8	
4	J	1	Total	C	O	0
			72	64	8	

- Molecule 5 is GLUTAMIC ACID (three-letter code: GLU) (formula: C₅H₉NO₄) (labeled as "Ligand of Interest" by depositor).



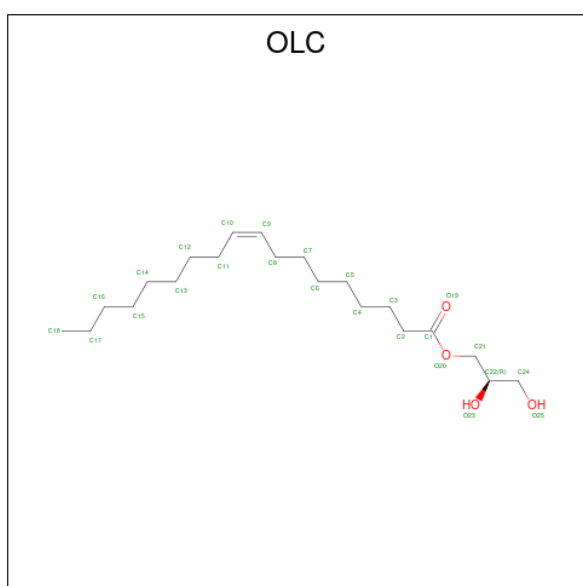
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
5	A	1	Total	C	N	O	0
			10	5	1	4	
5	B	1	Total	C	N	O	0
			10	5	1	4	
5	C	1	Total	C	N	O	0
			10	5	1	4	
5	D	1	Total	C	N	O	0
			10	5	1	4	

- Molecule 6 is CYCLOTHIAZIDE (three-letter code: CYZ) (formula: C₁₄H₁₆ClN₃O₄S₂) (labeled as "Ligand of Interest" by depositor).



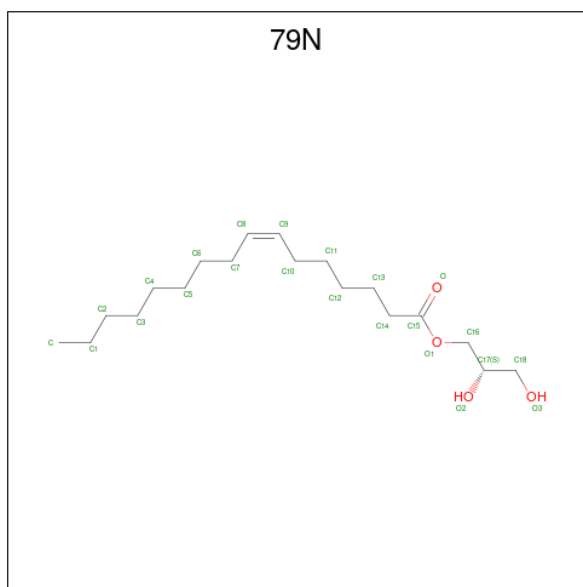
Mol	Chain	Residues	Atoms					AltConf	
			Total	C	Cl	N	O		S
6	A	1	24	14	1	3	4	2	0
6	B	1	24	14	1	3	4	2	0
6	C	1	24	14	1	3	4	2	0
6	D	1	24	14	1	3	4	2	0

- Molecule 7 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (three-letter code: OLC) (formula: C₂₁H₄₀O₄).

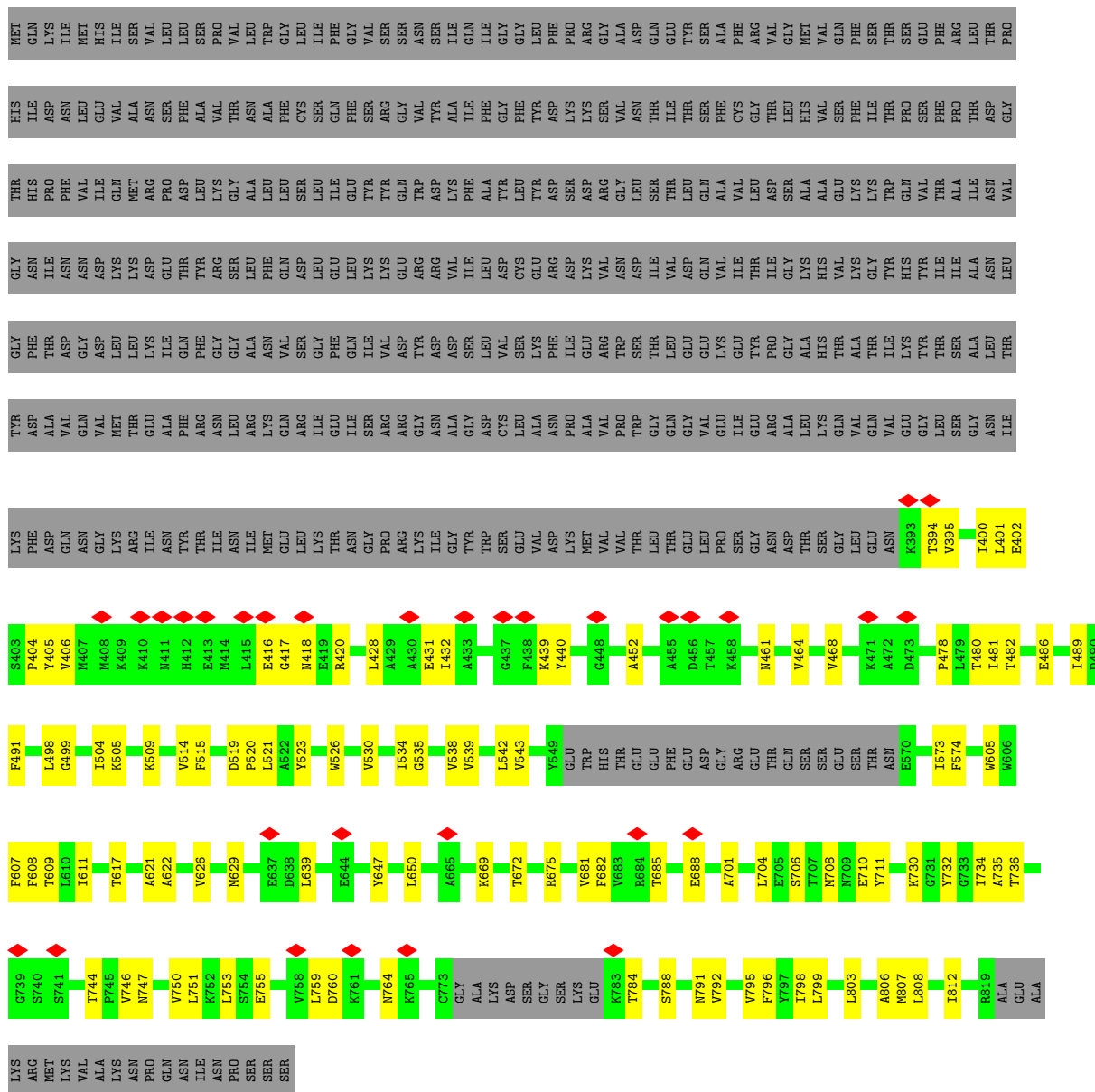


Mol	Chain	Residues	Atoms			AltConf
7	A	1	Total	C	O	0
			25	21	4	
7	C	1	Total	C	O	0
			25	21	4	

- Molecule 8 is (2S)-2,3-dihydroxypropyl (7Z)-hexadec-7-enoate (three-letter code: 79N) (formula: C₁₉H₃₆O₄).



Mol	Chain	Residues	Atoms			AltConf
8	A	1	Total	C	O	0
			23	19	4	
8	B	1	Total	C	O	0
			46	38	8	
8	B	1	Total	C	O	0
			46	38	8	
8	D	1	Total	C	O	0
			23	19	4	



- Molecule 2: Isoform Flip of Glutamate receptor 2

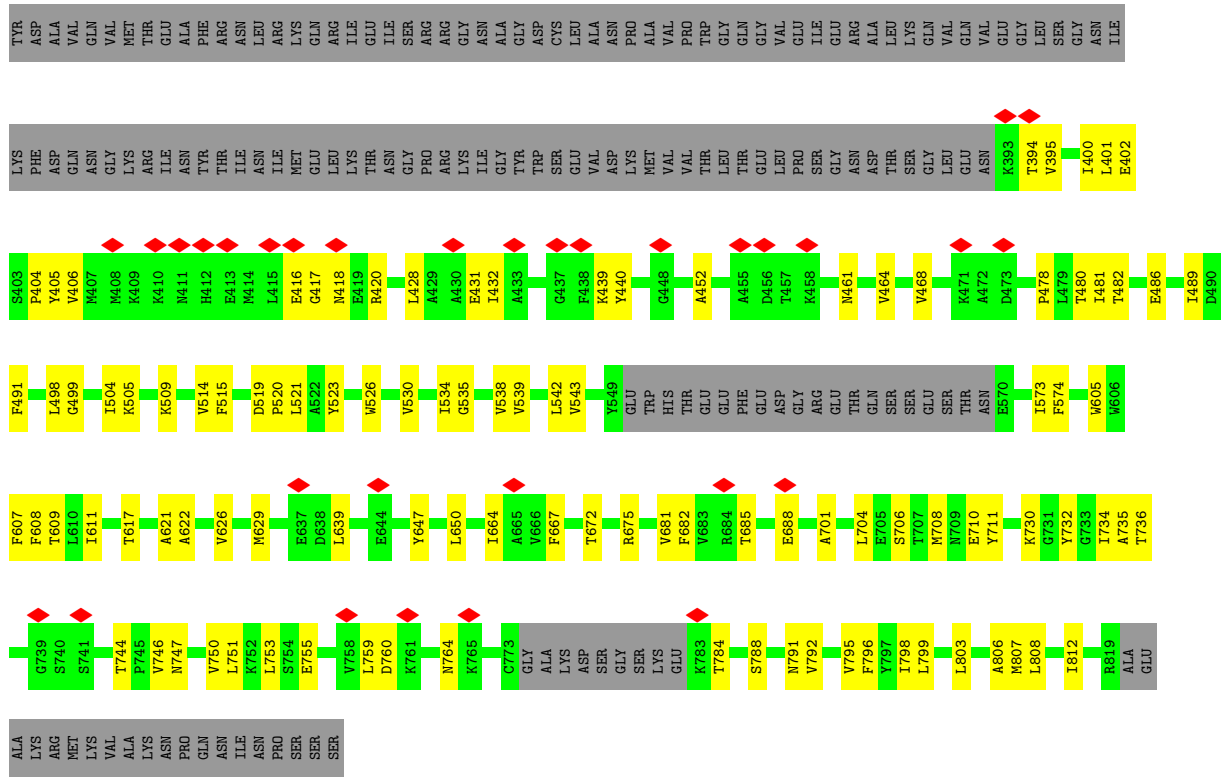
Chain D:

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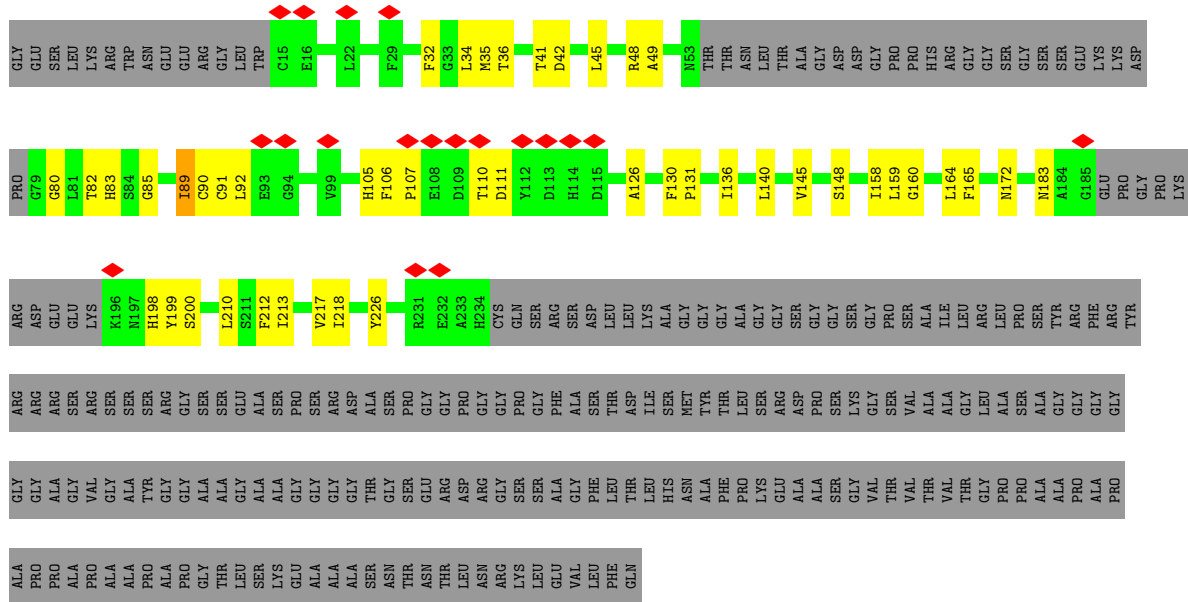
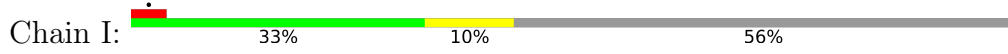
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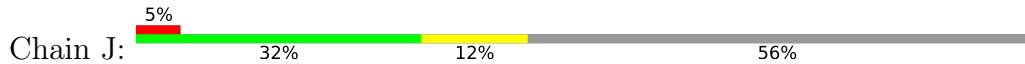




• Molecule 3: Voltage-dependent calcium channel gamma-8 subunit



• Molecule 3: Voltage-dependent calcium channel gamma-8 subunit



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	83344	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; CTF refinement was performed after 3D reconstruction	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	51	Depositor
Minimum defocus (nm)	340	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.206	Depositor
Minimum map value	-0.125	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0192	Depositor
Map size (\AA)	339.19998, 339.19998, 339.19998	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.06, 1.06, 1.06	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: CYZ, 79N, OLC, PAM

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	0.72	0/3001	0.55	0/4088
1	C	0.73	0/3001	0.55	0/4088
2	B	0.77	0/3064	0.55	0/4152
2	D	0.77	0/3064	0.55	0/4152
3	I	0.76	0/1353	0.59	0/1846
3	J	0.76	0/1353	0.59	0/1846
All	All	0.75	0/14836	0.56	0/20172

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	2934	0	2795	61	0
1	C	2934	0	2795	60	0
2	B	2999	0	2971	85	0
2	D	2999	0	2971	83	0
3	I	1328	0	1292	31	0
3	J	1328	0	1292	36	0
4	A	36	0	58	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	18	0	29	6	0
4	C	36	0	58	0	0
4	D	18	0	29	6	0
4	I	72	0	116	1	0
4	J	72	0	116	1	0
5	A	10	0	5	4	0
5	B	10	0	5	2	0
5	C	10	0	5	4	0
5	D	10	0	5	2	0
6	A	24	0	16	3	0
6	B	24	0	16	2	0
6	C	24	0	16	3	0
6	D	24	0	16	2	0
7	A	25	0	40	0	0
7	C	25	0	40	0	0
8	A	23	0	36	7	0
8	B	46	0	72	10	0
8	D	23	0	36	3	0
All	All	15052	0	14830	364	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 12.

All (364) 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)
8:A:1206:79N:H	4:D:904:PAM:H161	1.55	0.89
8:B:904:79N:H	4:B:905:PAM:H161	1.55	0.89
1:A:755:LEU:HB2	6:A:1203:CYZ:CL	2.19	0.80
1:C:755:LEU:HB2	6:C:1203:CYZ:CL	2.19	0.80
6:A:1203:CYZ:CL	6:A:1203:CYZ:N3	2.54	0.76
8:A:1206:79N:H	4:D:904:PAM:C15	2.15	0.76
6:C:1203:CYZ:CL	6:C:1203:CYZ:N3	2.54	0.76
8:A:1206:79N:H	4:D:904:PAM:C16	2.15	0.76
8:B:904:79N:H	4:B:905:PAM:C15	2.15	0.75
8:B:904:79N:H	4:B:905:PAM:C16	2.15	0.75
8:A:1206:79N:C	4:D:904:PAM:H161	2.18	0.72
8:B:904:79N:C	4:B:905:PAM:H161	2.18	0.72
8:B:904:79N:C1	4:B:905:PAM:H161	2.21	0.70
8:A:1206:79N:C1	4:D:904:PAM:H161	2.21	0.69
8:B:904:79N:O	1:C:595:ARG:NH1	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:595:ARG:NH1	8:A:1206:79N:O	2.26	0.68
2:D:498:LEU:HD12	2:D:499:GLY:N	2.08	0.68
2:B:498:LEU:HD12	2:B:499:GLY:N	2.08	0.67
1:A:745:ALA:O	1:A:749:LEU:HD23	1.94	0.66
1:C:745:ALA:O	1:C:749:LEU:HD23	1.94	0.66
1:A:749:LEU:HD12	1:A:754:VAL:HG11	1.78	0.66
1:C:749:LEU:HD12	1:C:754:VAL:HG11	1.78	0.66
2:B:498:LEU:HD12	2:B:499:GLY:CA	2.26	0.66
2:D:498:LEU:HD12	2:D:499:GLY:CA	2.26	0.65
1:C:448:ALA:N	1:C:457:ASN:OD1	2.29	0.65
3:J:45:LEU:HD12	3:J:200:SER:O	1.97	0.64
3:I:45:LEU:HD12	3:I:200:SER:O	1.98	0.63
1:A:448:ALA:N	1:A:457:ASN:OD1	2.29	0.63
3:I:148:SER:OG	3:I:158:ILE:HD11	1.98	0.63
1:C:791:VAL:CG1	2:D:608:PHE:HD1	2.12	0.62
3:J:148:SER:OG	3:J:158:ILE:HD11	1.98	0.62
1:A:791:VAL:CG1	2:B:608:PHE:HD1	2.11	0.62
2:B:478:PRO:O	5:B:901:GLU:N	2.33	0.62
2:D:395:VAL:N	2:D:439:LYS:O	2.32	0.62
2:D:498:LEU:HD22	2:D:732:TYR:CE1	2.35	0.62
2:D:478:PRO:O	5:D:901:GLU:N	2.33	0.62
2:D:605:TRP:O	2:D:609:THR:HG23	2.00	0.62
1:A:414:ASN:ND2	1:A:436:TYR:O	2.33	0.62
2:B:799:LEU:HA	1:C:600:VAL:CG1	2.30	0.61
2:B:395:VAL:N	2:B:439:LYS:O	2.32	0.61
2:B:498:LEU:HD22	2:B:732:TYR:CE1	2.35	0.61
3:I:110:THR:O	3:I:111:ASP:OD1	2.19	0.61
2:B:605:TRP:O	2:B:609:THR:HG23	2.00	0.61
3:J:91:CYS:SG	3:J:92:LEU:N	2.74	0.61
8:B:903:79N:O1	8:B:903:79N:O3	2.14	0.61
3:J:110:THR:O	3:J:111:ASP:OD1	2.19	0.60
3:I:91:CYS:SG	3:I:92:LEU:N	2.74	0.60
1:A:600:VAL:CG1	2:D:799:LEU:HA	2.31	0.60
2:B:621:ALA:HB2	1:C:614:ALA:HB1	1.84	0.60
2:B:799:LEU:HA	1:C:600:VAL:HG11	1.85	0.59
1:C:414:ASN:ND2	1:C:436:TYR:O	2.33	0.59
2:B:452:ALA:N	2:B:461:ASN:OD1	2.35	0.59
2:B:498:LEU:HD11	2:B:730:LYS:HB2	1.85	0.59
2:D:452:ALA:N	2:D:461:ASN:OD1	2.35	0.58
2:D:573:ILE:HG23	2:D:574:PHE:HD1	1.69	0.58
2:D:498:LEU:HD11	2:D:730:LYS:HB2	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:600:VAL:HG11	2:D:799:LEU:HA	1.86	0.57
1:A:614:ALA:HB1	2:D:621:ALA:HB2	1.85	0.57
2:D:535:GLY:O	2:D:539:VAL:HG23	2.05	0.57
2:B:573:ILE:HG23	2:B:574:PHE:HD1	1.69	0.57
2:D:514:VAL:HG12	2:D:515:PHE:CD1	2.40	0.57
3:I:41:THR:HG22	3:I:42:ASP:N	2.20	0.57
2:B:535:GLY:O	2:B:539:VAL:HG23	2.05	0.56
2:B:734:ILE:HG21	2:B:746:VAL:HG21	1.88	0.56
8:D:903:79N:O3	8:D:903:79N:O1	2.14	0.56
1:A:481:ARG:NH2	5:A:1202:GLU:OXT	2.38	0.56
2:D:734:ILE:HG21	2:D:746:VAL:HG21	1.88	0.56
1:A:791:VAL:HG12	2:B:608:PHE:HD1	1.71	0.56
3:J:41:THR:HG22	3:J:42:ASP:N	2.20	0.56
1:A:651:THR:OG1	5:A:1202:GLU:OE1	2.21	0.56
2:B:480:THR:HG1	5:B:901:GLU:N	2.03	0.56
2:B:514:VAL:HG12	2:B:515:PHE:CD1	2.40	0.56
1:C:481:ARG:NH2	5:C:1202:GLU:OXT	2.38	0.56
2:D:480:THR:HG1	5:D:901:GLU:N	2.04	0.56
2:B:539:VAL:O	2:B:543:VAL:HG23	2.06	0.55
2:D:539:VAL:O	2:D:543:VAL:HG23	2.06	0.55
1:C:738:LEU:O	1:C:742:VAL:HG23	2.07	0.55
1:C:791:VAL:HG12	2:D:608:PHE:HD1	1.72	0.55
2:B:491:PHE:CE1	2:B:735:ALA:HB2	2.42	0.55
2:B:759:LEU:HB3	6:B:902:CYZ:CL	2.43	0.55
2:B:792:VAL:O	2:B:792:VAL:HG22	2.07	0.55
1:C:596:ILE:O	1:C:600:VAL:HG23	2.07	0.55
2:D:759:LEU:HB3	6:D:902:CYZ:CL	2.44	0.55
2:D:792:VAL:O	2:D:792:VAL:HG22	2.07	0.54
2:D:491:PHE:CE1	2:D:735:ALA:HB2	2.41	0.54
2:B:498:LEU:HD12	2:B:498:LEU:C	2.28	0.54
1:A:754:VAL:O	1:A:757:LYS:N	2.41	0.53
2:D:704:LEU:HD23	2:D:704:LEU:H	1.74	0.53
1:A:596:ILE:O	1:A:600:VAL:HG23	2.07	0.53
1:C:651:THR:OG1	5:C:1202:GLU:OE1	2.21	0.53
1:A:738:LEU:O	1:A:742:VAL:HG23	2.07	0.53
2:B:704:LEU:H	2:B:704:LEU:HD23	1.74	0.53
2:D:498:LEU:HD12	2:D:498:LEU:C	2.28	0.53
1:C:401:TYR:CD2	1:C:474:PRO:HG3	2.44	0.53
1:A:494:LEU:HD23	1:A:494:LEU:N	2.24	0.53
2:B:428:LEU:HD21	2:B:734:ILE:HD11	1.91	0.52
1:C:754:VAL:O	1:C:757:LYS:N	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:401:TYR:CD2	1:A:474:PRO:HG3	2.44	0.52
1:A:650:SER:N	5:A:1202:GLU:OXT	2.37	0.52
2:D:428:LEU:HD21	2:D:734:ILE:HD11	1.91	0.52
1:A:538:LEU:HD23	1:A:542:PHE:HE1	1.75	0.52
1:C:650:SER:N	5:C:1202:GLU:OXT	2.37	0.52
1:C:538:LEU:HD23	1:C:542:PHE:HE1	1.75	0.52
3:J:165:PHE:CD2	3:J:218:ILE:HG22	2.45	0.52
1:C:494:LEU:N	1:C:494:LEU:HD23	2.24	0.52
2:D:432:ILE:HG21	2:D:746:VAL:HG23	1.92	0.51
2:B:432:ILE:HG21	2:B:746:VAL:HG23	1.92	0.51
2:B:431:GLU:OE1	2:B:753:LEU:HD11	2.11	0.51
3:I:165:PHE:CD2	3:I:218:ILE:HG22	2.45	0.51
2:B:417:GLY:O	2:B:420:ARG:HD3	2.11	0.51
2:B:784:THR:HG23	2:B:784:THR:O	2.11	0.51
2:D:605:TRP:CZ3	2:D:608:PHE:CD2	2.99	0.51
2:D:504:ILE:HG22	2:D:505:LYS:N	2.26	0.50
3:I:106:PHE:N	3:I:107:PRO:CD	2.74	0.50
2:B:464:VAL:O	2:B:468:VAL:HG22	2.12	0.50
2:D:431:GLU:OE1	2:D:753:LEU:HD11	2.11	0.50
2:D:464:VAL:O	2:D:468:VAL:HG22	2.12	0.50
2:B:605:TRP:CZ3	2:B:608:PHE:CD2	2.99	0.50
3:J:49:ALA:HB3	3:J:82:THR:HG21	1.93	0.50
3:J:106:PHE:N	3:J:107:PRO:CD	2.74	0.50
3:J:106:PHE:CD1	3:J:107:PRO:HD3	2.47	0.50
2:B:788:SER:N	2:B:791:ASN:OD1	2.39	0.50
1:C:683:GLU:O	1:C:687:ILE:HD12	2.12	0.49
2:D:784:THR:HG23	2:D:784:THR:O	2.11	0.49
3:I:106:PHE:CD1	3:I:107:PRO:HD3	2.47	0.49
2:B:402:GLU:OE1	2:B:402:GLU:HA	2.12	0.49
1:C:515:ASP:N	1:C:516:PRO:CD	2.75	0.49
4:I:1503:PAM:H111	4:I:1503:PAM:C7	2.42	0.49
2:D:607:PHE:O	2:D:611:ILE:HG12	2.13	0.49
1:A:405:LYS:NZ	1:A:415:ASP:O	2.45	0.49
1:A:515:ASP:N	1:A:516:PRO:CD	2.75	0.49
1:C:718:LYS:NZ	1:C:722:ASN:OD1	2.37	0.49
2:D:417:GLY:O	2:D:420:ARG:HD3	2.11	0.49
1:A:683:GLU:O	1:A:687:ILE:HD12	2.12	0.49
4:J:1703:PAM:H111	4:J:1703:PAM:C7	2.42	0.49
2:B:504:ILE:HG22	2:B:505:LYS:N	2.26	0.49
2:D:402:GLU:OE1	2:D:402:GLU:HA	2.12	0.49
2:B:607:PHE:O	2:B:611:ILE:HG12	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:49:ALA:HB3	3:I:82:THR:HG21	1.93	0.49
2:D:428:LEU:O	2:D:432:ILE:HG12	2.13	0.49
2:D:519:ASP:N	2:D:520:PRO:HD2	2.28	0.49
2:D:803:LEU:O	2:D:807:MET:HG3	2.13	0.49
3:J:213:ILE:O	3:J:217:VAL:HG23	2.12	0.48
3:I:213:ILE:O	3:I:217:VAL:HG23	2.12	0.48
2:D:788:SER:N	2:D:791:ASN:OD1	2.39	0.48
2:B:428:LEU:O	2:B:432:ILE:HG12	2.13	0.48
1:C:742:VAL:O	1:C:746:VAL:HG23	2.14	0.48
2:B:498:LEU:HD12	2:B:499:GLY:HA2	1.96	0.48
1:C:788:VAL:HG22	1:C:788:VAL:O	2.14	0.48
1:A:788:VAL:HG22	1:A:788:VAL:O	2.14	0.48
3:J:106:PHE:N	3:J:107:PRO:HD3	2.29	0.48
2:B:405:TYR:CD2	2:B:478:PRO:HB3	2.49	0.48
2:B:639:LEU:HD22	2:B:647:TYR:HD2	1.79	0.48
1:C:424:LEU:HG	1:C:428:ILE:HD11	1.96	0.48
1:A:718:LYS:NZ	1:A:722:ASN:OD1	2.37	0.47
1:A:742:VAL:O	1:A:746:VAL:HG23	2.14	0.47
1:A:801:LEU:O	1:A:805:VAL:HG23	2.14	0.47
2:B:519:ASP:N	2:B:520:PRO:HD2	2.28	0.47
2:B:803:LEU:O	2:B:807:MET:HG3	2.13	0.47
2:D:405:TYR:CD2	2:D:478:PRO:HB3	2.49	0.47
3:I:106:PHE:N	3:I:107:PRO:HD3	2.29	0.47
1:C:460:VAL:O	1:C:464:VAL:HG23	2.14	0.47
2:D:498:LEU:HD12	2:D:499:GLY:HA2	1.96	0.47
2:B:650:LEU:HD11	2:B:685:THR:HA	1.96	0.47
1:C:494:LEU:HD13	1:C:728:TYR:CE1	2.49	0.47
1:C:801:LEU:O	1:C:805:VAL:HG23	2.14	0.47
1:A:424:LEU:HG	1:A:428:ILE:HD11	1.96	0.47
1:A:494:LEU:HD13	1:A:728:TYR:CE1	2.49	0.47
1:A:658:SER:HG	1:A:663:PHE:HD2	1.62	0.47
2:B:795:VAL:HG23	1:C:603:PHE:CE2	2.50	0.47
2:D:639:LEU:HD22	2:D:647:TYR:HD2	1.79	0.47
2:D:650:LEU:HD11	2:D:685:THR:HA	1.96	0.47
1:A:460:VAL:O	1:A:464:VAL:HG23	2.14	0.47
2:B:526:TRP:O	2:B:530:VAL:HG23	2.15	0.47
2:D:672:THR:HG22	2:D:675:ARG:NH2	2.29	0.47
3:I:35:MET:CE	3:I:131:PRO:HB3	2.45	0.46
2:B:639:LEU:HD22	2:B:647:TYR:CD2	2.51	0.46
2:B:669:LYS:O	2:B:672:THR:OG1	2.31	0.46
1:C:603:PHE:O	1:C:607:ILE:HG12	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:538:VAL:O	2:B:542:LEU:HG	2.15	0.46
1:C:497:SER:HB2	1:C:718:LYS:HE3	1.98	0.46
1:A:603:PHE:O	1:A:607:ILE:HG12	2.15	0.46
2:B:672:THR:HG22	2:B:675:ARG:NH2	2.30	0.46
3:J:35:MET:CE	3:J:131:PRO:HB3	2.45	0.46
1:A:603:PHE:CE2	2:D:795:VAL:HG23	2.50	0.46
2:D:639:LEU:HD22	2:D:647:TYR:CD2	2.51	0.46
1:C:641:ILE:HG22	1:C:642:ALA:N	2.31	0.46
2:D:481:ILE:O	2:D:482:THR:HG23	2.16	0.46
1:A:497:SER:HB2	1:A:718:LYS:HE3	1.97	0.46
2:D:538:VAL:O	2:D:542:LEU:HG	2.15	0.46
2:D:747:ASN:O	2:D:751:LEU:HD13	2.15	0.46
2:D:526:TRP:O	2:D:530:VAL:HG23	2.15	0.46
1:A:518:ALA:HB1	1:A:520:GLU:OE1	2.17	0.45
1:A:755:LEU:CB	6:A:1203:CYZ:CL	2.98	0.45
2:B:481:ILE:O	2:B:482:THR:HG23	2.16	0.45
2:B:760:ASP:OD1	2:B:764:ASN:ND2	2.50	0.45
1:C:405:LYS:NZ	1:C:415:ASP:O	2.45	0.45
2:D:760:ASP:OD1	2:D:764:ASN:ND2	2.50	0.45
6:D:902:CYZ:CL	6:D:902:CYZ:O4	2.71	0.45
2:B:747:ASN:O	2:B:751:LEU:HD13	2.15	0.45
2:B:704:LEU:HD12	2:B:708:MET:HB2	1.99	0.45
2:D:681:VAL:HG23	2:D:682:PHE:CD1	2.52	0.45
3:I:145:VAL:O	3:I:148:SER:HB3	2.17	0.45
1:A:406:LYS:O	1:A:407:ASN:HB2	2.17	0.45
2:B:681:VAL:HG23	2:B:682:PHE:CD1	2.52	0.45
1:C:518:ALA:HB1	1:C:520:GLU:OE1	2.17	0.44
6:B:902:CYZ:CL	6:B:902:CYZ:O4	2.71	0.44
8:B:903:79N:HO3	8:B:903:79N:C15	2.30	0.44
1:C:730:ILE:HG22	1:C:731:ALA:N	2.32	0.44
2:B:573:ILE:HG23	2:B:574:PHE:CD1	2.50	0.44
1:C:406:LYS:O	1:C:407:ASN:HB2	2.17	0.44
1:C:446:TYR:CD2	5:C:1202:GLU:HB2	2.53	0.44
3:J:105:HIS:CB	3:J:126:ALA:HB2	2.47	0.44
1:A:480:VAL:HG23	1:A:481:ARG:N	2.33	0.44
1:A:641:ILE:HG22	1:A:642:ALA:N	2.31	0.44
1:A:749:LEU:HD12	1:A:754:VAL:CG1	2.46	0.44
8:D:903:79N:HO3	8:D:903:79N:C15	2.30	0.44
3:I:105:HIS:CB	3:I:126:ALA:HB2	2.47	0.44
2:B:400:ILE:HG13	2:B:401:LEU:N	2.33	0.44
2:B:617:THR:HG22	1:C:610:SER:OG	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:145:VAL:O	3:J:148:SER:HB3	2.17	0.44
1:A:423:GLU:O	1:A:426:ALA:HB3	2.18	0.44
2:B:647:TYR:HA	2:B:701:ALA:O	2.17	0.44
1:C:423:GLU:O	1:C:426:ALA:HB3	2.18	0.44
3:J:127:SER:O	3:J:128:SER:OG	2.35	0.44
3:J:159:LEU:HD12	3:J:226:TYR:CE2	2.53	0.44
1:A:730:ILE:HG22	1:A:731:ALA:N	2.32	0.44
1:A:749:LEU:HD13	1:A:754:VAL:HG21	2.00	0.44
1:C:749:LEU:HD12	1:C:754:VAL:CG1	2.47	0.44
2:D:400:ILE:HG13	2:D:401:LEU:N	2.33	0.44
2:D:751:LEU:O	2:D:755:GLU:HG2	2.18	0.44
2:B:751:LEU:O	2:B:755:GLU:HG2	2.18	0.43
1:C:532:VAL:HG21	1:C:601:TRP:CE3	2.53	0.43
1:C:755:LEU:CB	6:C:1203:CYZ:CL	2.98	0.43
2:D:704:LEU:HD12	2:D:708:MET:HB2	1.99	0.43
2:D:404:PRO:HD3	2:D:711:TYR:CD2	2.53	0.43
2:D:647:TYR:HA	2:D:701:ALA:O	2.17	0.43
1:A:392:ILE:HB	1:A:469:ASP:H	1.84	0.43
1:A:610:SER:OG	2:D:617:THR:HG22	2.18	0.43
2:B:706:SER:O	2:B:710:GLU:HG3	2.18	0.43
3:J:160:GLY:O	3:J:164:LEU:HG	2.19	0.43
3:J:89:ILE:HG13	3:J:90:CYS:N	2.34	0.43
1:C:510:VAL:HG23	1:C:511:PHE:CD1	2.54	0.43
1:A:393:VAL:O	1:A:393:VAL:HG12	2.18	0.43
1:A:446:TYR:CD2	5:A:1202:GLU:HB2	2.53	0.43
2:B:404:PRO:HD3	2:B:711:TYR:CD2	2.53	0.43
1:C:419:GLY:O	1:C:423:GLU:OE1	2.37	0.43
2:B:808:LEU:HD21	2:B:812:ILE:HD11	2.00	0.43
1:C:392:ILE:HB	1:C:469:ASP:H	1.84	0.43
3:I:41:THR:CG2	3:I:42:ASP:N	2.82	0.43
2:B:498:LEU:CD2	2:B:732:TYR:CE1	3.02	0.43
2:D:573:ILE:HG23	2:D:574:PHE:CD1	2.50	0.43
3:I:159:LEU:HD12	3:I:226:TYR:CE2	2.53	0.43
3:I:160:GLY:O	3:I:164:LEU:HG	2.19	0.43
3:I:89:ILE:HG13	3:I:90:CYS:N	2.34	0.43
3:J:34:LEU:HD13	3:J:210:LEU:HD23	2.01	0.43
1:A:532:VAL:HG21	1:A:601:TRP:CE3	2.53	0.43
2:B:486:GLU:OE1	2:B:491:PHE:CD2	2.71	0.43
2:B:808:LEU:C	2:B:808:LEU:HD23	2.39	0.43
1:C:480:VAL:HG23	1:C:481:ARG:N	2.33	0.43
2:D:746:VAL:O	2:D:750:VAL:HG23	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:792:VAL:O	2:D:795:VAL:HG12	2.19	0.43
2:D:808:LEU:HD23	2:D:808:LEU:C	2.39	0.43
1:A:510:VAL:HG23	1:A:511:PHE:CD1	2.54	0.42
3:I:34:LEU:HD13	3:I:210:LEU:HD23	2.01	0.42
3:J:41:THR:CG2	3:J:42:ASP:N	2.82	0.42
2:B:806:ALA:O	2:B:807:MET:C	2.58	0.42
1:C:500:ILE:HG22	1:C:501:LYS:N	2.34	0.42
2:D:808:LEU:HD21	2:D:812:ILE:HD11	2.00	0.42
3:I:32:PHE:O	3:I:36:THR:HG23	2.19	0.42
3:J:32:PHE:O	3:J:36:THR:HG23	2.19	0.42
2:B:746:VAL:O	2:B:750:VAL:HG23	2.19	0.42
1:C:393:VAL:HG12	1:C:393:VAL:O	2.18	0.42
2:D:798:ILE:O	2:D:799:LEU:C	2.57	0.42
3:I:82:THR:HB	3:I:89:ILE:HD11	2.01	0.42
3:J:183:ASN:OD1	3:J:183:ASN:O	2.38	0.42
1:C:688:ARG:O	1:C:692:SER:N	2.53	0.42
1:A:419:GLY:O	1:A:423:GLU:OE1	2.37	0.42
1:A:660:ILE:HG22	1:A:661:ALA:N	2.35	0.42
2:B:792:VAL:O	2:B:795:VAL:HG12	2.19	0.42
2:D:486:GLU:OE1	2:D:491:PHE:CD2	2.71	0.42
2:D:706:SER:O	2:D:710:GLU:HG3	2.18	0.42
2:D:795:VAL:HG13	2:D:796:PHE:N	2.35	0.42
3:I:83:HIS:H	3:I:92:LEU:HD22	1.84	0.42
1:A:500:ILE:HG22	1:A:501:LYS:N	2.34	0.42
1:C:749:LEU:HD13	1:C:754:VAL:HG21	2.00	0.42
2:D:480:THR:HG22	2:D:481:ILE:N	2.35	0.42
2:D:672:THR:HA	2:D:675:ARG:HG2	2.01	0.42
2:D:534:ILE:O	2:D:538:VAL:HG23	2.20	0.42
3:I:183:ASN:OD1	3:I:183:ASN:O	2.38	0.42
1:A:688:ARG:O	1:A:692:SER:N	2.53	0.42
8:A:1206:79N:H	4:D:904:PAM:H151	2.00	0.42
3:I:83:HIS:CD2	3:I:83:HIS:O	2.73	0.42
3:I:172:ASN:HD22	3:I:212:PHE:HB2	1.85	0.42
3:J:82:THR:HB	3:J:89:ILE:HD11	2.01	0.42
3:J:174:ILE:HG21	3:J:174:ILE:HD13	1.78	0.42
2:B:480:THR:HG22	2:B:481:ILE:N	2.35	0.42
2:B:795:VAL:HG13	2:B:796:PHE:N	2.35	0.41
8:B:904:79N:H	4:B:905:PAM:H151	2.00	0.41
3:J:80:GLY:O	3:J:82:THR:HG23	2.20	0.41
2:D:520:PRO:O	2:D:521:LEU:HD23	2.20	0.41
3:J:83:HIS:O	3:J:83:HIS:CD2	2.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:432:VAL:O	1:C:432:VAL:HG12	2.21	0.41
2:D:394:THR:HG22	2:D:395:VAL:N	2.35	0.41
2:D:491:PHE:CD1	2:D:735:ALA:HB2	2.56	0.41
2:D:685:THR:HG23	2:D:688:GLU:H	1.85	0.41
2:D:806:ALA:O	2:D:807:MET:C	2.58	0.41
3:I:80:GLY:O	3:I:82:THR:HG23	2.20	0.41
3:I:198:HIS:ND1	3:I:199:TYR:N	2.68	0.41
3:J:42:ASP:HA	3:J:85:GLY:HA3	2.02	0.41
3:J:83:HIS:H	3:J:92:LEU:HD22	1.84	0.41
2:B:418:ASN:ND2	2:B:440:TYR:CE1	2.88	0.41
2:B:523:TYR:HD2	8:B:903:79N:H12	1.86	0.41
2:B:685:THR:HG23	2:B:688:GLU:H	1.85	0.41
3:I:89:ILE:HG13	3:I:90:CYS:H	1.86	0.41
2:B:520:PRO:O	2:B:521:LEU:HD23	2.20	0.41
2:D:523:TYR:HD2	8:D:903:79N:H12	1.86	0.41
2:B:609:THR:HG23	2:B:609:THR:H	1.72	0.41
2:B:622:ALA:O	2:B:626:VAL:N	2.54	0.41
1:C:660:ILE:HG22	1:C:661:ALA:N	2.35	0.41
2:D:498:LEU:CD2	2:D:732:TYR:CE1	3.02	0.41
3:J:198:HIS:ND1	3:J:199:TYR:N	2.68	0.41
2:D:416:GLU:HA	2:D:420:ARG:HD2	2.03	0.41
2:D:489:ILE:HB	2:D:736:THR:O	2.21	0.41
1:A:432:VAL:HG12	1:A:432:VAL:O	2.20	0.41
1:A:494:LEU:HD12	1:A:701:GLU:HB3	2.03	0.41
1:A:749:LEU:CD1	1:A:754:VAL:HG11	2.50	0.41
2:B:394:THR:HG22	2:B:395:VAL:N	2.36	0.41
2:B:400:ILE:O	2:B:406:VAL:HB	2.21	0.41
2:B:489:ILE:HB	2:B:736:THR:O	2.21	0.41
2:B:491:PHE:CD1	2:B:735:ALA:HB2	2.56	0.41
2:B:534:ILE:O	2:B:538:VAL:HG23	2.20	0.41
2:B:798:ILE:O	2:B:799:LEU:C	2.57	0.41
1:C:395:THR:OG1	1:C:473:ALA:HB2	2.21	0.41
2:D:509:LYS:HG2	2:D:629:MET:SD	2.61	0.41
3:I:42:ASP:HA	3:I:85:GLY:HA3	2.02	0.41
3:J:110:THR:O	3:J:112:TYR:N	2.53	0.41
3:J:148:SER:OG	3:J:158:ILE:CD1	2.69	0.41
2:B:416:GLU:HA	2:B:420:ARG:HD2	2.03	0.41
2:D:418:ASN:ND2	2:D:440:TYR:CE1	2.88	0.41
3:J:130:PHE:HB2	3:J:131:PRO:HD3	2.03	0.41
2:B:509:LYS:HG2	2:B:629:MET:SD	2.61	0.40
2:B:672:THR:HA	2:B:675:ARG:HG2	2.01	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:799:LEU:CD2	2:B:803:LEU:HD11	2.52	0.40
1:C:498:ILE:HB	1:C:719:VAL:HG13	2.03	0.40
2:D:400:ILE:O	2:D:406:VAL:HB	2.21	0.40
3:I:130:PHE:HB2	3:I:131:PRO:HD3	2.03	0.40
3:I:136:ILE:HG22	3:I:140:LEU:HD12	2.02	0.40
3:J:136:ILE:HG22	3:J:140:LEU:HD12	2.02	0.40
1:A:395:THR:OG1	1:A:473:ALA:HB2	2.21	0.40
1:A:706:GLU:O	1:A:710:GLN:HG2	2.22	0.40
3:J:172:ASN:HD22	3:J:212:PHE:HB2	1.85	0.40
1:A:707:TYR:O	1:A:711:ARG:HG2	2.22	0.40
1:C:425:ALA:HA	1:C:428:ILE:HD12	2.04	0.40
1:C:643:TYR:O	1:C:643:TYR:CD1	2.75	0.40
1:C:707:TYR:O	1:C:711:ARG:HG2	2.22	0.40
2:D:622:ALA:O	2:D:626:VAL:N	2.54	0.40
3:J:148:SER:OG	3:J:158:ILE:CG1	2.70	0.40
3:J:173:ILE:HG13	3:J:174:ILE:N	2.37	0.40
1:A:425:ALA:HA	1:A:428:ILE:HD12	2.04	0.40
1:A:643:TYR:CD1	1:A:643:TYR:O	2.75	0.40
1:C:500:ILE:HG22	1:C:501:LYS:O	2.21	0.40
1:C:789:ALA:HA	1:C:792:PHE:HD2	1.87	0.40
2:D:664:ILE:HB	2:D:667:PHE:HD2	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [\(i\)](#)

5.3.1 Protein backbone [\(i\)](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	392/915 (43%)	353 (90%)	39 (10%)	0	100	100
1	C	392/915 (43%)	354 (90%)	38 (10%)	0	100	100
2	B	392/860 (46%)	362 (92%)	30 (8%)	0	100	100
2	D	392/860 (46%)	362 (92%)	30 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	I	179/423 (42%)	160 (89%)	19 (11%)	0	100	100
3	J	179/423 (42%)	160 (89%)	19 (11%)	0	100	100
All	All	1926/4396 (44%)	1751 (91%)	175 (9%)	0	100	100

There are no Ramachandran outliers to report.

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	285/778 (37%)	284 (100%)	1 (0%)	91	96
1	C	285/778 (37%)	284 (100%)	1 (0%)	91	96
2	B	309/737 (42%)	308 (100%)	1 (0%)	92	97
2	D	309/737 (42%)	308 (100%)	1 (0%)	92	97
3	I	128/309 (41%)	126 (98%)	2 (2%)	62	83
3	J	128/309 (41%)	126 (98%)	2 (2%)	62	83
All	All	1444/3648 (40%)	1436 (99%)	8 (1%)	86	94

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	765	ASP
2	B	744	THR
1	C	765	ASP
2	D	744	THR
3	I	48	ARG
3	I	89	ILE
3	J	48	ARG
3	J	89	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
3	I	83	HIS
3	I	105	HIS
3	J	83	HIS
3	J	105	HIS

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](#)

28 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
4	PAM	C	1205	-	14,17,17	0.31	0	13,17,17	0.60	0
4	PAM	J	1704	-	14,17,17	0.24	0	13,17,17	0.55	0
4	PAM	B	905	-	14,17,17	0.29	0	13,17,17	0.79	0
8	79N	B	904	-	22,22,22	0.85	2 (9%)	23,23,23	1.20	2 (8%)
5	GLU	D	901	-	2,9,9	0.35	0	2,11,11	0.14	0
8	79N	A	1206	-	22,22,22	0.85	2 (9%)	23,23,23	1.20	2 (8%)
8	79N	B	903	-	22,22,22	0.82	1 (4%)	23,23,23	0.97	1 (4%)
4	PAM	A	1201	-	14,17,17	0.27	0	13,17,17	0.71	0
4	PAM	I	1504	-	14,17,17	0.25	0	13,17,17	0.55	0
5	GLU	B	901	-	2,9,9	0.35	0	2,11,11	0.14	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	79N	D	903	-	22,22,22	0.82	1 (4%)	23,23,23	0.97	1 (4%)
4	PAM	J	1701	-	14,17,17	0.32	0	13,17,17	0.71	0
6	CYZ	A	1203	-	26,27,27	0.56	0	38,44,44	0.51	0
7	OLC	C	1204	-	24,24,24	0.81	2 (8%)	25,25,25	0.82	1 (4%)
4	PAM	C	1201	-	14,17,17	0.27	0	13,17,17	0.71	0
6	CYZ	B	902	-	26,27,27	0.50	0	38,44,44	0.66	1 (2%)
4	PAM	I	1503	-	14,17,17	0.29	0	13,17,17	0.80	0
4	PAM	J	1703	-	14,17,17	0.29	0	13,17,17	0.80	0
4	PAM	D	904	-	14,17,17	0.29	0	13,17,17	0.79	0
6	CYZ	C	1203	-	26,27,27	0.56	0	38,44,44	0.50	0
4	PAM	I	1502	-	14,17,17	0.32	0	13,17,17	0.70	0
5	GLU	C	1202	-	2,9,9	0.56	0	2,11,11	0.27	0
4	PAM	I	1501	-	14,17,17	0.26	0	13,17,17	0.66	0
4	PAM	A	1205	-	14,17,17	0.31	0	13,17,17	0.60	0
6	CYZ	D	902	-	26,27,27	0.50	0	38,44,44	0.66	1 (2%)
7	OLC	A	1204	-	24,24,24	0.80	2 (8%)	25,25,25	0.82	1 (4%)
5	GLU	A	1202	-	2,9,9	0.54	0	2,11,11	0.28	0
4	PAM	J	1702	-	14,17,17	0.26	0	13,17,17	0.66	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
4	PAM	C	1205	-	-	7/13/15/15	-
4	PAM	J	1704	-	-	5/13/15/15	-
4	PAM	B	905	-	-	6/13/15/15	-
8	79N	B	904	-	-	11/22/22/22	-
5	GLU	D	901	-	-	1/3/9/9	-
8	79N	A	1206	-	-	11/22/22/22	-
8	79N	B	903	-	-	14/22/22/22	-
4	PAM	A	1201	-	-	8/13/15/15	-
4	PAM	I	1504	-	-	5/13/15/15	-
5	GLU	B	901	-	-	1/3/9/9	-
8	79N	D	903	-	-	14/22/22/22	-
4	PAM	J	1701	-	-	8/13/15/15	-
6	CYZ	A	1203	-	-	6/6/42/42	0/5/4/4
7	OLC	C	1204	-	-	11/24/24/24	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PAM	C	1201	-	-	8/13/15/15	-
6	CYZ	B	902	-	-	6/6/42/42	0/5/4/4
4	PAM	I	1503	-	-	8/13/15/15	-
4	PAM	J	1703	-	-	8/13/15/15	-
4	PAM	D	904	-	-	6/13/15/15	-
6	CYZ	C	1203	-	-	6/6/42/42	0/5/4/4
4	PAM	I	1502	-	-	8/13/15/15	-
5	GLU	C	1202	-	-	1/3/9/9	-
4	PAM	I	1501	-	-	6/13/15/15	-
4	PAM	A	1205	-	-	7/13/15/15	-
6	CYZ	D	902	-	-	6/6/42/42	0/5/4/4
7	OLC	A	1204	-	-	11/24/24/24	-
5	GLU	A	1202	-	-	1/3/9/9	-
4	PAM	J	1702	-	-	6/13/15/15	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	903	79N	O1-C15	2.52	1.40	1.33
8	D	903	79N	O1-C15	2.52	1.40	1.33
8	A	1206	79N	O1-C16	-2.38	1.39	1.45
8	B	904	79N	O1-C16	-2.36	1.39	1.45
7	A	1204	OLC	O20-C1	2.31	1.40	1.33
7	C	1204	OLC	O20-C1	2.31	1.40	1.33
7	C	1204	OLC	O20-C21	-2.28	1.39	1.45
8	A	1206	79N	O1-C15	2.26	1.39	1.33
8	B	904	79N	O1-C15	2.26	1.39	1.33
7	A	1204	OLC	O20-C21	-2.26	1.40	1.45

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	902	CYZ	C2-C1-C8	3.17	119.33	114.81
6	D	902	CYZ	C2-C1-C8	3.13	119.27	114.81
8	A	1206	79N	O1-C15-C14	3.05	121.47	111.91
8	B	904	79N	O1-C15-C14	3.05	121.47	111.91
8	B	903	79N	O1-C15-C14	2.82	120.75	111.91
8	D	903	79N	O1-C15-C14	2.82	120.75	111.91
7	A	1204	OLC	O20-C1-C2	2.39	119.41	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	1204	OLC	O20-C1-C2	2.39	119.41	111.91
8	A	1206	79N	C10-C9-C8	2.20	141.59	124.73
8	B	904	79N	C10-C9-C8	2.20	141.59	124.73

There are no chirality outliers.

All (196) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1205	PAM	C1-C2-C3-C4
4	B	905	PAM	C1-C2-C3-C4
4	C	1205	PAM	C1-C2-C3-C4
4	D	904	PAM	C1-C2-C3-C4
4	I	1502	PAM	C1-C2-C3-C4
4	I	1503	PAM	C1-C2-C3-C4
4	I	1504	PAM	C1-C2-C3-C4
4	J	1701	PAM	C1-C2-C3-C4
4	J	1703	PAM	C1-C2-C3-C4
4	J	1704	PAM	C1-C2-C3-C4
6	A	1203	CYZ	C11-C12-S2-O3
6	A	1203	CYZ	C11-C12-S2-O4
6	A	1203	CYZ	C11-C12-S2-N3
6	A	1203	CYZ	C13-C12-S2-O3
6	A	1203	CYZ	C13-C12-S2-O4
6	A	1203	CYZ	C13-C12-S2-N3
6	B	902	CYZ	C13-C12-S2-O3
6	C	1203	CYZ	C11-C12-S2-O3
6	C	1203	CYZ	C11-C12-S2-O4
6	C	1203	CYZ	C11-C12-S2-N3
6	C	1203	CYZ	C13-C12-S2-O3
6	C	1203	CYZ	C13-C12-S2-O4
6	C	1203	CYZ	C13-C12-S2-N3
6	D	902	CYZ	C13-C12-S2-O3
8	B	903	79N	C16-C17-C18-O3
8	D	903	79N	C16-C17-C18-O3
8	B	903	79N	C14-C15-O1-C16
8	D	903	79N	C14-C15-O1-C16
8	A	1206	79N	O-C15-O1-C16
8	B	903	79N	O-C15-O1-C16
8	B	904	79N	O-C15-O1-C16
8	D	903	79N	O-C15-O1-C16
8	A	1206	79N	C14-C15-O1-C16
8	B	904	79N	C14-C15-O1-C16

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Mol	Chain	Res	Type	Atoms
6	B	902	CYZ	C13-C12-S2-O4
6	D	902	CYZ	C13-C12-S2-O4
7	A	1204	OLC	C2-C1-O20-C21
7	C	1204	OLC	C2-C1-O20-C21
8	A	1206	79N	O1-C16-C17-O2
8	B	904	79N	O1-C16-C17-O2
8	B	903	79N	C12-C13-C14-C15
8	D	903	79N	C12-C13-C14-C15
6	B	902	CYZ	C13-C12-S2-N3
6	D	902	CYZ	C13-C12-S2-N3
7	A	1204	OLC	O19-C1-O20-C21
7	C	1204	OLC	O19-C1-O20-C21
7	A	1204	OLC	C1-C2-C3-C4
7	C	1204	OLC	C1-C2-C3-C4
8	B	903	79N	C9-C10-C11-C12
8	D	903	79N	C9-C10-C11-C12
4	A	1205	PAM	C5-C6-C7-C8
4	C	1205	PAM	C5-C6-C7-C8
4	I	1501	PAM	C4-C5-C6-C7
4	J	1702	PAM	C4-C5-C6-C7
8	A	1206	79N	O1-C16-C17-C18
8	B	904	79N	O1-C16-C17-C18
4	A	1201	PAM	C4-C5-C6-C7
4	A	1205	PAM	C12-C13-C14-C15
4	C	1205	PAM	C12-C13-C14-C15
4	C	1201	PAM	C4-C5-C6-C7
4	I	1502	PAM	C4-C5-C6-C7
4	J	1701	PAM	C4-C5-C6-C7
4	A	1205	PAM	C4-C5-C6-C7
4	C	1205	PAM	C4-C5-C6-C7
4	I	1501	PAM	C2-C3-C4-C5
4	J	1702	PAM	C2-C3-C4-C5
4	I	1504	PAM	C3-C4-C5-C6
4	I	1504	PAM	C5-C6-C7-C8
4	J	1704	PAM	C3-C4-C5-C6
4	J	1704	PAM	C5-C6-C7-C8
4	A	1201	PAM	C5-C6-C7-C8
4	A	1205	PAM	C3-C4-C5-C6
4	C	1201	PAM	C5-C6-C7-C8
4	C	1205	PAM	C3-C4-C5-C6
7	A	1204	OLC	C2-C3-C4-C5
7	C	1204	OLC	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
4	A	1205	PAM	C2-C3-C4-C5
4	C	1205	PAM	C2-C3-C4-C5
8	A	1206	79N	C1-C2-C3-C4
8	B	904	79N	C1-C2-C3-C4
8	B	903	79N	C1-C2-C3-C4
8	D	903	79N	C1-C2-C3-C4
8	B	903	79N	O2-C17-C18-O3
8	D	903	79N	O2-C17-C18-O3
8	A	1206	79N	C9-C10-C11-C12
8	B	904	79N	C9-C10-C11-C12
4	A	1201	PAM	C2-C3-C4-C5
4	C	1201	PAM	C2-C3-C4-C5
4	B	905	PAM	C11-C12-C13-C14
4	D	904	PAM	C11-C12-C13-C14
7	A	1204	OLC	C4-C5-C6-C7
7	C	1204	OLC	C4-C5-C6-C7
5	B	901	GLU	CA-CB-CG-CD
5	D	901	GLU	CA-CB-CG-CD
4	A	1201	PAM	C9-C10-C11-C12
4	C	1201	PAM	C9-C10-C11-C12
4	I	1502	PAM	C6-C7-C8-C9
4	I	1502	PAM	C10-C11-C12-C13
4	J	1701	PAM	C6-C7-C8-C9
4	J	1701	PAM	C10-C11-C12-C13
4	B	905	PAM	C3-C4-C5-C6
4	D	904	PAM	C3-C4-C5-C6
4	B	905	PAM	C6-C7-C8-C9
4	D	904	PAM	C6-C7-C8-C9
8	B	903	79N	C5-C6-C7-C8
8	D	903	79N	C5-C6-C7-C8
4	I	1503	PAM	C4-C5-C6-C7
4	J	1703	PAM	C4-C5-C6-C7
4	I	1503	PAM	C10-C11-C12-C13
4	J	1703	PAM	C10-C11-C12-C13
8	A	1206	79N	C5-C6-C7-C8
8	B	904	79N	C5-C6-C7-C8
4	B	905	PAM	C2-C3-C4-C5
4	D	904	PAM	C2-C3-C4-C5
4	I	1502	PAM	C3-C4-C5-C6
4	J	1701	PAM	C3-C4-C5-C6
4	I	1503	PAM	C12-C13-C14-C15
4	J	1703	PAM	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
6	B	902	CYZ	C11-C12-S2-O4
4	I	1502	PAM	C12-C13-C14-C15
4	J	1701	PAM	C12-C13-C14-C15
6	D	902	CYZ	C11-C12-S2-O4
4	I	1501	PAM	C5-C6-C7-C8
4	J	1702	PAM	C5-C6-C7-C8
4	A	1201	PAM	C11-C12-C13-C14
4	C	1201	PAM	C11-C12-C13-C14
4	B	905	PAM	C12-C13-C14-C15
4	D	904	PAM	C12-C13-C14-C15
6	D	902	CYZ	C11-C12-S2-O3
7	A	1204	OLC	C12-C13-C14-C15
7	C	1204	OLC	C12-C13-C14-C15
4	A	1201	PAM	C7-C8-C9-C10
4	C	1201	PAM	C7-C8-C9-C10
8	B	903	79N	C3-C4-C5-C6
8	D	903	79N	C3-C4-C5-C6
4	I	1501	PAM	C10-C11-C12-C13
4	J	1702	PAM	C10-C11-C12-C13
8	B	903	79N	O1-C16-C17-O2
8	D	903	79N	O1-C16-C17-O2
4	I	1503	PAM	C7-C8-C9-C10
4	J	1703	PAM	C7-C8-C9-C10
4	I	1503	PAM	C11-C12-C13-C14
4	J	1703	PAM	C11-C12-C13-C14
6	B	902	CYZ	C11-C12-S2-O3
7	A	1204	OLC	C10-C11-C12-C13
7	C	1204	OLC	C10-C11-C12-C13
4	I	1503	PAM	C3-C4-C5-C6
4	J	1703	PAM	C3-C4-C5-C6
8	B	904	79N	C11-C12-C13-C14
8	A	1206	79N	C11-C12-C13-C14
4	I	1502	PAM	C11-C12-C13-C14
4	J	1701	PAM	C11-C12-C13-C14
4	I	1501	PAM	C11-C12-C13-C14
4	J	1702	PAM	C11-C12-C13-C14
6	D	902	CYZ	C11-C12-S2-N3
8	A	1206	79N	C12-C13-C14-C15
8	B	904	79N	C12-C13-C14-C15
6	B	902	CYZ	C11-C12-S2-N3
4	A	1201	PAM	C6-C7-C8-C9
4	I	1501	PAM	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
4	I	1504	PAM	C6-C7-C8-C9
4	J	1702	PAM	C6-C7-C8-C9
4	J	1704	PAM	C6-C7-C8-C9
8	B	903	79N	O1-C16-C17-C18
8	D	903	79N	O1-C16-C17-C18
4	C	1201	PAM	C6-C7-C8-C9
5	A	1202	GLU	CA-CB-CG-CD
4	I	1503	PAM	C5-C6-C7-C8
4	J	1703	PAM	C5-C6-C7-C8
8	B	903	79N	C4-C5-C6-C7
8	D	903	79N	C4-C5-C6-C7
4	A	1205	PAM	C7-C8-C9-C10
4	C	1205	PAM	C7-C8-C9-C10
8	B	903	79N	C10-C11-C12-C13
8	D	903	79N	C10-C11-C12-C13
5	C	1202	GLU	CA-CB-CG-CD
4	C	1201	PAM	C12-C13-C14-C15
7	A	1204	OLC	C6-C7-C8-C9
7	C	1204	OLC	C6-C7-C8-C9
4	A	1201	PAM	C12-C13-C14-C15
7	A	1204	OLC	C9-C10-C11-C12
7	C	1204	OLC	C9-C10-C11-C12
8	A	1206	79N	C6-C7-C8-C9
8	A	1206	79N	C11-C10-C9-C8
8	B	903	79N	C6-C7-C8-C9
8	B	904	79N	C6-C7-C8-C9
8	B	904	79N	C11-C10-C9-C8
8	D	903	79N	C6-C7-C8-C9
7	A	1204	OLC	C7-C8-C9-C10
7	C	1204	OLC	C7-C8-C9-C10
4	I	1504	PAM	C2-C3-C4-C5
4	J	1704	PAM	C2-C3-C4-C5
4	I	1502	PAM	C13-C14-C15-C16
4	J	1701	PAM	C13-C14-C15-C16
7	A	1204	OLC	O23-C22-C24-O25
7	C	1204	OLC	O23-C22-C24-O25

There are no ring outliers.

16 monomers are involved in 44 short contacts:

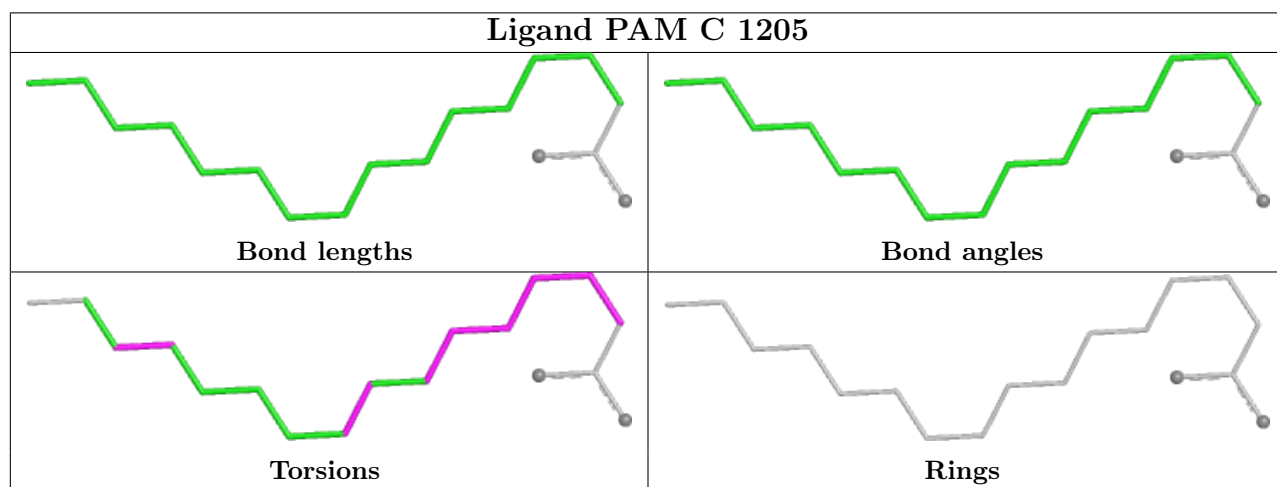
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	905	PAM	6	0

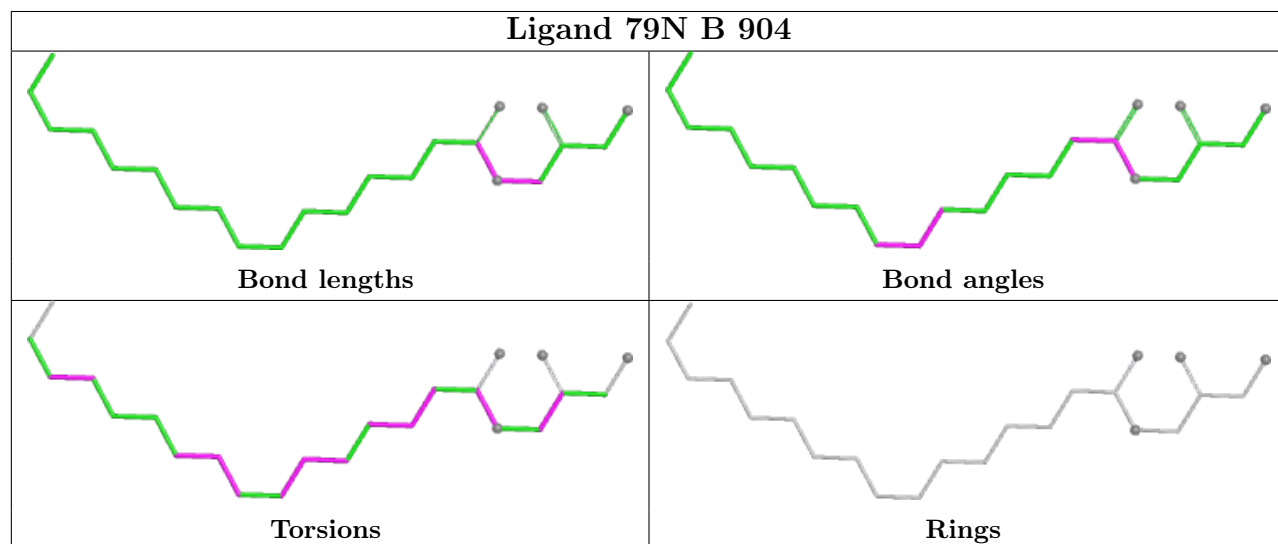
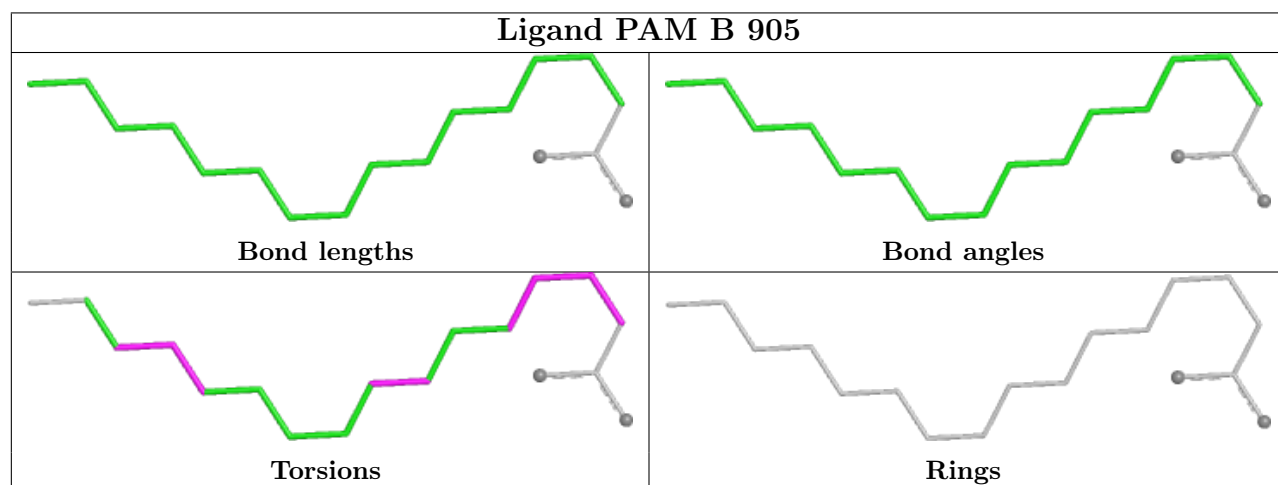
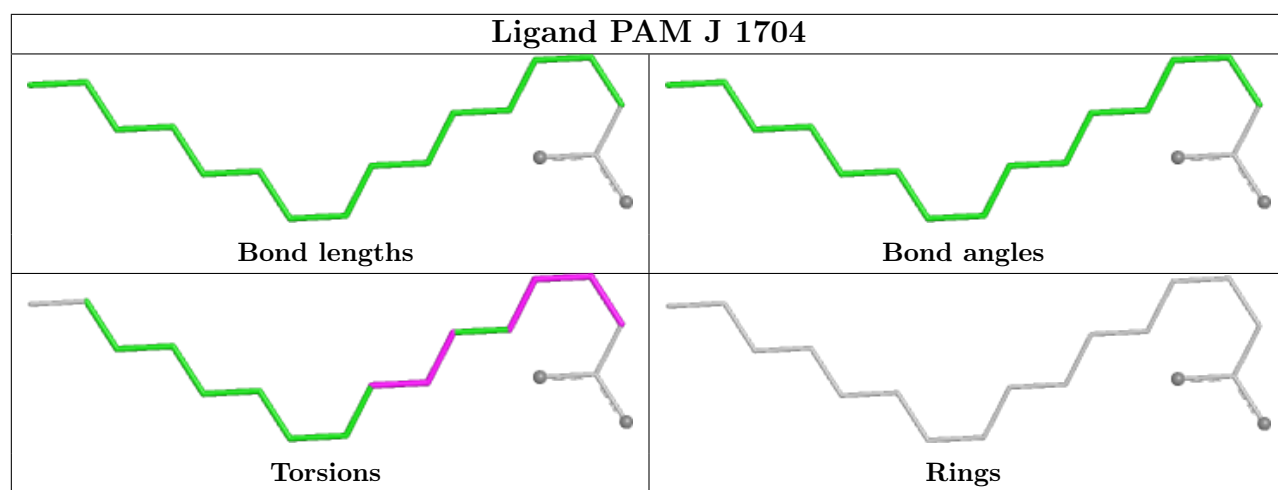
Continued on next page...

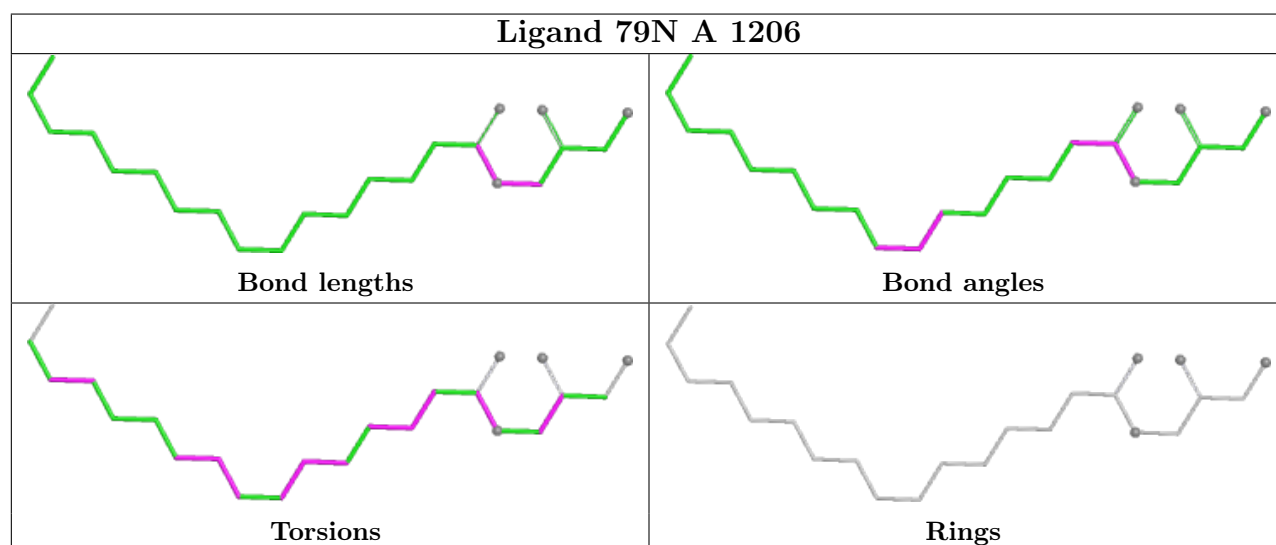
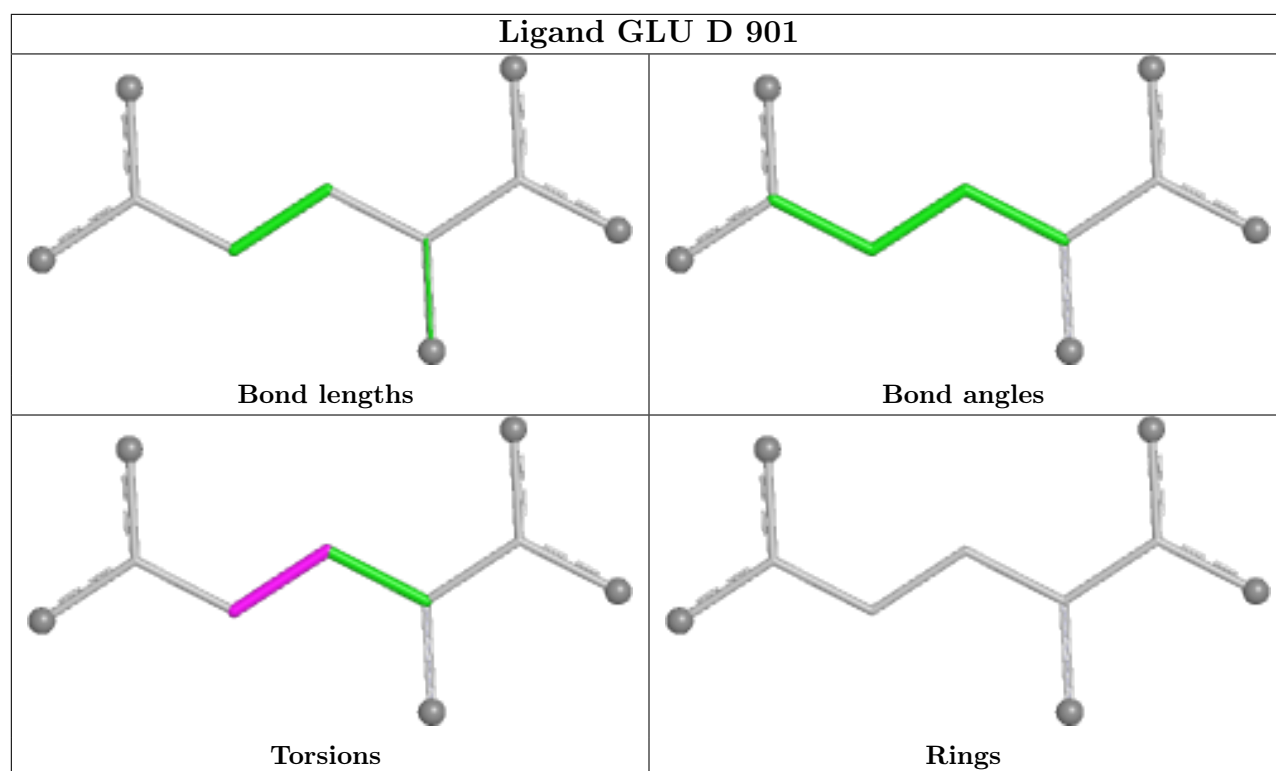
Continued from previous page...

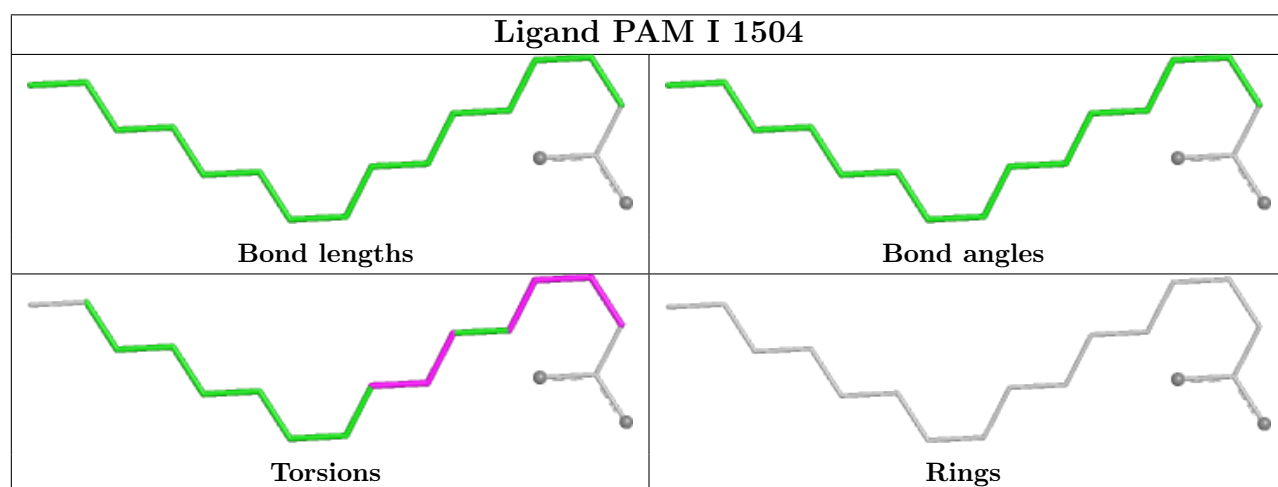
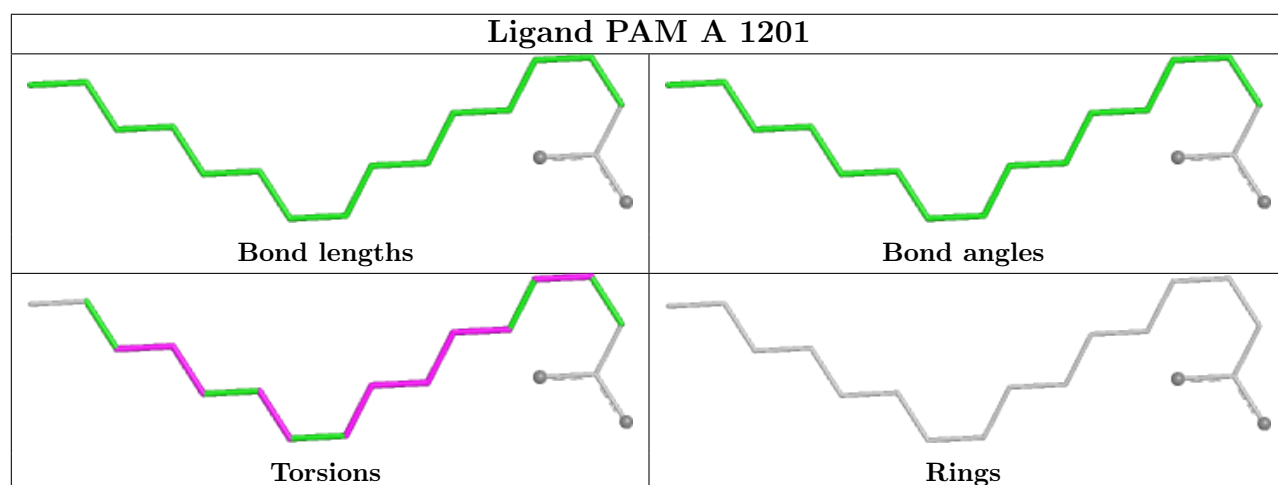
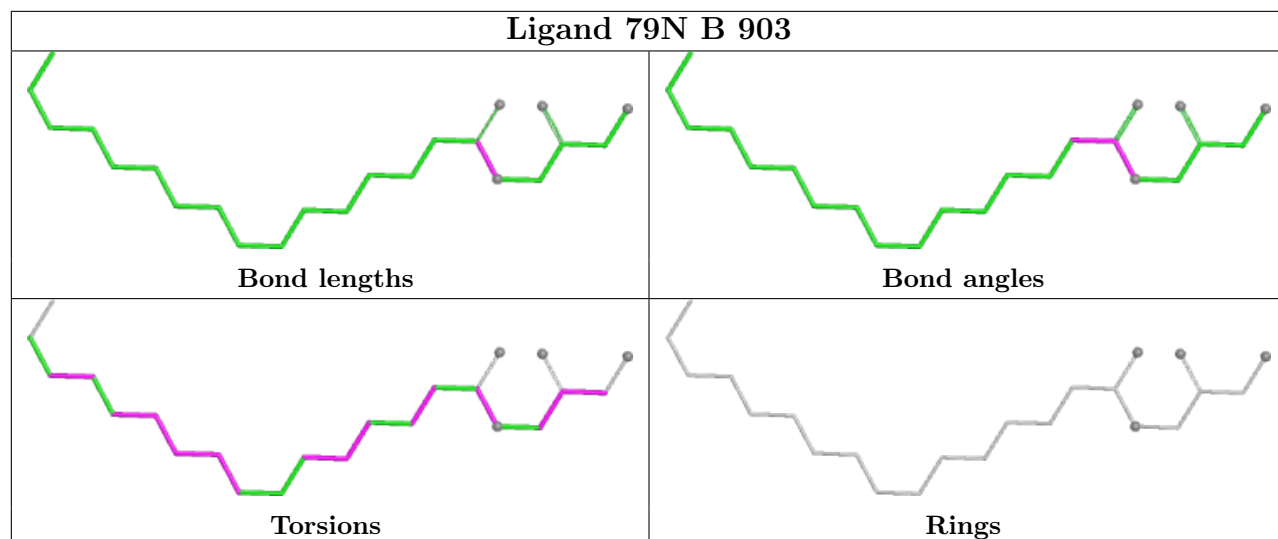
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	904	79N	7	0
5	D	901	GLU	2	0
8	A	1206	79N	7	0
8	B	903	79N	3	0
5	B	901	GLU	2	0
8	D	903	79N	3	0
6	A	1203	CYZ	3	0
6	B	902	CYZ	2	0
4	I	1503	PAM	1	0
4	J	1703	PAM	1	0
4	D	904	PAM	6	0
6	C	1203	CYZ	3	0
5	C	1202	GLU	4	0
6	D	902	CYZ	2	0
5	A	1202	GLU	4	0

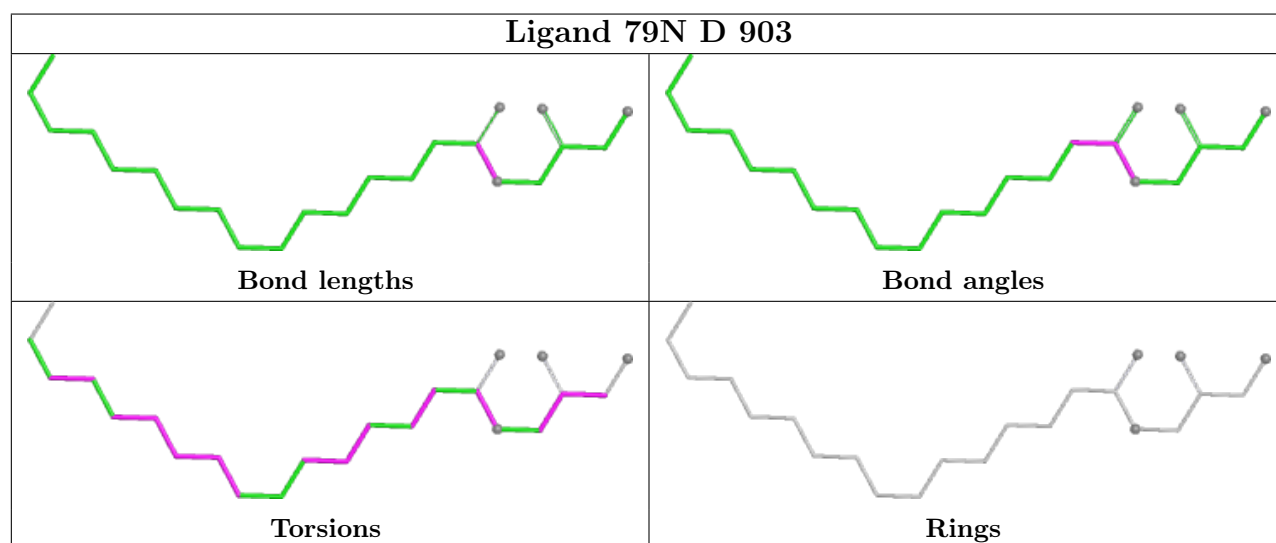
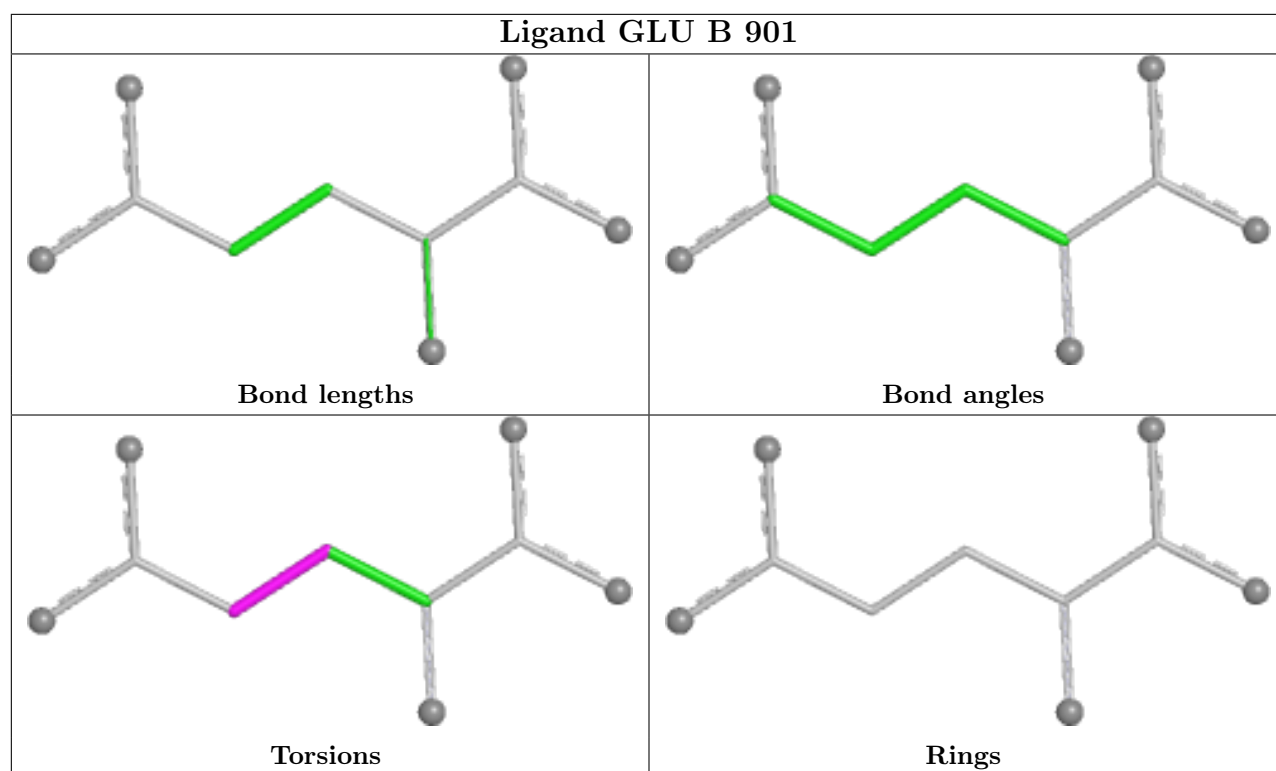
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

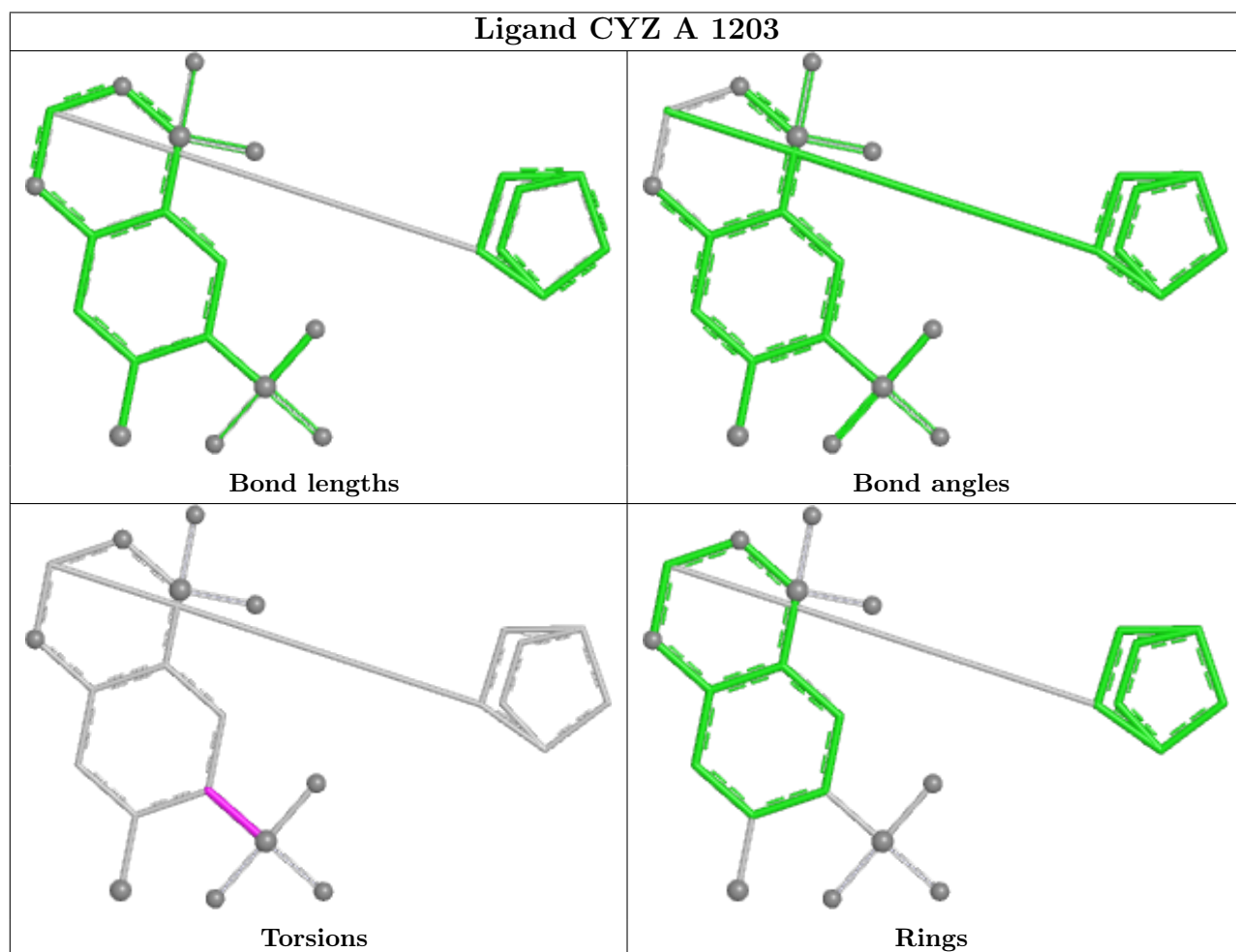
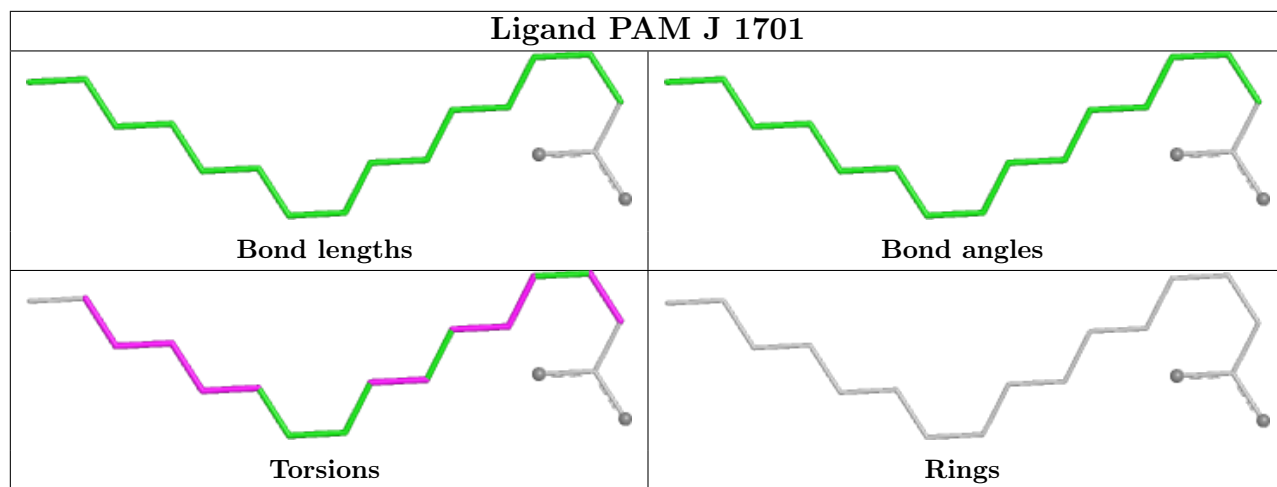


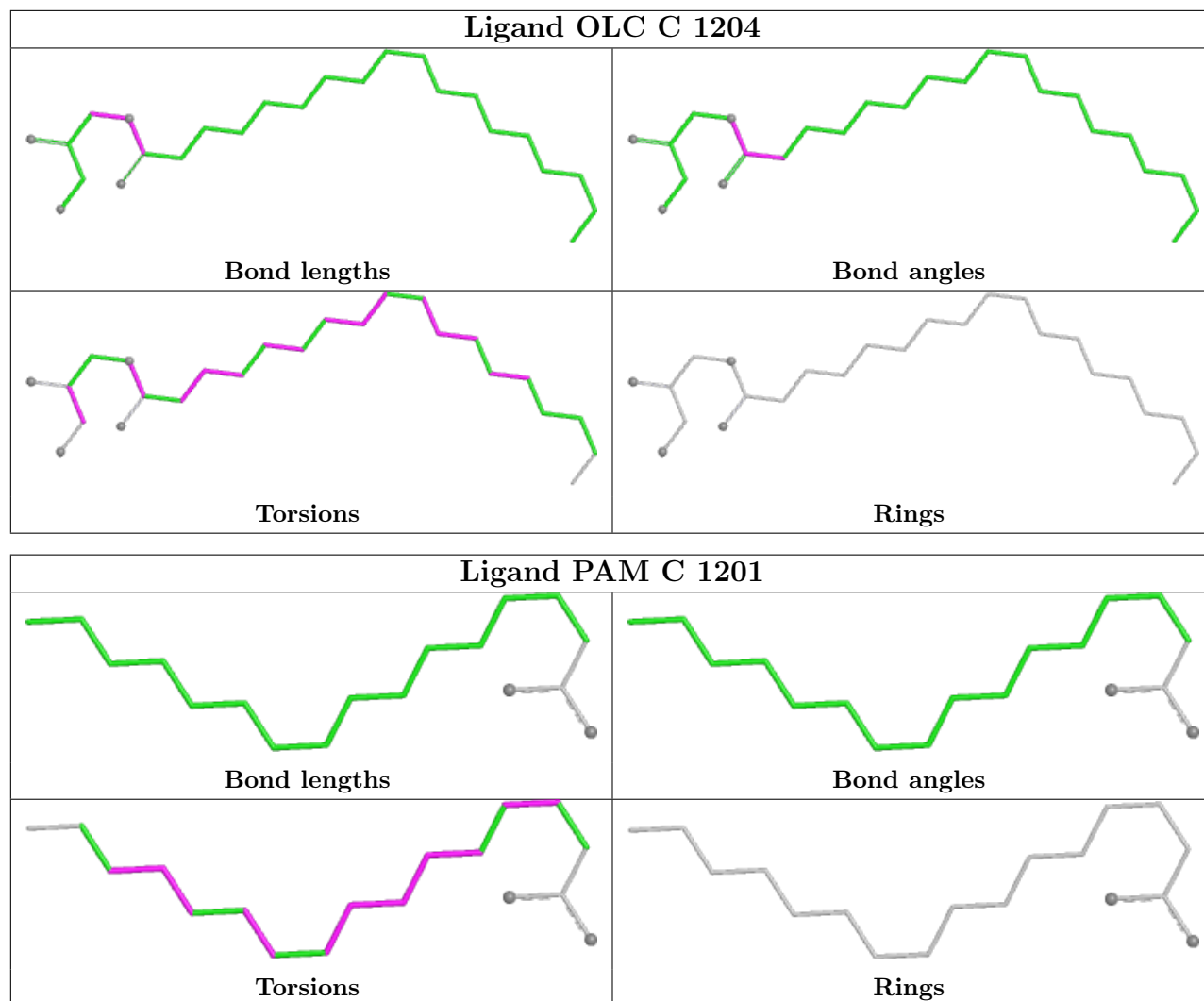


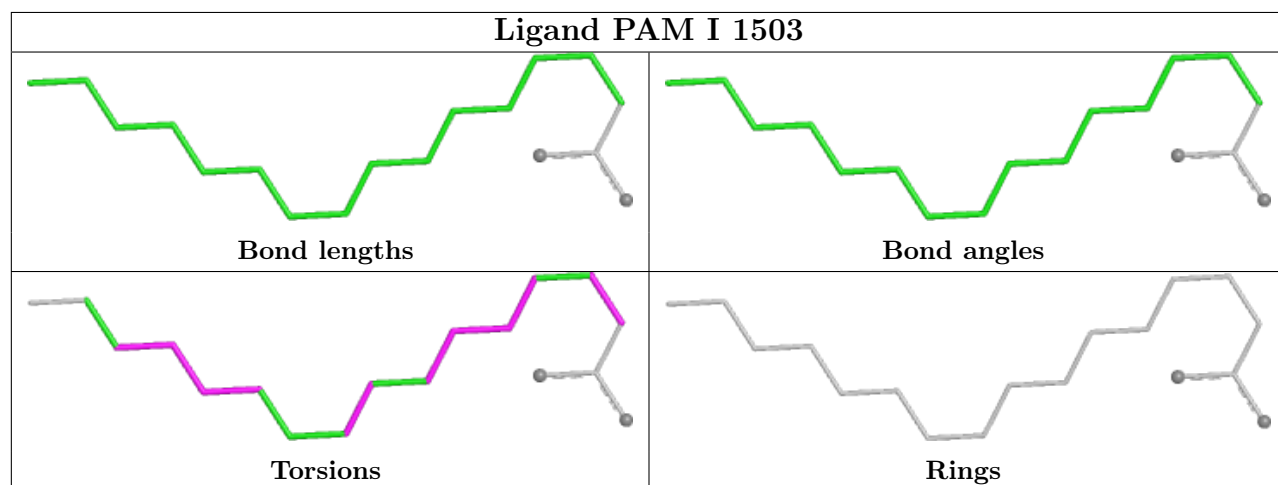
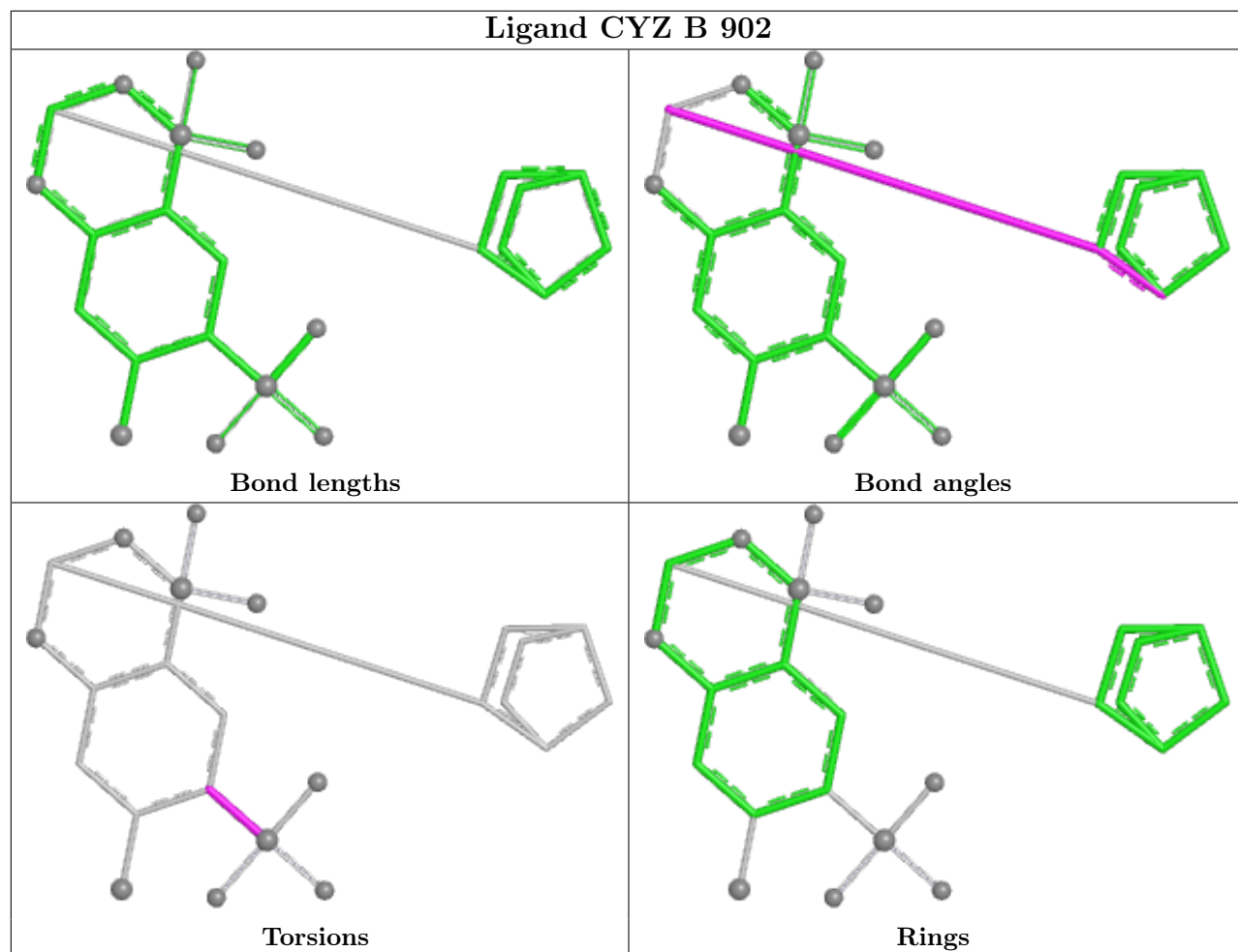


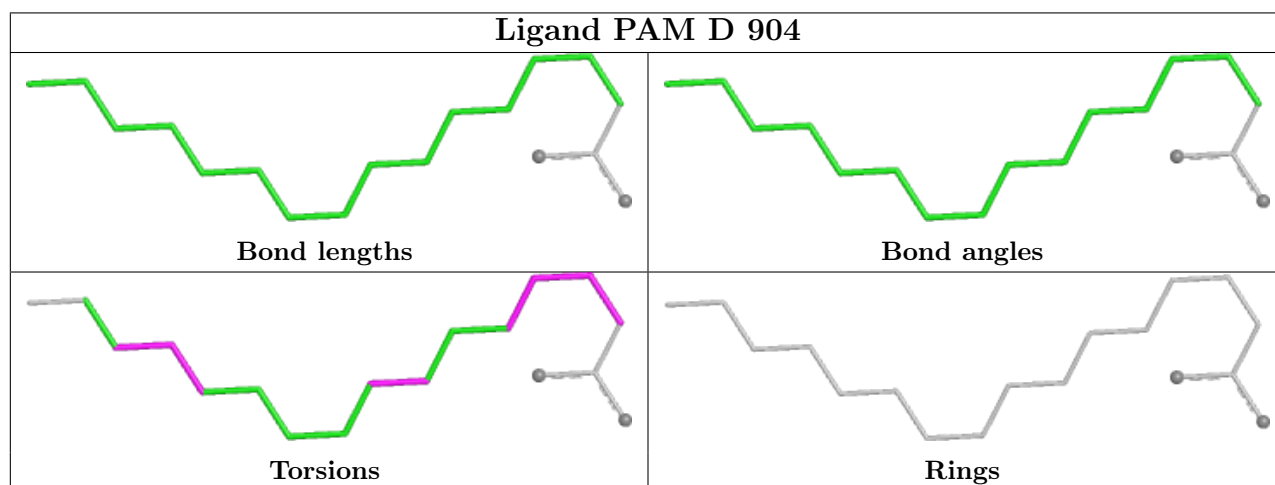
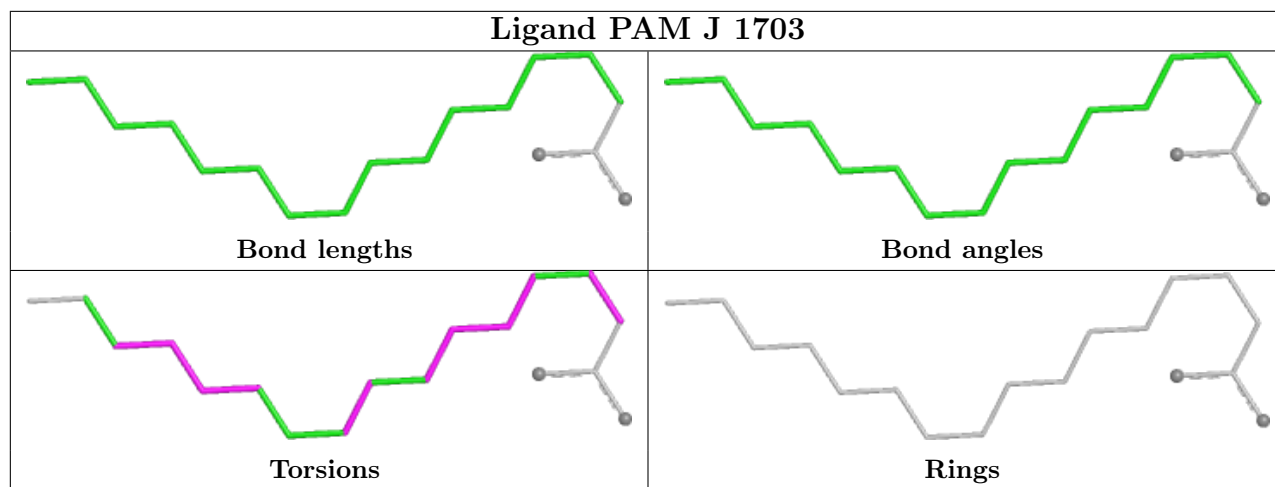


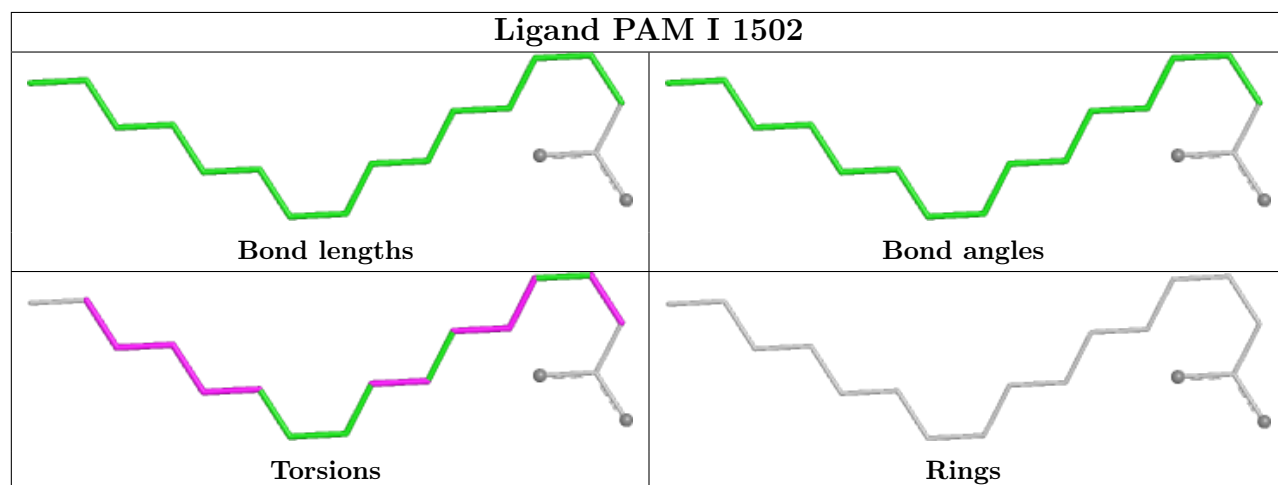
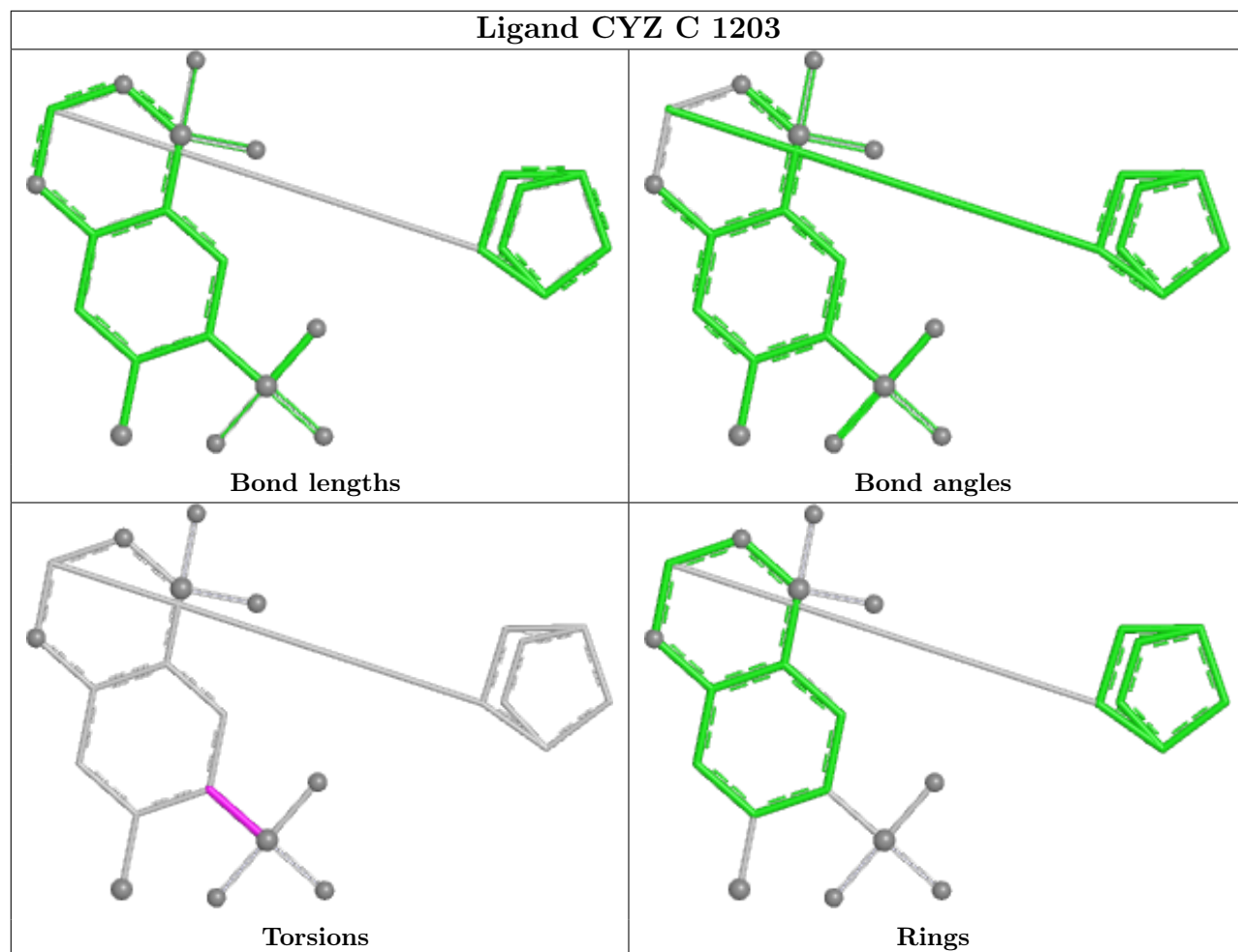


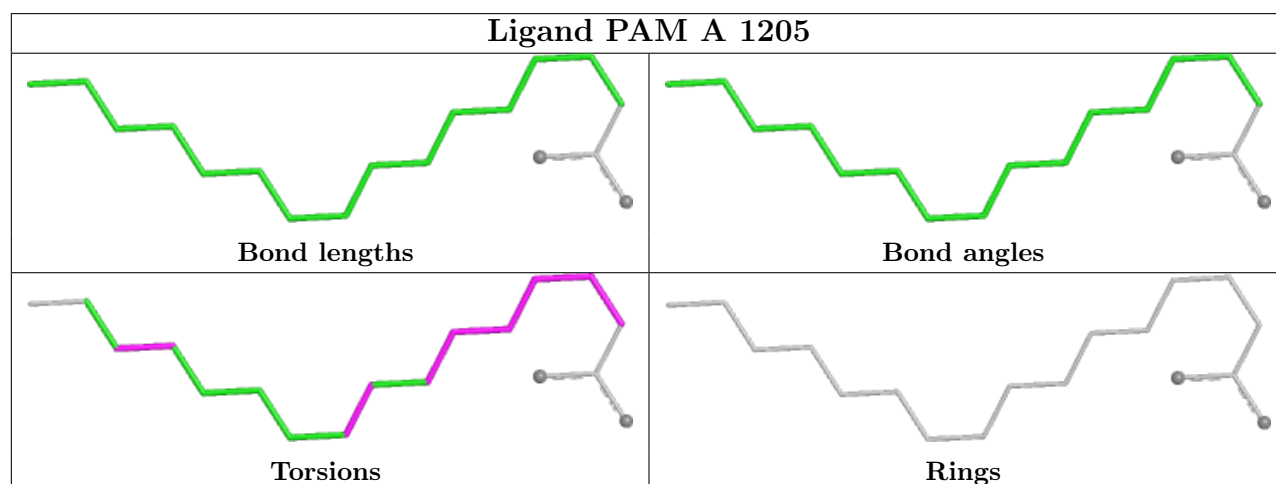
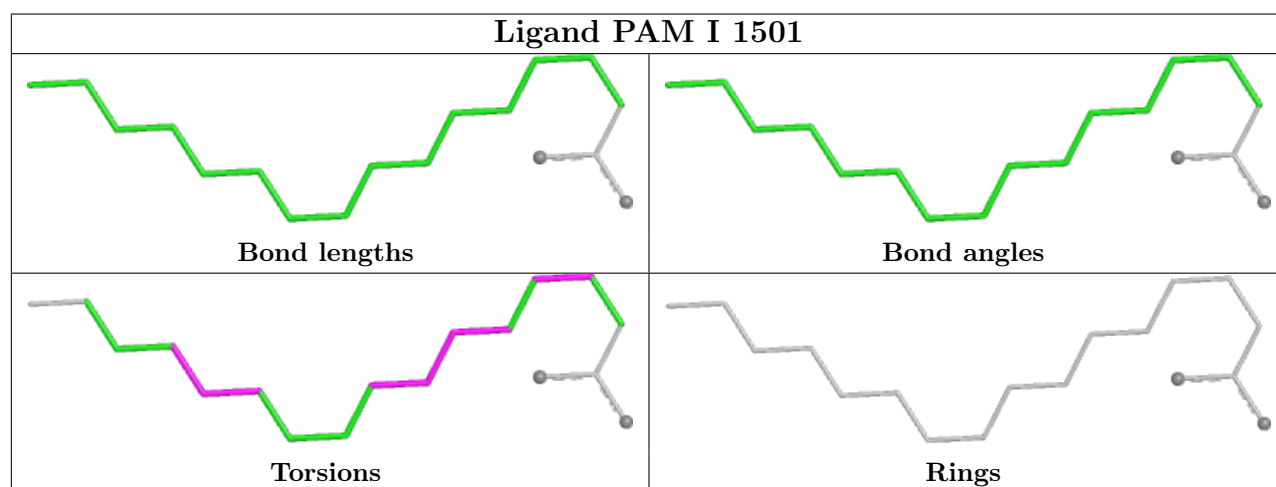
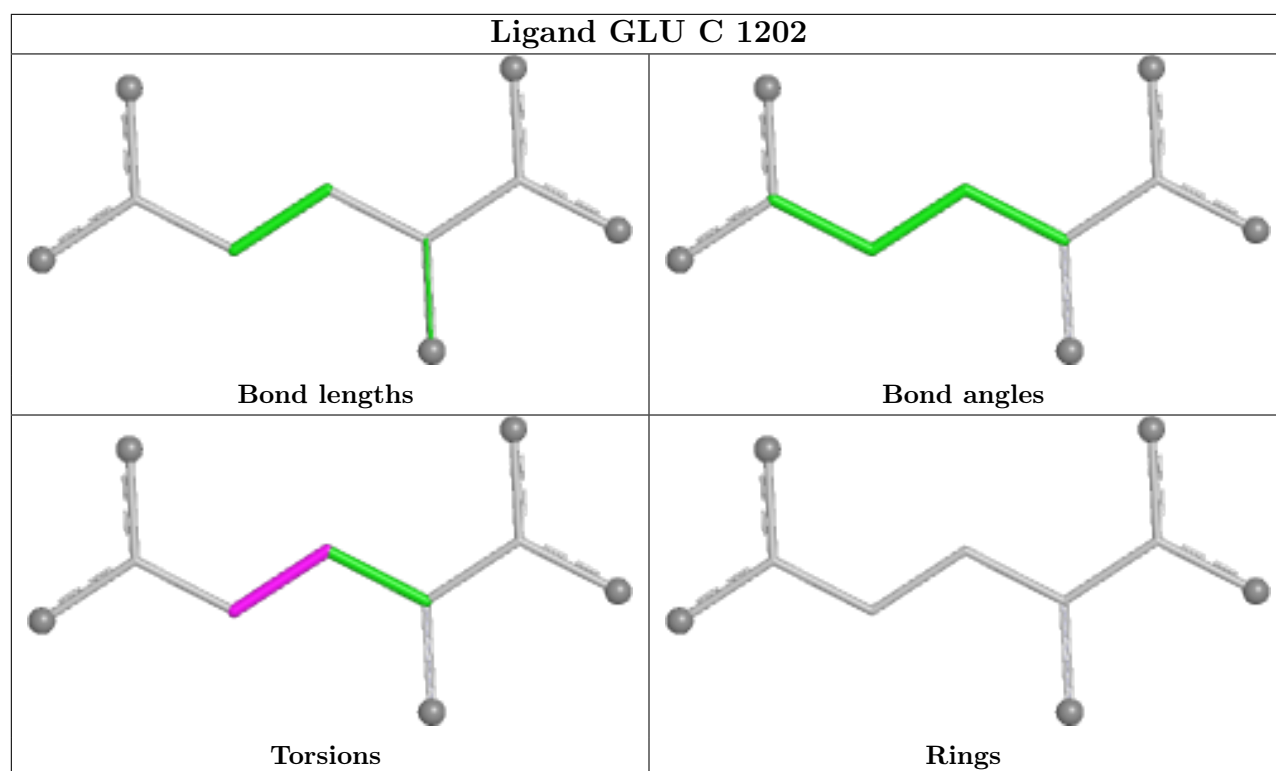


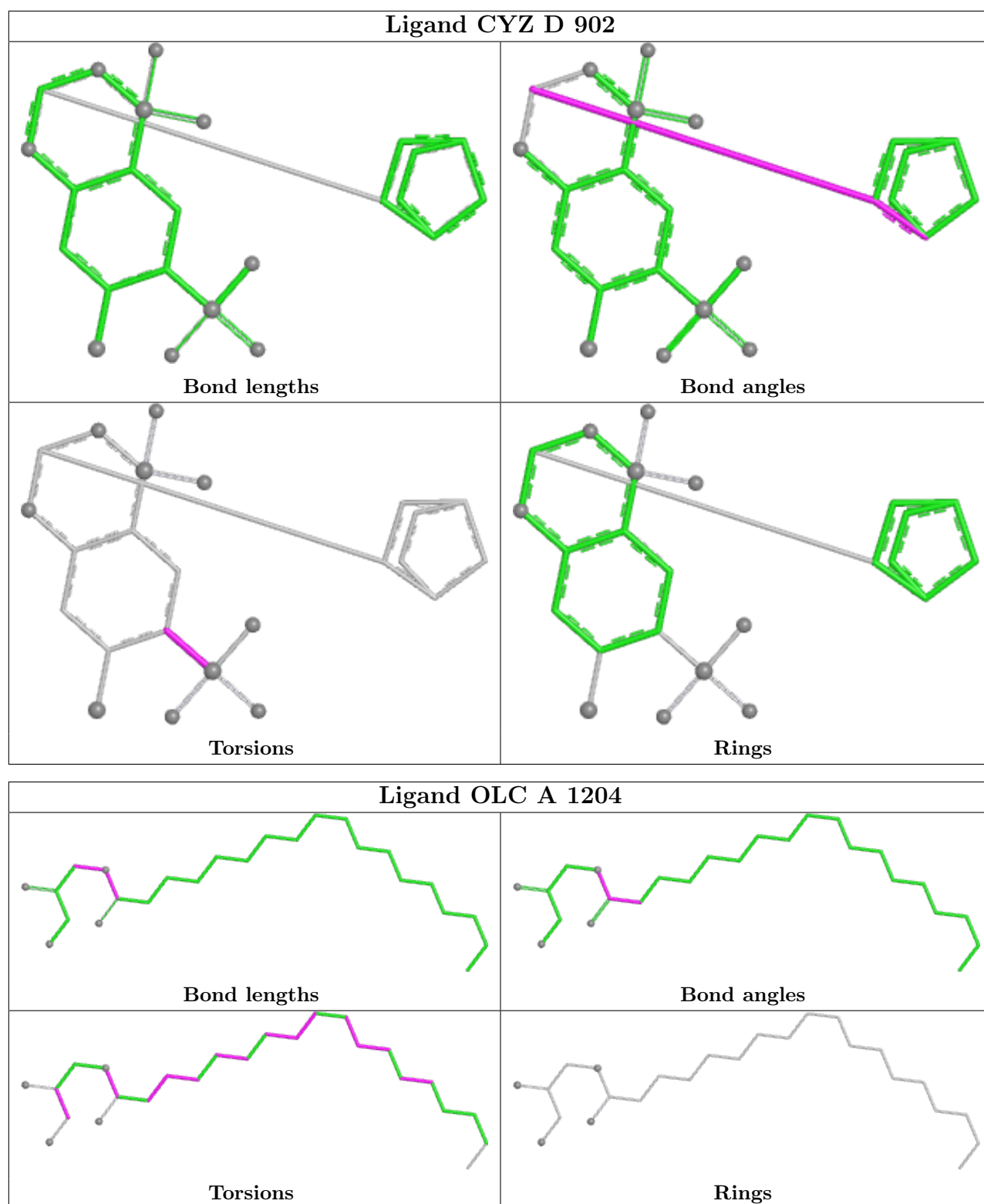


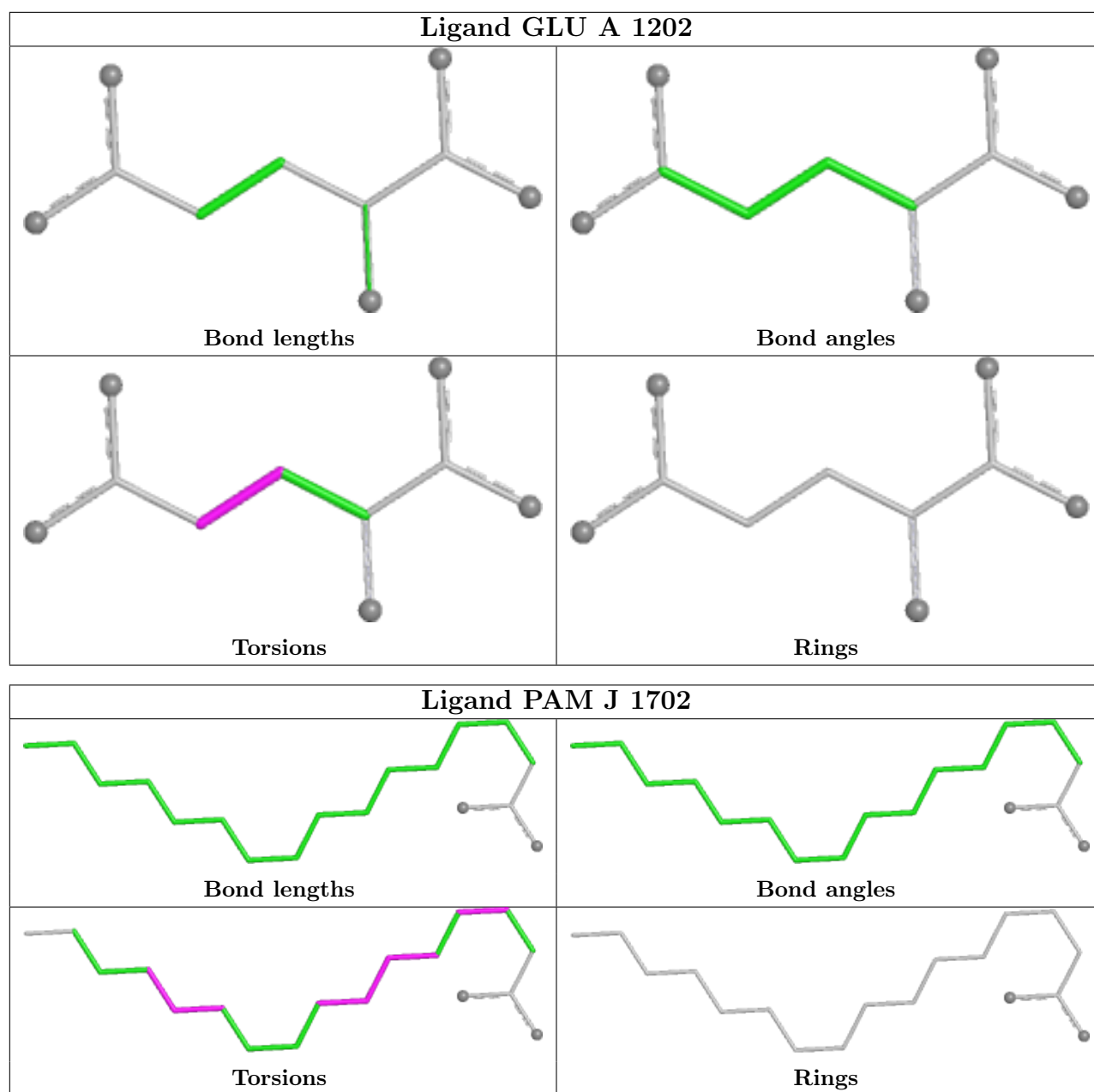












5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

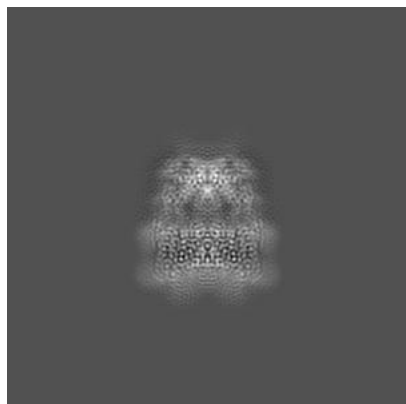
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13969. These allow visual inspection of the internal detail of the map and identification of artifacts.

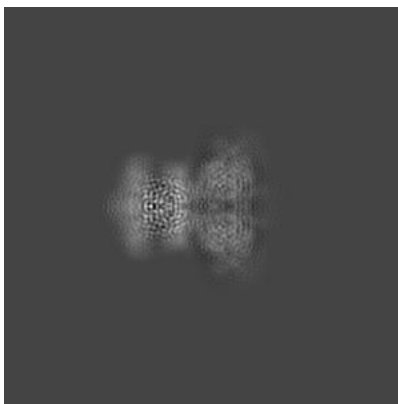
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

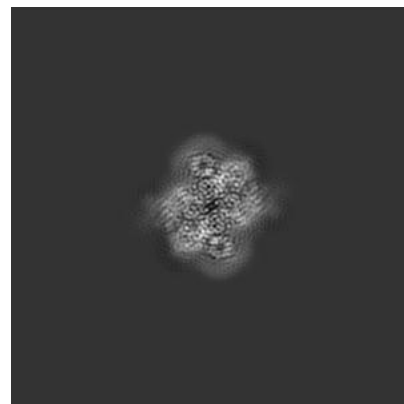
6.1.1 Primary map



X

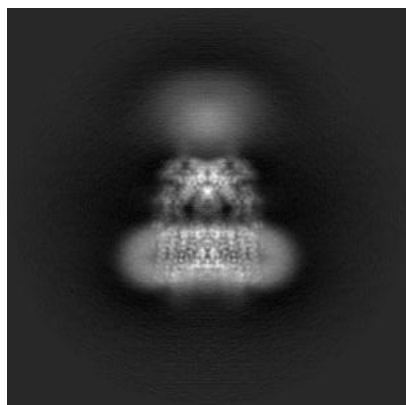


Y

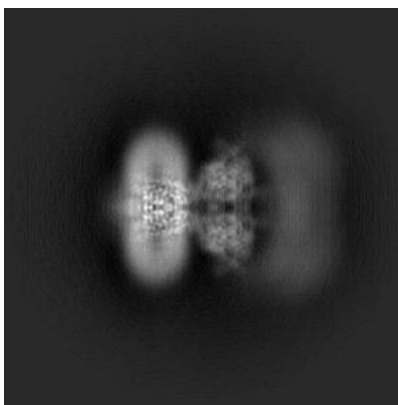


Z

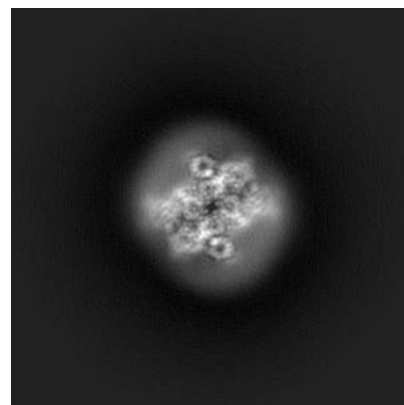
6.1.2 Raw map



X



Y

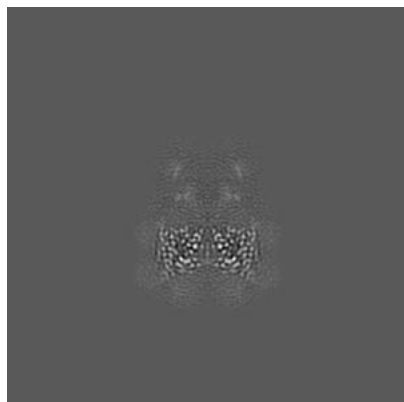


Z

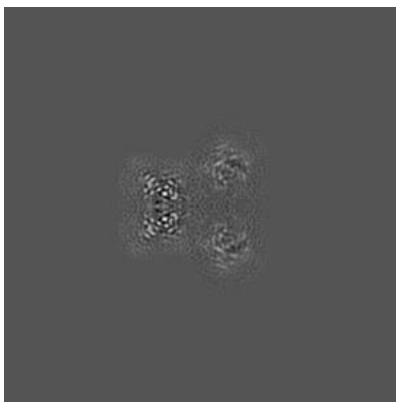
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

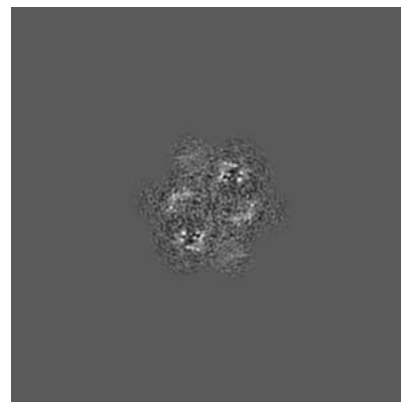
6.2.1 Primary map



X Index: 160

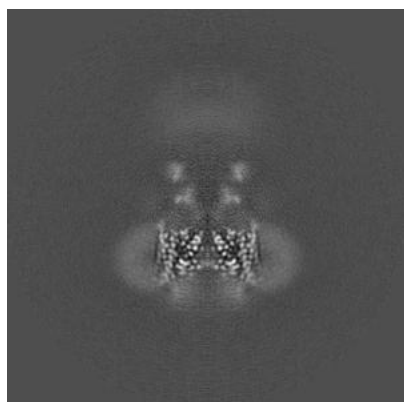


Y Index: 160

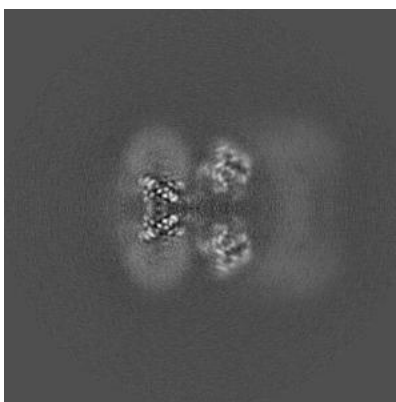


Z Index: 160

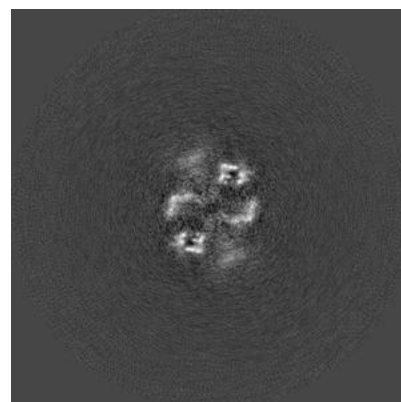
6.2.2 Raw map



X Index: 160



Y Index: 160

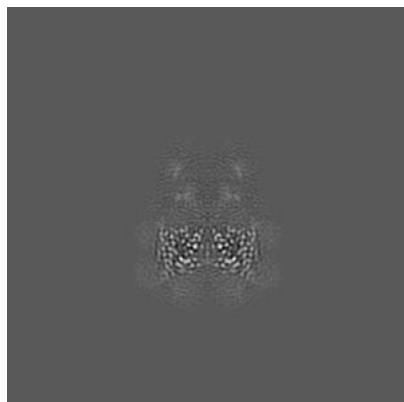


Z Index: 160

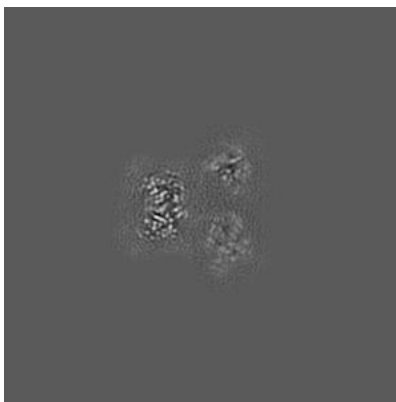
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

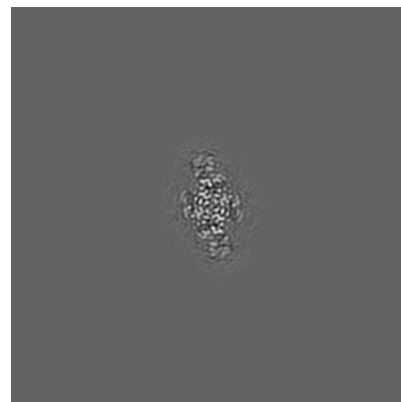
6.3.1 Primary map



X Index: 160

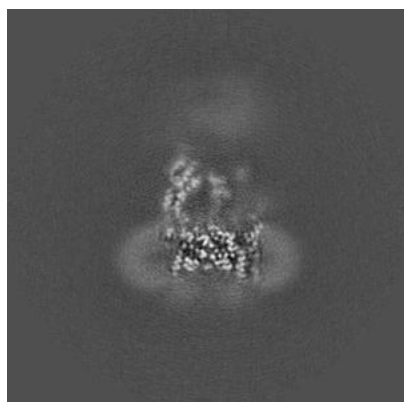


Y Index: 164

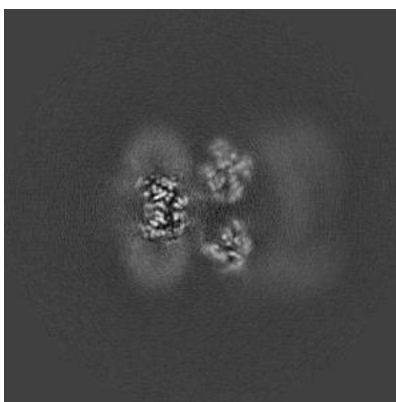


Z Index: 122

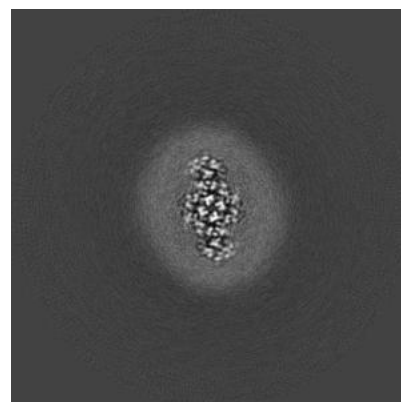
6.3.2 Raw map



X Index: 152



Y Index: 156

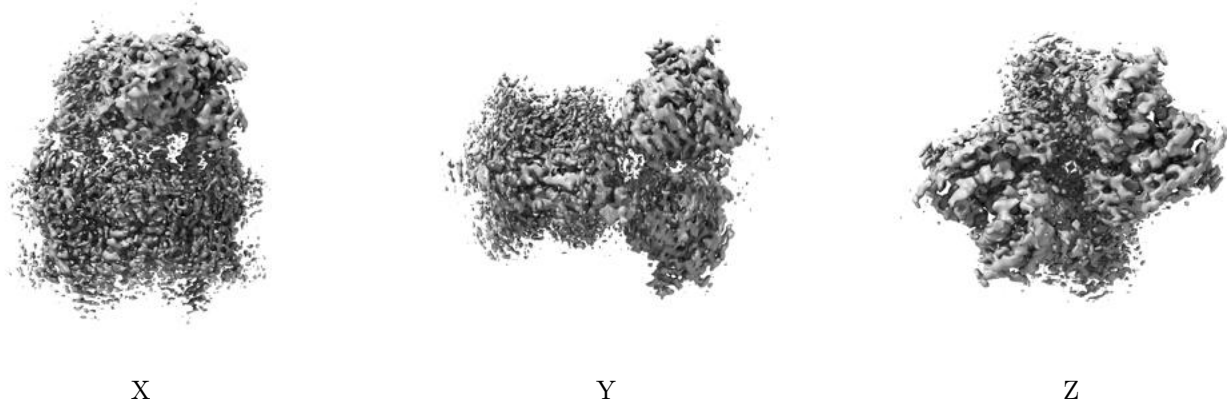


Z Index: 137

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

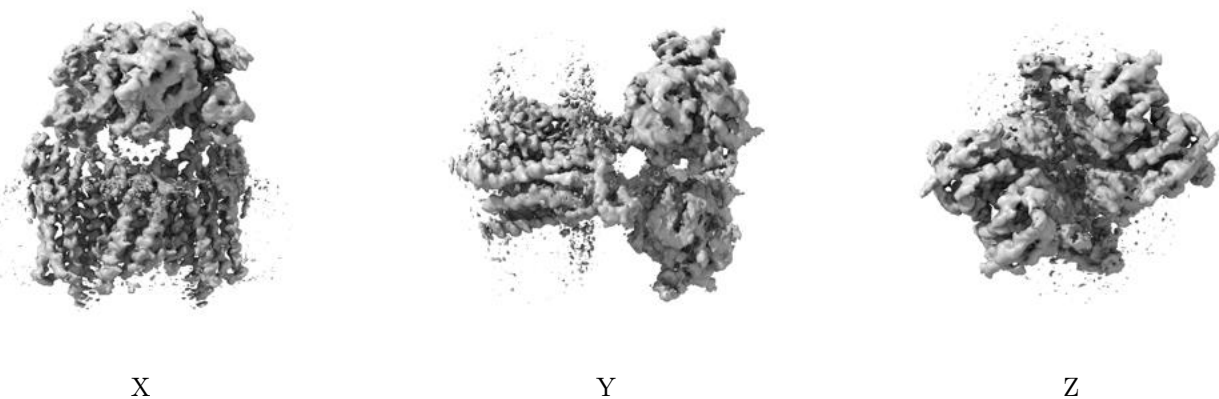
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0192. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

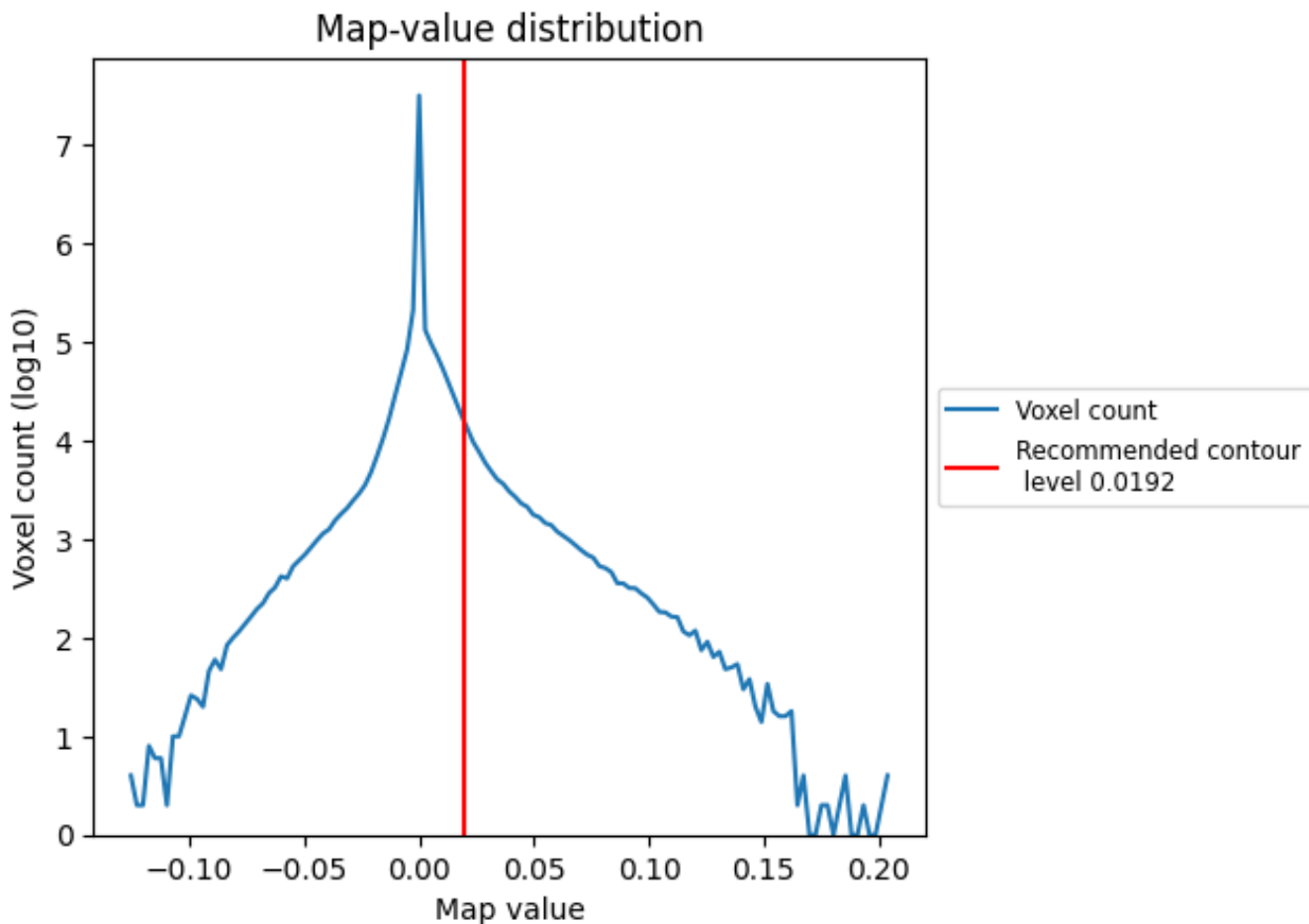
6.5 Mask visualisation [i](#)

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

7 Map analysis [i](#)

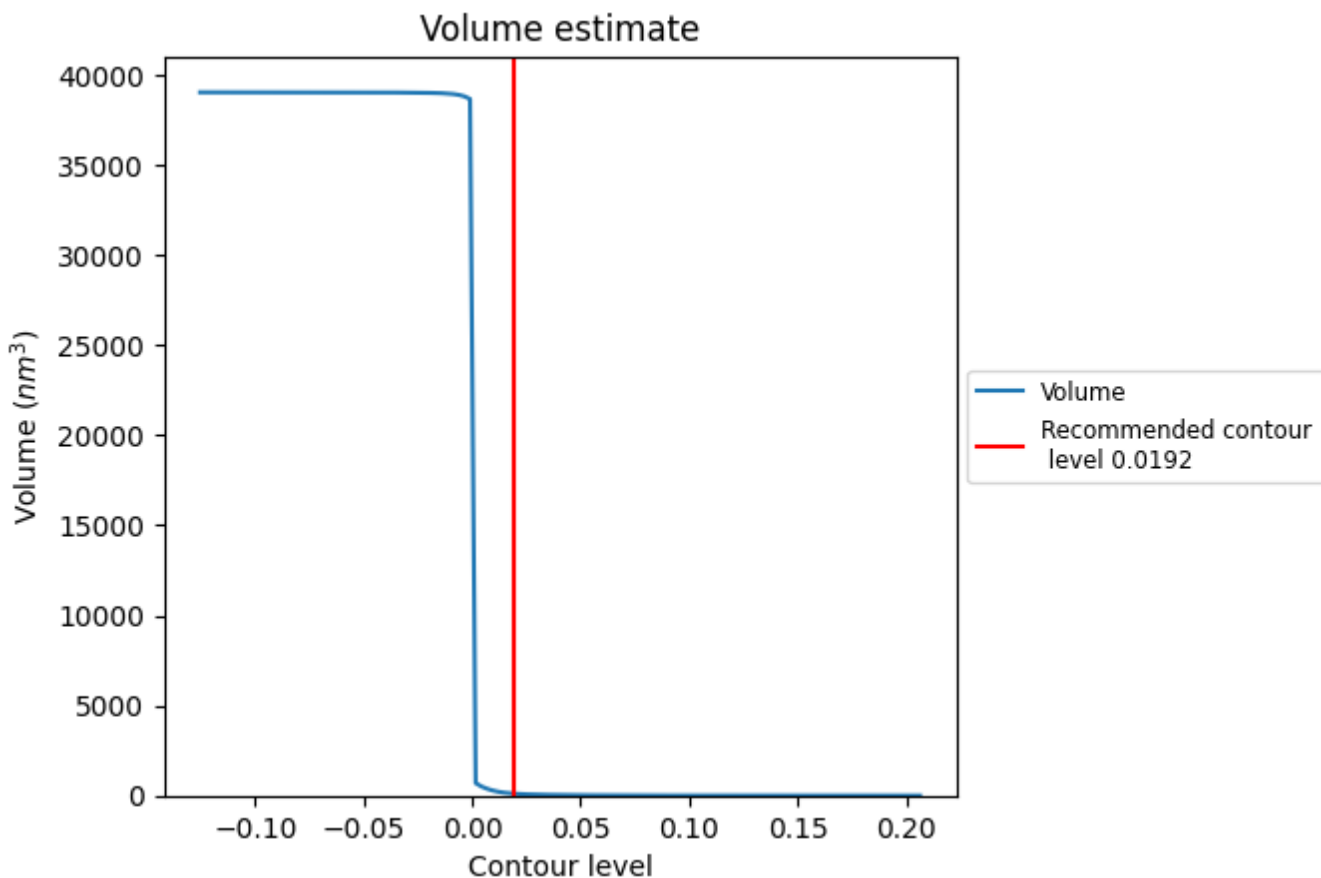
This section contains the results of statistical analysis of the map.

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.

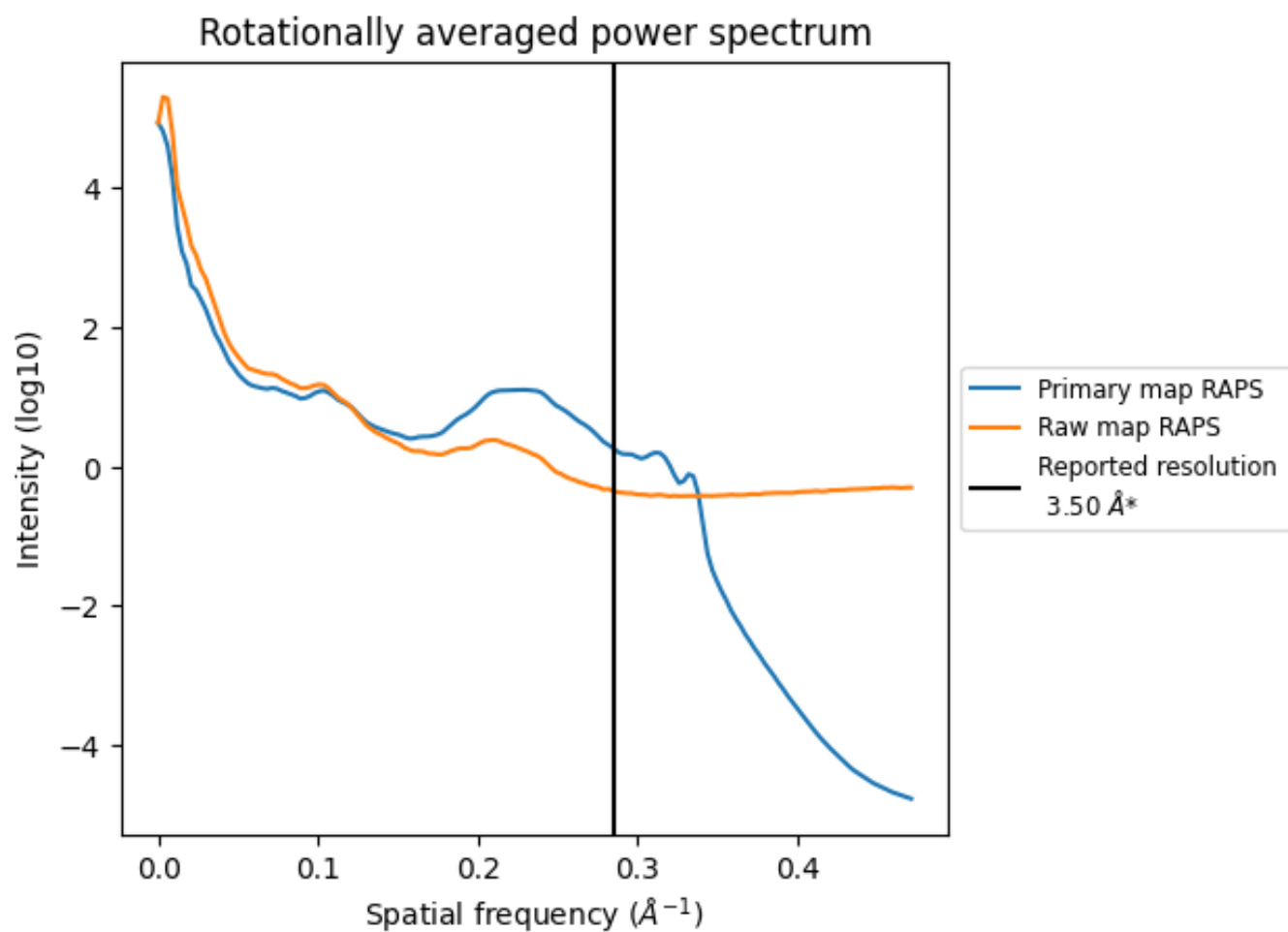
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 106 nm³; this corresponds to an approximate mass of 96 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

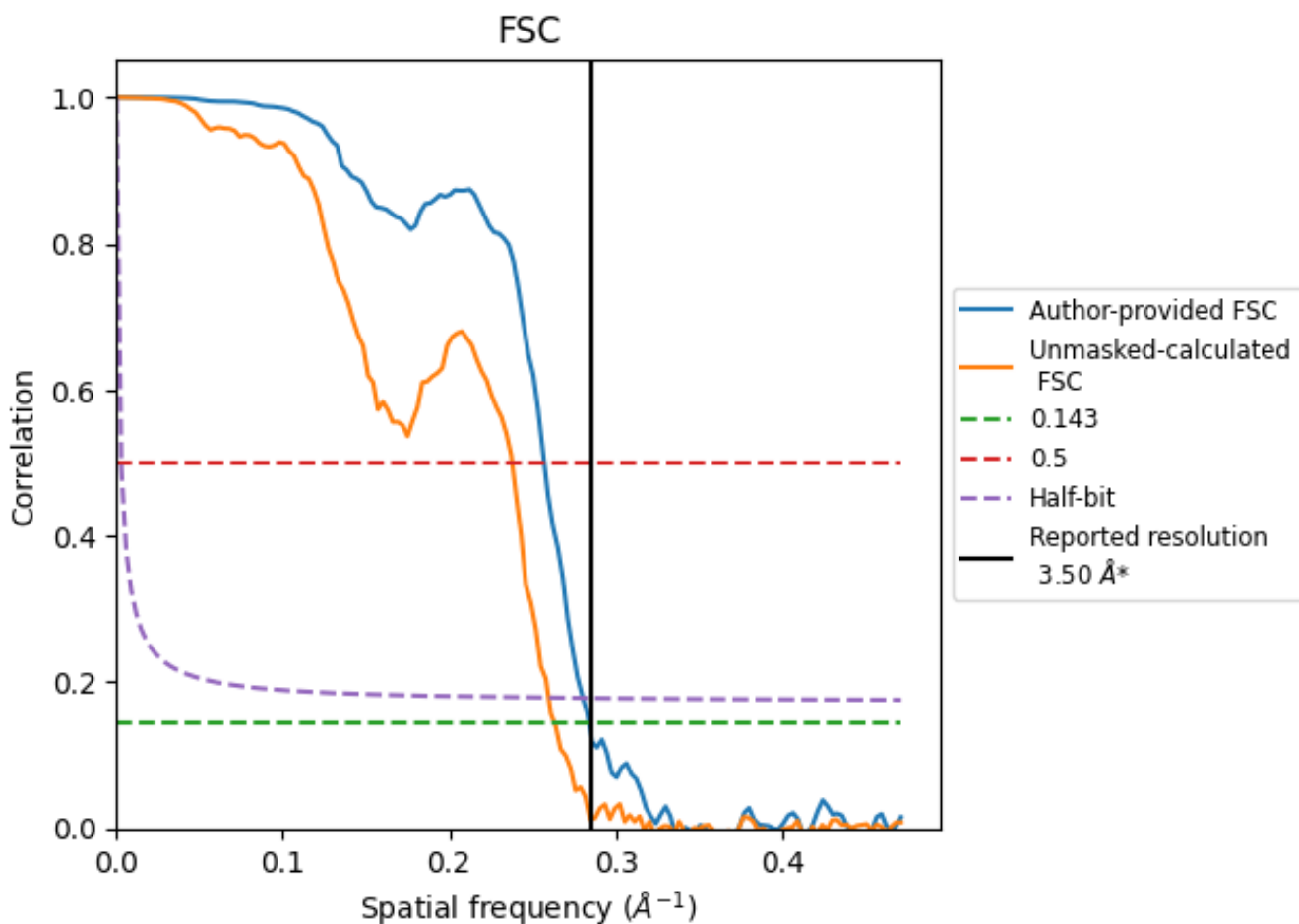


*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

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 0.286 Å⁻¹

8.2 Resolution estimates [i](#)

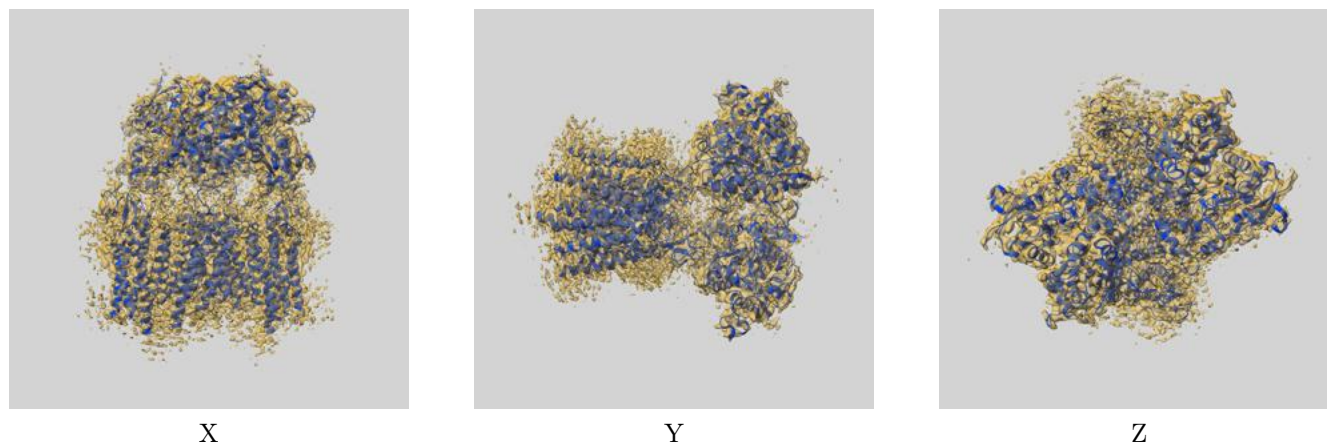
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.52	3.89	3.57
Unmasked-calculated*	3.80	4.20	3.85

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

9 Map-model fit [i](#)

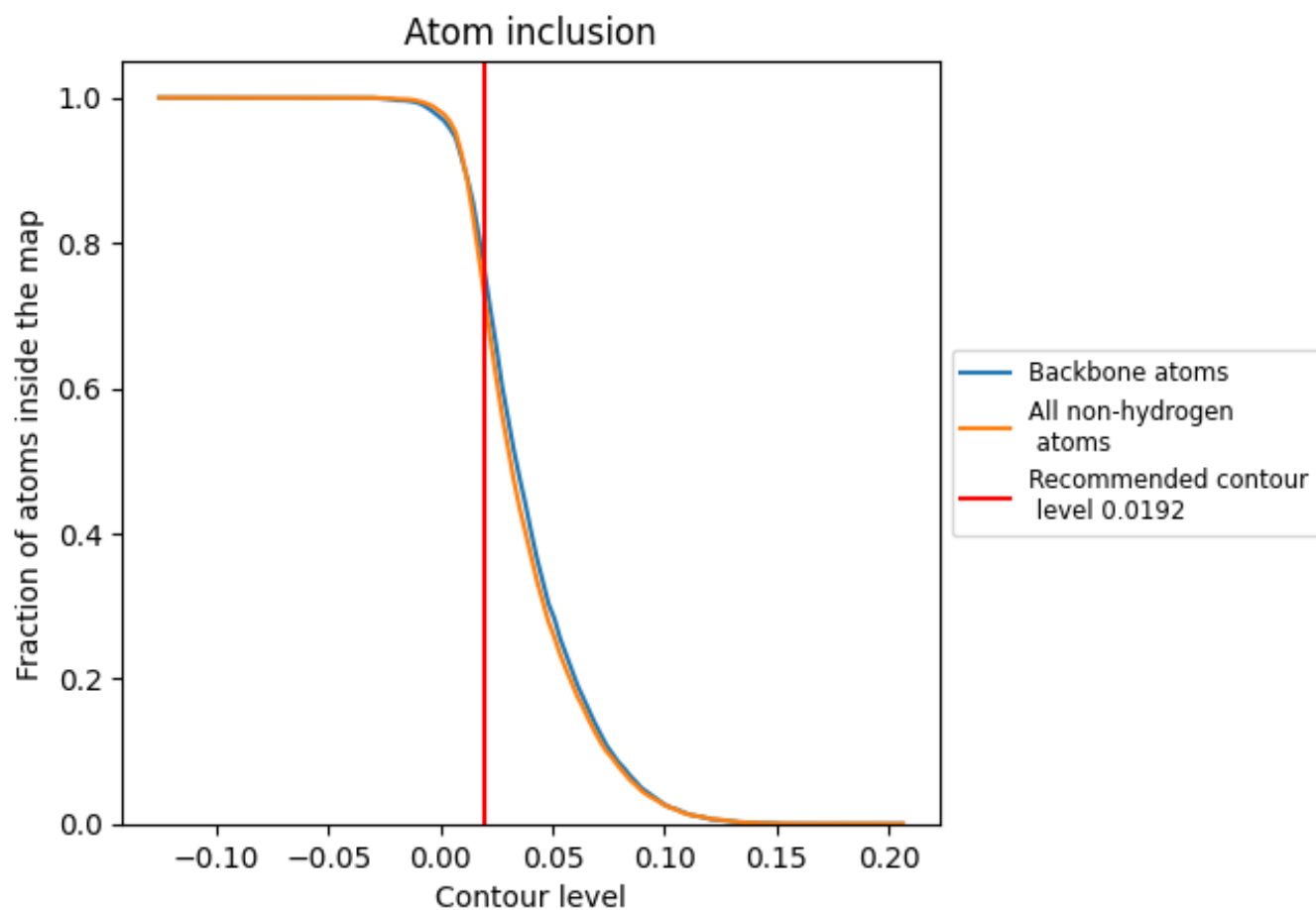
This section contains information regarding the fit between EMDB map EMD-13969 and PDB model 7QHB. Per-residue inclusion information can be found in section [3](#) on page [10](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.0192 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 Atom inclusion [i](#)



At the recommended contour level, 77% of all backbone atoms, 74% of all non-hydrogen atoms, are inside the map.