



Full wwPDB EM Validation Report ⓘ

Oct 15, 2024 – 03:40 AM EDT

PDB ID : 8V6N
EMDB ID : EMD-42997
Title : Open-state cryo-EM structure of human TRPV3 in presence of 2-APB in cNW30 nanodiscs
Authors : Nadezhdin, K.D.; Neuberger, A.; Sobolevsky, A.I.
Deposited on : 2023-12-01
Resolution : 2.59 Å(reported)

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 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

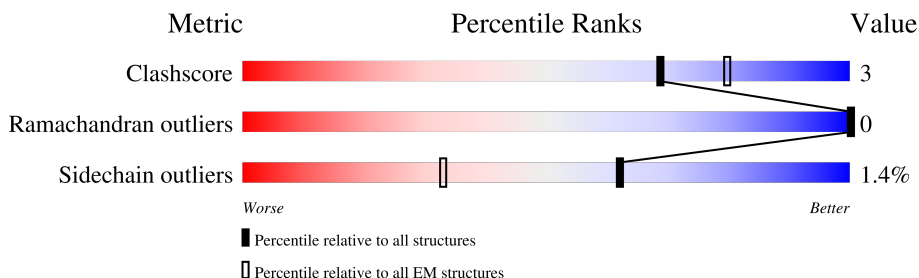
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.59 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	808	<div> <div>16%</div> <div>72%</div> <div>7%</div> <div>21%</div> </div>
1	B	808	<div> <div>17%</div> <div>72%</div> <div>7%</div> <div>21%</div> </div>
1	C	808	<div> <div>17%</div> <div>72%</div> <div>7%</div> <div>21%</div> </div>
1	D	808	<div> <div>17%</div> <div>72%</div> <div>7%</div> <div>21%</div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 22185 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 Transient receptor potential cation channel subfamily V member 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	636	Total	C	N	O	S	0	0
			5184	3367	858	926	33		
1	B	636	Total	C	N	O	S	0	0
			5184	3367	858	926	33		
1	C	636	Total	C	N	O	S	0	0
			5184	3367	858	926	33		
1	D	636	Total	C	N	O	S	0	0
			5184	3367	858	926	33		

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	792	LEU	-	expression tag	UNP Q8NET8
A	793	VAL	-	expression tag	UNP Q8NET8
A	794	PRO	-	expression tag	UNP Q8NET8
A	795	ARG	-	expression tag	UNP Q8NET8
A	796	GLY	-	expression tag	UNP Q8NET8
A	797	SER	-	expression tag	UNP Q8NET8
A	798	ALA	-	expression tag	UNP Q8NET8
A	799	ALA	-	expression tag	UNP Q8NET8
A	800	ALA	-	expression tag	UNP Q8NET8
A	801	TRP	-	expression tag	UNP Q8NET8
A	802	SER	-	expression tag	UNP Q8NET8
A	803	HIS	-	expression tag	UNP Q8NET8
A	804	PRO	-	expression tag	UNP Q8NET8
A	805	GLN	-	expression tag	UNP Q8NET8
A	806	PHE	-	expression tag	UNP Q8NET8
A	807	GLU	-	expression tag	UNP Q8NET8
A	808	LYS	-	expression tag	UNP Q8NET8
B	792	LEU	-	expression tag	UNP Q8NET8
B	793	VAL	-	expression tag	UNP Q8NET8
B	794	PRO	-	expression tag	UNP Q8NET8
B	795	ARG	-	expression tag	UNP Q8NET8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	796	GLY	-	expression tag	UNP Q8NET8
B	797	SER	-	expression tag	UNP Q8NET8
B	798	ALA	-	expression tag	UNP Q8NET8
B	799	ALA	-	expression tag	UNP Q8NET8
B	800	ALA	-	expression tag	UNP Q8NET8
B	801	TRP	-	expression tag	UNP Q8NET8
B	802	SER	-	expression tag	UNP Q8NET8
B	803	HIS	-	expression tag	UNP Q8NET8
B	804	PRO	-	expression tag	UNP Q8NET8
B	805	GLN	-	expression tag	UNP Q8NET8
B	806	PHE	-	expression tag	UNP Q8NET8
B	807	GLU	-	expression tag	UNP Q8NET8
B	808	LYS	-	expression tag	UNP Q8NET8
C	792	LEU	-	expression tag	UNP Q8NET8
C	793	VAL	-	expression tag	UNP Q8NET8
C	794	PRO	-	expression tag	UNP Q8NET8
C	795	ARG	-	expression tag	UNP Q8NET8
C	796	GLY	-	expression tag	UNP Q8NET8
C	797	SER	-	expression tag	UNP Q8NET8
C	798	ALA	-	expression tag	UNP Q8NET8
C	799	ALA	-	expression tag	UNP Q8NET8
C	800	ALA	-	expression tag	UNP Q8NET8
C	801	TRP	-	expression tag	UNP Q8NET8
C	802	SER	-	expression tag	UNP Q8NET8
C	803	HIS	-	expression tag	UNP Q8NET8
C	804	PRO	-	expression tag	UNP Q8NET8
C	805	GLN	-	expression tag	UNP Q8NET8
C	806	PHE	-	expression tag	UNP Q8NET8
C	807	GLU	-	expression tag	UNP Q8NET8
C	808	LYS	-	expression tag	UNP Q8NET8
D	792	LEU	-	expression tag	UNP Q8NET8
D	793	VAL	-	expression tag	UNP Q8NET8
D	794	PRO	-	expression tag	UNP Q8NET8
D	795	ARG	-	expression tag	UNP Q8NET8
D	796	GLY	-	expression tag	UNP Q8NET8
D	797	SER	-	expression tag	UNP Q8NET8
D	798	ALA	-	expression tag	UNP Q8NET8
D	799	ALA	-	expression tag	UNP Q8NET8
D	800	ALA	-	expression tag	UNP Q8NET8
D	801	TRP	-	expression tag	UNP Q8NET8
D	802	SER	-	expression tag	UNP Q8NET8
D	803	HIS	-	expression tag	UNP Q8NET8

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Chain	Residue	Modelled	Actual	Comment	Reference
D	804	PRO	-	expression tag	UNP Q8NET8
D	805	GLN	-	expression tag	UNP Q8NET8
D	806	PHE	-	expression tag	UNP Q8NET8
D	807	GLU	-	expression tag	UNP Q8NET8
D	808	LYS	-	expression tag	UNP Q8NET8

- Molecule 2 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylamm onio)ethyl phosphate (three-letter code: POV) (formula: C₄₂H₈₂NO₈P).



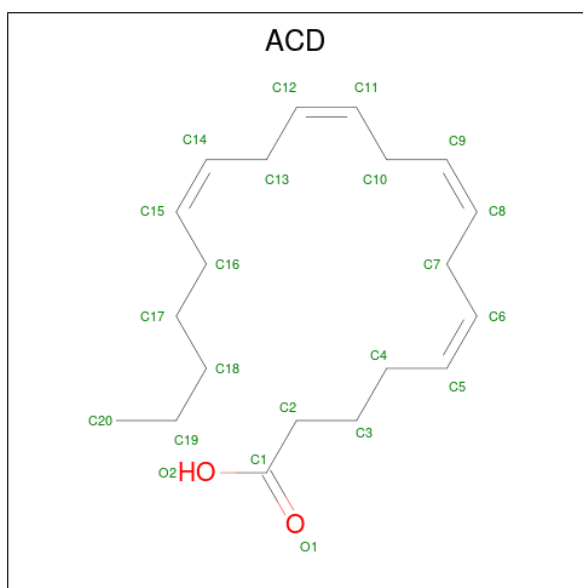
Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	B	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	B	1	Total	C	N	O	P	0
			52	42	1	8	1	

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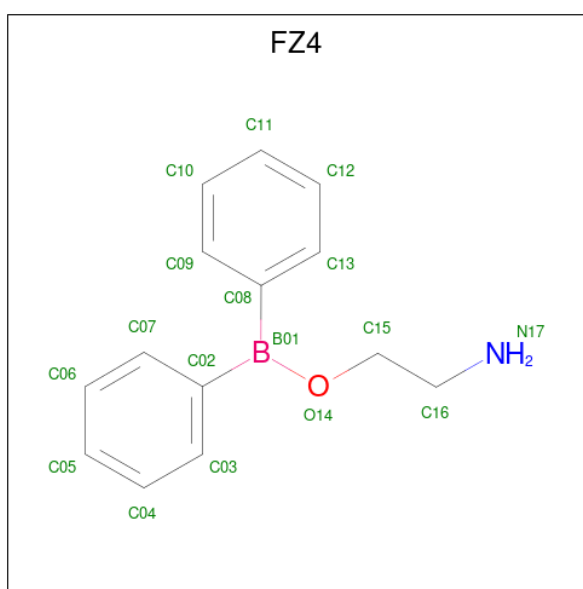
Mol	Chain	Residues	Atoms					AltConf
2	B	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	B	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	B	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	C	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	C	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	C	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	C	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	D	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	D	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	D	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	D	1	Total	C	N	O	P	0
			52	42	1	8	1	

- Molecule 3 is ARACHIDONIC ACID (three-letter code: ACD) (formula: $C_{20}H_{32}O_2$).



Mol	Chain	Residues	Atoms			AltConf
3	A	1	Total	C	O	0
			22	20	2	
3	B	1	Total	C	O	0
			22	20	2	
3	C	1	Total	C	O	0
			22	20	2	
3	D	1	Total	C	O	0
			22	20	2	

- Molecule 4 is 2-aminoethyl diphenylborinate (three-letter code: FZ4) (formula: C₁₄H₁₆BNO) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	B	C	N	O	0
			17	1	14	1	1	
4	A	1	Total	B	C	N	O	0
			17	1	14	1	1	
4	B	1	Total	B	C	N	O	0
			17	1	14	1	1	
4	B	1	Total	B	C	N	O	0
			17	1	14	1	1	
4	C	1	Total	B	C	N	O	0
			17	1	14	1	1	
4	C	1	Total	B	C	N	O	0
			17	1	14	1	1	
4	D	1	Total	B	C	N	O	0
			17	1	14	1	1	

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Mol	Chain	Residues	Atoms					AltConf
4	D	1	Total	B	C	N	O	0
			17	1	14	1	1	

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total	Na	0
			1	1	

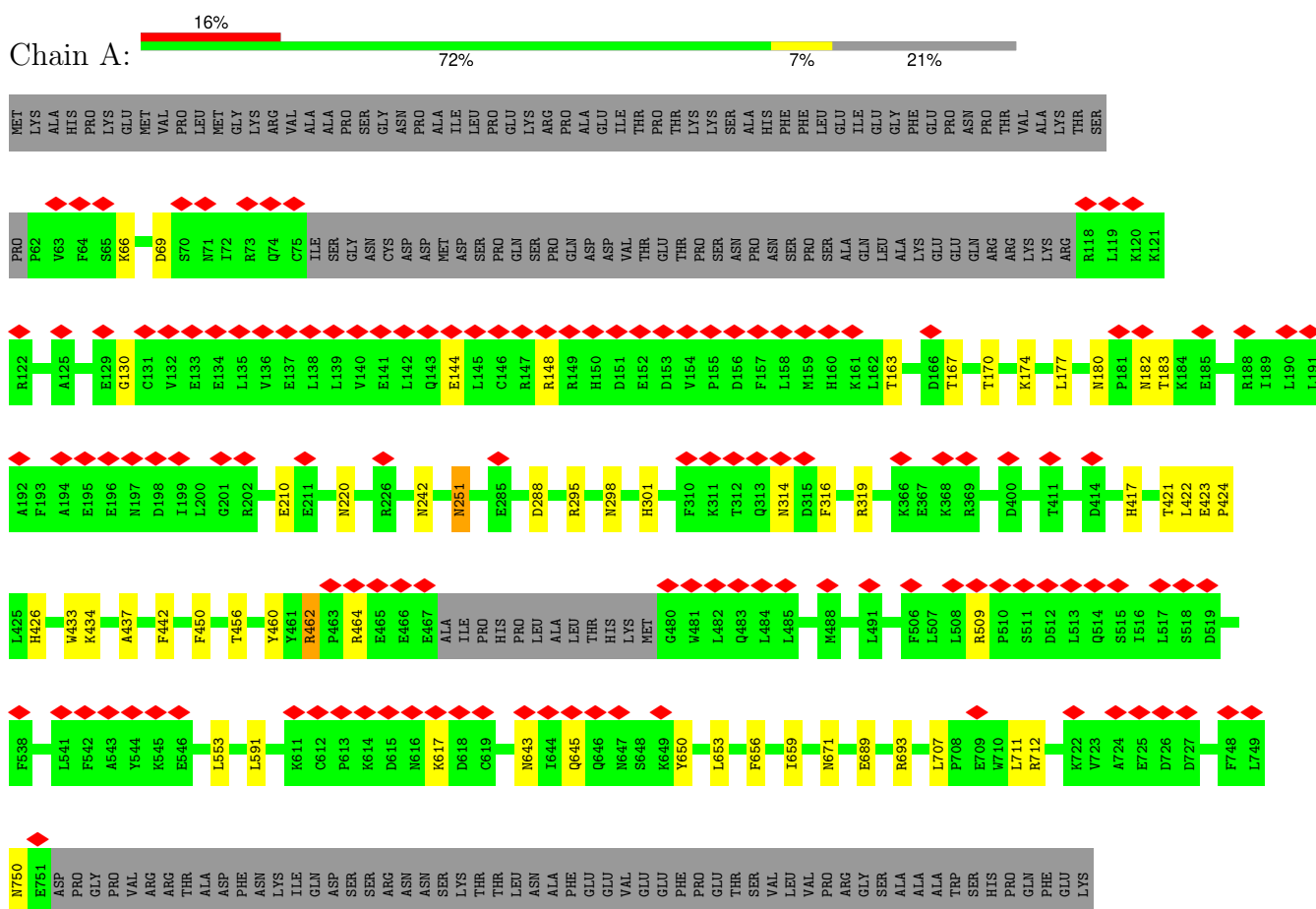
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		AltConf
6	A	46	Total	O	0
			46	46	
6	B	46	Total	O	0
			46	46	
6	C	46	Total	O	0
			46	46	
6	D	46	Total	O	0
			46	46	

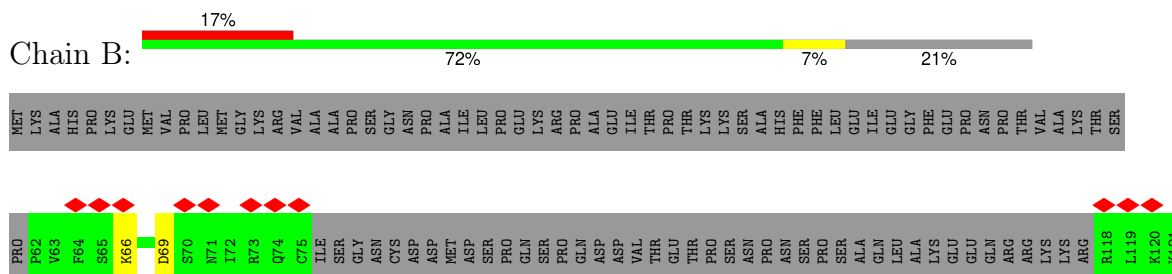
3 Residue-property plots

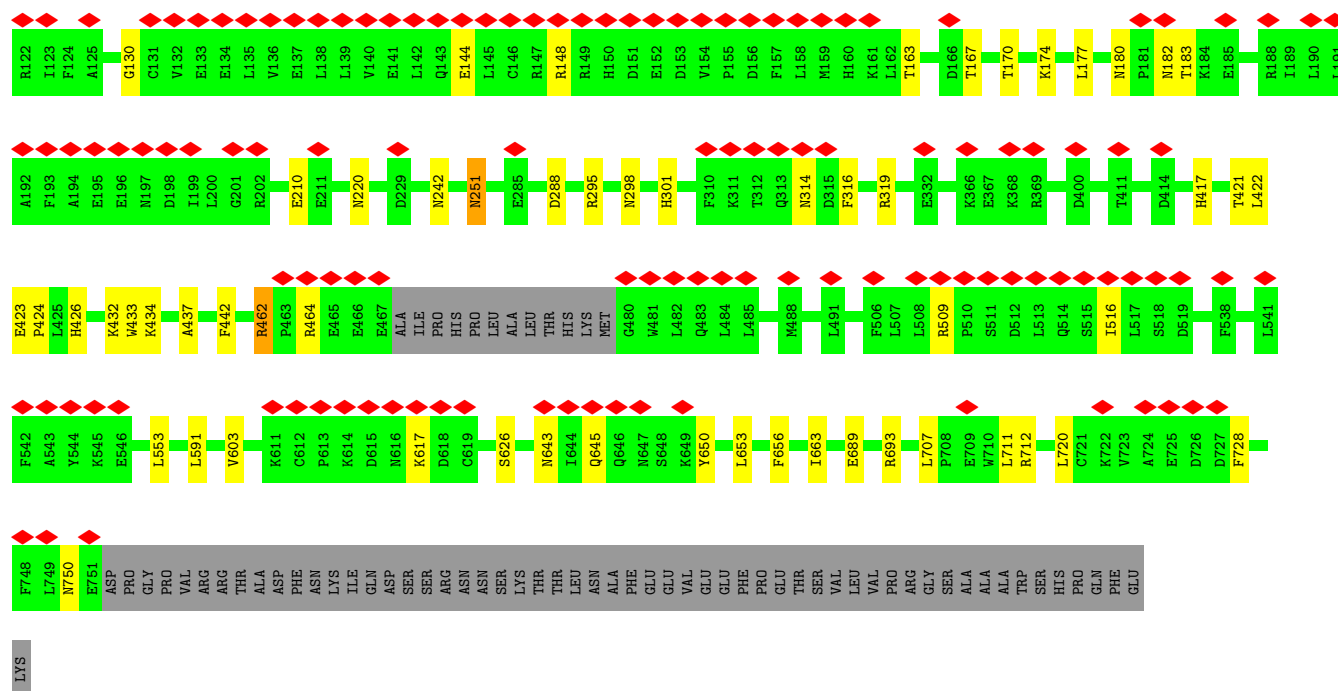
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: Transient receptor potential cation channel subfamily V member 3

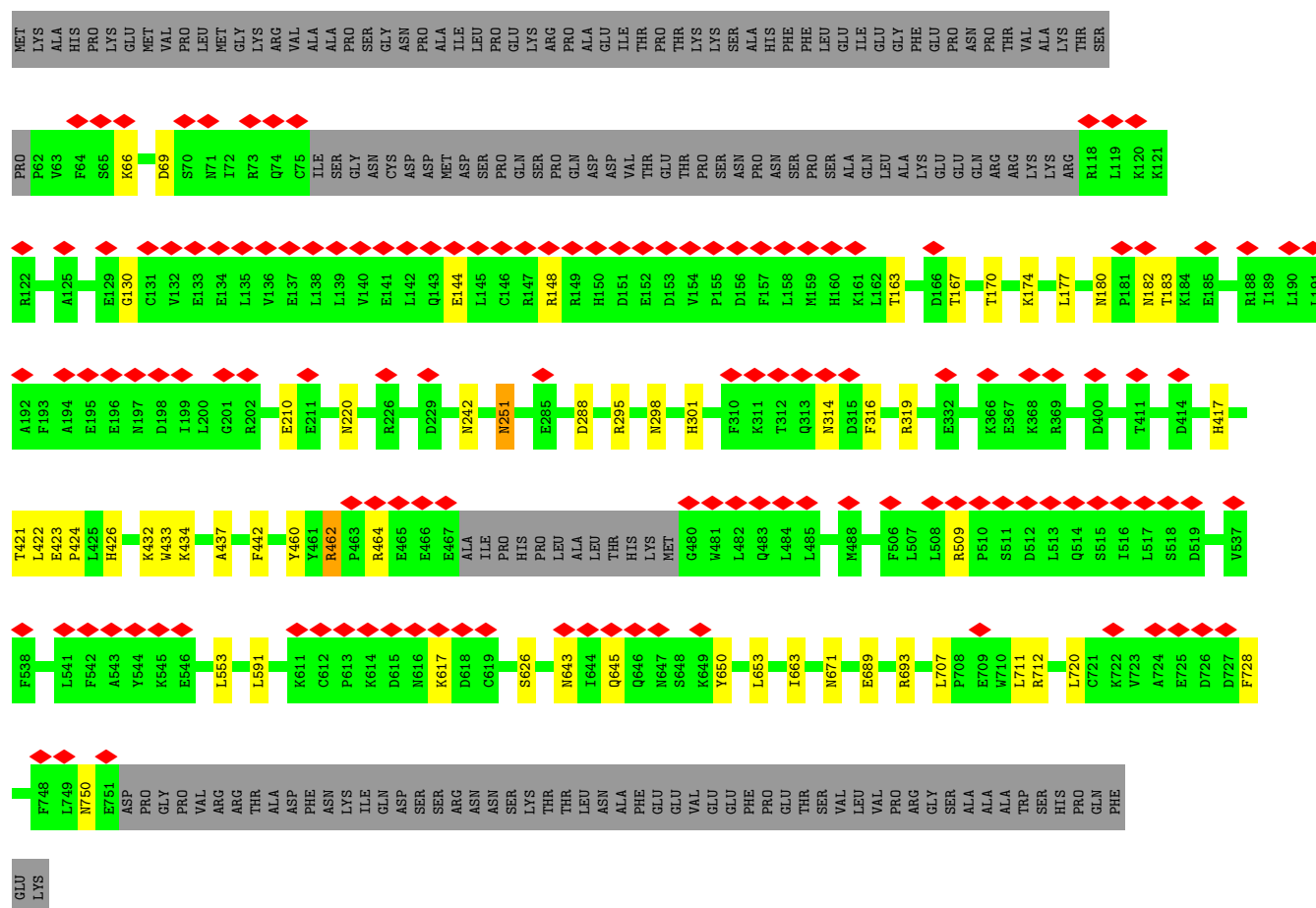


- Molecule 1: Transient receptor potential cation channel subfamily V member 3

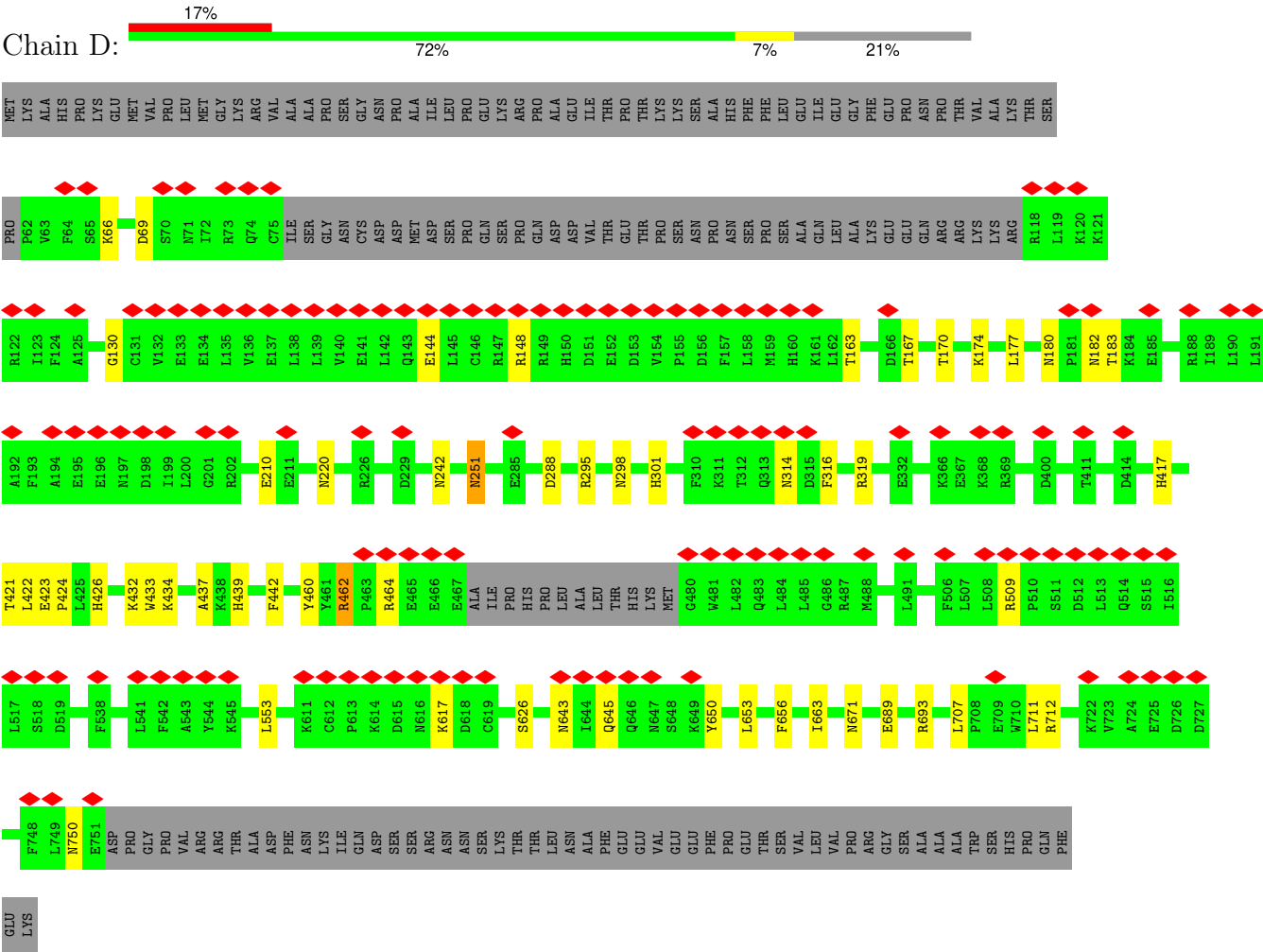




- Molecule 1: Transient receptor potential cation channel subfamily V member 3



● Molecule 1: Transient receptor potential cation channel subfamily V member 3



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	105954	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	750	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.825	Depositor
Minimum map value	-1.237	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.074	Depositor
Recommended contour level	0.241	Depositor
Map size (\AA)	204.8, 204.8, 204.8	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.8, 0.8, 0.8	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: POV, FZ4, ACD, NA

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	0.26	0/5295	0.50	0/7157
1	B	0.26	0/5295	0.50	0/7157
1	C	0.26	0/5295	0.50	0/7157
1	D	0.26	0/5295	0.50	0/7157
All	All	0.26	0/21180	0.50	0/28628

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
1	C	0	2
1	D	0	2
All	All	0	8

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	422	LEU	Peptide
1	A	645	GLN	Peptide
1	B	422	LEU	Peptide
1	B	645	GLN	Peptide
1	C	422	LEU	Peptide

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Mol	Chain	Res	Type	Group
1	C	645	GLN	Peptide
1	D	422	LEU	Peptide
1	D	645	GLN	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5184	0	5239	32	0
1	B	5184	0	5239	34	0
1	C	5184	0	5239	32	0
1	D	5184	0	5239	32	0
2	A	312	0	492	17	0
2	B	260	0	410	12	0
2	C	260	0	410	13	0
2	D	208	0	328	13	0
3	A	22	0	31	1	0
3	B	22	0	31	2	0
3	C	22	0	31	2	0
3	D	22	0	31	2	0
4	A	34	0	0	1	0
4	B	34	0	0	1	0
4	C	34	0	0	1	0
4	D	34	0	0	1	0
5	A	1	0	0	0	0
6	A	46	0	0	1	0
6	B	46	0	0	1	0
6	C	46	0	0	2	0
6	D	46	0	0	2	0
All	All	22185	0	22720	156	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 3.

All (156) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:242:ASN:HD21	1:C:288:ASP:H	1.47	0.62
1:D:242:ASN:HD21	1:D:288:ASP:H	1.47	0.62
1:A:242:ASN:HD21	1:A:288:ASP:H	1.47	0.61
1:B:242:ASN:HD21	1:B:288:ASP:H	1.47	0.61
1:C:433:TRP:HA	1:C:437:ALA:HB3	1.85	0.58
1:C:462:ARG:HE	1:C:464:ARG:HD3	1.69	0.58
1:D:433:TRP:HA	1:D:437:ALA:HB3	1.85	0.58
1:A:433:TRP:HA	1:A:437:ALA:HB3	1.85	0.58
1:B:433:TRP:HA	1:B:437:ALA:HB3	1.85	0.57
1:A:163:THR:HG22	1:A:170:THR:HG22	1.86	0.57
1:B:163:THR:HG22	1:B:170:THR:HG22	1.86	0.57
1:B:462:ARG:HE	1:B:464:ARG:HD3	1.69	0.57
1:D:462:ARG:HE	1:D:464:ARG:HD3	1.69	0.57
1:C:163:THR:HG22	1:C:170:THR:HG22	1.86	0.57
1:D:163:THR:HG22	1:D:170:THR:HG22	1.86	0.57
1:A:462:ARG:HE	1:A:464:ARG:HD3	1.69	0.56
1:C:298:ASN:OD1	1:C:301:HIS:ND1	2.38	0.56
2:B:901:POV:H36A	2:B:901:POV:H211	1.86	0.56
1:B:626:SER:HB2	2:B:902:POV:H15B	1.89	0.55
1:C:426:HIS:NE2	4:C:906:FZ4:O14	2.36	0.55
1:B:426:HIS:NE2	4:B:906:FZ4:O14	2.36	0.54
1:D:423:GLU:HG2	1:D:424:PRO:HD3	1.89	0.54
1:C:144:GLU:HG3	1:C:148:ARG:HH22	1.73	0.54
1:C:626:SER:HB2	2:C:902:POV:H15B	1.89	0.54
1:D:144:GLU:HG3	1:D:148:ARG:HH22	1.73	0.54
2:A:908:POV:H15B	1:D:626:SER:HB2	1.90	0.53
1:B:423:GLU:HG2	1:B:424:PRO:HD3	1.89	0.53
1:A:423:GLU:HG2	1:A:424:PRO:HD3	1.89	0.53
1:A:144:GLU:HG3	1:A:148:ARG:HH22	1.73	0.53
1:B:144:GLU:HG3	1:B:148:ARG:HH22	1.73	0.53
1:C:423:GLU:HG2	1:C:424:PRO:HD3	1.89	0.53
1:B:298:ASN:OD1	1:B:301:HIS:ND1	2.38	0.53
1:A:298:ASN:OD1	1:A:301:HIS:ND1	2.38	0.52
3:B:903:ACD:H12	2:C:901:POV:H21B	1.90	0.52
1:C:130:GLY:O	1:C:182:ASN:ND2	2.43	0.52
3:C:903:ACD:H12	2:D:902:POV:H21B	1.91	0.51
1:D:426:HIS:NE2	4:D:906:FZ4:O14	2.36	0.51
1:D:130:GLY:O	1:D:182:ASN:ND2	2.43	0.51
1:A:69:ASP:OD1	1:A:174:LYS:NZ	2.44	0.51
1:B:130:GLY:O	1:B:182:ASN:ND2	2.43	0.51
1:A:130:GLY:O	1:A:182:ASN:ND2	2.43	0.51
2:A:909:POV:H21B	3:D:903:ACD:H12	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:69:ASP:OD1	1:D:174:LYS:NZ	2.44	0.50
1:D:689:GLU:O	1:D:693:ARG:NH1	2.44	0.50
1:B:69:ASP:OD1	1:B:174:LYS:NZ	2.44	0.50
1:D:66:LYS:HD2	1:D:210:GLU:HG3	1.94	0.50
1:A:689:GLU:O	1:A:693:ARG:NH1	2.44	0.50
1:D:66:LYS:HD3	1:D:167:THR:HG22	1.93	0.50
1:A:66:LYS:HD2	1:A:210:GLU:HG3	1.94	0.50
1:D:298:ASN:OD1	1:D:301:HIS:ND1	2.38	0.50
1:B:689:GLU:O	1:B:693:ARG:NH1	2.44	0.49
1:C:316:PHE:HA	1:C:319:ARG:HE	1.78	0.49
1:D:316:PHE:HA	1:D:319:ARG:HE	1.78	0.49
1:A:426:HIS:NE2	4:A:905:FZ4:O14	2.34	0.49
1:B:66:LYS:HD3	1:B:167:THR:HG22	1.93	0.49
1:B:66:LYS:HD2	1:B:210:GLU:HG3	1.94	0.49
1:C:66:LYS:HD2	1:C:210:GLU:HG3	1.94	0.49
1:B:316:PHE:HA	1:B:319:ARG:HE	1.78	0.49
1:A:66:LYS:HD3	1:A:167:THR:HG22	1.93	0.48
1:C:689:GLU:O	1:C:693:ARG:NH1	2.44	0.48
2:A:909:POV:H21A	1:D:553:LEU:HD23	1.95	0.48
1:C:69:ASP:OD1	1:C:174:LYS:NZ	2.44	0.48
1:B:553:LEU:HD23	2:C:901:POV:H21A	1.94	0.48
1:C:66:LYS:HD3	1:C:167:THR:HG22	1.93	0.48
1:B:711:LEU:HD21	2:B:904:POV:H27	1.96	0.48
1:D:442:PHE:HD1	2:D:904:POV:H39	1.79	0.48
1:A:251:ASN:HD21	1:A:295:ARG:HE	1.63	0.47
1:A:316:PHE:HA	1:A:319:ARG:HE	1.78	0.47
1:B:251:ASN:HD21	1:B:295:ARG:HE	1.63	0.47
1:C:417:HIS:O	1:C:421:THR:OG1	2.31	0.47
1:C:553:LEU:HD23	2:D:902:POV:H21A	1.96	0.47
1:A:671:ASN:ND2	6:A:1004:HOH:O	2.48	0.46
1:C:442:PHE:HD1	2:C:904:POV:H39	1.80	0.46
1:A:417:HIS:O	1:A:421:THR:OG1	2.31	0.46
1:D:711:LEU:HD21	2:D:904:POV:H27	1.97	0.46
1:C:251:ASN:HD21	1:C:295:ARG:HE	1.63	0.46
1:B:432:LYS:NZ	6:B:1003:HOH:O	2.43	0.46
1:D:251:ASN:HD21	1:D:295:ARG:HE	1.62	0.46
1:A:180:ASN:O	1:A:183:THR:OG1	2.34	0.46
1:C:711:LEU:HD21	2:C:904:POV:H27	1.98	0.46
2:A:908:POV:H23A	2:D:905:POV:H28	1.98	0.45
1:B:442:PHE:HD1	2:B:904:POV:H39	1.80	0.45
1:D:180:ASN:O	1:D:183:THR:OG1	2.34	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:656:PHE:HZ	2:A:909:POV:H310	1.80	0.45
1:B:180:ASN:O	1:B:183:THR:OG1	2.34	0.45
1:A:689:GLU:HB3	1:A:693:ARG:HH12	1.81	0.45
2:D:901:POV:H31A	2:D:901:POV:H37A	1.79	0.45
3:A:902:ACD:H42	3:A:902:ACD:H71	1.80	0.45
1:D:689:GLU:HB3	1:D:693:ARG:HH12	1.81	0.45
1:B:689:GLU:HB3	1:B:693:ARG:HH12	1.81	0.44
1:A:591:LEU:HD11	2:A:904:POV:H216	1.99	0.44
1:B:591:LEU:HD11	2:B:905:POV:H216	2.00	0.44
2:C:904:POV:H38A	2:C:904:POV:H311	1.85	0.44
2:C:901:POV:H36A	2:C:901:POV:H211	1.99	0.44
2:A:901:POV:H313	1:B:663:ILE:HD12	2.00	0.44
2:A:908:POV:H27A	2:D:905:POV:H21C	1.99	0.44
1:C:689:GLU:HB3	1:C:693:ARG:HH12	1.81	0.44
1:A:707:LEU:O	1:A:712:ARG:NH2	2.51	0.44
1:C:180:ASN:O	1:C:183:THR:OG1	2.34	0.44
1:A:69:ASP:HB2	1:A:177:LEU:HD13	2.00	0.44
1:D:69:ASP:HB2	1:D:177:LEU:HD13	2.00	0.44
2:A:901:POV:H210	2:A:901:POV:H213	1.92	0.44
1:B:417:HIS:O	1:B:421:THR:OG1	2.31	0.44
1:B:707:LEU:O	1:B:712:ARG:NH2	2.51	0.44
2:C:902:POV:H23A	2:C:905:POV:H28	2.00	0.44
1:D:671:ASN:ND2	6:D:1006:HOH:O	2.50	0.44
1:D:707:LEU:O	1:D:712:ARG:NH2	2.51	0.44
1:D:432:LYS:NZ	6:D:1003:HOH:O	2.43	0.43
2:B:904:POV:H38A	2:B:904:POV:H311	1.87	0.43
1:C:707:LEU:O	1:C:712:ARG:NH2	2.51	0.43
1:D:314:ASN:OD1	1:D:319:ARG:NH1	2.51	0.43
1:B:650:TYR:HB3	1:B:653:LEU:HB3	2.01	0.43
1:C:432:LYS:NZ	6:C:1003:HOH:O	2.43	0.43
1:A:553:LEU:HD11	1:B:653:LEU:HD21	2.01	0.43
1:A:650:TYR:HB3	1:A:653:LEU:HB3	2.01	0.43
1:A:711:LEU:HD21	2:A:903:POV:H27	2.01	0.43
1:C:69:ASP:HB2	1:C:177:LEU:HD13	2.00	0.43
1:A:314:ASN:OD1	1:A:319:ARG:NH1	2.51	0.43
2:A:908:POV:H21G	2:A:908:POV:H21D	1.84	0.43
1:B:314:ASN:OD1	1:B:319:ARG:NH1	2.51	0.43
1:C:314:ASN:OD1	1:C:319:ARG:NH1	2.51	0.43
1:B:69:ASP:HB2	1:B:177:LEU:HD13	2.00	0.43
1:A:456:THR:HG23	1:B:603:VAL:HG11	2.01	0.43
2:B:902:POV:H27A	2:B:905:POV:H21C	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:903:ACD:H71	3:C:903:ACD:H42	1.79	0.42
1:C:460:TYR:OH	2:D:905:POV:O14	2.37	0.42
3:D:903:ACD:H42	3:D:903:ACD:H71	1.80	0.42
3:B:903:ACD:H42	3:B:903:ACD:H71	1.79	0.42
1:B:516:ILE:H	1:B:516:ILE:HG13	1.74	0.42
1:D:439:HIS:HB2	2:D:904:POV:H3A	2.01	0.42
1:A:460:TYR:OH	2:B:905:POV:O14	2.36	0.42
2:B:902:POV:H21D	2:B:902:POV:H21G	1.85	0.42
2:C:902:POV:H21D	2:C:902:POV:H21G	1.84	0.42
2:C:902:POV:H27A	2:C:905:POV:H21C	2.01	0.42
1:D:417:HIS:O	1:D:421:THR:OG1	2.31	0.42
1:D:650:TYR:HB3	1:D:653:LEU:HB3	2.01	0.42
2:A:901:POV:H27A	2:A:904:POV:H21C	2.01	0.42
2:A:904:POV:O14	1:D:460:TYR:OH	2.35	0.42
1:C:671:ASN:ND2	6:C:1006:HOH:O	2.51	0.42
2:A:907:POV:H37A	2:A:907:POV:H31A	1.79	0.41
2:B:901:POV:H11	2:B:901:POV:H14B	1.82	0.41
1:A:442:PHE:HD1	2:A:903:POV:H39	1.85	0.41
1:A:450:PHE:HB2	2:A:907:POV:H21D	2.02	0.41
2:B:902:POV:H313	1:C:663:ILE:HD12	2.02	0.41
2:C:902:POV:H313	1:D:663:ILE:HD12	2.01	0.41
1:C:650:TYR:HB3	1:C:653:LEU:HB3	2.01	0.41
1:B:656:PHE:HZ	2:B:901:POV:H310	1.86	0.41
1:C:591:LEU:HD11	2:C:905:POV:H216	2.03	0.41
1:D:656:PHE:HZ	2:D:902:POV:H310	1.87	0.40
1:C:720:LEU:HD11	1:C:728:PHE:HB3	2.03	0.40
2:C:905:POV:H11A	2:C:905:POV:H15B	1.91	0.40
2:D:902:POV:H36A	2:D:902:POV:H211	2.02	0.40
1:A:659:ILE:HD12	2:A:908:POV:H37A	2.03	0.40
1:B:720:LEU:HD11	1:B:728:PHE:HB3	2.03	0.40
2:D:902:POV:H312	2:D:902:POV:H315	1.82	0.40
2:D:905:POV:H11A	2:D:905:POV:H15B	1.92	0.40

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	630/808 (78%)	594 (94%)	36 (6%)	0	100	100
1	B	630/808 (78%)	595 (94%)	35 (6%)	0	100	100
1	C	630/808 (78%)	595 (94%)	35 (6%)	0	100	100
1	D	630/808 (78%)	595 (94%)	35 (6%)	0	100	100
All	All	2520/3232 (78%)	2379 (94%)	141 (6%)	0	100	100

There are no Ramachandran outliers to report.

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	566/716 (79%)	558 (99%)	8 (1%)	62	82
1	B	566/716 (79%)	558 (99%)	8 (1%)	62	82
1	C	566/716 (79%)	558 (99%)	8 (1%)	62	82
1	D	566/716 (79%)	558 (99%)	8 (1%)	62	82
All	All	2264/2864 (79%)	2232 (99%)	32 (1%)	62	82

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	220	ASN
1	A	251	ASN
1	A	434	LYS
1	A	462	ARG
1	A	509	ARG
1	A	617	LYS
1	A	643	ASN
1	A	750	ASN

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Mol	Chain	Res	Type
1	B	220	ASN
1	B	251	ASN
1	B	434	LYS
1	B	462	ARG
1	B	509	ARG
1	B	617	LYS
1	B	643	ASN
1	B	750	ASN
1	C	220	ASN
1	C	251	ASN
1	C	434	LYS
1	C	462	ARG
1	C	509	ARG
1	C	617	LYS
1	C	643	ASN
1	C	750	ASN
1	D	220	ASN
1	D	251	ASN
1	D	434	LYS
1	D	462	ARG
1	D	509	ARG
1	D	617	LYS
1	D	643	ASN
1	D	750	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	ASN
1	A	182	ASN
1	A	205	ASN
1	A	220	ASN
1	A	242	ASN
1	A	412	ASN
1	A	585	HIS
1	A	643	ASN
1	A	671	ASN
1	A	750	ASN
1	B	71	ASN
1	B	182	ASN
1	B	205	ASN
1	B	220	ASN

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Mol	Chain	Res	Type
1	B	242	ASN
1	B	412	ASN
1	B	585	HIS
1	B	643	ASN
1	B	671	ASN
1	B	750	ASN
1	C	71	ASN
1	C	182	ASN
1	C	205	ASN
1	C	220	ASN
1	C	242	ASN
1	C	412	ASN
1	C	585	HIS
1	C	643	ASN
1	C	671	ASN
1	C	750	ASN
1	D	71	ASN
1	D	182	ASN
1	D	205	ASN
1	D	220	ASN
1	D	242	ASN
1	D	412	ASN
1	D	585	HIS
1	D	643	ASN
1	D	671	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 33 ligands modelled in this entry, 1 is monoatomic - leaving 32 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ACD	B	903	-	21,21,21	0.54	0	21,21,21	0.65	0
2	POV	B	905	-	51,51,51	1.14	3 (5%)	57,59,59	0.87	3 (5%)
4	FZ4	D	906	-	17,18,18	0.52	0	18,22,22	1.36	3 (16%)
2	POV	B	908	-	51,51,51	1.14	3 (5%)	57,59,59	0.91	3 (5%)
4	FZ4	B	907	-	17,18,18	0.51	0	18,22,22	1.10	2 (11%)
4	FZ4	C	907	-	17,18,18	0.51	0	18,22,22	1.14	2 (11%)
2	POV	A	901	-	51,51,51	1.14	3 (5%)	57,59,59	0.92	3 (5%)
2	POV	D	904	-	51,51,51	1.14	3 (5%)	57,59,59	0.93	2 (3%)
2	POV	A	904	-	51,51,51	1.14	3 (5%)	57,59,59	0.88	3 (5%)
4	FZ4	A	906	-	17,18,18	0.49	0	18,22,22	1.02	2 (11%)
4	FZ4	D	907	-	17,18,18	0.51	0	18,22,22	1.15	2 (11%)
2	POV	C	904	-	51,51,51	1.15	3 (5%)	57,59,59	0.99	2 (3%)
4	FZ4	C	906	-	17,18,18	0.52	0	18,22,22	1.38	2 (11%)
2	POV	A	907	-	51,51,51	1.14	3 (5%)	57,59,59	0.91	3 (5%)
2	POV	C	908	-	51,51,51	1.14	3 (5%)	57,59,59	0.91	3 (5%)
2	POV	B	901	-	51,51,51	1.14	3 (5%)	57,59,59	0.89	2 (3%)
2	POV	B	904	-	51,51,51	1.15	3 (5%)	57,59,59	0.96	2 (3%)
2	POV	D	905	-	51,51,51	1.14	3 (5%)	57,59,59	0.88	3 (5%)
3	ACD	A	902	-	21,21,21	0.54	0	21,21,21	0.64	0
3	ACD	C	903	-	21,21,21	0.54	0	21,21,21	0.64	0
2	POV	C	902	-	51,51,51	1.14	3 (5%)	57,59,59	0.91	3 (5%)
2	POV	A	908	-	51,51,51	1.14	3 (5%)	57,59,59	0.91	3 (5%)
2	POV	A	909	-	51,51,51	1.14	3 (5%)	57,59,59	0.91	2 (3%)
2	POV	C	905	-	51,51,51	1.14	3 (5%)	57,59,59	0.87	3 (5%)
2	POV	D	901	-	51,51,51	1.14	3 (5%)	57,59,59	0.90	3 (5%)
2	POV	D	902	-	51,51,51	1.14	3 (5%)	57,59,59	0.89	2 (3%)
3	ACD	D	903	-	21,21,21	0.54	0	21,21,21	0.64	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	POV	A	903	-	51,51,51	1.16	3 (5%)	57,59,59	0.96	3 (5%)
2	POV	C	901	-	51,51,51	1.14	3 (5%)	57,59,59	0.89	3 (5%)
4	FZ4	A	905	-	17,18,18	0.53	0	18,22,22	1.41	3 (16%)
4	FZ4	B	906	-	17,18,18	0.52	0	18,22,22	1.36	2 (11%)
2	POV	B	902	-	51,51,51	1.14	3 (5%)	57,59,59	0.91	3 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ACD	B	903	-	-	5/19/19/19	-
2	POV	B	905	-	-	24/55/55/55	-
4	FZ4	D	906	-	-	5/12/12/12	0/2/2/2
2	POV	B	908	-	-	29/55/55/55	-
4	FZ4	B	907	-	-	7/12/12/12	0/2/2/2
4	FZ4	C	907	-	-	9/12/12/12	0/2/2/2
2	POV	A	901	-	-	33/55/55/55	-
2	POV	D	904	-	-	27/55/55/55	-
2	POV	A	904	-	-	24/55/55/55	-
4	FZ4	A	906	-	-	9/12/12/12	0/2/2/2
4	FZ4	D	907	-	-	9/12/12/12	0/2/2/2
2	POV	C	904	-	-	25/55/55/55	-
4	FZ4	C	906	-	-	6/12/12/12	0/2/2/2
2	POV	A	907	-	-	30/55/55/55	-
2	POV	C	908	-	-	30/55/55/55	-
2	POV	B	901	-	-	28/55/55/55	-
2	POV	B	904	-	-	26/55/55/55	-
2	POV	D	905	-	-	24/55/55/55	-
3	ACD	A	902	-	-	5/19/19/19	-
3	ACD	C	903	-	-	6/19/19/19	-
2	POV	C	902	-	-	32/55/55/55	-
2	POV	A	908	-	-	33/55/55/55	-
2	POV	A	909	-	-	30/55/55/55	-
2	POV	C	905	-	-	25/55/55/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	POV	D	901	-	-	31/55/55/55	-
2	POV	D	902	-	-	30/55/55/55	-
3	ACD	D	903	-	-	6/19/19/19	-
2	POV	A	903	-	-	27/55/55/55	-
2	POV	C	901	-	-	30/55/55/55	-
4	FZ4	A	905	-	-	5/12/12/12	0/2/2/2
4	FZ4	B	906	-	-	6/12/12/12	0/2/2/2
2	POV	B	902	-	-	33/55/55/55	-

All (60) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	903	POV	O31-C31	3.19	1.42	1.33
2	C	904	POV	O31-C31	3.15	1.42	1.33
2	B	904	POV	O31-C31	3.12	1.42	1.33
2	A	901	POV	O21-C21	3.09	1.43	1.34
2	A	908	POV	O21-C21	3.07	1.43	1.34
2	B	902	POV	O21-C21	3.07	1.43	1.34
2	C	902	POV	O21-C21	3.07	1.42	1.34
2	D	901	POV	O31-C31	3.04	1.42	1.33
2	B	908	POV	O31-C31	3.02	1.42	1.33
2	D	904	POV	O31-C31	3.01	1.42	1.33
2	C	908	POV	O31-C31	3.00	1.42	1.33
2	A	907	POV	O31-C31	2.98	1.42	1.33
2	A	901	POV	O31-C31	2.98	1.42	1.33
2	B	902	POV	O31-C31	2.96	1.42	1.33
2	A	904	POV	O31-C31	2.96	1.42	1.33
2	D	905	POV	O31-C31	2.94	1.41	1.33
2	A	908	POV	O31-C31	2.94	1.41	1.33
2	B	905	POV	O31-C31	2.93	1.41	1.33
2	D	902	POV	O31-C31	2.93	1.41	1.33
2	C	905	POV	O31-C31	2.93	1.41	1.33
2	C	902	POV	O31-C31	2.93	1.41	1.33
2	B	904	POV	O21-C21	2.92	1.42	1.34
2	C	901	POV	O31-C31	2.92	1.41	1.33
2	A	909	POV	O31-C31	2.92	1.41	1.33
2	B	901	POV	O31-C31	2.92	1.41	1.33
2	C	904	POV	O21-C21	2.91	1.42	1.34
2	D	904	POV	O21-C21	2.91	1.42	1.34
2	A	904	POV	O21-C21	2.90	1.42	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	905	POV	O21-C21	2.90	1.42	1.34
2	B	905	POV	O21-C21	2.88	1.42	1.34
2	D	905	POV	O21-C21	2.88	1.42	1.34
2	A	903	POV	O21-C21	2.88	1.42	1.34
2	C	901	POV	O21-C21	2.87	1.42	1.34
2	B	901	POV	O21-C21	2.87	1.42	1.34
2	A	909	POV	O21-C21	2.83	1.42	1.34
2	D	902	POV	O21-C21	2.83	1.42	1.34
2	C	908	POV	O21-C21	2.82	1.42	1.34
2	A	907	POV	O21-C21	2.81	1.42	1.34
2	B	908	POV	O21-C21	2.80	1.42	1.34
2	D	901	POV	O21-C21	2.79	1.42	1.34
2	C	908	POV	O21-C2	-2.65	1.40	1.46
2	A	903	POV	O21-C2	-2.64	1.40	1.46
2	B	908	POV	O21-C2	-2.62	1.40	1.46
2	A	907	POV	O21-C2	-2.61	1.40	1.46
2	B	905	POV	O21-C2	-2.60	1.40	1.46
2	C	905	POV	O21-C2	-2.59	1.40	1.46
2	A	904	POV	O21-C2	-2.59	1.40	1.46
2	D	901	POV	O21-C2	-2.59	1.40	1.46
2	D	902	POV	O21-C2	-2.58	1.40	1.46
2	C	901	POV	O21-C2	-2.57	1.40	1.46
2	A	909	POV	O21-C2	-2.56	1.40	1.46
2	B	901	POV	O21-C2	-2.56	1.40	1.46
2	B	904	POV	O21-C2	-2.55	1.40	1.46
2	D	905	POV	O21-C2	-2.55	1.40	1.46
2	C	904	POV	O21-C2	-2.52	1.40	1.46
2	D	904	POV	O21-C2	-2.52	1.40	1.46
2	A	908	POV	O21-C2	-2.12	1.41	1.46
2	C	902	POV	O21-C2	-2.11	1.41	1.46
2	B	902	POV	O21-C2	-2.06	1.41	1.46
2	A	901	POV	O21-C2	-2.05	1.41	1.46

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	904	POV	O21-C21-C22	4.02	120.17	111.48
2	B	904	POV	O21-C21-C22	4.01	120.15	111.48
2	D	904	POV	O21-C21-C22	4.01	120.15	111.48
2	B	901	POV	O21-C21-C22	3.91	119.95	111.48
2	A	907	POV	O21-C21-C22	3.89	119.89	111.48
2	A	909	POV	O21-C21-C22	3.87	119.86	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	901	POV	O21-C21-C22	3.87	119.84	111.48
2	D	902	POV	O21-C21-C22	3.85	119.81	111.48
2	C	908	POV	O21-C21-C22	3.84	119.79	111.48
2	B	908	POV	O21-C21-C22	3.82	119.74	111.48
2	D	901	POV	O21-C21-C22	3.76	119.61	111.48
2	A	903	POV	O21-C21-C22	3.76	119.61	111.48
2	A	904	POV	O21-C21-C22	3.71	119.51	111.48
2	D	905	POV	O21-C21-C22	3.68	119.44	111.48
2	B	905	POV	O21-C21-C22	3.67	119.41	111.48
2	C	905	POV	O21-C21-C22	3.62	119.31	111.48
2	A	901	POV	O21-C21-C22	3.51	119.07	111.48
2	B	902	POV	O21-C21-C22	3.49	119.03	111.48
2	A	908	POV	O21-C21-C22	3.48	119.02	111.48
2	C	902	POV	O21-C21-C22	3.47	118.99	111.48
2	A	903	POV	O31-C31-C32	3.43	122.28	111.83
2	C	904	POV	O31-C31-C32	3.37	122.11	111.83
2	B	904	POV	O31-C31-C32	3.12	121.34	111.83
4	A	905	FZ4	C13-C08-C09	2.91	120.20	116.86
4	C	906	FZ4	C07-C02-C03	2.90	120.19	116.86
2	A	901	POV	C13-N-C12	2.86	121.28	109.91
2	C	902	POV	C13-N-C12	2.85	121.23	109.91
2	A	908	POV	C13-N-C12	2.84	121.19	109.91
2	B	902	POV	C13-N-C12	2.83	121.17	109.91
4	B	906	FZ4	C07-C02-C03	2.82	120.09	116.86
4	D	906	FZ4	C07-C02-C03	2.80	120.08	116.86
4	D	906	FZ4	C13-C08-C09	2.80	120.08	116.86
4	A	905	FZ4	C07-C02-C03	2.79	120.06	116.86
4	C	906	FZ4	C13-C08-C09	2.78	120.05	116.86
4	B	906	FZ4	C13-C08-C09	2.77	120.04	116.86
2	B	908	POV	O31-C31-C32	2.75	120.23	111.83
2	C	908	POV	O31-C31-C32	2.75	120.22	111.83
2	D	901	POV	O31-C31-C32	2.71	120.09	111.83
2	A	907	POV	O31-C31-C32	2.69	120.04	111.83
2	C	905	POV	O31-C31-C32	2.67	119.96	111.83
2	B	905	POV	O31-C31-C32	2.65	119.93	111.83
2	D	905	POV	O31-C31-C32	2.65	119.91	111.83
2	A	904	POV	O31-C31-C32	2.65	119.90	111.83
2	D	902	POV	O31-C31-C32	2.62	119.81	111.83
2	C	901	POV	O31-C31-C32	2.61	119.78	111.83
2	A	909	POV	O31-C31-C32	2.60	119.77	111.83
2	A	901	POV	O31-C31-C32	2.56	119.66	111.83
2	A	908	POV	O31-C31-C32	2.56	119.64	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	902	POV	O31-C31-C32	2.56	119.63	111.83
2	B	901	POV	O31-C31-C32	2.54	119.58	111.83
2	B	902	POV	O31-C31-C32	2.54	119.58	111.83
2	D	904	POV	O31-C31-C32	2.53	119.54	111.83
4	C	907	FZ4	C07-C02-C03	2.44	119.66	116.86
4	D	907	FZ4	C13-C08-C09	2.44	119.66	116.86
4	D	907	FZ4	C07-C02-C03	2.42	119.64	116.86
4	C	907	FZ4	C13-C08-C09	2.38	119.59	116.86
4	B	907	FZ4	C13-C08-C09	2.33	119.53	116.86
4	B	907	FZ4	C07-C02-C03	2.31	119.51	116.86
4	A	905	FZ4	C10-C09-C08	-2.16	119.51	121.58
2	A	903	POV	C13-N-C12	2.14	118.44	109.91
2	D	901	POV	C13-N-C12	2.14	118.41	109.91
4	A	906	FZ4	C07-C02-C03	2.14	119.31	116.86
4	A	906	FZ4	C13-C08-C09	2.12	119.30	116.86
2	B	908	POV	C13-N-C12	2.12	118.33	109.91
2	C	908	POV	C13-N-C12	2.12	118.32	109.91
2	C	905	POV	C13-N-C12	2.10	118.24	109.91
2	B	905	POV	C13-N-C12	2.10	118.24	109.91
2	A	904	POV	C13-N-C12	2.09	118.23	109.91
2	D	905	POV	C13-N-C12	2.09	118.23	109.91
2	A	907	POV	C13-N-C12	2.09	118.23	109.91
2	C	901	POV	C13-N-C12	2.01	117.89	109.91
4	D	906	FZ4	C10-C09-C08	-2.00	119.66	121.58

There are no chirality outliers.

All (649) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	901	POV	C11-O12-P-O11
2	A	901	POV	C11-O12-P-O13
2	A	901	POV	C11-O12-P-O14
2	A	903	POV	C1-O11-P-O12
2	A	903	POV	C1-O11-P-O13
2	A	903	POV	C32-C31-O31-C3
2	A	903	POV	O32-C31-O31-C3
2	A	904	POV	C11-O12-P-O11
2	A	904	POV	C11-O12-P-O13
2	A	904	POV	C11-O12-P-O14
2	A	904	POV	O12-C11-C12-N
2	A	907	POV	C1-O11-P-O12
2	A	907	POV	C1-O11-P-O13

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Mol	Chain	Res	Type	Atoms
2	A	907	POV	C1-O11-P-O14
2	A	907	POV	C11-O12-P-O11
2	A	907	POV	C11-O12-P-O13
2	A	907	POV	C11-O12-P-O14
2	A	907	POV	C22-C21-O21-C2
2	A	908	POV	C11-O12-P-O11
2	A	908	POV	C11-O12-P-O13
2	A	908	POV	C11-O12-P-O14
2	A	909	POV	C1-O11-P-O12
2	A	909	POV	C1-O11-P-O14
2	B	901	POV	C1-O11-P-O14
2	B	901	POV	O21-C2-C3-O31
2	B	901	POV	C22-C21-O21-C2
2	B	902	POV	C11-O12-P-O11
2	B	902	POV	C11-O12-P-O13
2	B	904	POV	C1-O11-P-O12
2	B	904	POV	C1-O11-P-O13
2	B	904	POV	C2-C1-O11-P
2	B	904	POV	C32-C31-O31-C3
2	B	904	POV	O32-C31-O31-C3
2	B	905	POV	C11-O12-P-O11
2	B	905	POV	C11-O12-P-O13
2	B	905	POV	C11-O12-P-O14
2	B	905	POV	O12-C11-C12-N
2	B	908	POV	C1-O11-P-O12
2	B	908	POV	C1-O11-P-O13
2	B	908	POV	C1-O11-P-O14
2	B	908	POV	C11-O12-P-O11
2	B	908	POV	C11-O12-P-O13
2	B	908	POV	C11-O12-P-O14
2	B	908	POV	C22-C21-O21-C2
2	C	901	POV	C1-O11-P-O14
2	C	901	POV	O21-C2-C3-O31
2	C	901	POV	C22-C21-O21-C2
2	C	902	POV	C11-O12-P-O11
2	C	902	POV	C11-O12-P-O13
2	C	904	POV	C1-O11-P-O12
2	C	904	POV	C1-O11-P-O13
2	C	904	POV	C2-C1-O11-P
2	C	904	POV	C32-C31-O31-C3
2	C	904	POV	O32-C31-O31-C3
2	C	905	POV	C11-O12-P-O11

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Mol	Chain	Res	Type	Atoms
2	C	905	POV	C11-O12-P-O13
2	C	905	POV	C11-O12-P-O14
2	C	905	POV	O12-C11-C12-N
2	C	908	POV	C1-O11-P-O12
2	C	908	POV	C1-O11-P-O13
2	C	908	POV	C1-O11-P-O14
2	C	908	POV	C11-O12-P-O11
2	C	908	POV	C11-O12-P-O13
2	C	908	POV	C11-O12-P-O14
2	C	908	POV	C22-C21-O21-C2
2	D	901	POV	C1-O11-P-O12
2	D	901	POV	C1-O11-P-O13
2	D	901	POV	C1-O11-P-O14
2	D	901	POV	C11-O12-P-O11
2	D	901	POV	C11-O12-P-O13
2	D	901	POV	C11-O12-P-O14
2	D	901	POV	O12-C11-C12-N
2	D	901	POV	C22-C21-O21-C2
2	D	902	POV	C1-O11-P-O14
2	D	902	POV	O21-C2-C3-O31
2	D	902	POV	C22-C21-O21-C2
2	D	904	POV	C1-O11-P-O12
2	D	904	POV	C1-O11-P-O13
2	D	904	POV	O12-C11-C12-N
2	D	905	POV	C11-O12-P-O11
2	D	905	POV	C11-O12-P-O13
2	D	905	POV	C11-O12-P-O14
2	D	905	POV	O12-C11-C12-N
3	A	902	ACD	C11-C10-C9-C8
3	B	903	ACD	C11-C10-C9-C8
3	C	903	ACD	C11-C10-C9-C8
3	D	903	ACD	C11-C10-C9-C8
4	A	905	FZ4	O14-B01-C08-C09
4	A	905	FZ4	O14-B01-C08-C13
4	A	905	FZ4	C02-B01-O14-C15
4	A	905	FZ4	C08-B01-O14-C15
4	A	905	FZ4	O14-C15-C16-N17
4	A	906	FZ4	O14-B01-C08-C09
4	A	906	FZ4	O14-B01-C08-C13
4	A	906	FZ4	C02-B01-O14-C15
4	A	906	FZ4	C08-B01-O14-C15
4	A	906	FZ4	O14-C15-C16-N17

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Mol	Chain	Res	Type	Atoms
4	B	906	FZ4	O14-B01-C08-C09
4	B	906	FZ4	O14-B01-C08-C13
4	B	906	FZ4	C02-B01-O14-C15
4	B	906	FZ4	C08-B01-O14-C15
4	B	906	FZ4	O14-C15-C16-N17
4	B	907	FZ4	O14-B01-C08-C09
4	B	907	FZ4	O14-B01-C08-C13
4	B	907	FZ4	C02-B01-O14-C15
4	B	907	FZ4	C08-B01-O14-C15
4	B	907	FZ4	O14-C15-C16-N17
4	C	906	FZ4	O14-B01-C08-C09
4	C	906	FZ4	O14-B01-C08-C13
4	C	906	FZ4	C02-B01-O14-C15
4	C	906	FZ4	C08-B01-O14-C15
4	C	906	FZ4	O14-C15-C16-N17
4	C	907	FZ4	O14-B01-C08-C09
4	C	907	FZ4	O14-B01-C08-C13
4	C	907	FZ4	C02-B01-O14-C15
4	C	907	FZ4	C08-B01-O14-C15
4	C	907	FZ4	O14-C15-C16-N17
4	D	906	FZ4	O14-B01-C08-C09
4	D	906	FZ4	O14-B01-C08-C13
4	D	906	FZ4	C02-B01-O14-C15
4	D	906	FZ4	C08-B01-O14-C15
4	D	906	FZ4	O14-C15-C16-N17
4	D	907	FZ4	O14-B01-C08-C09
4	D	907	FZ4	O14-B01-C08-C13
4	D	907	FZ4	C02-B01-O14-C15
4	D	907	FZ4	C08-B01-O14-C15
4	D	907	FZ4	O14-C15-C16-N17
2	A	909	POV	O32-C31-O31-C3
2	B	901	POV	O32-C31-O31-C3
2	C	901	POV	O32-C31-O31-C3
2	D	902	POV	O32-C31-O31-C3
2	D	904	POV	O32-C31-O31-C3
2	A	909	POV	O22-C21-O21-C2
2	B	901	POV	O22-C21-O21-C2
2	B	908	POV	O22-C21-O21-C2
2	C	901	POV	O22-C21-O21-C2
2	C	908	POV	O22-C21-O21-C2
2	D	901	POV	O22-C21-O21-C2
2	D	902	POV	O22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
2	A	909	POV	C32-C31-O31-C3
2	B	901	POV	C32-C31-O31-C3
2	C	901	POV	C32-C31-O31-C3
2	D	902	POV	C32-C31-O31-C3
2	D	904	POV	C32-C31-O31-C3
2	A	909	POV	C22-C21-O21-C2
2	B	905	POV	C32-C31-O31-C3
2	C	905	POV	C32-C31-O31-C3
2	A	907	POV	O22-C21-O21-C2
2	A	903	POV	C11-C12-N-C14
2	A	904	POV	C32-C31-O31-C3
2	D	905	POV	C32-C31-O31-C3
2	A	904	POV	O32-C31-O31-C3
2	B	905	POV	O32-C31-O31-C3
2	C	905	POV	O32-C31-O31-C3
2	A	903	POV	C2-C1-O11-P
2	D	904	POV	C2-C1-O11-P
2	D	905	POV	O32-C31-O31-C3
2	A	908	POV	C32-C31-O31-C3
2	B	902	POV	C32-C31-O31-C3
2	C	902	POV	C32-C31-O31-C3
2	A	908	POV	C11-C12-N-C13
2	B	902	POV	C11-C12-N-C13
2	A	901	POV	C32-C31-O31-C3
2	A	903	POV	C21-C22-C23-C24
2	A	909	POV	C31-C32-C33-C34
2	B	902	POV	O32-C31-O31-C3
2	B	904	POV	C21-C22-C23-C24
2	C	904	POV	C21-C22-C23-C24
2	D	904	POV	C21-C22-C23-C24
2	C	902	POV	O32-C31-O31-C3
2	A	908	POV	O32-C31-O31-C3
2	A	908	POV	O22-C21-O21-C2
2	D	905	POV	C31-C32-C33-C34
2	B	908	POV	C32-C31-O31-C3
2	C	908	POV	C32-C31-O31-C3
2	D	901	POV	C32-C31-O31-C3
2	A	908	POV	C22-C21-O21-C2
2	B	902	POV	C22-C21-O21-C2
2	C	902	POV	C22-C21-O21-C2
2	A	901	POV	O32-C31-O31-C3
2	D	902	POV	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
2	A	901	POV	O22-C21-O21-C2
2	B	902	POV	O22-C21-O21-C2
2	C	902	POV	O22-C21-O21-C2
2	A	901	POV	C11-C12-N-C13
2	A	901	POV	C11-C12-N-C14
2	A	901	POV	C11-C12-N-C15
2	A	903	POV	C11-C12-N-C13
2	A	908	POV	C11-C12-N-C14
2	A	908	POV	C11-C12-N-C15
2	B	902	POV	C11-C12-N-C14
2	B	902	POV	C11-C12-N-C15
2	B	904	POV	C11-C12-N-C13
2	B	904	POV	C11-C12-N-C14
2	B	904	POV	C11-C12-N-C15
2	C	902	POV	C11-C12-N-C13
2	C	902	POV	C11-C12-N-C14
2	C	904	POV	C11-C12-N-C13
2	C	904	POV	C11-C12-N-C14
2	C	904	POV	C11-C12-N-C15
2	D	904	POV	C11-C12-N-C14
2	C	905	POV	C31-C32-C33-C34
2	A	907	POV	C32-C31-O31-C3
2	A	901	POV	C22-C21-O21-C2
2	C	908	POV	O32-C31-O31-C3
2	A	901	POV	C311-C310-C39-C38
2	B	908	POV	O32-C31-O31-C3
2	A	909	POV	O21-C2-C3-O31
2	A	903	POV	C11-C12-N-C15
2	C	902	POV	C11-C12-N-C15
2	D	904	POV	C11-C12-N-C15
2	D	901	POV	O32-C31-O31-C3
2	D	901	POV	C35-C36-C37-C38
2	A	904	POV	C39-C310-C311-C312
2	A	907	POV	C35-C36-C37-C38
2	A	909	POV	C35-C36-C37-C38
2	B	908	POV	C24-C25-C26-C27
2	C	908	POV	C24-C25-C26-C27
2	B	905	POV	C39-C310-C311-C312
2	C	901	POV	C33-C34-C35-C36
2	D	902	POV	C33-C34-C35-C36
2	B	901	POV	C34-C35-C36-C37
2	B	908	POV	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
2	C	905	POV	C39-C310-C311-C312
2	A	909	POV	C23-C24-C25-C26
2	C	908	POV	C35-C36-C37-C38
2	D	905	POV	C39-C310-C311-C312
2	C	901	POV	C31-C32-C33-C34
2	A	909	POV	C310-C311-C312-C313
2	B	901	POV	C23-C24-C25-C26
2	C	901	POV	C211-C212-C213-C214
2	B	901	POV	C310-C311-C312-C313
2	A	903	POV	C35-C36-C37-C38
2	C	901	POV	C23-C24-C25-C26
2	C	904	POV	C211-C212-C213-C214
2	D	904	POV	C211-C212-C213-C214
2	A	903	POV	C211-C212-C213-C214
2	A	907	POV	C24-C25-C26-C27
2	D	902	POV	C23-C24-C25-C26
2	D	904	POV	C35-C36-C37-C38
2	B	902	POV	C1-C2-C3-O31
2	B	904	POV	C211-C212-C213-C214
2	C	901	POV	C310-C311-C312-C313
2	C	904	POV	C35-C36-C37-C38
2	D	902	POV	C310-C311-C312-C313
2	B	901	POV	C31-C32-C33-C34
2	B	905	POV	C31-C32-C33-C34
2	A	908	POV	C311-C310-C39-C38
2	A	909	POV	C32-C33-C34-C35
2	B	901	POV	C211-C212-C213-C214
2	B	904	POV	C35-C36-C37-C38
2	C	901	POV	C24-C25-C26-C27
2	A	907	POV	O32-C31-O31-C3
2	D	902	POV	C211-C212-C213-C214
2	A	903	POV	C36-C37-C38-C39
2	B	902	POV	C311-C310-C39-C38
2	D	904	POV	C11-C12-N-C13
2	A	903	POV	C24-C25-C26-C27
2	C	902	POV	C311-C310-C39-C38
2	D	902	POV	C24-C25-C26-C27
2	D	904	POV	C312-C313-C314-C315
2	D	904	POV	C36-C37-C38-C39
2	A	909	POV	C211-C212-C213-C214
2	D	902	POV	C32-C33-C34-C35
2	B	904	POV	C312-C313-C314-C315

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Mol	Chain	Res	Type	Atoms
2	C	901	POV	C32-C33-C34-C35
2	C	904	POV	C312-C313-C314-C315
2	C	904	POV	C36-C37-C38-C39
2	A	903	POV	C312-C313-C314-C315
2	B	901	POV	C35-C36-C37-C38
2	A	904	POV	C212-C213-C214-C215
2	B	905	POV	C212-C213-C214-C215
2	A	904	POV	C31-C32-C33-C34
2	A	904	POV	C310-C311-C312-C313
2	D	905	POV	C213-C214-C215-C216
2	A	909	POV	C33-C34-C35-C36
2	C	905	POV	C212-C213-C214-C215
2	D	902	POV	C39-C310-C311-C312
2	D	902	POV	C35-C36-C37-C38
2	C	901	POV	C35-C36-C37-C38
2	D	901	POV	C24-C25-C26-C27
2	A	901	POV	C26-C27-C28-C29
2	A	908	POV	C26-C27-C28-C29
2	C	904	POV	C26-C27-C28-C29
2	D	904	POV	C26-C27-C28-C29
2	D	905	POV	C212-C213-C214-C215
2	B	901	POV	C33-C34-C35-C36
2	B	905	POV	C213-C214-C215-C216
2	C	905	POV	C213-C214-C215-C216
2	A	907	POV	C211-C212-C213-C214
2	B	901	POV	C39-C310-C311-C312
2	C	901	POV	C39-C310-C311-C312
2	A	903	POV	C212-C213-C214-C215
2	D	904	POV	C311-C310-C39-C38
2	B	904	POV	C36-C37-C38-C39
2	A	904	POV	C213-C214-C215-C216
2	A	909	POV	C39-C310-C311-C312
2	B	901	POV	C32-C33-C34-C35
2	B	904	POV	C212-C213-C214-C215
2	C	904	POV	C212-C213-C214-C215
2	D	904	POV	C212-C213-C214-C215
2	B	902	POV	C26-C27-C28-C29
2	B	904	POV	C26-C27-C28-C29
2	B	904	POV	C24-C25-C26-C27
2	D	901	POV	C211-C212-C213-C214
2	A	903	POV	C39-C310-C311-C312
2	C	908	POV	C211-C212-C213-C214

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Mol	Chain	Res	Type	Atoms
2	B	908	POV	C211-C212-C213-C214
2	A	907	POV	C36-C37-C38-C39
2	D	905	POV	C33-C34-C35-C36
2	D	905	POV	C37-C38-C39-C310
2	A	909	POV	C213-C214-C215-C216
2	D	901	POV	C36-C37-C38-C39
2	A	903	POV	C26-C27-C28-C29
2	A	907	POV	C26-C27-C28-C29
2	B	908	POV	C26-C27-C28-C29
2	C	902	POV	C26-C27-C28-C29
2	C	908	POV	C26-C27-C28-C29
3	D	903	ACD	C15-C16-C17-C18
2	B	905	POV	C37-C38-C39-C310
2	C	905	POV	C37-C38-C39-C310
2	A	904	POV	C37-C38-C39-C310
2	C	904	POV	C24-C25-C26-C27
2	D	904	POV	C22-C23-C24-C25
2	C	908	POV	C25-C26-C27-C28
2	A	907	POV	C25-C26-C27-C28
2	A	909	POV	C24-C25-C26-C27
2	A	909	POV	C37-C38-C39-C310
2	C	905	POV	C33-C34-C35-C36
2	C	904	POV	C311-C310-C39-C38
2	B	904	POV	C311-C310-C39-C38
2	B	905	POV	C310-C311-C312-C313
2	A	907	POV	C1-C2-C3-O31
2	A	908	POV	C1-C2-C3-O31
2	B	901	POV	C1-C2-C3-O31
2	B	908	POV	C1-C2-C3-O31
2	C	901	POV	C1-C2-C3-O31
2	C	902	POV	C1-C2-C3-O31
2	C	908	POV	C1-C2-C3-O31
2	D	901	POV	C1-C2-C3-O31
2	D	902	POV	C1-C2-C3-O31
2	D	904	POV	C1-C2-C3-O31
2	C	904	POV	C22-C23-C24-C25
2	D	901	POV	C26-C27-C28-C29
2	A	909	POV	C36-C37-C38-C39
2	D	904	POV	C24-C25-C26-C27
2	B	901	POV	C24-C25-C26-C27
2	B	908	POV	C25-C26-C27-C28
2	A	904	POV	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
2	C	904	POV	C213-C214-C215-C216
2	C	901	POV	C34-C35-C36-C37
2	A	903	POV	C213-C214-C215-C216
2	B	904	POV	C22-C23-C24-C25
2	D	904	POV	C213-C214-C215-C216
2	A	904	POV	C34-C35-C36-C37
2	B	904	POV	C213-C214-C215-C216
2	A	908	POV	C23-C24-C25-C26
2	B	905	POV	C33-C34-C35-C36
2	D	902	POV	O11-C1-C2-O21
2	D	905	POV	C310-C311-C312-C313
2	A	907	POV	C23-C24-C25-C26
2	B	905	POV	C34-C35-C36-C37
2	A	903	POV	C22-C23-C24-C25
3	C	903	ACD	C15-C16-C17-C18
2	D	901	POV	C25-C26-C27-C28
2	D	902	POV	C213-C214-C215-C216
2	C	905	POV	C310-C311-C312-C313
2	D	904	POV	C39-C310-C311-C312
2	D	901	POV	C39-C310-C311-C312
2	C	904	POV	C39-C310-C311-C312
3	B	903	ACD	C15-C16-C17-C18
2	B	901	POV	C214-C215-C216-C217
2	B	904	POV	C39-C310-C311-C312
2	C	901	POV	C213-C214-C215-C216
2	B	901	POV	C213-C214-C215-C216
2	C	908	POV	C23-C24-C25-C26
2	B	908	POV	C23-C24-C25-C26
2	A	901	POV	C31-C32-C33-C34
2	A	907	POV	C215-C216-C217-C218
3	A	902	ACD	C15-C16-C17-C18
2	B	902	POV	C31-C32-C33-C34
2	D	901	POV	C34-C35-C36-C37
2	D	902	POV	C34-C35-C36-C37
2	A	901	POV	C1-C2-C3-O31
2	A	909	POV	C1-C2-C3-O31
2	B	904	POV	C1-C2-C3-O31
2	D	901	POV	C37-C38-C39-C310
2	C	902	POV	C31-C32-C33-C34
2	B	905	POV	C35-C36-C37-C38
2	C	902	POV	C23-C24-C25-C26
2	A	904	POV	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
2	A	908	POV	O11-C1-C2-O21
2	A	909	POV	O11-C1-C2-O21
2	C	901	POV	O11-C1-C2-O21
2	D	902	POV	C37-C38-C39-C310
2	A	901	POV	C212-C213-C214-C215
2	A	907	POV	O21-C2-C3-O31
2	B	908	POV	O21-C2-C3-O31
2	C	908	POV	O21-C2-C3-O31
2	D	901	POV	O21-C2-C3-O31
3	D	903	ACD	C9-C10-C11-C12
2	A	904	POV	C214-C215-C216-C217
2	B	908	POV	C34-C35-C36-C37
2	C	908	POV	C34-C35-C36-C37
2	A	907	POV	C37-C38-C39-C310
2	C	902	POV	C212-C213-C214-C215
2	A	908	POV	C31-C32-C33-C34
2	B	902	POV	C212-C213-C214-C215
2	D	901	POV	C23-C24-C25-C26
2	C	901	POV	C37-C38-C39-C310
2	A	904	POV	C210-C211-C212-C213
2	D	905	POV	C210-C211-C212-C213
2	A	909	POV	O11-C1-C2-C3
2	B	902	POV	O11-C1-C2-C3
2	A	907	POV	C39-C310-C311-C312
2	A	901	POV	C32-C33-C34-C35
2	B	902	POV	C23-C24-C25-C26
2	A	908	POV	C212-C213-C214-C215
2	A	908	POV	C214-C215-C216-C217
4	A	906	FZ4	C02-B01-C08-C13
2	A	901	POV	C1-C2-O21-C21
2	A	908	POV	C1-C2-O21-C21
2	B	902	POV	C1-C2-O21-C21
2	C	902	POV	C1-C2-O21-C21
2	A	908	POV	C211-C212-C213-C214
2	B	905	POV	C210-C211-C212-C213
2	C	905	POV	C210-C211-C212-C213
2	B	905	POV	C24-C25-C26-C27
2	A	901	POV	O11-C1-C2-O21
2	B	901	POV	O11-C1-C2-O21
2	B	902	POV	O11-C1-C2-O21
2	C	902	POV	O11-C1-C2-O21
2	C	902	POV	C211-C212-C213-C214

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Mol	Chain	Res	Type	Atoms
2	C	901	POV	C214-C215-C216-C217
2	A	908	POV	O21-C2-C3-O31
2	C	902	POV	O21-C2-C3-O31
2	D	904	POV	O21-C2-C3-O31
2	C	905	POV	C34-C35-C36-C37
2	A	907	POV	C34-C35-C36-C37
2	D	905	POV	C35-C36-C37-C38
2	C	905	POV	C35-C36-C37-C38
2	D	905	POV	C34-C35-C36-C37
2	A	901	POV	O12-C11-C12-N
2	A	907	POV	O12-C11-C12-N
2	A	908	POV	O12-C11-C12-N
2	B	904	POV	O12-C11-C12-N
2	B	908	POV	O12-C11-C12-N
2	C	904	POV	O12-C11-C12-N
2	C	908	POV	O12-C11-C12-N
2	C	908	POV	C215-C216-C217-C218
2	A	901	POV	C23-C24-C25-C26
2	A	901	POV	C211-C212-C213-C214
2	A	909	POV	C22-C23-C24-C25
2	B	902	POV	C211-C212-C213-C214
2	B	905	POV	C36-C37-C38-C39
2	C	902	POV	C214-C215-C216-C217
2	A	901	POV	O11-C1-C2-C3
2	A	908	POV	O11-C1-C2-C3
2	B	901	POV	O11-C1-C2-C3
2	C	901	POV	O11-C1-C2-C3
2	C	902	POV	O11-C1-C2-C3
2	D	902	POV	O11-C1-C2-C3
2	C	905	POV	C313-C314-C315-C316
2	B	901	POV	C37-C38-C39-C310
2	B	902	POV	C32-C33-C34-C35
2	C	908	POV	C212-C213-C214-C215
2	A	909	POV	C212-C213-C214-C215
2	D	905	POV	C313-C314-C315-C316
2	A	907	POV	O11-C1-C2-O21
2	D	902	POV	C36-C37-C38-C39
2	D	901	POV	C213-C214-C215-C216
2	A	908	POV	C33-C34-C35-C36
2	D	902	POV	C214-C215-C216-C217
2	B	904	POV	O21-C2-C3-O31
2	C	902	POV	C39-C310-C311-C312

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Mol	Chain	Res	Type	Atoms
2	B	908	POV	C212-C213-C214-C215
2	B	901	POV	C313-C314-C315-C316
2	A	907	POV	C212-C213-C214-C215
2	B	902	POV	C214-C215-C216-C217
2	C	902	POV	C32-C33-C34-C35
2	A	903	POV	C1-O11-P-O14
2	B	902	POV	C11-O12-P-O14
2	B	904	POV	C1-O11-P-O14
2	C	902	POV	C11-O12-P-O14
2	C	904	POV	C1-O11-P-O14
2	D	904	POV	C1-O11-P-O14
2	C	905	POV	C24-C25-C26-C27
2	B	905	POV	C214-C215-C216-C217
2	C	901	POV	C313-C314-C315-C316
2	B	905	POV	C313-C314-C315-C316
2	B	902	POV	C39-C310-C311-C312
2	B	908	POV	C213-C214-C215-C216
2	C	908	POV	C213-C214-C215-C216
2	D	905	POV	C29-C210-C211-C212
2	D	901	POV	C215-C216-C217-C218
2	C	905	POV	O11-C1-C2-C3
2	C	901	POV	C36-C37-C38-C39
2	B	905	POV	C29-C210-C211-C212
2	C	901	POV	C29-C210-C211-C212
2	C	905	POV	C29-C210-C211-C212
2	A	903	POV	C31-C32-C33-C34
2	D	905	POV	C24-C25-C26-C27
2	C	908	POV	O11-C1-C2-O21
2	B	901	POV	C22-C23-C24-C25
2	A	908	POV	C2-C1-O11-P
2	B	908	POV	C215-C216-C217-C218
2	B	902	POV	O21-C2-C3-O31
2	A	908	POV	C35-C36-C37-C38
2	D	901	POV	C33-C34-C35-C36
2	A	904	POV	C29-C210-C211-C212
2	D	902	POV	C29-C210-C211-C212
4	A	906	FZ4	C02-B01-C08-C09
4	B	907	FZ4	C02-B01-C08-C09
4	B	907	FZ4	C02-B01-C08-C13
4	C	907	FZ4	C02-B01-C08-C09
4	C	907	FZ4	C02-B01-C08-C13
4	D	907	FZ4	C02-B01-C08-C09

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Mol	Chain	Res	Type	Atoms
4	D	907	FZ4	C02-B01-C08-C13
2	D	902	POV	C313-C314-C315-C316
2	A	903	POV	C311-C310-C39-C38
2	A	909	POV	C29-C210-C211-C212
2	C	905	POV	C214-C215-C216-C217
2	C	902	POV	C310-C311-C312-C313
2	A	904	POV	C313-C314-C315-C316
2	C	901	POV	C22-C23-C24-C25
2	C	902	POV	C33-C34-C35-C36
2	C	908	POV	C33-C34-C35-C36
2	A	907	POV	C213-C214-C215-C216
2	B	908	POV	C33-C34-C35-C36
2	D	901	POV	C212-C213-C214-C215
2	D	902	POV	C22-C23-C24-C25
2	A	904	POV	C36-C37-C38-C39
2	B	902	POV	C2-C1-O11-P
2	C	902	POV	C2-C1-O11-P
2	A	908	POV	C39-C310-C311-C312
2	B	905	POV	C311-C312-C313-C314
2	D	905	POV	C214-C215-C216-C217
2	B	901	POV	C36-C37-C38-C39
2	D	901	POV	C27-C28-C29-C210
2	A	907	POV	C33-C34-C35-C36
2	B	902	POV	C33-C34-C35-C36
2	A	901	POV	C33-C34-C35-C36
2	C	901	POV	C311-C312-C313-C314
2	C	905	POV	C36-C37-C38-C39
2	C	908	POV	C311-C310-C39-C38
2	C	902	POV	C37-C38-C39-C310
2	B	908	POV	O11-C1-C2-O21
2	B	902	POV	C310-C311-C312-C313
2	B	908	POV	C27-C28-C29-C210
2	A	901	POV	C2-C1-O11-P
2	A	908	POV	C32-C33-C34-C35
2	A	904	POV	O11-C1-C2-C3
2	A	907	POV	O11-C1-C2-C3
2	C	908	POV	C27-C28-C29-C210
3	D	903	ACD	C14-C15-C16-C17
2	A	901	POV	O21-C2-C3-O31
2	B	902	POV	C37-C38-C39-C310
3	C	903	ACD	C9-C10-C11-C12
2	B	901	POV	C311-C312-C313-C314

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Mol	Chain	Res	Type	Atoms
2	A	901	POV	C39-C310-C311-C312
2	A	908	POV	C310-C311-C312-C313
2	A	904	POV	C32-C33-C34-C35
2	A	903	POV	O22-C21-O21-C2
2	D	902	POV	C212-C213-C214-C215
2	A	901	POV	C35-C36-C37-C38
2	A	909	POV	C210-C211-C212-C213
2	C	905	POV	O11-C1-C2-O21
2	D	901	POV	O11-C1-C2-O21
3	A	902	ACD	O2-C1-C2-C3
2	A	904	POV	C311-C312-C313-C314
2	D	905	POV	C36-C37-C38-C39
2	A	907	POV	C27-C28-C29-C210
3	B	903	ACD	C14-C15-C16-C17
2	A	909	POV	C313-C314-C315-C316
2	B	902	POV	C35-C36-C37-C38
3	B	903	ACD	O2-C1-C2-C3
3	D	903	ACD	O2-C1-C2-C3
3	C	903	ACD	O2-C1-C2-C3
2	B	908	POV	C36-C37-C38-C39
2	C	902	POV	C35-C36-C37-C38
2	B	908	POV	C311-C310-C39-C38
2	B	905	POV	O11-C1-C2-C3
2	D	905	POV	O11-C1-C2-C3
3	A	902	ACD	O1-C1-C2-C3
3	D	903	ACD	O1-C1-C2-C3
2	A	908	POV	C37-C38-C39-C310
3	C	903	ACD	O1-C1-C2-C3
2	C	901	POV	C210-C211-C212-C213
2	C	908	POV	C36-C37-C38-C39
3	B	903	ACD	O1-C1-C2-C3
2	A	903	POV	C29-C210-C211-C212
2	B	904	POV	C29-C210-C211-C212
2	C	904	POV	C29-C210-C211-C212
3	C	903	ACD	C14-C15-C16-C17
2	A	908	POV	C22-C23-C24-C25
2	A	909	POV	C11-C12-N-C14
2	B	901	POV	C29-C210-C211-C212
2	D	904	POV	C29-C210-C211-C212
3	A	902	ACD	C14-C15-C16-C17
2	D	902	POV	C210-C211-C212-C213
2	C	901	POV	C212-C213-C214-C215

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Mol	Chain	Res	Type	Atoms
2	D	905	POV	C22-C23-C24-C25
2	A	909	POV	C312-C313-C314-C315
2	C	904	POV	C1-C2-C3-O31
2	B	902	POV	O21-C21-C22-C23
2	A	904	POV	C22-C23-C24-C25
2	C	905	POV	C311-C312-C313-C314
2	A	901	POV	O21-C21-C22-C23
2	C	902	POV	O21-C21-C22-C23
2	B	908	POV	O11-C1-C2-C3
2	C	908	POV	O11-C1-C2-C3
2	D	904	POV	C313-C314-C315-C316
2	C	905	POV	C22-C23-C24-C25
2	C	908	POV	C22-C23-C24-C25
2	A	903	POV	C22-C21-O21-C2
2	D	905	POV	C311-C312-C313-C314
2	B	902	POV	O12-C11-C12-N
2	C	902	POV	O12-C11-C12-N
2	D	902	POV	C311-C312-C313-C314
4	A	906	FZ4	O14-B01-C02-C03
4	A	906	FZ4	O14-B01-C02-C07
4	C	907	FZ4	O14-B01-C02-C03
4	C	907	FZ4	O14-B01-C02-C07
4	D	907	FZ4	O14-B01-C02-C03
4	D	907	FZ4	O14-B01-C02-C07
2	A	903	POV	C25-C26-C27-C28
2	A	908	POV	O21-C21-C22-C23
2	A	901	POV	C21-C22-C23-C24
2	A	901	POV	C36-C37-C38-C39
2	C	904	POV	C25-C26-C27-C28
2	B	905	POV	C22-C23-C24-C25
2	D	904	POV	C25-C26-C27-C28
2	A	901	POV	C310-C311-C312-C313
2	C	902	POV	O22-C21-C22-C23
2	A	908	POV	O22-C21-C22-C23
2	B	902	POV	O22-C21-C22-C23
2	D	902	POV	C312-C313-C314-C315
2	A	901	POV	C37-C38-C39-C310
2	D	901	POV	C29-C210-C211-C212
2	A	901	POV	O22-C21-C22-C23
4	B	906	FZ4	C02-B01-C08-C13
4	C	906	FZ4	C02-B01-C08-C13
2	B	901	POV	C312-C313-C314-C315

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Mol	Chain	Res	Type	Atoms
2	C	901	POV	C312-C313-C314-C315
2	A	909	POV	C11-C12-N-C15
2	D	901	POV	O11-C1-C2-C3
2	A	903	POV	O21-C21-C22-C23
2	B	904	POV	C25-C26-C27-C28
2	B	902	POV	C21-C22-C23-C24

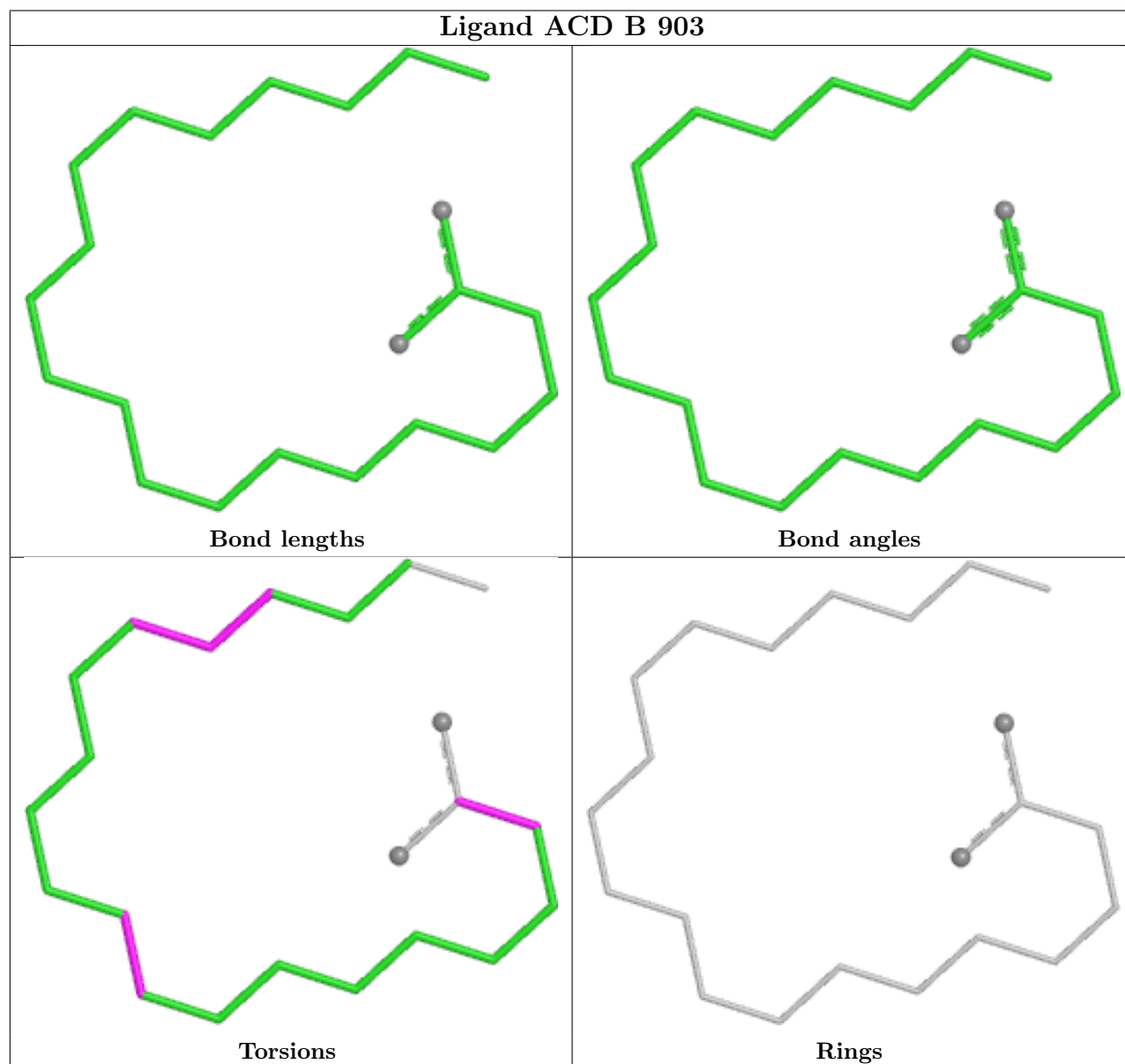
There are no ring outliers.

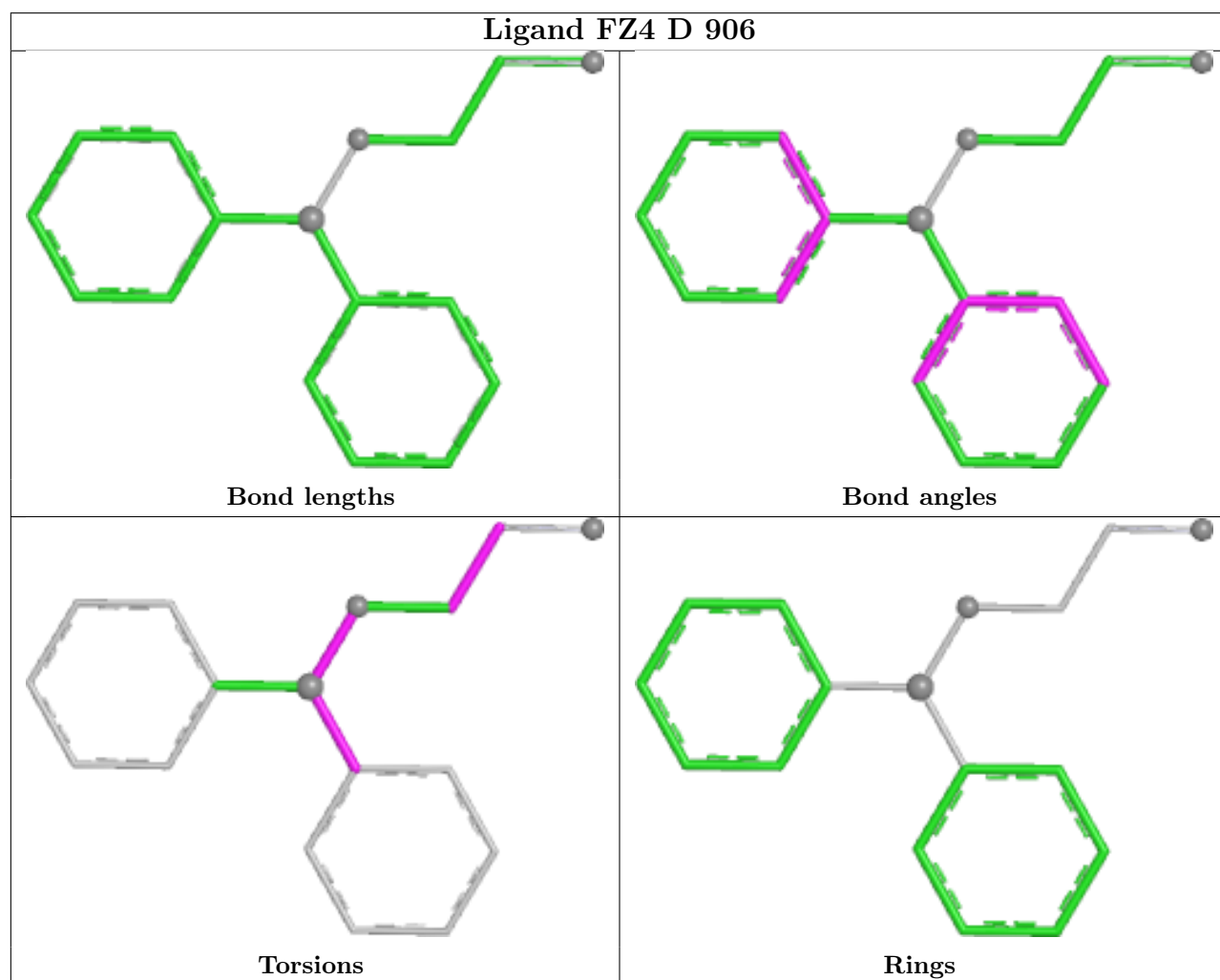
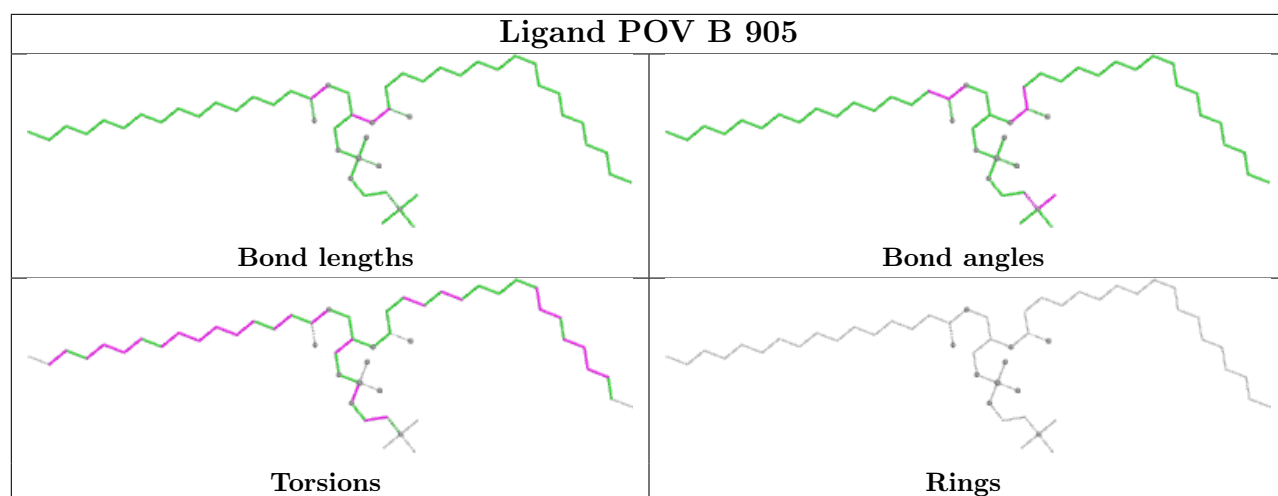
26 monomers are involved in 61 short contacts:

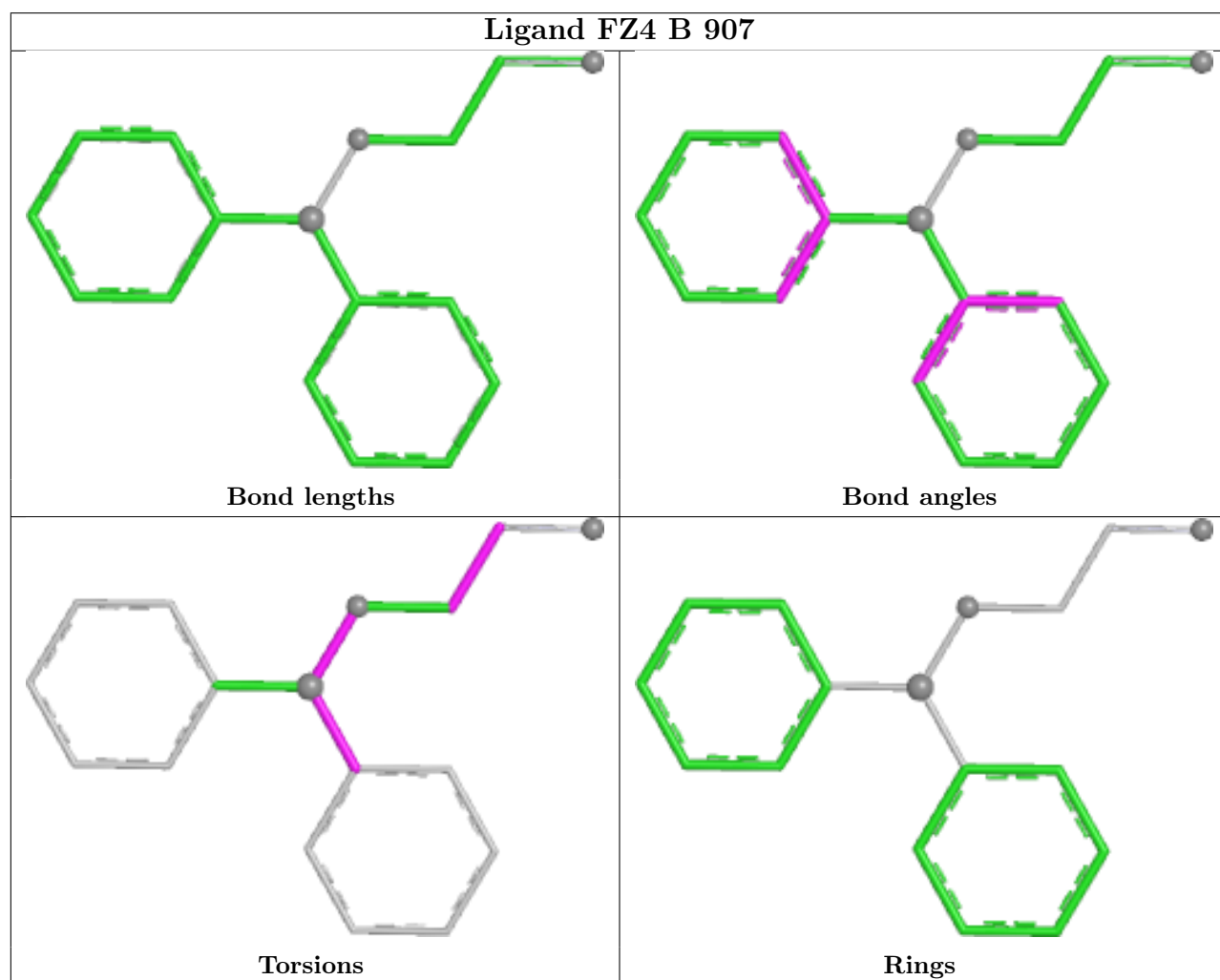
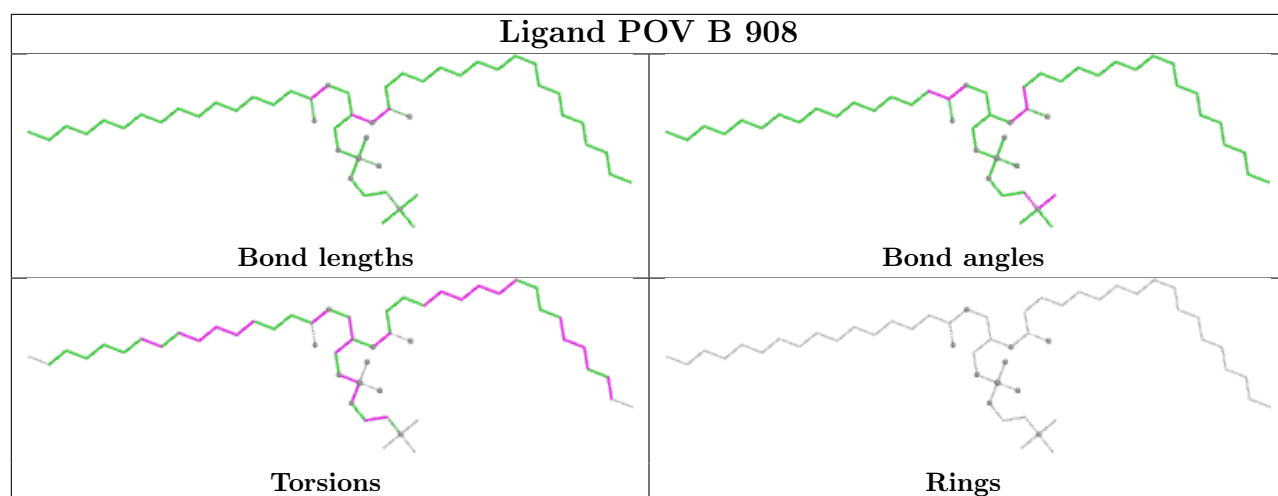
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	903	ACD	2	0
2	B	905	POV	3	0
4	D	906	FZ4	1	0
2	A	901	POV	3	0
2	D	904	POV	3	0
2	A	904	POV	3	0
2	C	904	POV	3	0
4	C	906	FZ4	1	0
2	A	907	POV	2	0
2	B	901	POV	3	0
2	B	904	POV	3	0
2	D	905	POV	4	0
3	A	902	ACD	1	0
3	C	903	ACD	2	0
2	C	902	POV	5	0
2	A	908	POV	5	0
2	A	909	POV	3	0
2	C	905	POV	4	0
2	D	901	POV	1	0
2	D	902	POV	5	0
3	D	903	ACD	2	0
2	A	903	POV	2	0
2	C	901	POV	3	0
4	A	905	FZ4	1	0
4	B	906	FZ4	1	0
2	B	902	POV	4	0

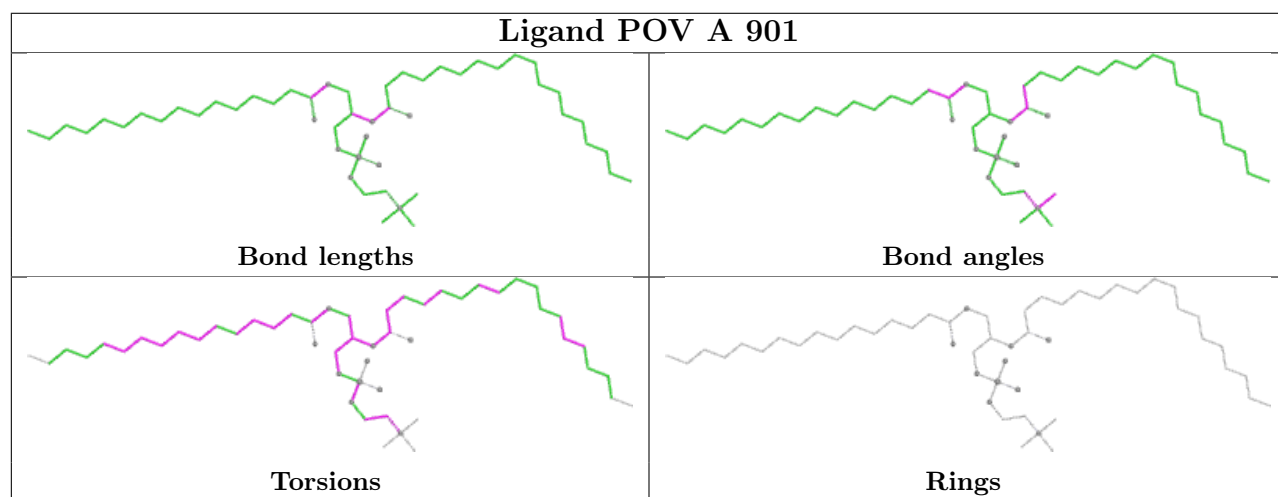
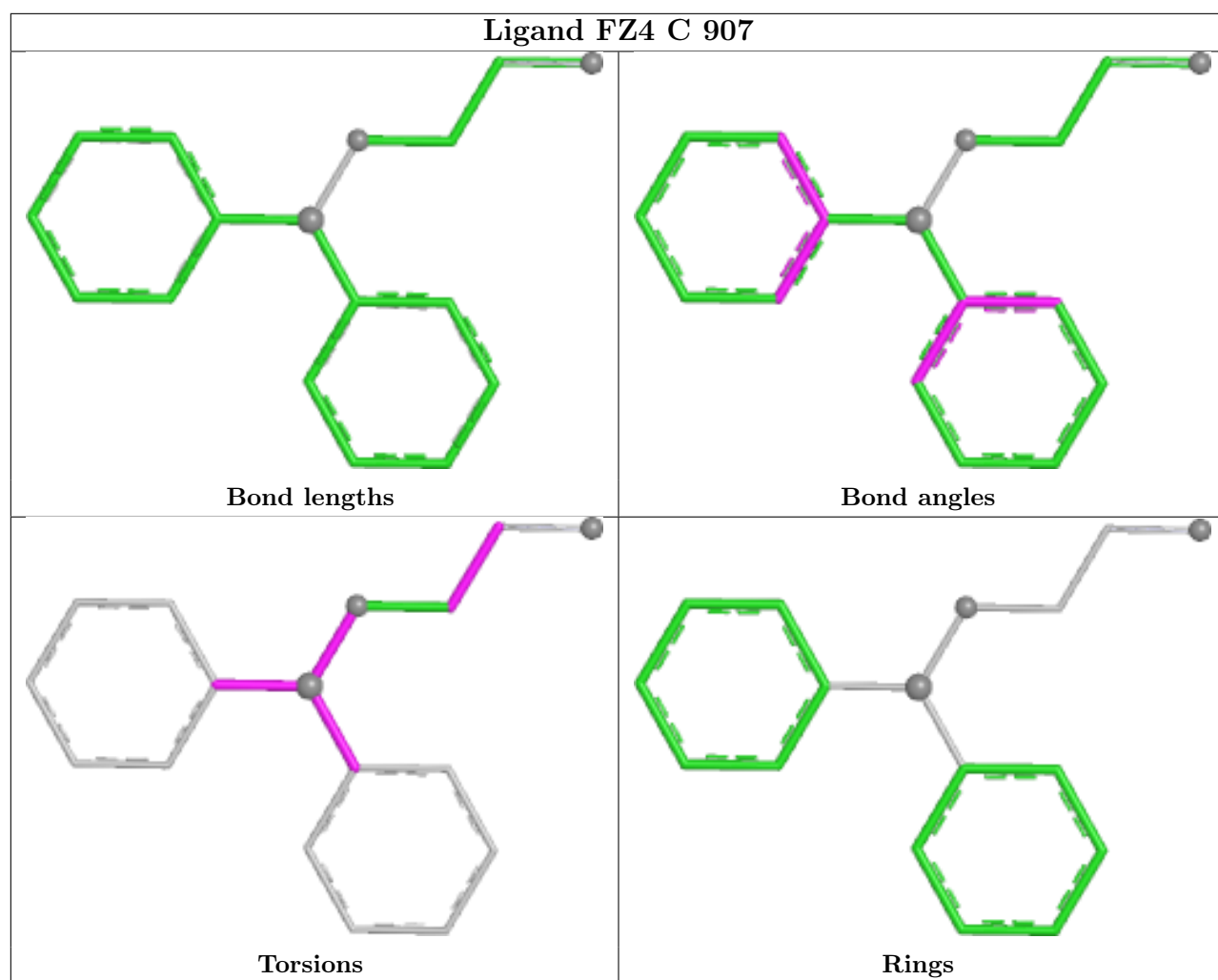
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

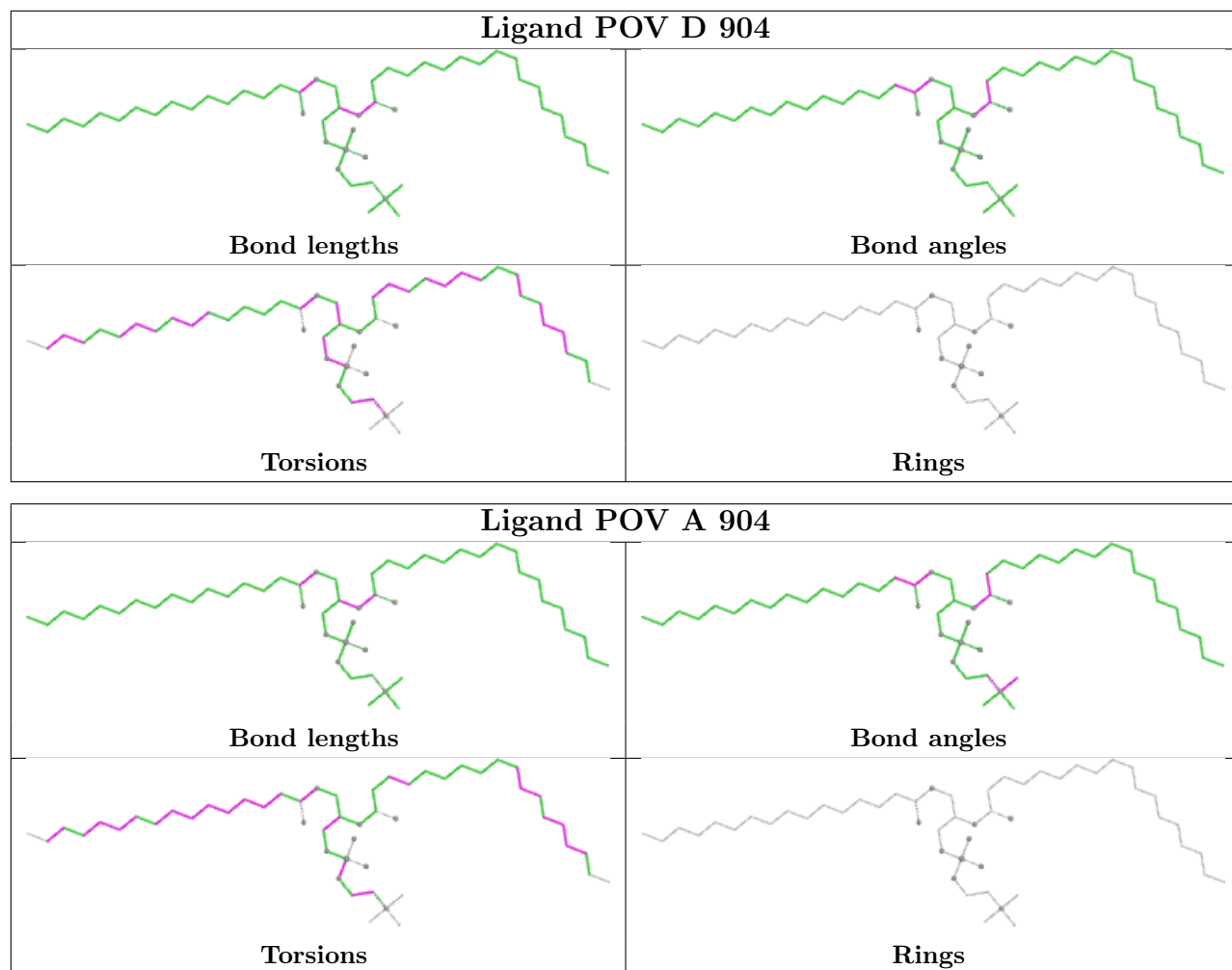
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question 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.

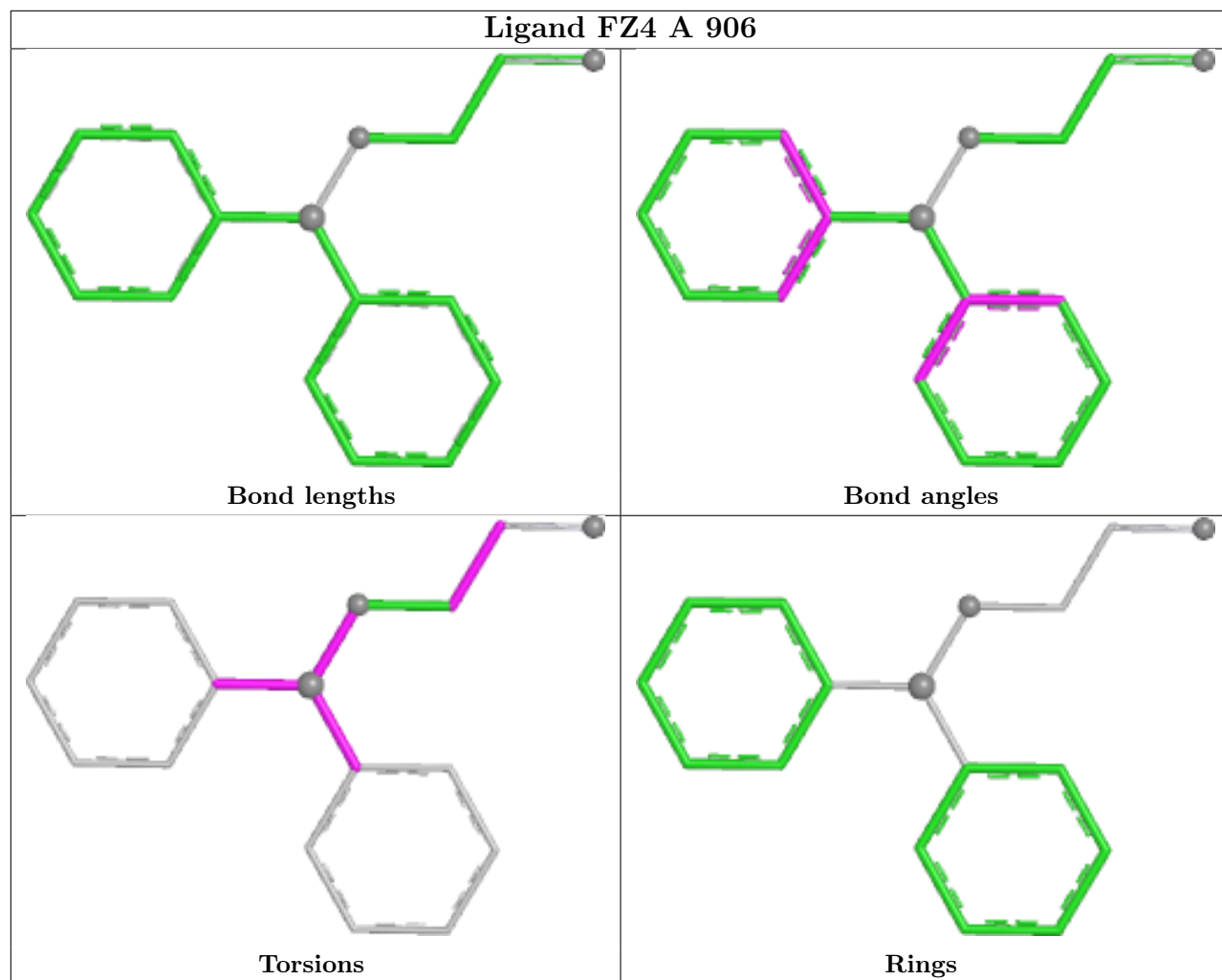


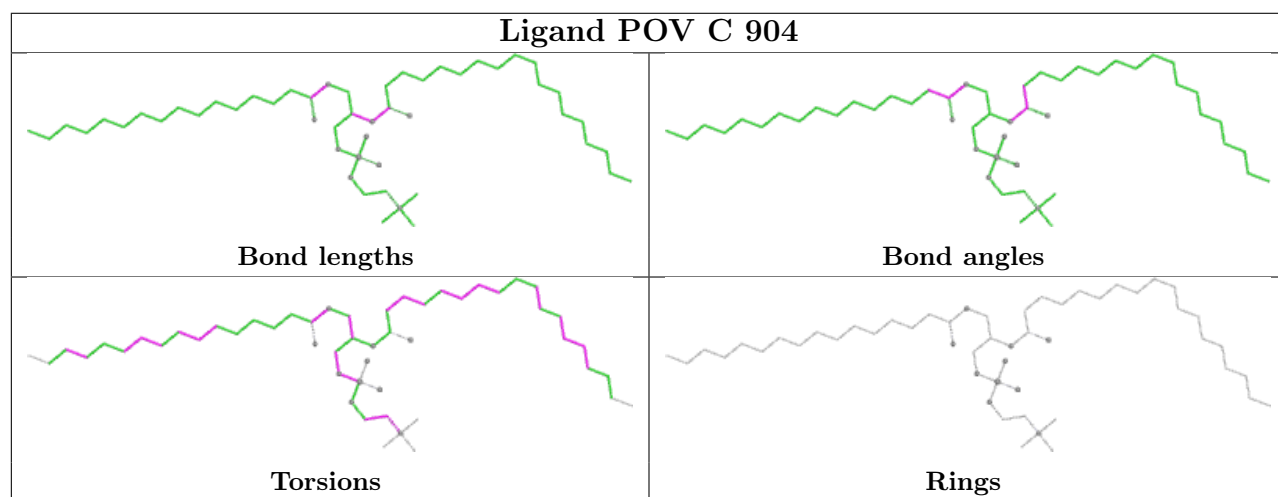
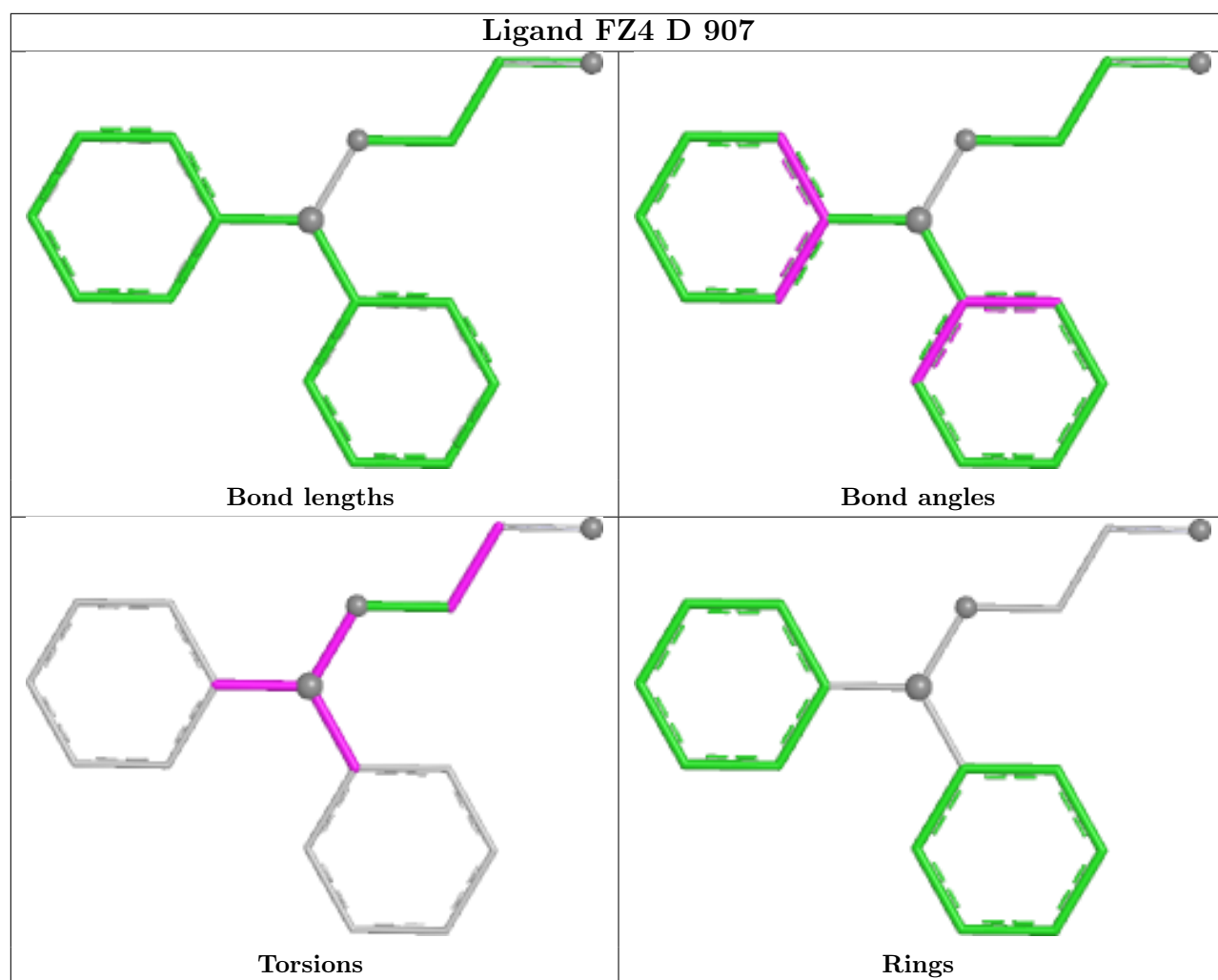


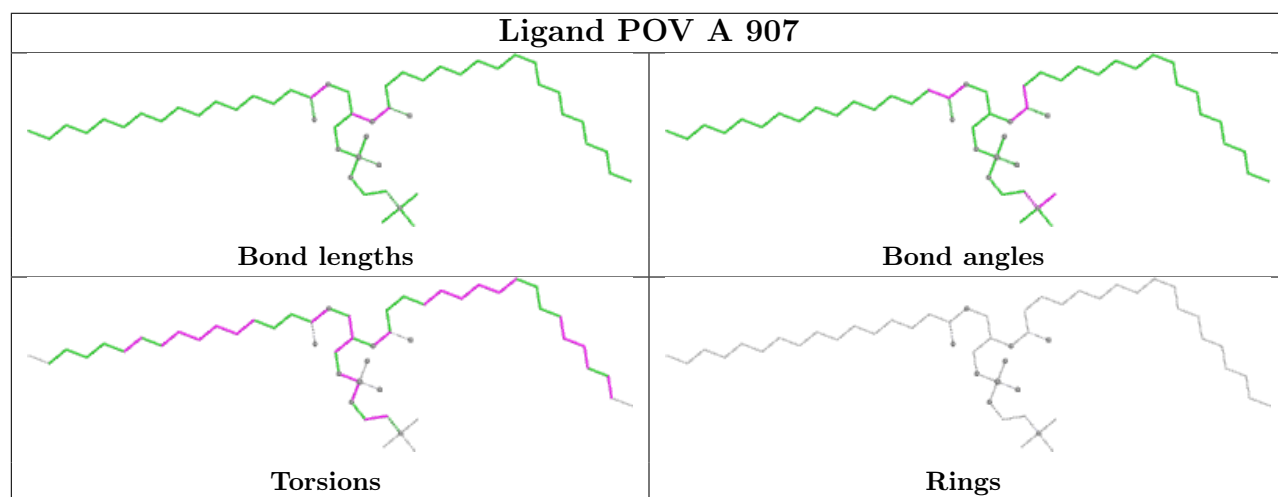
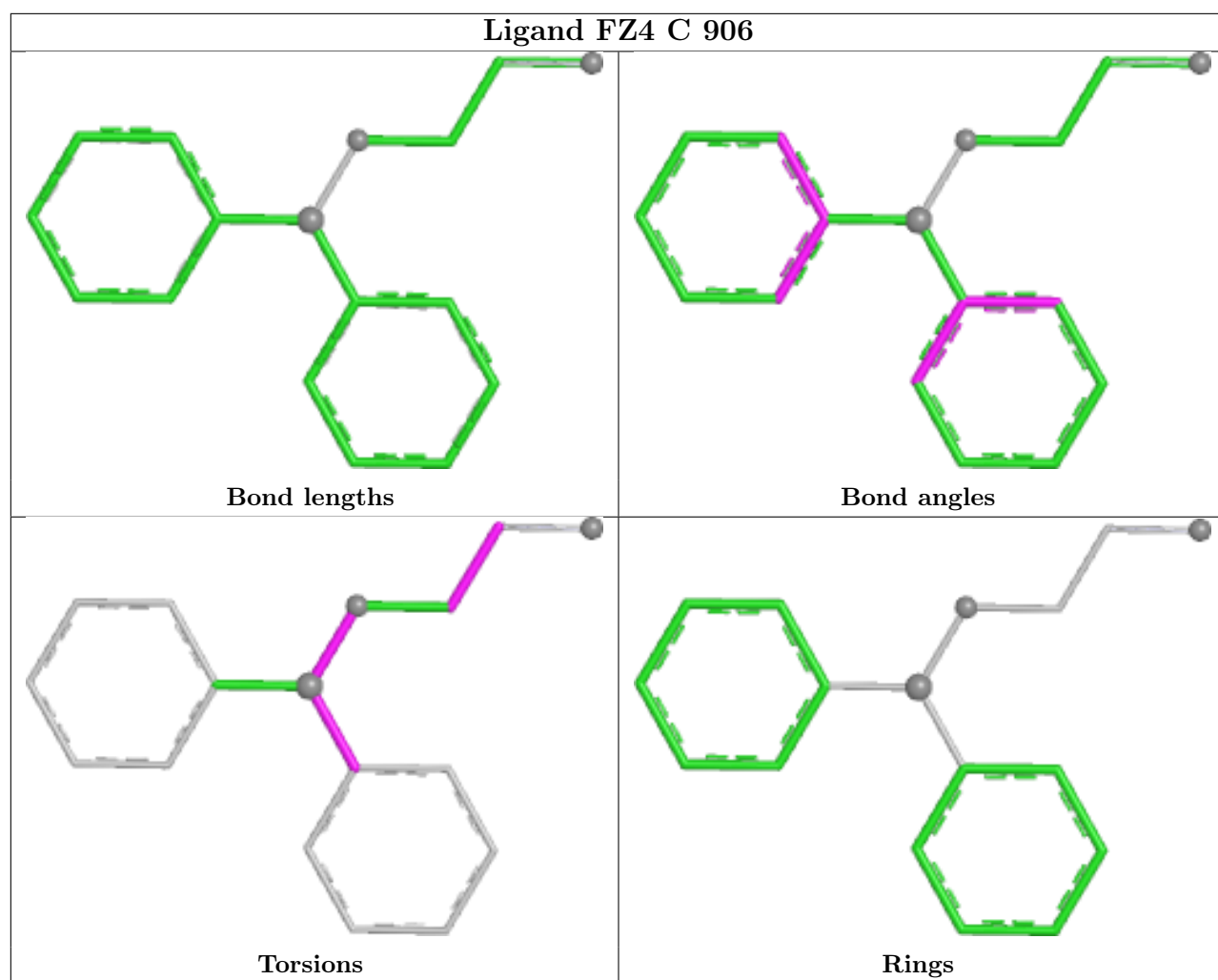


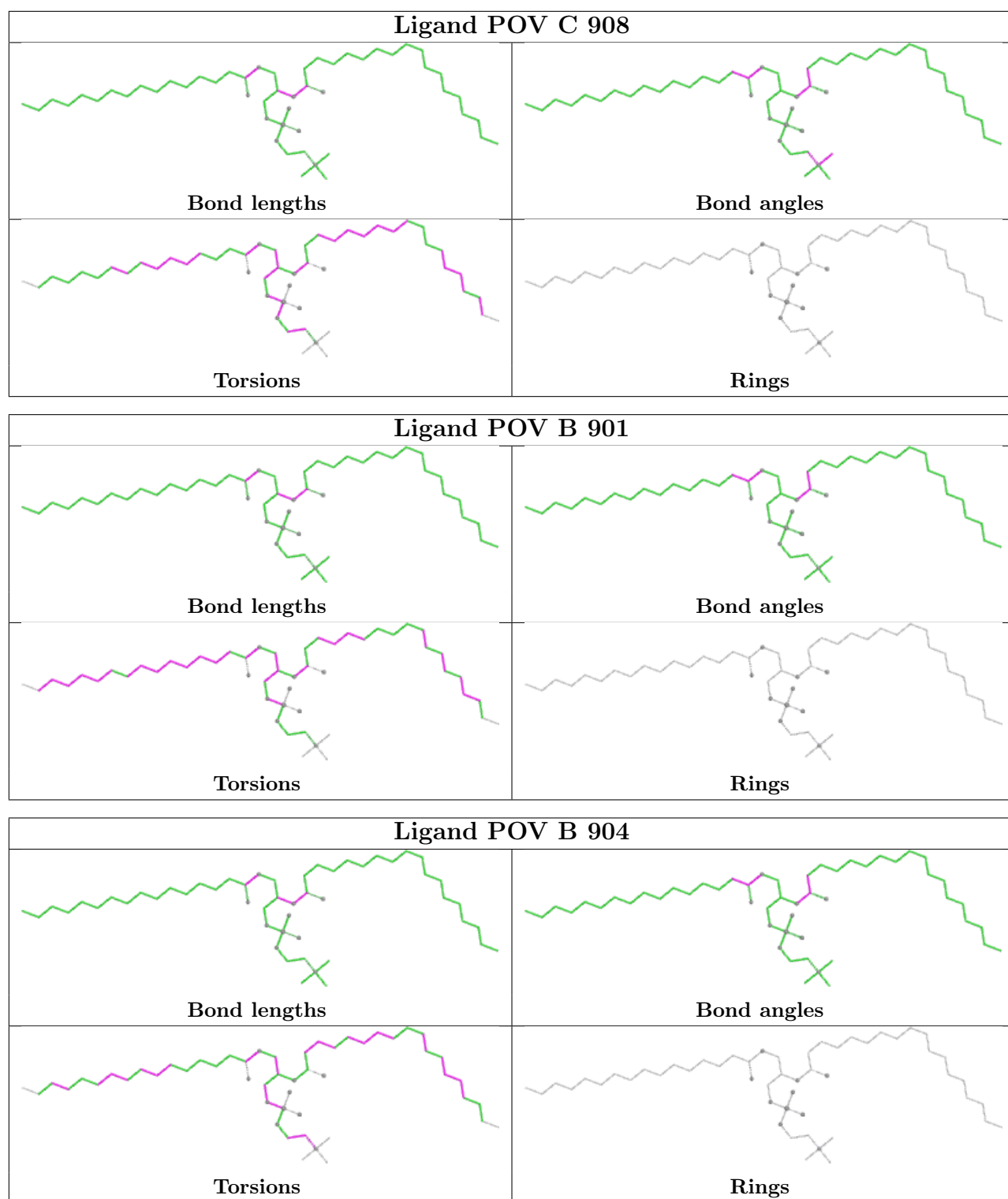


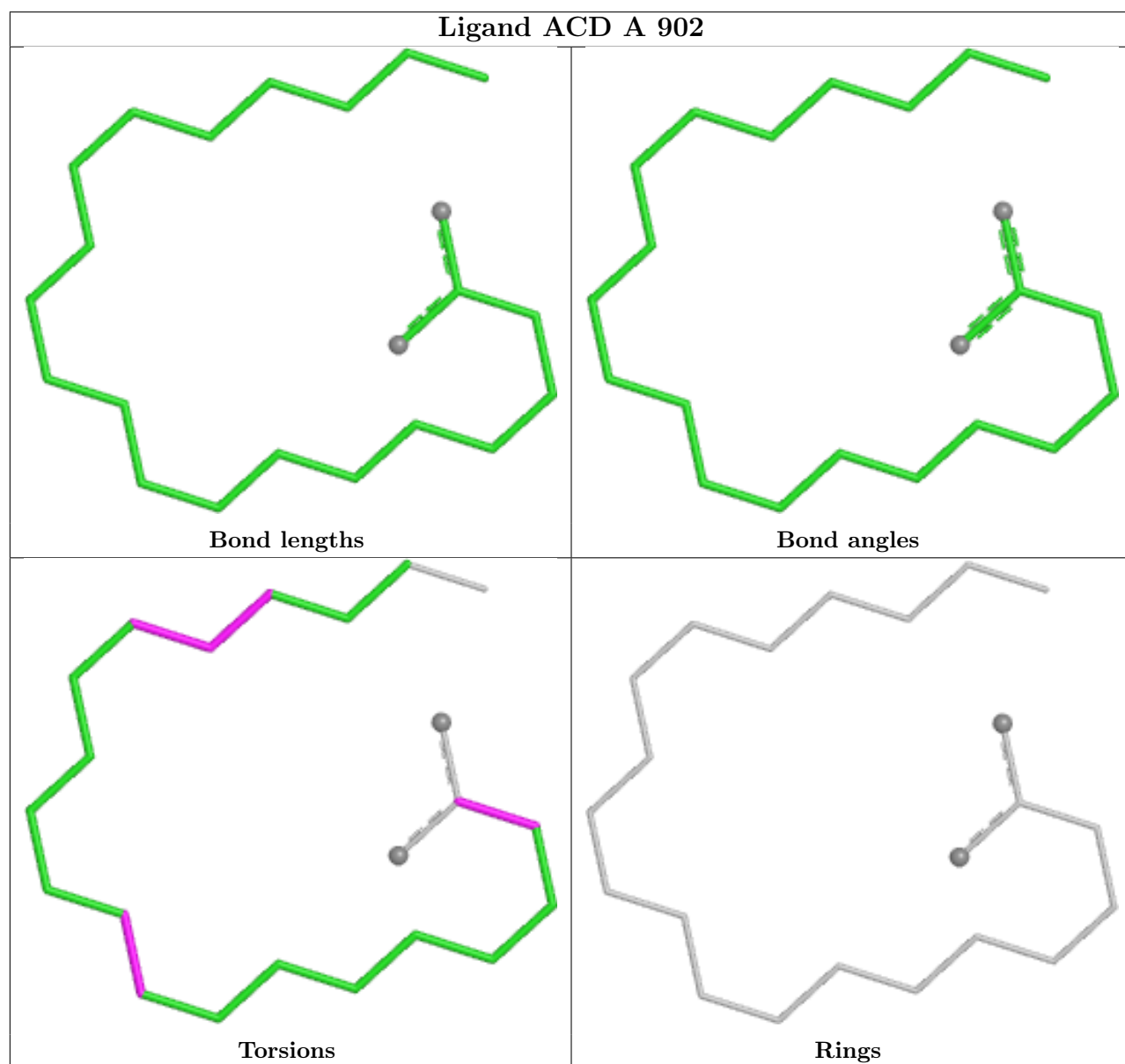
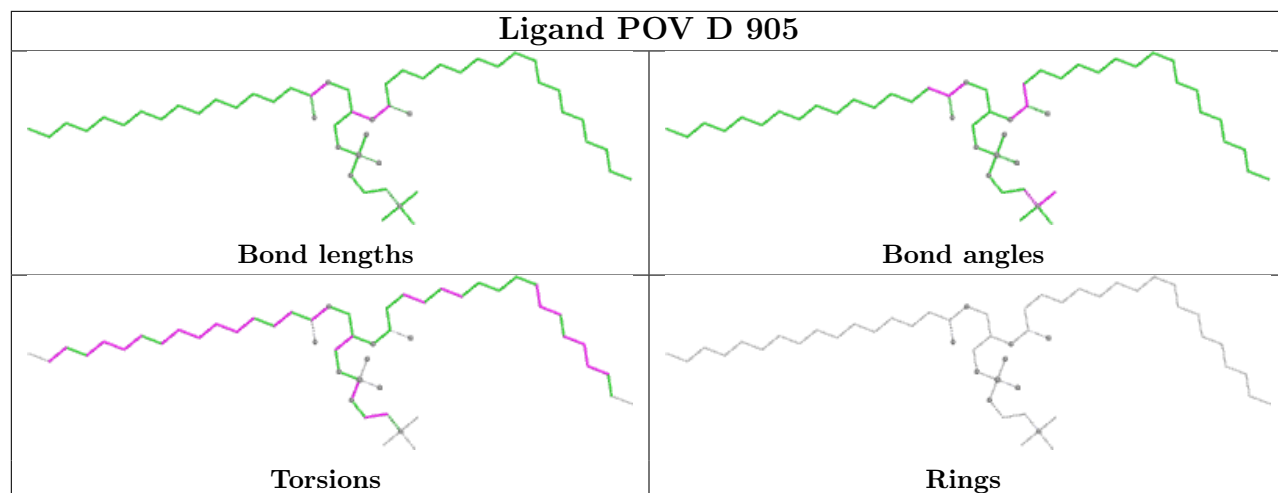


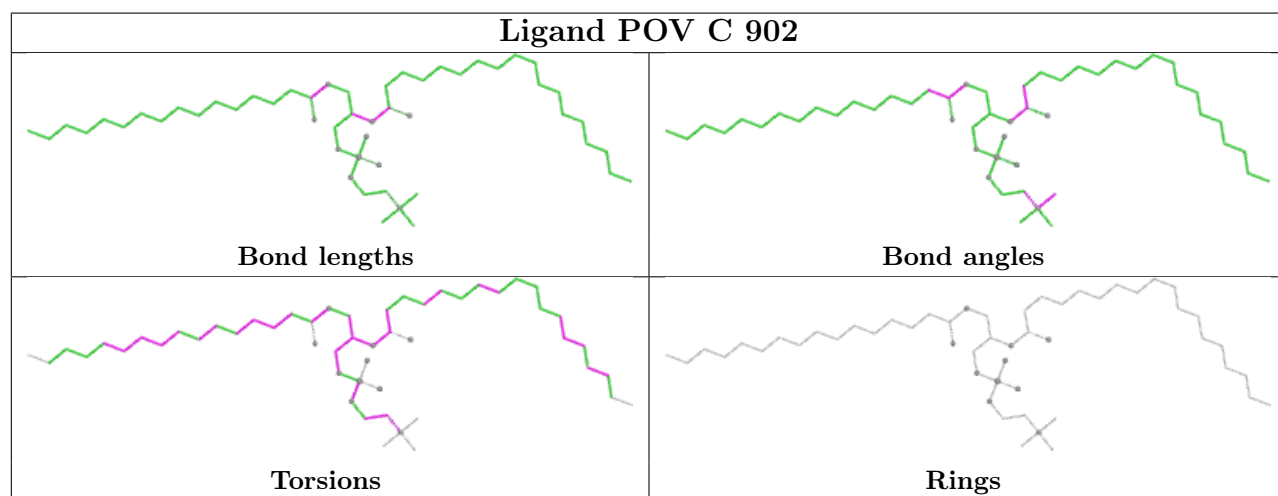
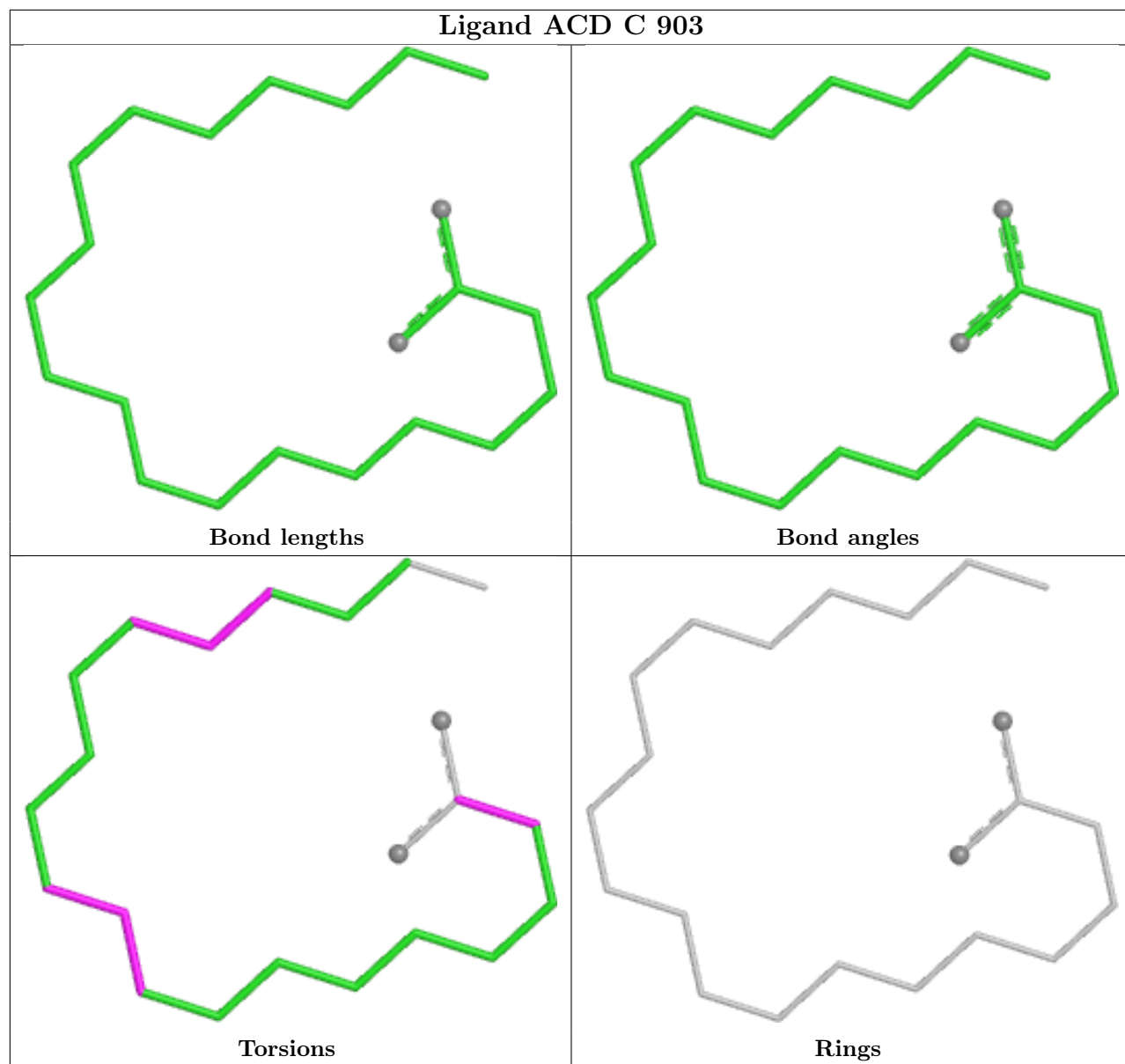


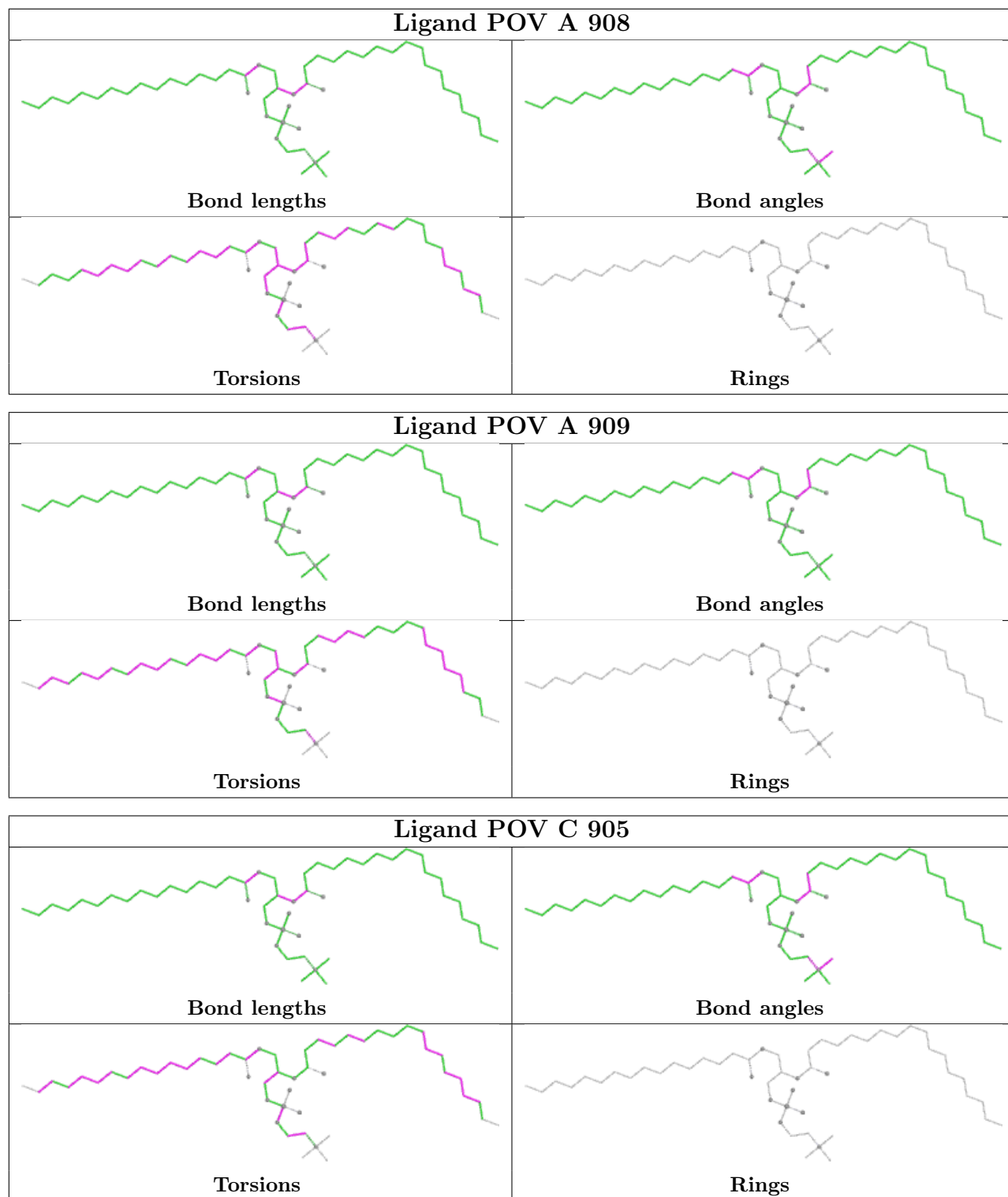


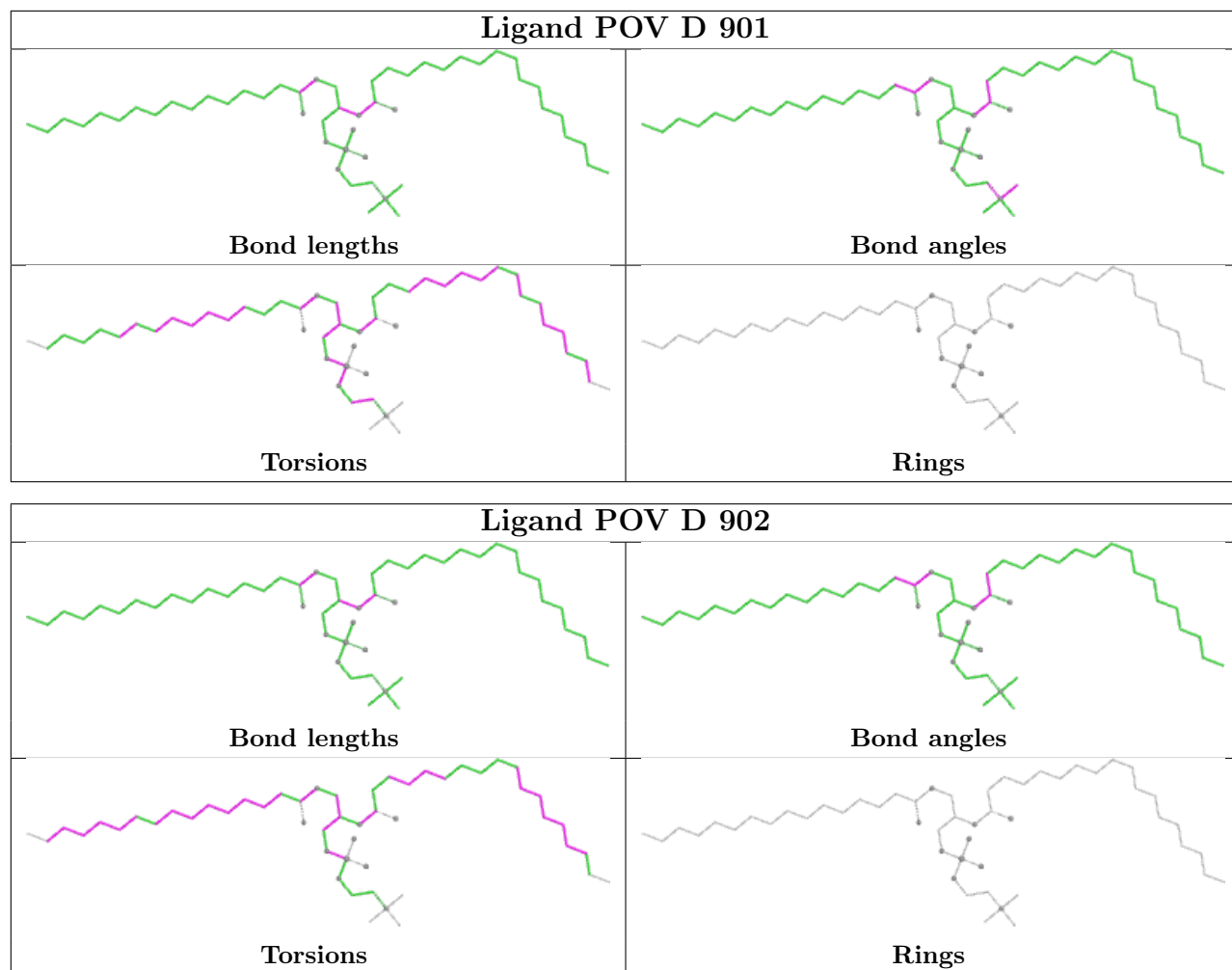


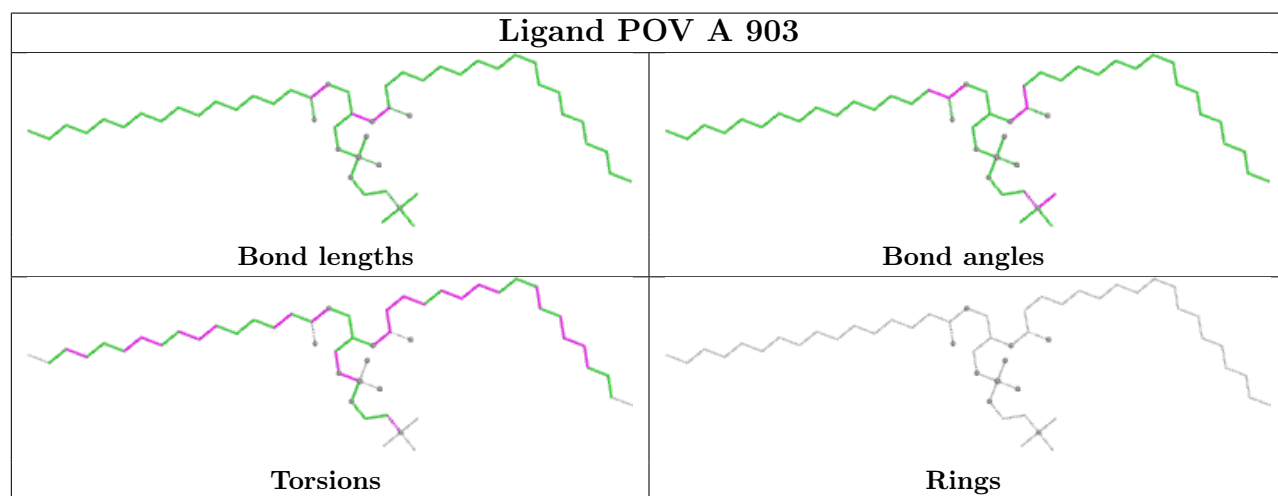
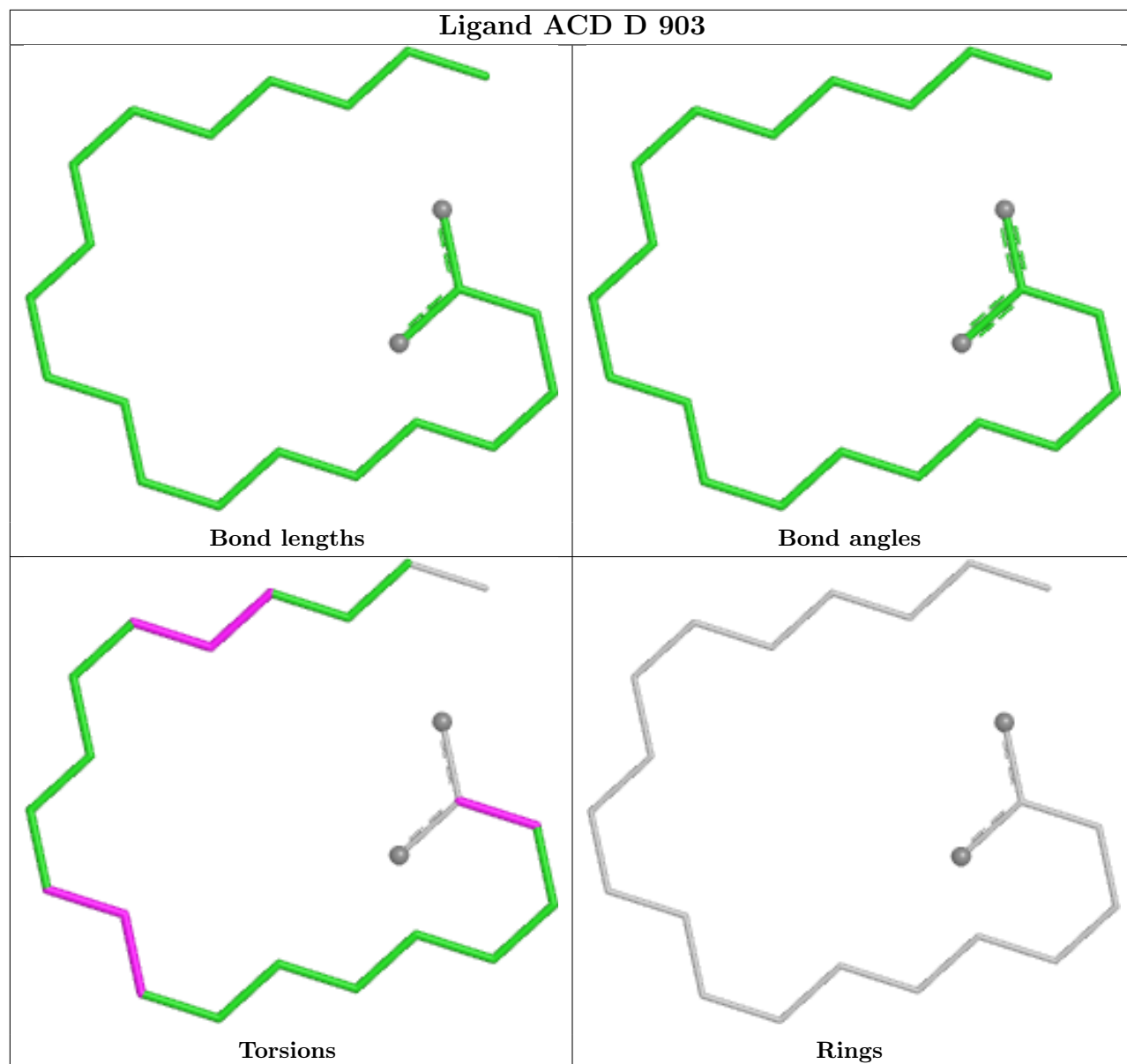


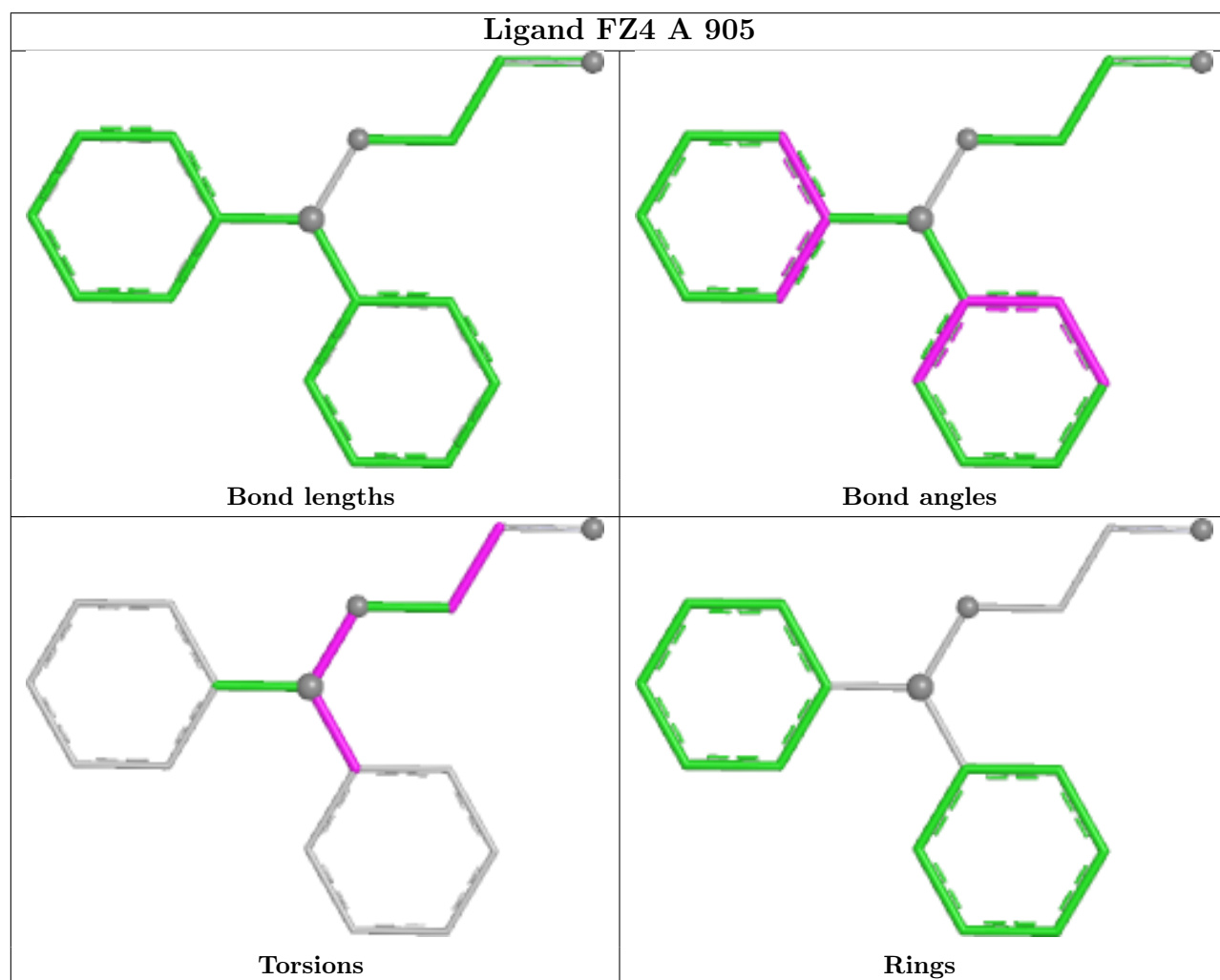
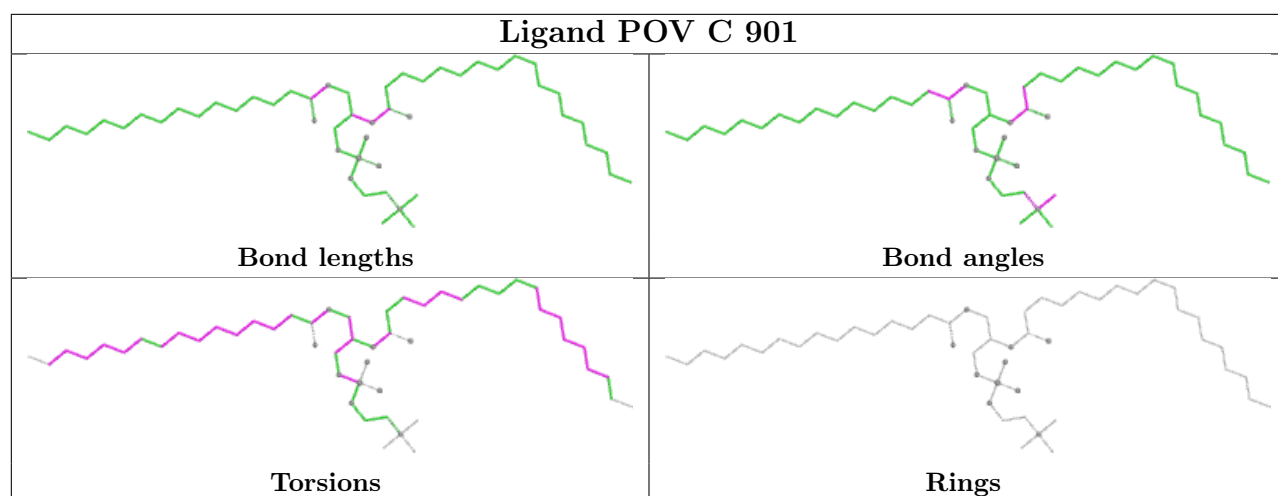


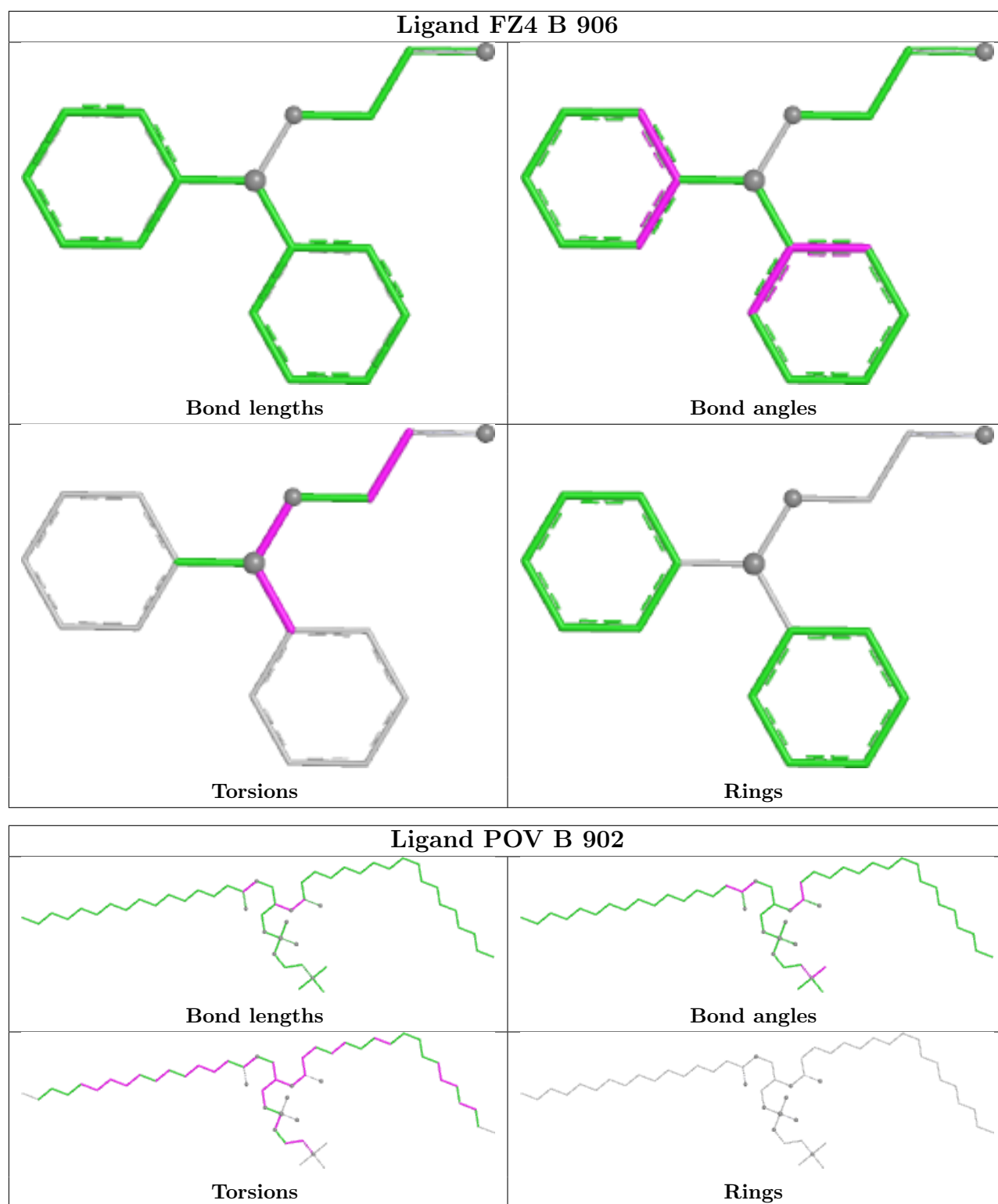












5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

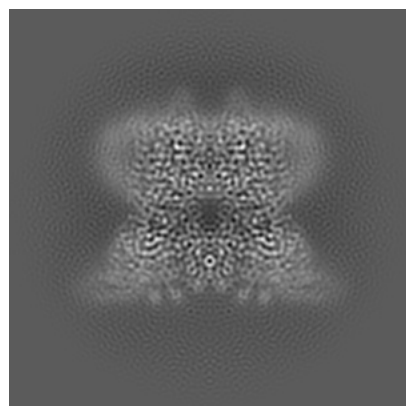
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-42997. These allow visual inspection of the internal detail of the map and identification of artifacts.

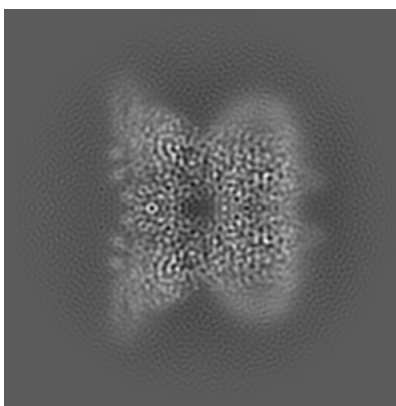
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

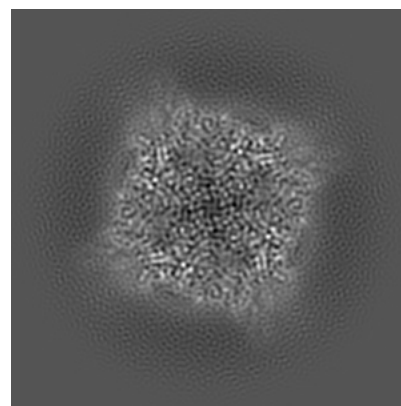
6.1.1 Primary map



X

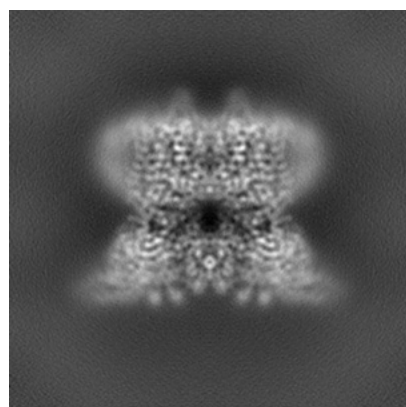


Y

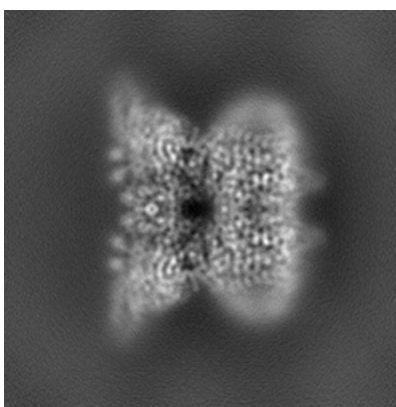


Z

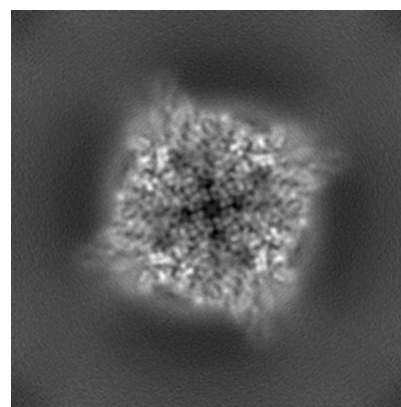
6.1.2 Raw map



X



Y

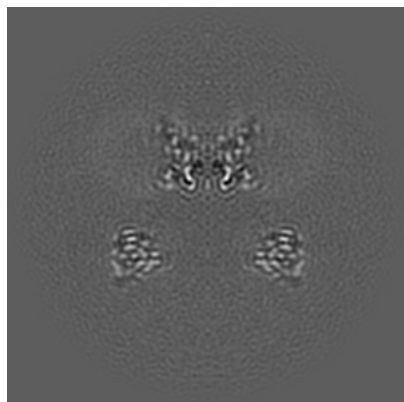


Z

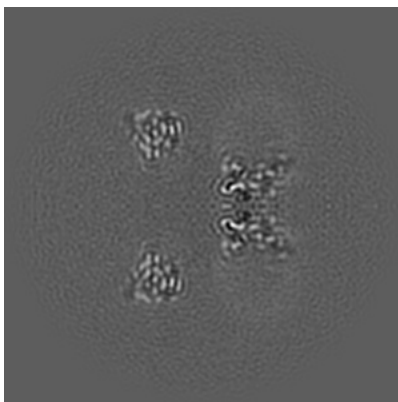
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

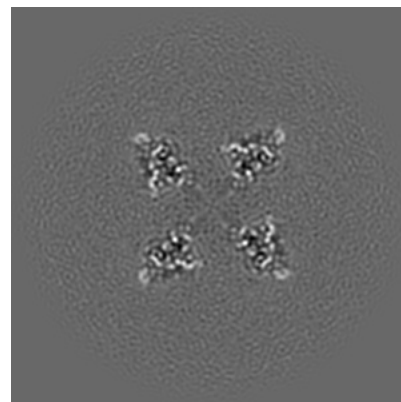
6.2.1 Primary map



X Index: 128

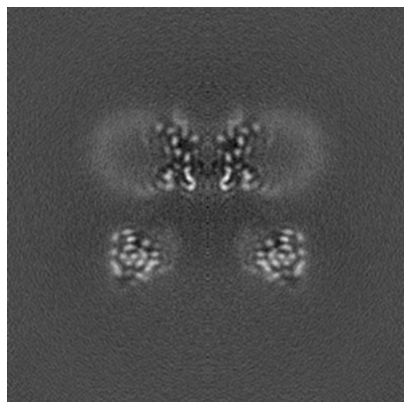


Y Index: 128

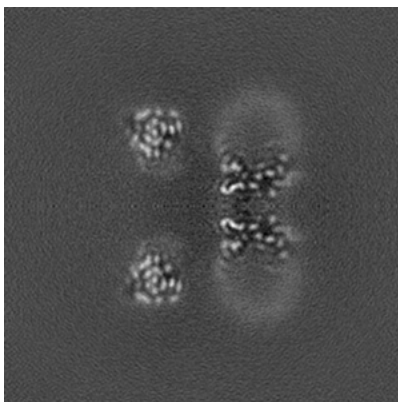


Z Index: 128

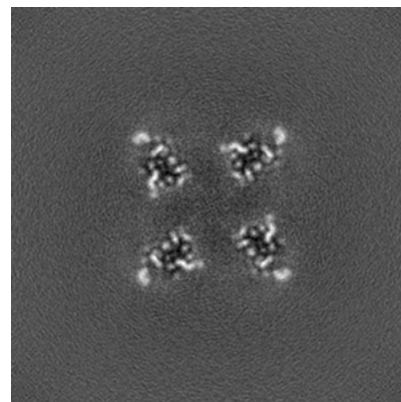
6.2.2 Raw map



X Index: 128



Y Index: 128

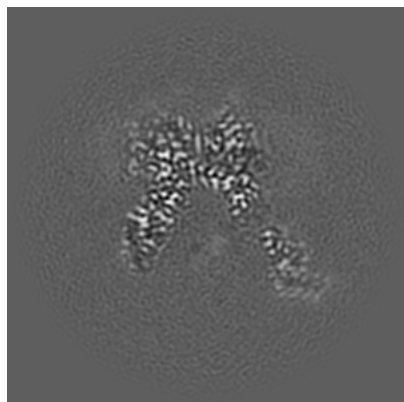


Z Index: 128

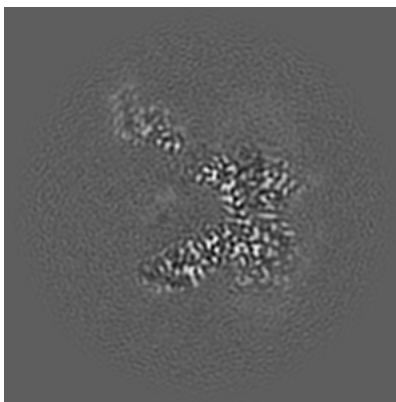
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

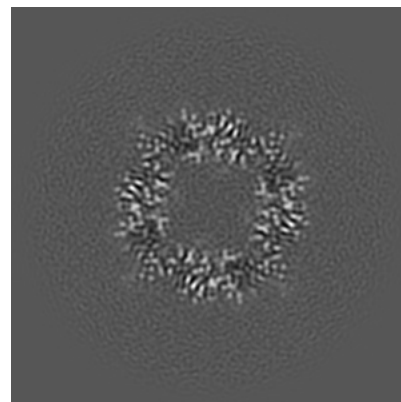
6.3.1 Primary map



X Index: 106

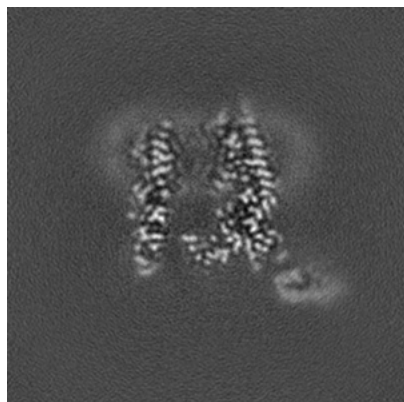


Y Index: 150

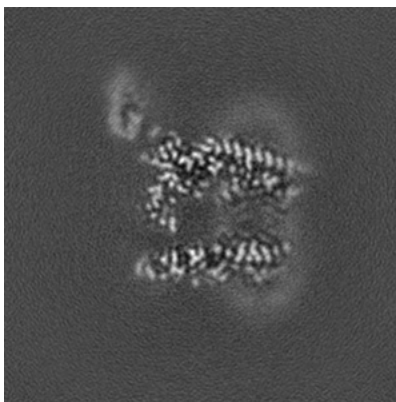


Z Index: 107

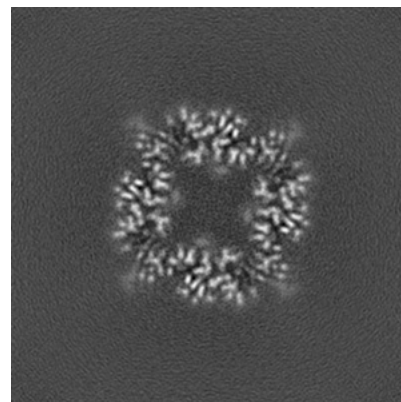
6.3.2 Raw map



X Index: 95



Y Index: 161

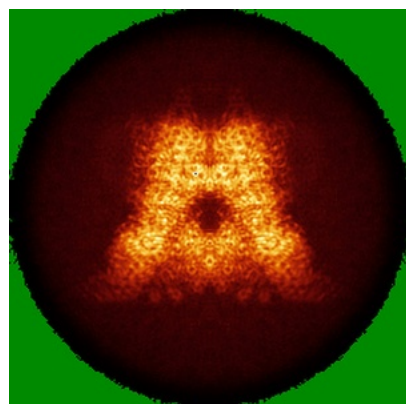


Z Index: 107

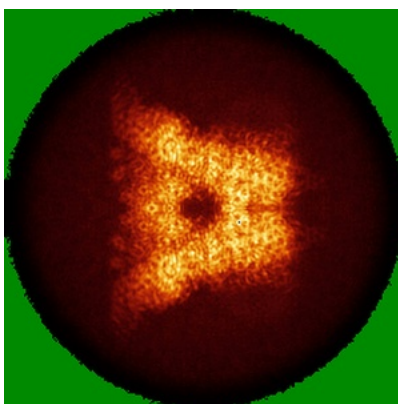
The images above show the largest variance slices of the map in three orthogonal directions.

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

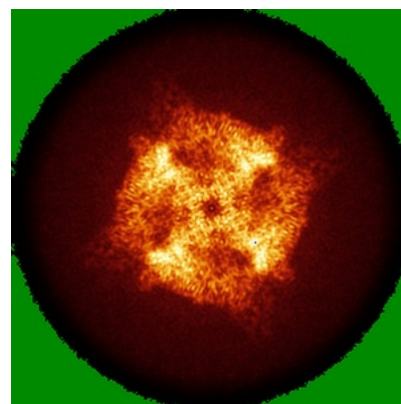
6.4.1 Primary map



X

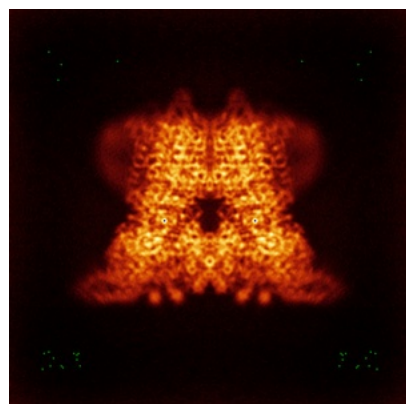


Y

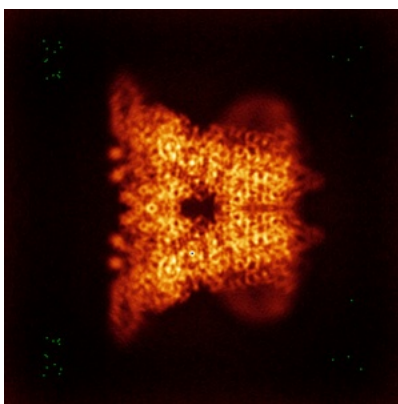


Z

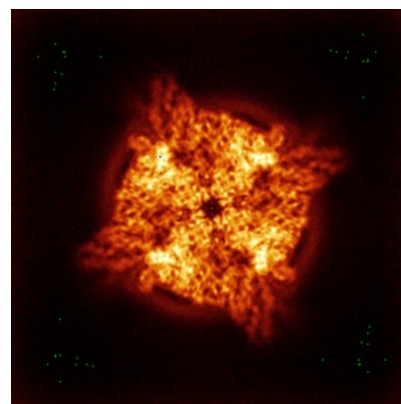
6.4.2 Raw map



X



Y

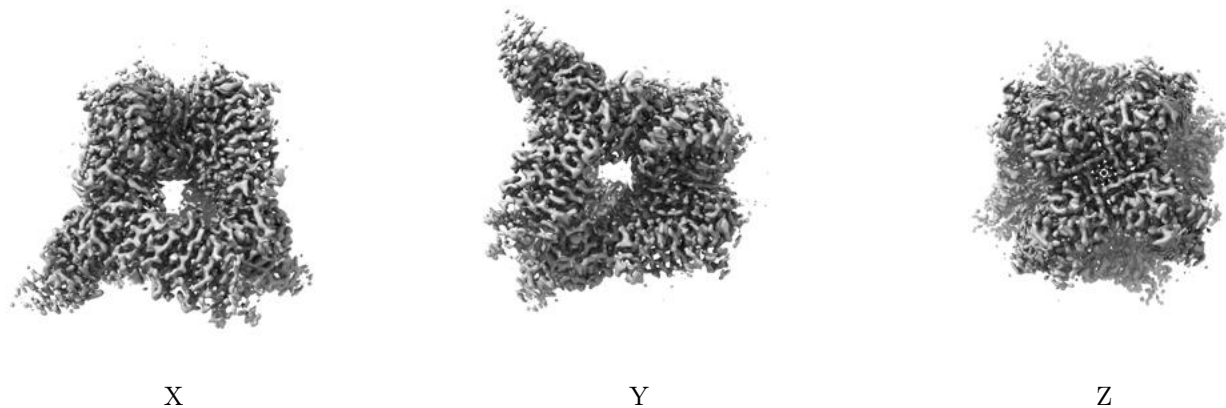


Z

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.

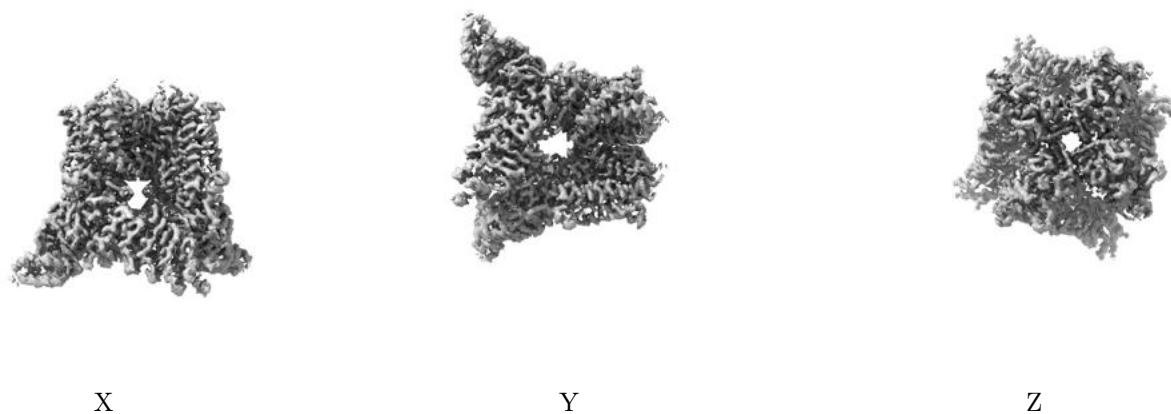
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.241. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 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.

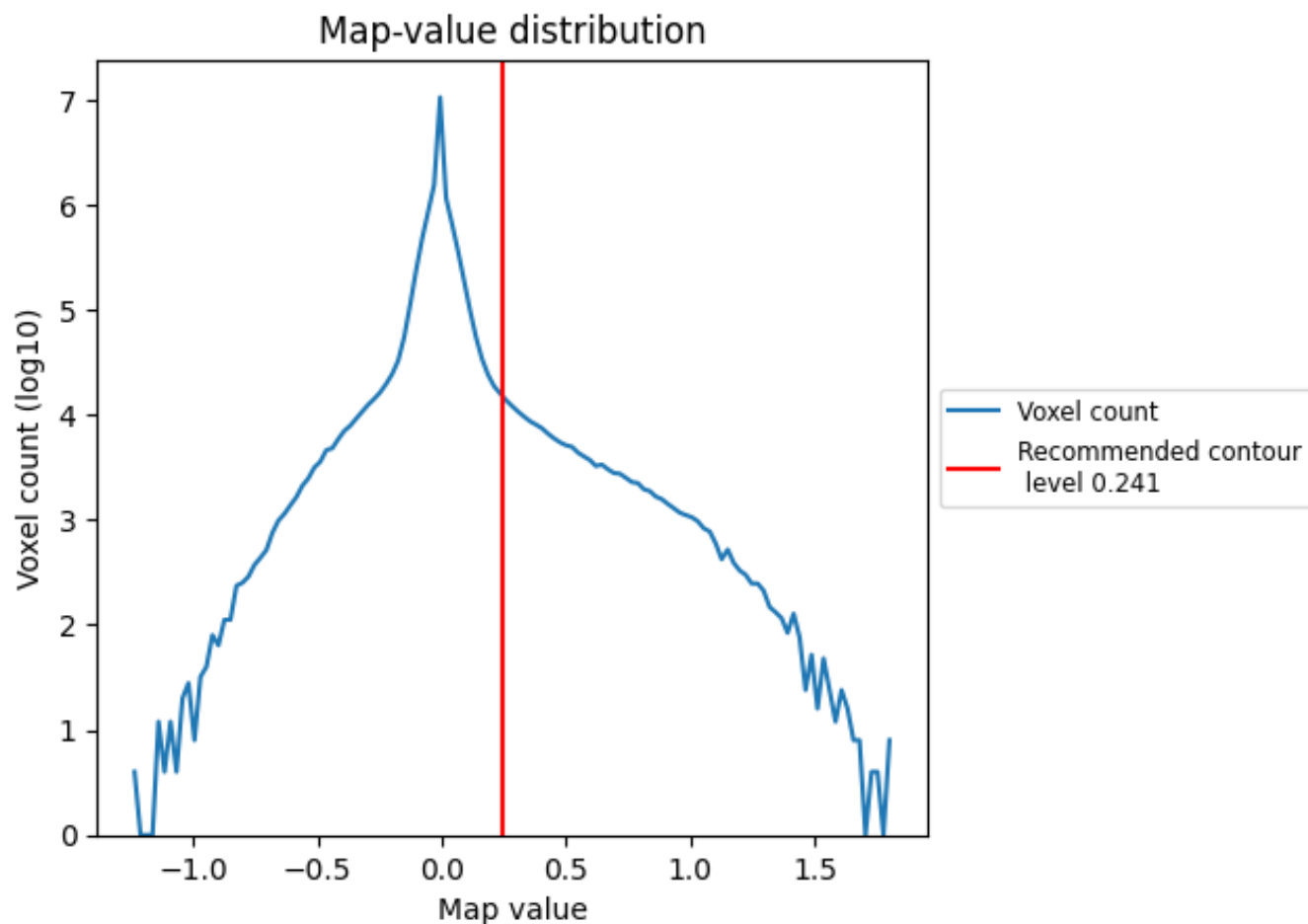
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

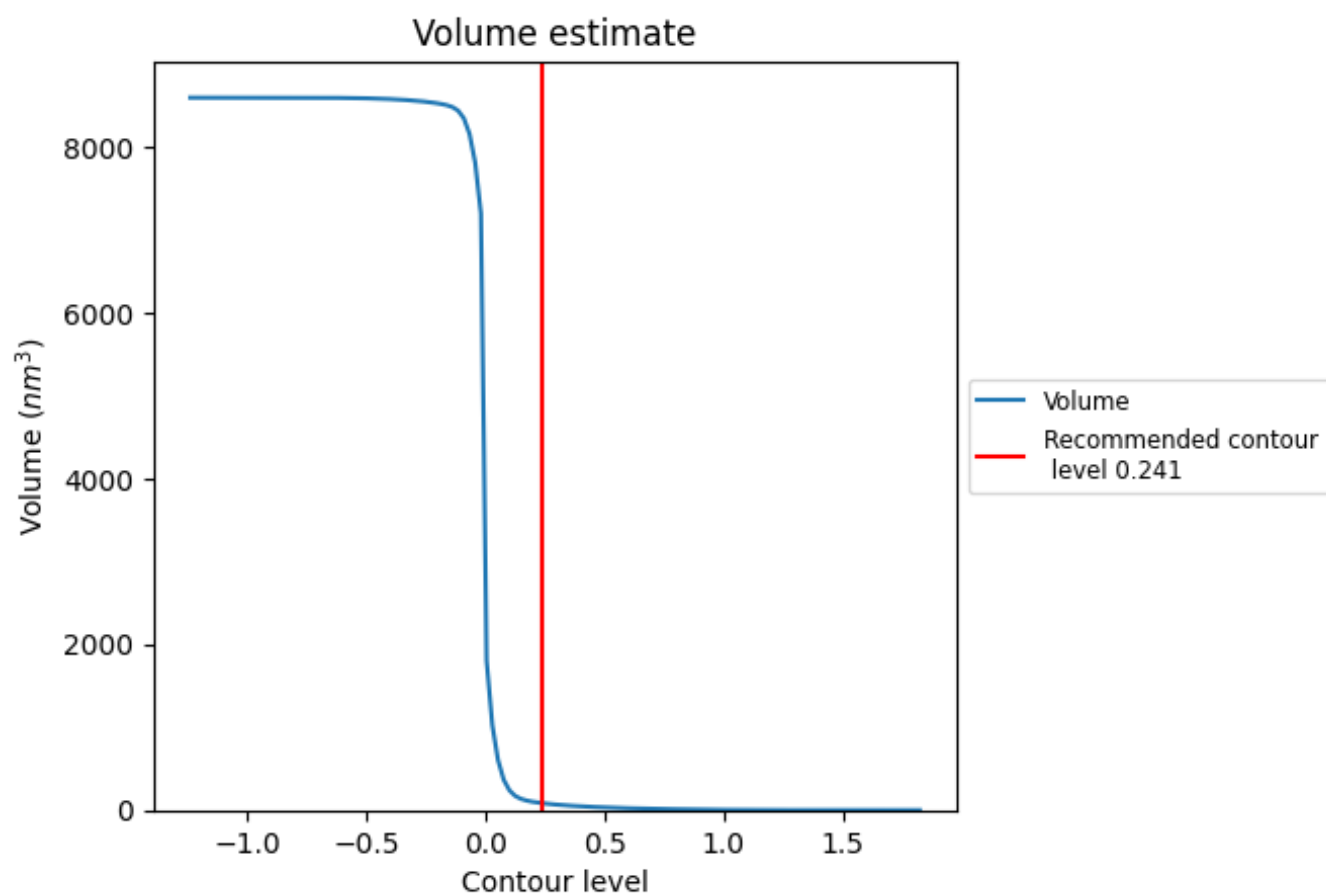
This section contains the results of statistical analysis of the map.

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.

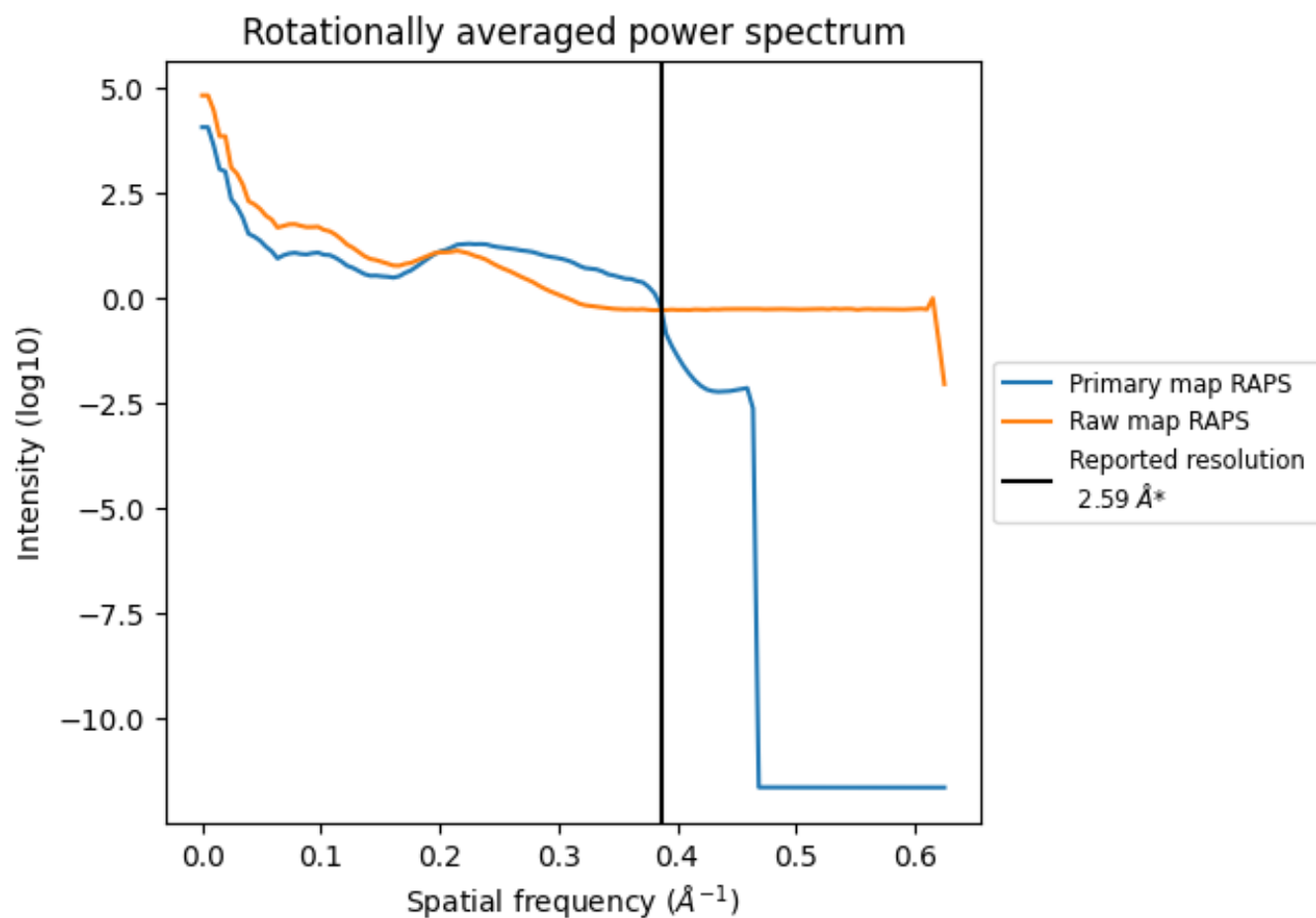
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 84 nm³; this corresponds to an approximate mass of 76 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 ⓘ

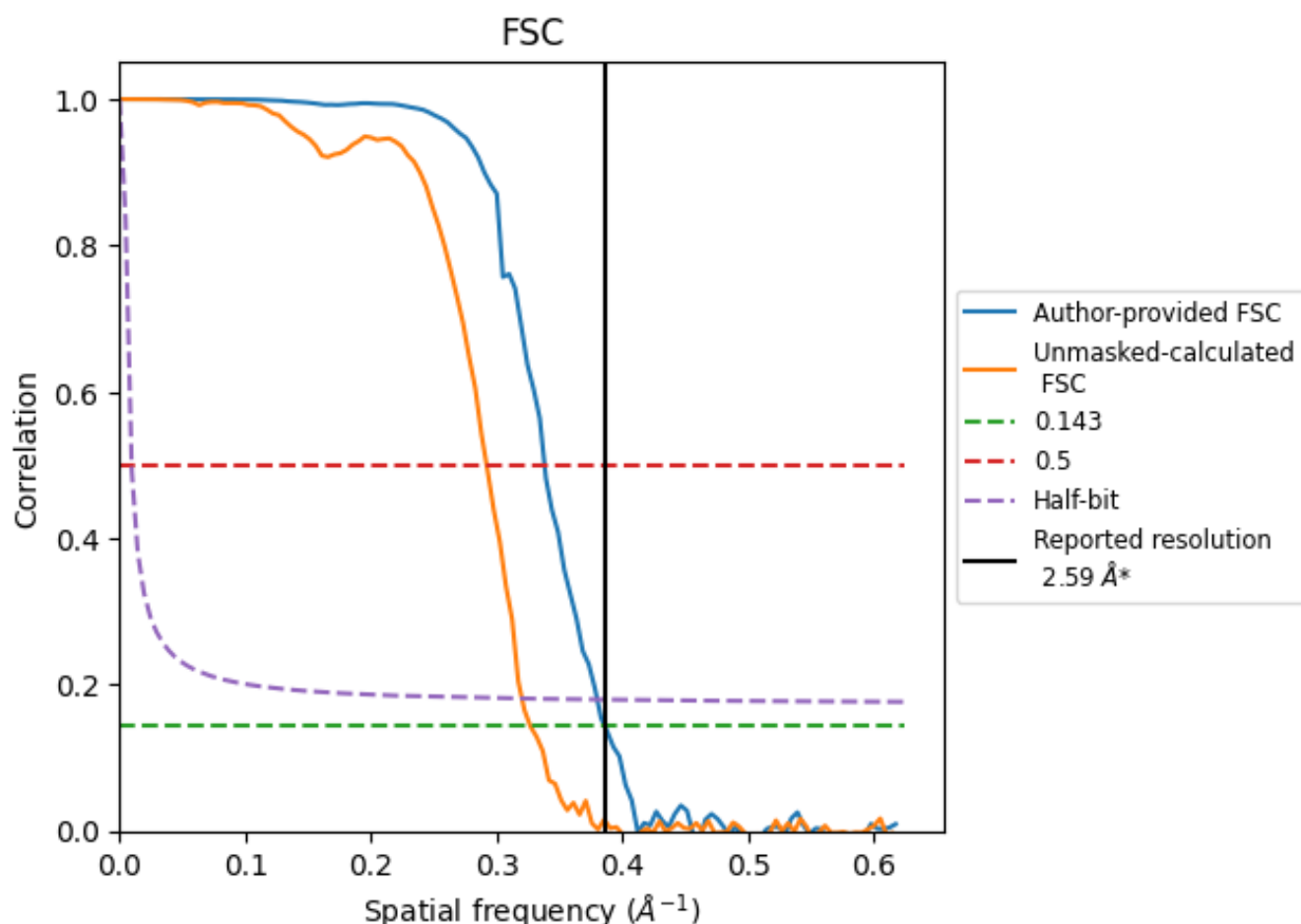


*Reported resolution corresponds to spatial frequency of 0.386 Å⁻¹

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 0.386 \AA^{-1}

8.2 Resolution estimates [i](#)

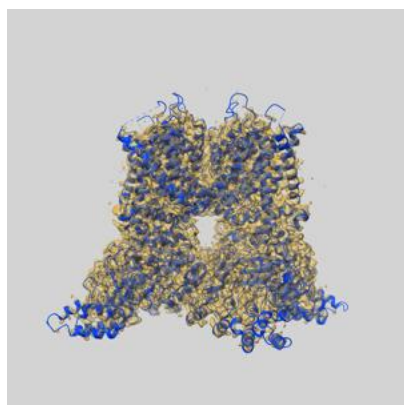
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.59	-	-
Author-provided FSC curve	2.59	2.96	2.63
Unmasked-calculated*	3.06	3.42	3.12

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.06 differs from the reported value 2.59 by more than 10 %

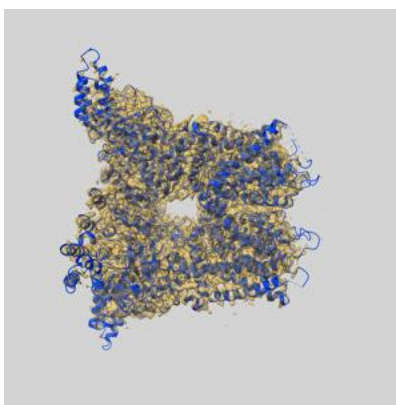
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-42997 and PDB model 8V6N. Per-residue inclusion information can be found in section [3](#) on page [9](#).

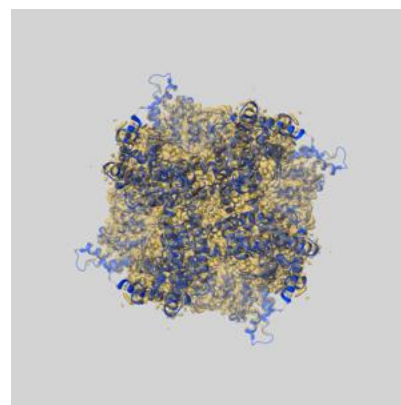
9.1 Map-model overlay [i](#)



X



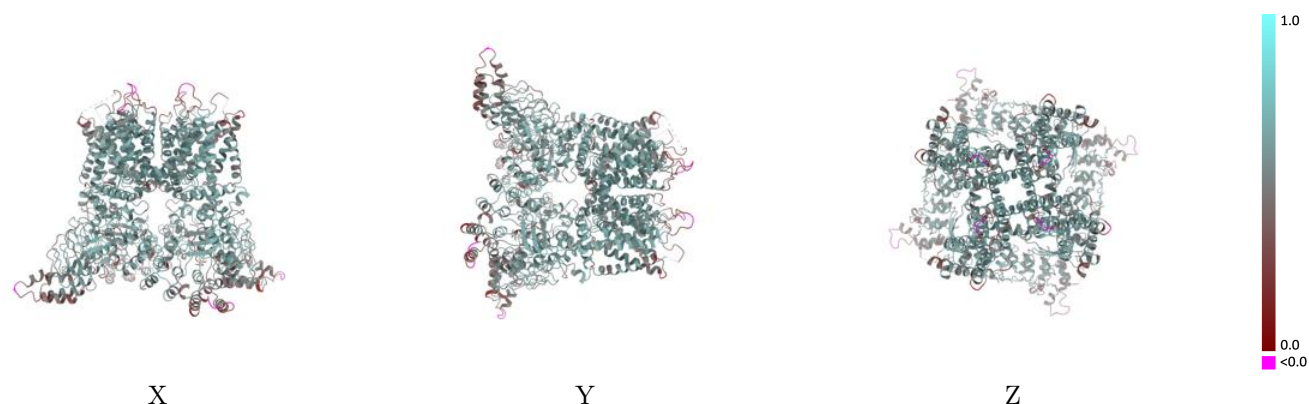
Y



Z

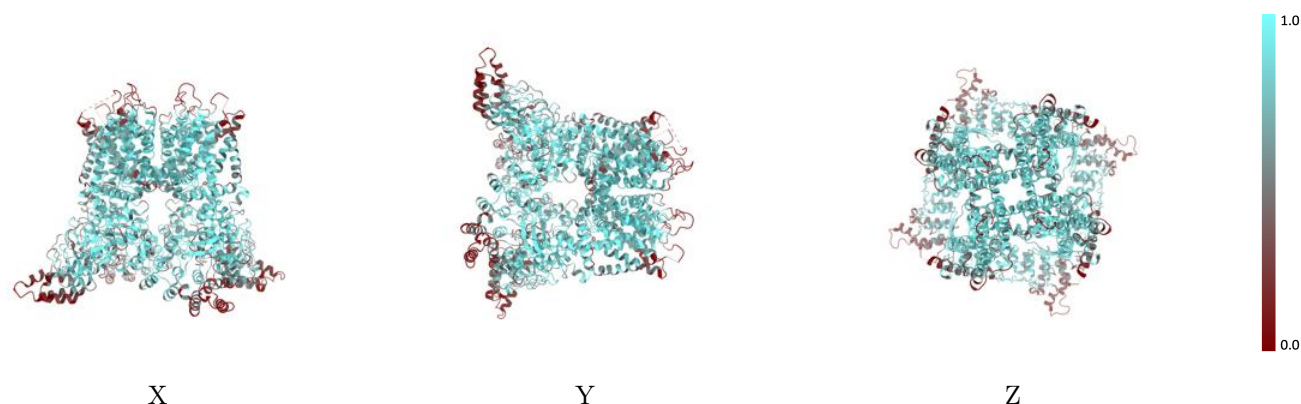
The images above show the 3D surface view of the map at the recommended contour level 0.241 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



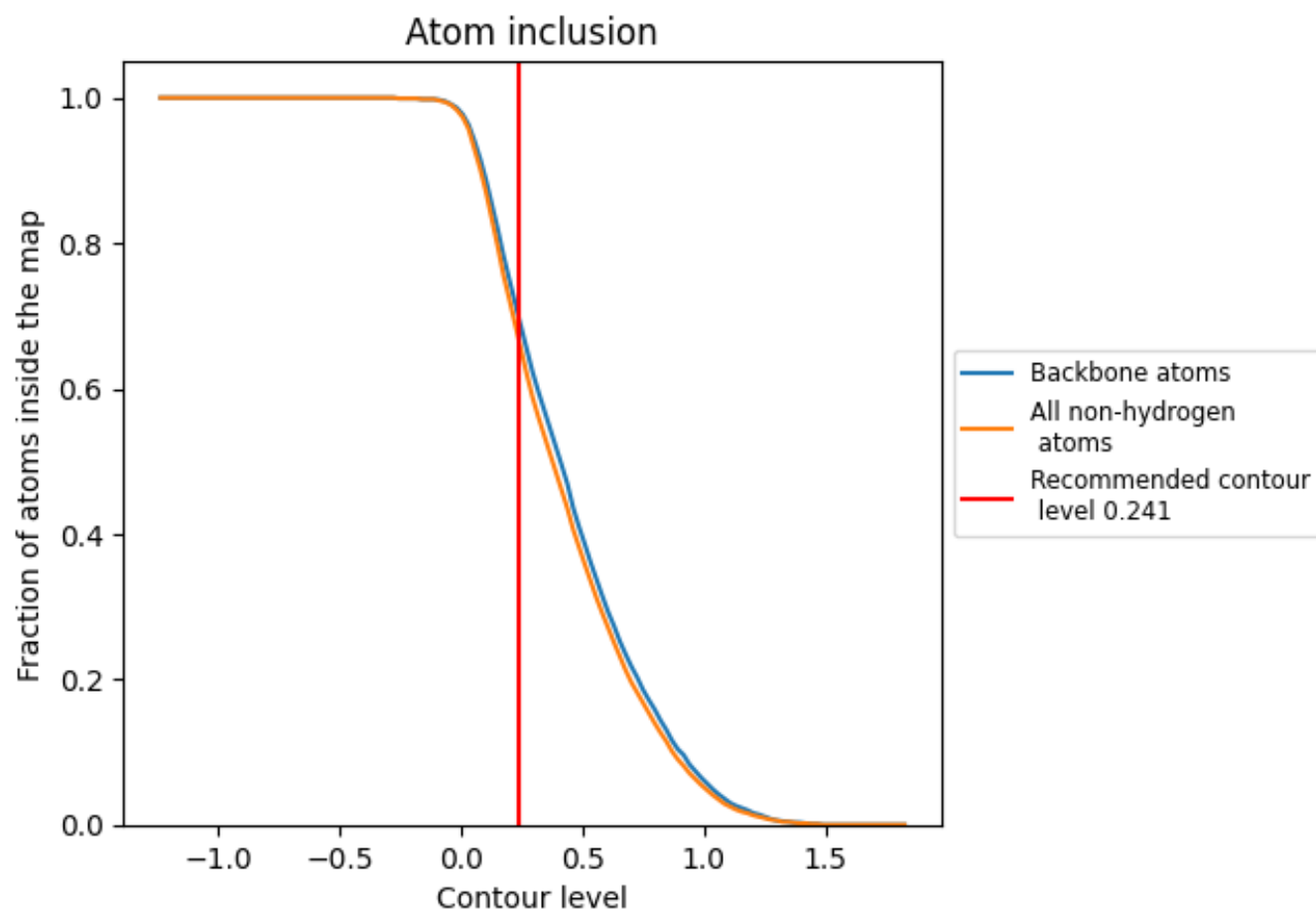
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.241).

9.4 Atom inclusion [i](#)



At the recommended contour level, 69% of all backbone atoms, 66% 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 (0.241) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6610	<div></div> 0.5340
A	<div></div> 0.6650	<div></div> 0.5360
B	<div></div> 0.6630	<div></div> 0.5330
C	<div></div> 0.6640	<div></div> 0.5340
D	<div></div> 0.6660	<div></div> 0.5330

