



## Full wwPDB EM Validation Report ⓘ

Aug 4, 2025 – 05:42 PM EDT

PDB ID : 9CUR / pdb\_00009cur  
EMDB ID : EMD-45939  
Title : BmrCD in the inward-facing conformation bound to Hoechst and lipids  
Authors : Qingyu, T.; Hassane, S.M.  
Deposited on : 2024-07-26  
Resolution : 3.40 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](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev126  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0rc1  
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) : 2.45.1

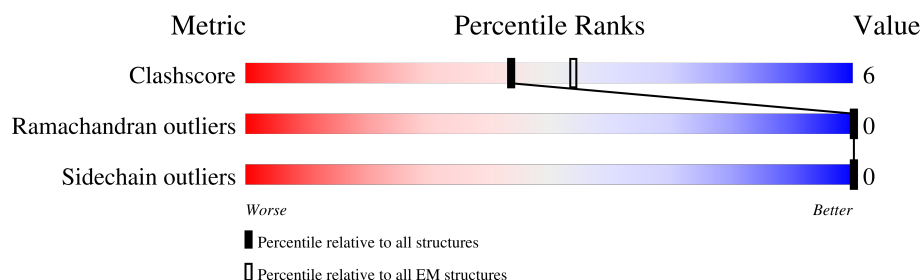
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.40 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	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  $\geq 3$ , 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	D	681	
2	C	607	

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 22040 atoms, of which 11209 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 Probable multidrug resistance ABC transporter ATP-binding/permease protein YheH.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	D	657	10535	3373	5289	892	961	20	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	674	LEU	-	expression tag	UNP O07549
D	675	GLU	-	expression tag	UNP O07549
D	676	HIS	-	expression tag	UNP O07549
D	677	HIS	-	expression tag	UNP O07549
D	678	HIS	-	expression tag	UNP O07549
D	679	HIS	-	expression tag	UNP O07549
D	680	HIS	-	expression tag	UNP O07549
D	681	HIS	-	expression tag	UNP O07549

- Molecule 2 is a protein called Probable multidrug resistance ABC transporter ATP-binding/permease protein YheI.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	C	568	9015	2890	4545	745	812	23	0	0

There are 23 discrepancies between the modelled and reference sequences:

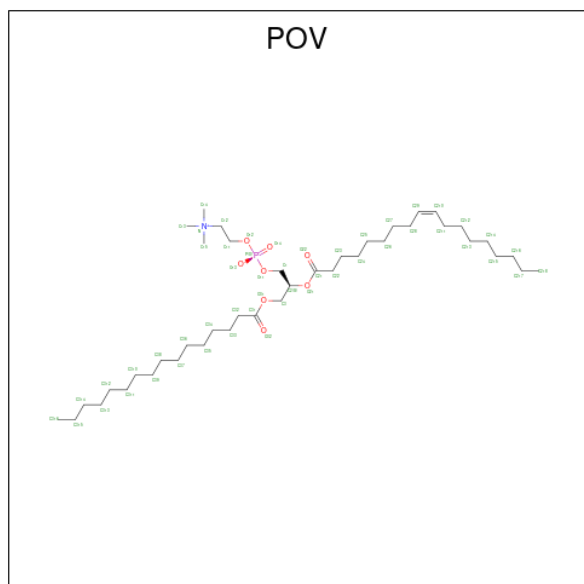
Chain	Residue	Modelled	Actual	Comment	Reference
C	-21	MET	-	expression tag	UNP O07550
C	-20	GLY	-	expression tag	UNP O07550
C	-19	SER	-	expression tag	UNP O07550
C	-18	SER	-	expression tag	UNP O07550
C	-17	HIS	-	expression tag	UNP O07550
C	-16	HIS	-	expression tag	UNP O07550
C	-15	HIS	-	expression tag	UNP O07550

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-14	HIS	-	expression tag	UNP O07550
C	-13	HIS	-	expression tag	UNP O07550
C	-12	HIS	-	expression tag	UNP O07550
C	-11	SER	-	expression tag	UNP O07550
C	-10	SER	-	expression tag	UNP O07550
C	-9	GLY	-	expression tag	UNP O07550
C	-8	LEU	-	expression tag	UNP O07550
C	-7	VAL	-	expression tag	UNP O07550
C	-6	PRO	-	expression tag	UNP O07550
C	-5	ARG	-	expression tag	UNP O07550
C	-4	GLY	-	expression tag	UNP O07550
C	-3	SER	-	expression tag	UNP O07550
C	-2	HIS	-	expression tag	UNP O07550
C	-1	MET	-	expression tag	UNP O07550
C	0	LEU	-	expression tag	UNP O07550
C	1	GLU	-	expression tag	UNP O07550

- Molecule 3 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylammonio)ethyl phosphate (CCD ID: POV) (formula: C<sub>42</sub>H<sub>82</sub>NO<sub>8</sub>P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf	
3	D	1	Total	C	H	N	O	P	0
			119	39	70	1	8	1	
3	D	1	Total	C	H	N	O	P	0
			125	40	75	1	8	1	

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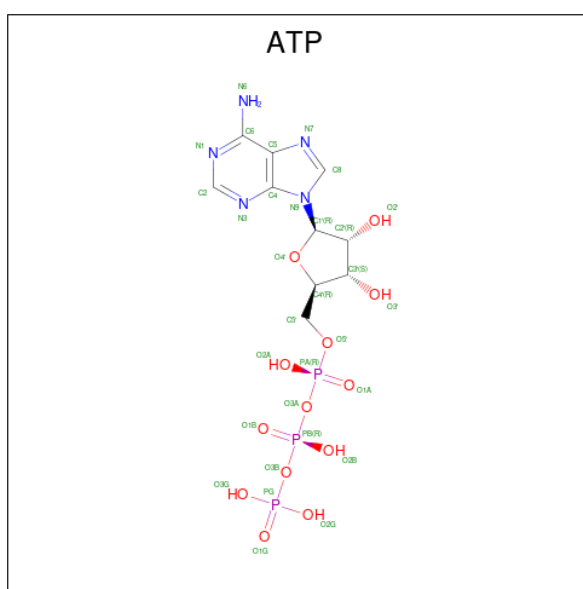
Mol	Chain	Residues	Atoms						AltConf
3	D	1	Total	C	H	N	O	P	0
			68	22	36	1	8	1	
3	D	1	Total	C	H	O	P		0
			25	8	10	6	1		
3	D	1	Total	C	H	O	P		0
			115	37	69	8	1		
3	D	1	Total	C	H	O	P		0
			91	30	52	8	1		
3	D	1	Total	C	H	N	O	P	0
			66	21	37	1	6	1	
3	D	1	Total	C	H	O	P		0
			88	30	49	8	1		
3	D	1	Total	C	H	N	O	P	0
			98	32	56	1	8	1	
3	D	1	Total	C	H	N	O	P	0
			89	28	51	1	8	1	
3	D	1	Total	C	H	N	O	P	0
			98	31	57	1	8	1	
3	D	1	Total	C	H	O	P		0
			73	24	40	8	1		
3	D	1	Total	C	H	N	O	P	0
			85	27	48	1	8	1	
3	C	1	Total	C	H	O	P		0
			30	10	11	8	1		
3	C	1	Total	C	H	O	P		0
			24	8	7	8	1		
3	C	1	Total	C	H	O	P		0
			54	18	27	8	1		
3	C	1	Total	C	H	N	O	P	0
			77	25	42	1	8	1	
3	C	1	Total	C	H	O	P		0
			91	31	51	8	1		
3	C	1	Total	C	H	N	O	P	0
			110	35	65	1	8	1	
3	C	1	Total	C	H	O	P		0
			115	37	69	8	1		
3	C	1	Total	C	H	N	O	P	0
			64	20	34	1	8	1	
3	C	1	Total	C	H	N	O	P	0
			79	25	44	1	8	1	
3	C	1	Total	C	H	N	O	P	0
			73	23	40	1	8	1	

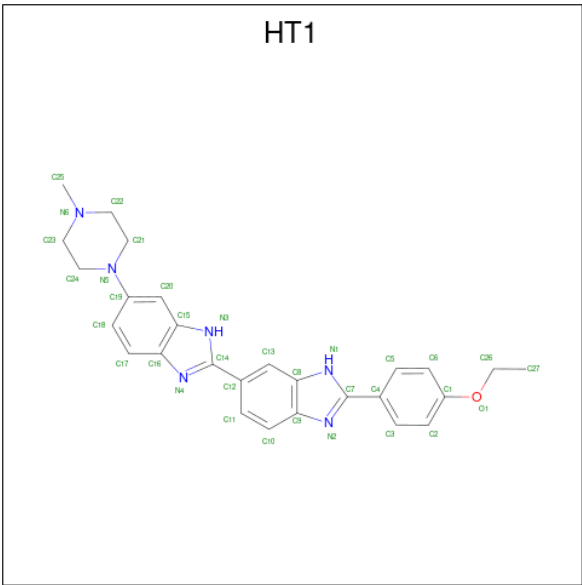
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Mol	Chain	Residues	Atoms					AltConf
3	C	1	Total	C	H	O		0
			41	15	24	2		
3	C	1	Total	C	H	N	O	P
			134	42	82	1	8	1
3	C	1	Total	C	H	N	O	P
			134	42	82	1	8	1
3	C	1	Total	C	H	N	O	P
			113	36	67	1	8	1

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).





Mol	Chain	Residues	Atoms					AltConf
5	D	1	Total	C	H	N	O	0
			62	27	28	6	1	
5	D	1	Total	C	H	N	O	0
			62	27	28	6	1	

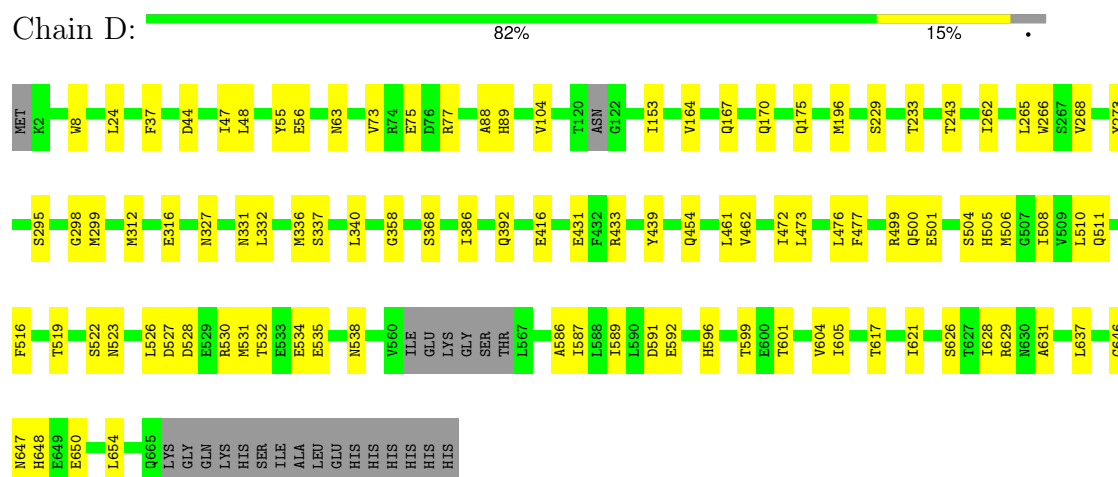
- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
6	D	1	Total	Mg	0
			1	1	

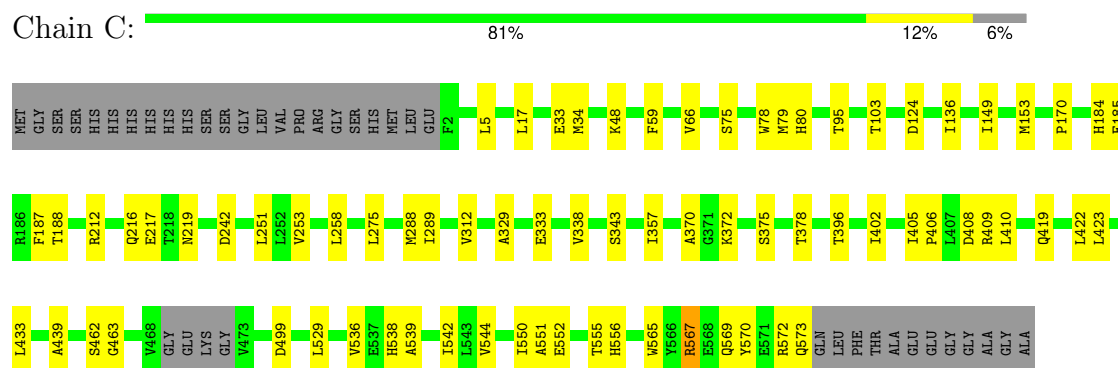
### 3 Residue-property plots

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: Probable multidrug resistance ABC transporter ATP-binding/permease protein YheH



- Molecule 2: Probable multidrug resistance ABC transporter ATP-binding/permease protein YheI





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	74260	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	15	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.517	Depositor
Minimum map value	-0.408	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.036	Depositor
Map size ( $\text{\AA}$ )	310.56, 310.56, 310.56	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.647, 0.647, 0.647	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: HT1, ATP, POV, MG

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	D	0.17	0/5344	0.33	0/7215
2	C	0.20	0/4562	0.39	1/6175 (0.0%)
All	All	0.18	0/9906	0.36	1/13390 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	567	ARG	N-CA-C	-8.20	103.41	113.41

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	D	5246	5289	5286	82	0
2	C	4470	4545	4543	67	0
3	C	494	645	645	13	0
3	D	490	650	650	8	0
4	C	31	12	12	1	0
4	D	31	12	12	2	0
5	D	68	56	56	2	0
6	D	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	10831	11209	11204	139	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 6.

All (139) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:47:ILE:HG21	2:C:275:LEU:HD21	1.62	0.81
1:D:646:GLY:O	1:D:647:ASN:ND2	2.19	0.75
1:D:48:LEU:CD1	2:C:275:LEU:HD11	2.16	0.75
1:D:316:GLU:OE2	2:C:95:THR:HG23	1.87	0.74
2:C:258:LEU:HD22	3:C:605:POV:H21B	1.76	0.67
1:D:599:THR:O	1:D:599:THR:HG22	1.95	0.65
1:D:416:GLU:OE1	1:D:499:ARG:NE	2.30	0.64
1:D:500:GLN:OE1	1:D:500:GLN:N	2.32	0.63
5:D:715:HT1:H17	2:C:79:MET:HE2	1.81	0.62
1:D:56:GLU:N	1:D:56:GLU:OE1	2.33	0.60
1:D:153:ILE:HG23	2:C:258:LEU:HD21	1.82	0.60
1:D:531:MET:HG2	1:D:532:THR:H	1.66	0.60
1:D:621:ILE:O	1:D:621:ILE:HG22	2.01	0.60
2:C:572:ARG:O	2:C:573:GLN:HB2	2.03	0.58
1:D:528:ASP:OD2	2:C:216:GLN:NE2	2.37	0.58
1:D:48:LEU:HD11	2:C:275:LEU:HD11	1.85	0.57
2:C:408:ASP:OD1	2:C:409:ARG:N	2.36	0.57
1:D:505:HIS:O	1:D:586:ALA:N	2.37	0.57
2:C:75:SER:HA	2:C:78:TRP:CD1	2.39	0.57
2:C:80:HIS:ND1	3:C:608:POV:H14B	2.19	0.57
1:D:262:ILE:HG23	3:D:705:POV:H21H	1.86	0.56
2:C:333:GLU:N	2:C:333:GLU:OE1	2.40	0.55
1:D:48:LEU:HD11	2:C:275:LEU:CD1	2.37	0.55
1:D:519:THR:O	1:D:522:SER:OG	2.23	0.54
2:C:433:LEU:HD21	2:C:439:ALA:CB	2.38	0.54
1:D:104:VAL:HG22	1:D:104:VAL:O	2.09	0.53
1:D:516:PHE:N	1:D:523:ASN:OD1	2.39	0.53
1:D:647:ASN:CG	1:D:650:GLU:OE2	2.52	0.52
1:D:527:ASP:O	2:C:219:ASN:ND2	2.43	0.51
1:D:631:ALA:O	1:D:647:ASN:CG	2.53	0.51
1:D:506:MET:HB2	1:D:587:ILE:HB	1.93	0.51
2:C:565:TRP:CE3	2:C:567:ARG:CZ	2.94	0.51
1:D:530:ARG:HB3	1:D:534:GLU:HG3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:433:LEU:HD21	2:C:439:ALA:HB2	1.93	0.50
2:C:343:SER:O	2:C:343:SER:OG	2.29	0.50
1:D:587:ILE:O	1:D:617:THR:O	2.29	0.50
1:D:596:HIS:O	1:D:596:HIS:CG	2.65	0.50
2:C:48:LYS:HD3	2:C:275:LEU:HD12	1.94	0.49
1:D:273:TYR:HB3	1:D:332:LEU:HD22	1.94	0.49
1:D:501:GLU:O	1:D:504:SER:OG	2.31	0.49
1:D:477:PHE:HE2	1:D:508:ILE:HD12	1.78	0.49
1:D:511:GLN:N	1:D:591:ASP:OD2	2.46	0.49
1:D:604:VAL:HG12	1:D:604:VAL:O	2.13	0.49
2:C:124:ASP:HB3	2:C:312:VAL:HG23	1.94	0.49
2:C:185:GLU:O	2:C:188:THR:HG22	2.13	0.49
2:C:258:LEU:C	2:C:258:LEU:HD23	2.38	0.48
2:C:34:MET:N	2:C:34:MET:HE2	2.28	0.48
2:C:372:LYS:HG2	2:C:565:TRP:CZ3	2.48	0.48
2:C:103:THR:HG22	2:C:103:THR:O	2.13	0.48
1:D:164:VAL:HG21	2:C:251:LEU:HB2	1.95	0.48
1:D:331:ASN:HB2	3:C:608:POV:H14A	1.95	0.48
1:D:648:HIS:CE1	1:D:654:LEU:HB2	2.48	0.48
1:D:522:SER:O	1:D:526:LEU:N	2.47	0.48
2:C:33:GLU:C	2:C:34:MET:HE2	2.38	0.48
2:C:536:VAL:O	2:C:542:ILE:HD11	2.13	0.48
1:D:462:VAL:O	1:D:637:LEU:N	2.44	0.48
2:C:170:PRO:HG3	3:C:611:POV:H212	1.95	0.48
2:C:136:ILE:HD12	3:C:609:POV:H35	1.95	0.47
2:C:402:ILE:HG23	2:C:410:LEU:CD1	2.43	0.47
1:D:55:TYR:OH	1:D:75:GLU:OE2	2.23	0.47
1:D:266:TRP:CZ2	1:D:337:SER:HA	2.48	0.47
1:D:266:TRP:HE1	1:D:336:MET:HB3	1.79	0.47
1:D:88:ALA:O	1:D:89:HIS:ND1	2.48	0.47
1:D:591:ASP:OD1	1:D:592:GLU:N	2.48	0.47
2:C:572:ARG:O	2:C:573:GLN:OE1	2.32	0.46
1:D:586:ALA:C	1:D:587:ILE:HD13	2.40	0.46
2:C:378:THR:HG22	2:C:378:THR:O	2.16	0.46
1:D:431:GLU:OE1	1:D:433:ARG:NH2	2.48	0.46
2:C:372:LYS:O	2:C:375:SER:OG	2.32	0.46
1:D:531:MET:HG2	1:D:532:THR:N	2.30	0.46
1:D:392:GLN:HA	1:D:392:GLN:OE1	2.16	0.46
1:D:508:ILE:HD11	1:D:510:LEU:HD21	1.97	0.46
1:D:628:ILE:HG22	1:D:628:ILE:O	2.16	0.46
4:D:714:ATP:PA	4:D:714:ATP:O4'	2.74	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:266:TRP:HZ3	1:D:386:ILE:HG22	1.81	0.45
1:D:63:ASN:O	1:D:73:VAL:HG23	2.17	0.45
2:C:433:LEU:CD2	2:C:439:ALA:HB2	2.46	0.45
2:C:66:VAL:HG21	3:C:606:POV:H310	1.98	0.44
2:C:462:SER:OG	2:C:463:GLY:N	2.50	0.44
1:D:175:GLN:NE2	2:C:242:ASP:OD2	2.50	0.44
1:D:531:MET:CG	1:D:532:THR:H	2.30	0.44
2:C:555:THR:OG1	2:C:556:HIS:N	2.49	0.44
1:D:591:ASP:CG	1:D:592:GLU:N	2.75	0.44
1:D:77:ARG:N	1:D:77:ARG:CD	2.81	0.44
2:C:499:ASP:OD1	2:C:529:LEU:HD12	2.17	0.44
5:D:715:HT1:H17	2:C:79:MET:CE	2.48	0.44
1:D:229:SER:O	1:D:233:THR:HB	2.18	0.43
1:D:626:SER:O	1:D:629:ARG:HG2	2.17	0.43
2:C:567:ARG:O	2:C:570:TYR:HB2	2.19	0.43
1:D:243:THR:HG21	3:D:702:POV:H31E	1.99	0.43
2:C:149:ILE:HG21	2:C:288:MET:HB2	2.01	0.43
1:D:37:PHE:HB3	3:D:702:POV:H23	2.01	0.43
1:D:295:SER:O	1:D:299:MET:HE2	2.18	0.43
3:C:607:POV:H35A	3:C:608:POV:H2	2.00	0.43
1:D:461:LEU:HD11	1:D:472:ILE:HG21	2.00	0.43
1:D:24:LEU:HD11	3:D:701:POV:H313	2.01	0.43
2:C:5:LEU:HD22	2:C:136:ILE:HD11	2.01	0.43
1:D:265:LEU:O	1:D:268:VAL:HG12	2.18	0.43
1:D:340:LEU:HD11	3:D:705:POV:H31F	2.00	0.43
1:D:648:HIS:O	1:D:654:LEU:HB3	2.19	0.43
2:C:338:VAL:HG13	2:C:396:THR:HB	2.00	0.43
2:C:405:ILE:HG23	2:C:406:PRO:CD	2.49	0.43
1:D:535:GLU:HA	1:D:538:ASN:ND2	2.33	0.43
1:D:454:GLN:O	1:D:617:THR:OG1	2.31	0.43
1:D:631:ALA:O	1:D:647:ASN:OD1	2.36	0.42
1:D:312:MET:O	1:D:316:GLU:HG2	2.20	0.42
2:C:184:HIS:HA	3:C:614:POV:H3	2.01	0.42
2:C:253:VAL:HG13	2:C:289:ILE:HD11	2.02	0.42
1:D:439:TYR:CE1	4:D:714:ATP:C8	3.08	0.42
1:D:599:THR:O	1:D:599:THR:CG2	2.66	0.42
2:C:17:LEU:HB3	3:C:604:POV:H1	2.00	0.42
2:C:149:ILE:O	2:C:153:MET:HG3	2.19	0.42
1:D:358:GLY:HA3	3:D:703:POV:H11A	2.01	0.42
2:C:551:ALA:O	2:C:552:GLU:HG3	2.20	0.42
2:C:569:GLN:OE1	2:C:569:GLN:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:298:GLY:HA2	2:C:422:LEU:HD13	2.02	0.42
2:C:59:PHE:HA	3:C:606:POV:C36	2.49	0.42
1:D:8:TRP:CH2	3:D:708:POV:H23	2.55	0.41
2:C:329:ALA:O	2:C:409:ARG:NH2	2.52	0.41
2:C:59:PHE:HA	3:C:606:POV:H36	2.02	0.41
1:D:601:THR:OG1	1:D:605:ILE:N	2.54	0.41
1:D:500:GLN:NE2	2:C:217:GLU:OE2	2.48	0.41
2:C:423:LEU:HD12	2:C:423:LEU:C	2.45	0.41
2:C:187:PHE:CD1	2:C:187:PHE:C	2.98	0.41
1:D:196:MET:O	2:C:212:ARG:NH1	2.54	0.41
1:D:473:LEU:C	1:D:473:LEU:HD23	2.46	0.41
1:D:587:ILE:HD13	1:D:587:ILE:N	2.36	0.41
3:C:607:POV:H35	3:C:608:POV:H12	2.01	0.41
2:C:95:THR:O	2:C:95:THR:HG22	2.20	0.41
2:C:538:HIS:O	2:C:539:ALA:C	2.64	0.41
1:D:167:GLN:O	1:D:170:GLN:HG3	2.21	0.40
2:C:357:ILE:O	2:C:550:ILE:HD11	2.21	0.40
1:D:44:ASP:OD2	1:D:368:SER:OG	2.39	0.40
1:D:47:ILE:CG2	2:C:275:LEU:HD21	2.44	0.40
2:C:370:ALA:O	2:C:544:VAL:HA	2.21	0.40
1:D:476:LEU:CD2	1:D:589:ILE:HD11	2.51	0.40
2:C:419:GLN:OE1	4:C:615:ATP:O2G	2.39	0.40
1:D:327:ASN:HB3	3:C:608:POV:H15	2.04	0.40
3:D:711:POV:H25	3:D:711:POV:H1A	2.04	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	D	651/681 (96%)	616 (95%)	35 (5%)	0	<a href="#">100</a> <a href="#">100</a>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	C	564/607 (93%)	544 (96%)	20 (4%)	0	100	100
All	All	1215/1288 (94%)	1160 (96%)	55 (4%)	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	D	560/584 (96%)	560 (100%)	0	100	100
2	C	480/508 (94%)	480 (100%)	0	100	100
All	All	1040/1092 (95%)	1040 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	63	ASN
1	D	92	GLN
1	D	192	HIS
1	D	278	ASN
1	D	339	ASN
1	D	557	ASN
2	C	538	HIS
2	C	556	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 32 ligands modelled in this entry, 1 is monoatomic - leaving 31 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	POV	C	610	-	32,32,51	0.35	0	38,40,59	0.37	0
3	POV	C	611	-	16,16,51	0.41	0	16,16,59	0.30	0
3	POV	C	609	-	34,34,51	0.35	0	40,42,59	0.59	1 (2%)
3	POV	C	607	-	45,45,51	0.40	0	48,50,59	0.52	1 (2%)
5	HT1	D	716	-	37,39,39	0.73	0	34,56,56	0.94	1 (2%)
3	POV	D	702	-	49,49,51	0.36	0	55,57,59	0.36	0
3	POV	D	709	-	41,41,51	0.37	0	47,49,59	0.39	0
3	POV	D	705	-	45,45,51	0.41	0	48,50,59	0.52	1 (2%)
4	ATP	D	714	6	28,33,33	0.79	0	34,52,52	0.89	2 (5%)
3	POV	D	708	-	38,38,51	0.46	0	41,43,59	0.56	1 (2%)
3	POV	D	706	-	38,38,51	0.43	0	41,43,59	0.52	1 (2%)
3	POV	C	606	-	44,44,51	0.35	0	50,52,59	0.32	0
3	POV	C	602	-	16,16,51	0.57	0	19,21,59	0.76	1 (5%)
3	POV	D	707	-	28,28,51	0.41	0	33,34,59	0.46	0
3	POV	D	703	-	31,31,51	0.41	0	37,39,59	0.41	0
4	ATP	C	615	-	28,33,33	0.81	0	34,52,52	0.77	1 (2%)
3	POV	D	713	-	36,36,51	0.33	0	42,44,59	0.34	0
3	POV	C	601	-	18,18,51	0.54	0	21,23,59	0.82	1 (4%)
3	POV	D	710	-	37,37,51	0.35	0	43,45,59	0.37	0
3	POV	D	711	-	40,40,51	0.35	0	46,48,59	0.43	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	HT1	D	715	-	37,39,39	0.71	0	34,56,56	0.87	2 (5%)
3	POV	C	608	-	29,29,51	0.40	0	35,37,59	0.45	0
3	POV	C	605	-	39,39,51	0.48	0	42,44,59	0.55	1 (2%)
3	POV	C	613	-	51,51,51	0.34	0	57,59,59	0.43	0
3	POV	C	604	-	34,34,51	0.37	0	40,42,59	0.41	0
3	POV	C	614	-	45,45,51	0.34	0	51,53,59	0.44	0
3	POV	D	701	-	48,48,51	0.34	0	54,56,59	0.55	1 (1%)
3	POV	D	712	-	31,31,51	0.45	0	34,36,59	0.52	1 (2%)
3	POV	D	704	-	14,14,51	0.62	0	17,17,59	0.75	1 (5%)
3	POV	C	612	-	51,51,51	0.34	0	57,59,59	0.28	0
3	POV	C	603	-	26,26,51	0.49	0	29,31,59	0.63	1 (3%)

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	POV	C	610	-	-	9/36/36/55	-
3	POV	C	611	-	-	5/14/14/55	-
3	POV	C	609	-	-	11/38/38/55	-
3	POV	C	607	-	-	15/47/47/55	-
5	HT1	D	716	-	-	3/7/25/25	0/6/6/6
3	POV	D	702	-	-	21/53/53/55	-
3	POV	D	709	-	-	15/45/45/55	-
3	POV	D	705	-	-	12/47/47/55	-
4	ATP	D	714	6	-	5/18/38/38	0/3/3/3
3	POV	D	708	-	-	14/40/40/55	-
3	POV	D	706	-	-	3/40/40/55	-
3	POV	C	606	-	-	16/48/48/55	-
3	POV	C	602	-	-	8/17/17/55	-
3	POV	D	707	-	-	10/29/29/55	-
3	POV	D	703	-	-	8/35/35/55	-
4	ATP	C	615	-	-	5/18/38/38	0/3/3/3
3	POV	D	713	-	-	16/40/40/55	-
3	POV	C	601	-	-	6/19/19/55	-
3	POV	D	710	-	-	14/40/40/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	POV	D	711	-	-	16/44/44/55	-
5	HT1	D	715	-	-	3/7/25/25	0/6/6/6
3	POV	C	608	-	-	9/33/33/55	-
3	POV	C	605	-	-	15/41/41/55	-
3	POV	C	613	-	-	9/55/55/55	-
3	POV	C	604	-	-	13/37/37/55	-
3	POV	C	614	-	-	19/49/49/55	-
3	POV	D	701	-	-	15/52/52/55	-
3	POV	D	712	-	-	15/33/33/55	-
3	POV	D	704	-	-	3/13/13/55	-
3	POV	C	612	-	-	17/55/55/55	-
3	POV	C	603	-	-	5/28/28/55	-

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	701	POV	O21-C21-C22	3.02	118.01	111.48
3	C	607	POV	O13-P-O14	2.56	120.80	110.83
3	D	706	POV	O13-P-O14	2.41	120.23	110.83
3	C	605	POV	O13-P-O14	2.41	120.22	110.83
5	D	715	HT1	C24-N5-C19	2.37	124.56	118.11
3	D	712	POV	O13-P-O14	2.34	119.94	110.83
3	C	603	POV	O13-P-O14	2.33	119.92	110.83
3	D	708	POV	O13-P-O14	2.33	119.91	110.83
3	D	704	POV	O13-P-O14	2.29	119.76	110.83
3	C	602	POV	O13-P-O14	2.29	119.74	110.83
3	D	705	POV	O13-P-O14	2.26	119.64	110.83
4	D	714	ATP	C5-C6-N6	2.26	123.75	120.31
4	C	615	ATP	C5-C6-N6	2.21	123.67	120.31
5	D	716	HT1	C24-N5-C19	2.19	124.07	118.11
3	C	609	POV	O21-C21-C22	2.14	116.12	111.48
3	C	601	POV	O13-P-O14	2.14	119.18	110.83
5	D	715	HT1	C21-N5-C19	2.14	123.94	118.11
4	D	714	ATP	O3A-PB-O1B	-2.12	104.31	110.70

There are no chirality outliers.

All (335) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	701	POV	C22-C21-O21-C2
3	D	701	POV	O22-C21-O21-C2
3	D	702	POV	C1-O11-P-O12
3	D	702	POV	C1-O11-P-O14
3	D	702	POV	O12-C11-C12-N
3	D	702	POV	C22-C21-O21-C2
3	D	703	POV	O12-C11-C12-N
3	D	705	POV	C22-C21-O21-C2
3	D	707	POV	C1-O11-P-O14
3	D	708	POV	C1-O11-P-O13
3	D	708	POV	C1-O11-P-O14
3	D	708	POV	C22-C21-O21-C2
3	D	708	POV	O22-C21-O21-C2
3	D	709	POV	C11-O12-P-O14
3	D	709	POV	C22-C21-O21-C2
3	D	711	POV	C11-O12-P-O11
3	D	711	POV	C11-O12-P-O13
3	D	711	POV	C22-C21-O21-C2
3	D	712	POV	C2-C1-O11-P
3	D	713	POV	C11-O12-P-O11
3	D	713	POV	C11-O12-P-O14
3	C	601	POV	C22-C21-O21-C2
3	C	601	POV	O22-C21-O21-C2
3	C	602	POV	C22-C21-O21-C2
3	C	604	POV	C1-O11-P-O12
3	C	604	POV	C1-O11-P-O13
3	C	604	POV	C1-O11-P-O14
3	C	604	POV	O12-C11-C12-N
3	C	605	POV	C2-C1-O11-P
3	C	605	POV	C22-C21-O21-C2
3	C	606	POV	C11-O12-P-O14
3	C	606	POV	C22-C21-O21-C2
3	C	607	POV	C1-O11-P-O13
3	C	607	POV	C22-C21-O21-C2
3	C	607	POV	O22-C21-O21-C2
3	C	608	POV	O12-C11-C12-N
3	C	608	POV	C22-C21-O21-C2
3	C	608	POV	O22-C21-O21-C2
3	C	609	POV	C11-O12-P-O11
3	C	609	POV	C11-O12-P-O14
3	C	609	POV	C22-C21-O21-C2
3	C	609	POV	O22-C21-O21-C2
3	C	610	POV	O12-C11-C12-N

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Mol	Chain	Res	Type	Atoms
3	C	612	POV	C2-C1-O11-P
3	C	613	POV	C22-C21-O21-C2
4	D	714	ATP	C5'-O5'-PA-O2A
4	D	714	ATP	C5'-O5'-PA-O3A
4	D	714	ATP	C4'-C5'-O5'-PA
4	C	615	ATP	C4'-C5'-O5'-PA
3	D	710	POV	C32-C31-O31-C3
3	D	707	POV	O22-C21-O21-C2
3	D	709	POV	O32-C31-O31-C3
3	C	605	POV	O32-C31-O31-C3
3	C	612	POV	O32-C31-O31-C3
3	C	605	POV	C32-C31-O31-C3
3	C	609	POV	C32-C31-O31-C3
3	C	608	POV	O32-C31-O31-C3
3	C	609	POV	O32-C31-O31-C3
3	D	702	POV	O22-C21-O21-C2
3	D	705	POV	O22-C21-O21-C2
3	D	709	POV	O22-C21-O21-C2
3	D	711	POV	O22-C21-O21-C2
3	C	602	POV	O22-C21-O21-C2
3	C	606	POV	O22-C21-O21-C2
3	D	707	POV	C22-C21-O21-C2
3	D	709	POV	C32-C31-O31-C3
3	C	608	POV	C32-C31-O31-C3
3	C	612	POV	C32-C31-O31-C3
3	D	710	POV	O32-C31-O31-C3
3	D	712	POV	O32-C31-O31-C3
3	C	605	POV	O22-C21-O21-C2
3	C	613	POV	O22-C21-O21-C2
3	D	703	POV	C22-C21-O21-C2
3	D	712	POV	C32-C31-O31-C3
3	D	702	POV	C2-C1-O11-P
3	D	704	POV	C22-C21-O21-C2
3	D	713	POV	C32-C31-O31-C3
3	D	704	POV	O22-C21-O21-C2
3	C	614	POV	C32-C31-O31-C3
3	C	606	POV	C11-C12-N-C13
3	D	713	POV	O32-C31-O31-C3
3	C	610	POV	O21-C2-C3-O31
3	D	703	POV	O22-C21-O21-C2
3	C	607	POV	C312-C313-C314-C315
5	D	715	HT1	C2-C1-O1-C26

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Mol	Chain	Res	Type	Atoms
3	C	601	POV	C2-C1-O11-P
3	C	614	POV	O32-C31-O31-C3
5	D	715	HT1	C6-C1-O1-C26
3	C	614	POV	C212-C213-C214-C215
3	D	702	POV	C31-C32-C33-C34
3	D	711	POV	C32-C31-O31-C3
3	D	710	POV	C22-C21-O21-C2
3	C	603	POV	C22-C21-O21-C2
3	C	610	POV	C31-C32-C33-C34
3	D	710	POV	O22-C21-O21-C2
3	C	603	POV	O22-C21-O21-C2
3	D	707	POV	O11-C1-C2-O21
3	C	606	POV	C11-C12-N-C14
3	C	606	POV	C11-C12-N-C15
4	C	615	ATP	O4'-C4'-C5'-O5'
3	D	711	POV	O32-C31-O31-C3
3	C	604	POV	C21-C22-C23-C24
3	C	606	POV	C32-C33-C34-C35
3	D	705	POV	C311-C312-C313-C314
3	D	706	POV	C32-C33-C34-C35
4	C	615	ATP	C3'-C4'-C5'-O5'
3	D	701	POV	C32-C31-O31-C3
3	C	612	POV	C34-C35-C36-C37
3	C	614	POV	C35-C36-C37-C38
3	C	609	POV	C33-C34-C35-C36
3	D	709	POV	C22-C23-C24-C25
3	C	605	POV	C210-C211-C212-C213
3	D	713	POV	C2-C1-O11-P
3	D	707	POV	C211-C210-C29-C28
3	C	604	POV	C211-C210-C29-C28
3	D	701	POV	O32-C31-O31-C3
3	C	603	POV	C33-C34-C35-C36
3	D	701	POV	C24-C25-C26-C27
3	D	712	POV	C31-C32-C33-C34
3	D	711	POV	C24-C25-C26-C27
3	C	612	POV	C22-C21-O21-C2
3	C	613	POV	C31-C32-C33-C34
3	D	705	POV	C311-C310-C39-C38
3	C	612	POV	C310-C311-C312-C313
3	D	702	POV	C212-C213-C214-C215
3	C	610	POV	C37-C38-C39-C310
3	D	703	POV	O21-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
3	D	708	POV	C210-C211-C212-C213
3	D	709	POV	C26-C27-C28-C29
3	C	612	POV	O22-C21-O21-C2
3	C	603	POV	C32-C33-C34-C35
3	D	705	POV	C39-C310-C311-C312
3	D	708	POV	C22-C23-C24-C25
3	D	701	POV	C211-C210-C29-C28
3	C	614	POV	C213-C214-C215-C216
3	C	607	POV	C22-C23-C24-C25
3	C	607	POV	C35-C36-C37-C38
3	C	601	POV	O11-C1-C2-C3
3	D	713	POV	C31-C32-C33-C34
3	D	701	POV	C33-C34-C35-C36
3	D	703	POV	C1-C2-C3-O31
3	C	610	POV	C1-C2-C3-O31
3	D	708	POV	C26-C27-C28-C29
3	D	702	POV	C34-C35-C36-C37
3	C	604	POV	C32-C31-O31-C3
3	D	711	POV	C212-C213-C214-C215
3	C	605	POV	C21-C22-C23-C24
3	D	702	POV	C39-C310-C311-C312
3	C	608	POV	C1-C2-O21-C21
3	C	612	POV	C26-C27-C28-C29
3	D	710	POV	C211-C210-C29-C28
3	C	607	POV	C33-C34-C35-C36
3	D	701	POV	C37-C38-C39-C310
3	D	713	POV	C35-C36-C37-C38
4	C	615	ATP	PA-O3A-PB-O1B
3	D	712	POV	C22-C21-O21-C2
5	D	715	HT1	C27-C26-O1-C1
3	C	611	POV	C212-C213-C214-C215
3	C	613	POV	C35-C36-C37-C38
3	D	712	POV	O11-C1-C2-C3
3	D	711	POV	O31-C31-C32-C33
3	C	606	POV	C24-C25-C26-C27
3	D	711	POV	C211-C210-C29-C28
3	C	613	POV	C211-C210-C29-C28
3	D	707	POV	C2-C1-O11-P
3	C	610	POV	C32-C31-O31-C3
3	D	712	POV	C1-C2-C3-O31
3	C	608	POV	C1-C2-C3-O31
3	D	712	POV	C311-C312-C313-C314

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Mol	Chain	Res	Type	Atoms
3	C	602	POV	C32-C31-O31-C3
3	D	710	POV	C21-C22-C23-C24
3	D	702	POV	O11-C1-C2-O21
3	D	708	POV	O11-C1-C2-O21
3	D	701	POV	C2-C1-O11-P
3	D	712	POV	O21-C2-C3-O31
3	C	608	POV	O21-C2-C3-O31
3	C	612	POV	O21-C2-C3-O31
3	C	612	POV	C311-C310-C39-C38
3	D	705	POV	C25-C26-C27-C28
3	D	702	POV	C25-C26-C27-C28
3	C	613	POV	C34-C35-C36-C37
3	C	604	POV	C29-C210-C211-C212
3	C	614	POV	C31-C32-C33-C34
3	D	710	POV	C24-C25-C26-C27
3	D	708	POV	C1-O11-P-O12
3	C	605	POV	C1-O11-P-O13
3	D	712	POV	O22-C21-O21-C2
3	C	613	POV	C212-C213-C214-C215
3	D	708	POV	O32-C31-O31-C3
3	C	610	POV	O32-C31-O31-C3
3	D	712	POV	C3-C2-O21-C21
3	D	701	POV	C29-C210-C211-C212
3	D	710	POV	C23-C24-C25-C26
3	D	702	POV	C12-C11-O12-P
3	D	711	POV	C12-C11-O12-P
3	D	713	POV	C12-C11-O12-P
3	C	606	POV	C12-C11-O12-P
3	C	609	POV	C12-C11-O12-P
3	C	612	POV	C12-C11-O12-P
3	C	608	POV	C34-C35-C36-C37
3	D	712	POV	C33-C34-C35-C36
3	C	614	POV	C22-C21-O21-C2
3	D	707	POV	O12-C11-C12-N
3	D	709	POV	O12-C11-C12-N
3	D	713	POV	O12-C11-C12-N
3	C	606	POV	O12-C11-C12-N
3	C	612	POV	O12-C11-C12-N
3	C	613	POV	O12-C11-C12-N
4	D	714	ATP	PG-O3B-PB-O1B
3	C	604	POV	C27-C28-C29-C210
5	D	716	HT1	C27-C26-O1-C1

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Mol	Chain	Res	Type	Atoms
3	D	711	POV	C211-C212-C213-C214
3	C	605	POV	C35-C36-C37-C38
3	D	710	POV	C22-C23-C24-C25
3	C	605	POV	C22-C23-C24-C25
3	D	702	POV	O11-C1-C2-C3
3	D	708	POV	C32-C31-O31-C3
3	D	705	POV	C29-C210-C211-C212
3	D	709	POV	C29-C210-C211-C212
3	C	604	POV	C2-C1-O11-P
3	D	709	POV	C25-C26-C27-C28
3	C	607	POV	C214-C215-C216-C217
3	C	614	POV	O22-C21-O21-C2
3	D	712	POV	O11-C1-C2-O21
3	C	601	POV	O11-C1-C2-O21
3	D	712	POV	C310-C311-C312-C313
3	C	605	POV	C29-C210-C211-C212
3	D	709	POV	C1-C2-C3-O31
3	D	701	POV	C311-C310-C39-C38
3	D	702	POV	C11-O12-P-O14
3	D	703	POV	C11-O12-P-O14
3	D	707	POV	C11-O12-P-O14
3	D	709	POV	C1-O11-P-O14
3	D	710	POV	C11-C12-N-C15
3	D	710	POV	C11-O12-P-O14
3	D	713	POV	C11-O12-P-O13
3	C	606	POV	C11-O12-P-O11
3	C	609	POV	C11-O12-P-O13
3	C	612	POV	C1-O11-P-O14
3	C	614	POV	C11-C12-N-C14
3	C	614	POV	C11-O12-P-O14
3	D	707	POV	C27-C28-C29-C210
3	C	607	POV	C213-C214-C215-C216
3	D	701	POV	C1-C2-O21-C21
3	C	601	POV	C3-C2-O21-C21
3	C	607	POV	C3-C2-O21-C21
3	D	713	POV	C34-C35-C36-C37
3	D	707	POV	C29-C210-C211-C212
3	D	704	POV	O11-C1-C2-O21
3	D	708	POV	C21-C22-C23-C24
3	C	604	POV	O32-C31-O31-C3
3	D	713	POV	O22-C21-O21-C2
3	D	702	POV	C211-C210-C29-C28

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Mol	Chain	Res	Type	Atoms
3	C	612	POV	C1-C2-C3-O31
3	C	612	POV	C39-C310-C311-C312
4	D	714	ATP	PG-O3B-PB-O2B
3	D	711	POV	C29-C210-C211-C212
3	D	711	POV	C27-C28-C29-C210
3	C	614	POV	C27-C28-C29-C210
3	C	606	POV	C310-C311-C312-C313
3	C	611	POV	C27-C28-C29-C210
3	C	607	POV	C310-C311-C312-C313
3	D	713	POV	C310-C311-C312-C313
3	C	607	POV	C32-C33-C34-C35
3	D	702	POV	C213-C214-C215-C216
3	C	604	POV	C22-C23-C24-C25
3	D	705	POV	C32-C33-C34-C35
3	D	702	POV	C211-C212-C213-C214
3	D	709	POV	C3-C2-O21-C21
3	C	602	POV	C3-C2-O21-C21
3	C	603	POV	C3-C2-O21-C21
3	C	605	POV	C1-C2-O21-C21
3	D	713	POV	C33-C34-C35-C36
3	C	602	POV	O21-C21-C22-C23
3	D	713	POV	C22-C21-O21-C2
3	C	611	POV	O21-C21-C22-C23
3	C	614	POV	C33-C34-C35-C36
3	C	602	POV	O32-C31-O31-C3
3	C	609	POV	C36-C37-C38-C39
3	C	606	POV	C23-C24-C25-C26
3	D	710	POV	C11-C12-N-C14
3	C	611	POV	O22-C21-C22-C23
3	C	612	POV	C311-C312-C313-C314
3	D	711	POV	C2-C1-O11-P
3	C	602	POV	O22-C21-C22-C23
3	C	614	POV	C11-C12-N-C13
3	C	614	POV	C11-C12-N-C15
3	C	607	POV	C21-C22-C23-C24
3	C	607	POV	C1-C2-C3-O31
3	C	614	POV	C1-C2-C3-O31
3	D	701	POV	C311-C312-C313-C314
3	C	614	POV	O11-C1-C2-O21
5	D	716	HT1	C2-C1-O1-C26
3	C	606	POV	C311-C312-C313-C314
3	D	708	POV	O11-C1-C2-C3

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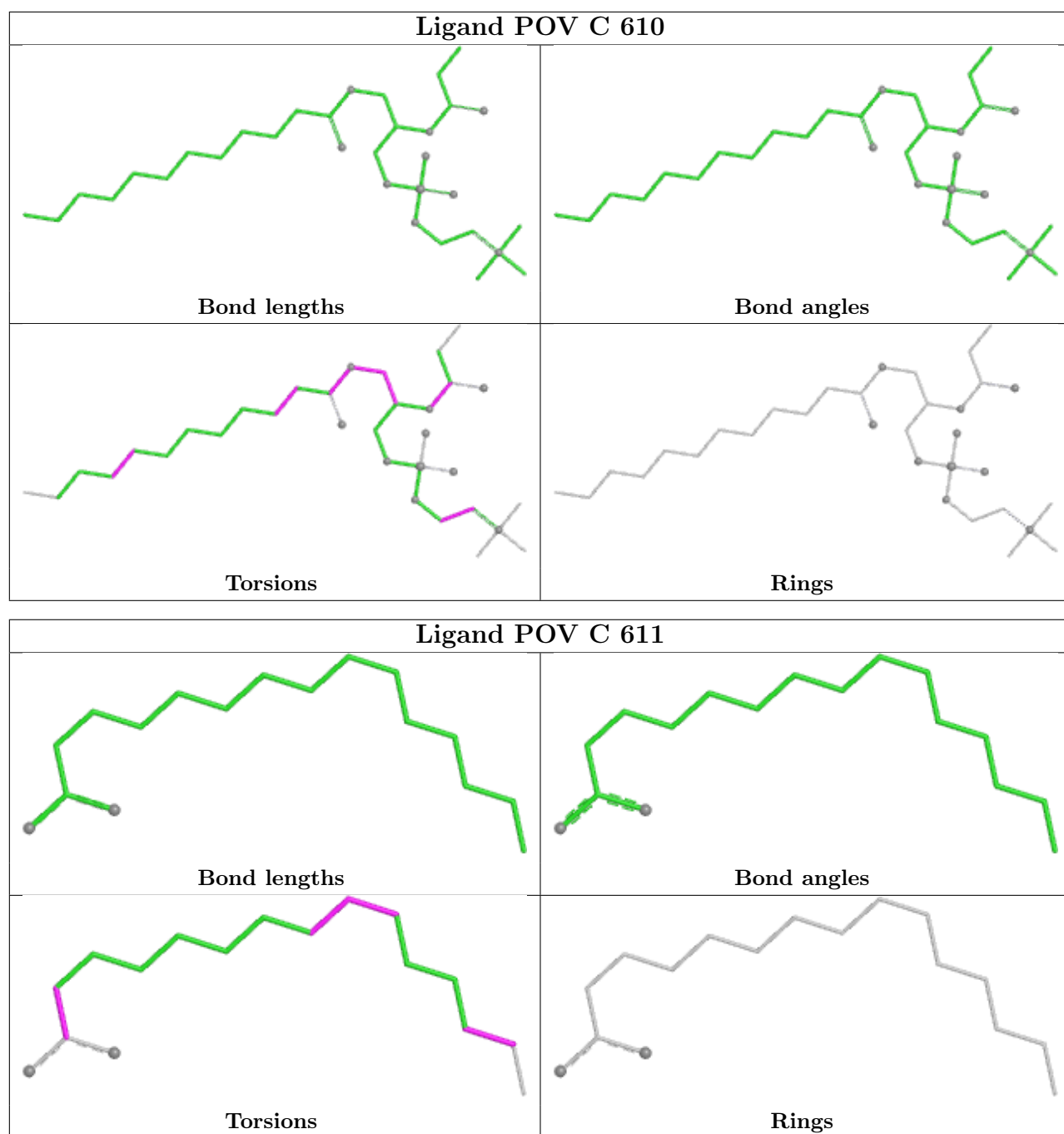
Mol	Chain	Res	Type	Atoms
3	C	614	POV	O21-C2-C3-O31
3	D	705	POV	C22-C23-C24-C25
3	C	607	POV	C1-O11-P-O12
5	D	716	HT1	C6-C1-O1-C26
3	C	604	POV	C25-C26-C27-C28
3	D	713	POV	C1-C2-O21-C21
3	C	602	POV	C1-C2-O21-C21
4	C	615	ATP	PB-O3B-PG-O2G
3	D	705	POV	C27-C28-C29-C210
3	D	711	POV	O32-C31-C32-C33
3	C	605	POV	O21-C2-C3-O31
3	C	606	POV	C35-C36-C37-C38
3	D	703	POV	C23-C24-C25-C26
3	D	710	POV	C11-C12-N-C13
3	D	706	POV	C34-C35-C36-C37
3	C	609	POV	C32-C33-C34-C35
3	D	702	POV	C311-C312-C313-C314
3	C	613	POV	C211-C212-C213-C214
3	C	614	POV	C25-C26-C27-C28
3	C	605	POV	C1-C2-C3-O31
3	C	610	POV	C2-C3-O31-C31
3	D	709	POV	O31-C31-C32-C33
3	D	712	POV	C35-C36-C37-C38
3	D	706	POV	C35-C36-C37-C38
3	D	701	POV	C3-C2-O21-C21
3	C	605	POV	C3-C2-O21-C21
3	C	614	POV	C3-C2-O21-C21
3	D	702	POV	C33-C34-C35-C36
3	D	702	POV	C24-C25-C26-C27
3	C	612	POV	C33-C34-C35-C36
3	D	709	POV	O32-C31-C32-C33
3	D	701	POV	C39-C310-C311-C312
3	C	610	POV	O22-C21-O21-C2
3	D	705	POV	C211-C210-C29-C28
3	C	611	POV	C211-C210-C29-C28
3	C	606	POV	C37-C38-C39-C310
3	D	708	POV	C31-C32-C33-C34
3	D	703	POV	O21-C21-C22-C23
3	D	710	POV	C29-C210-C211-C212
3	D	705	POV	C33-C34-C35-C36

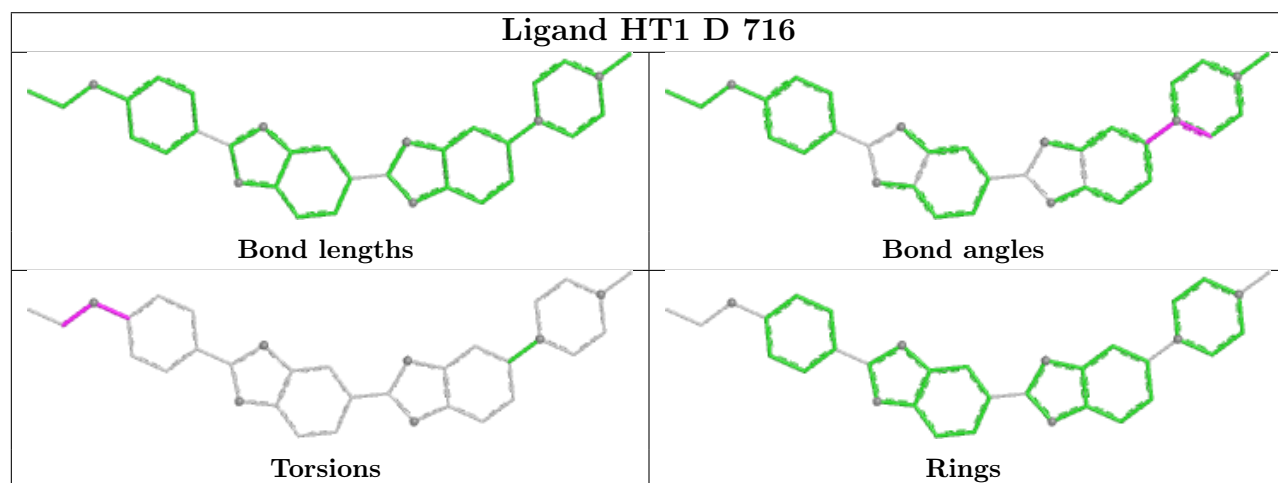
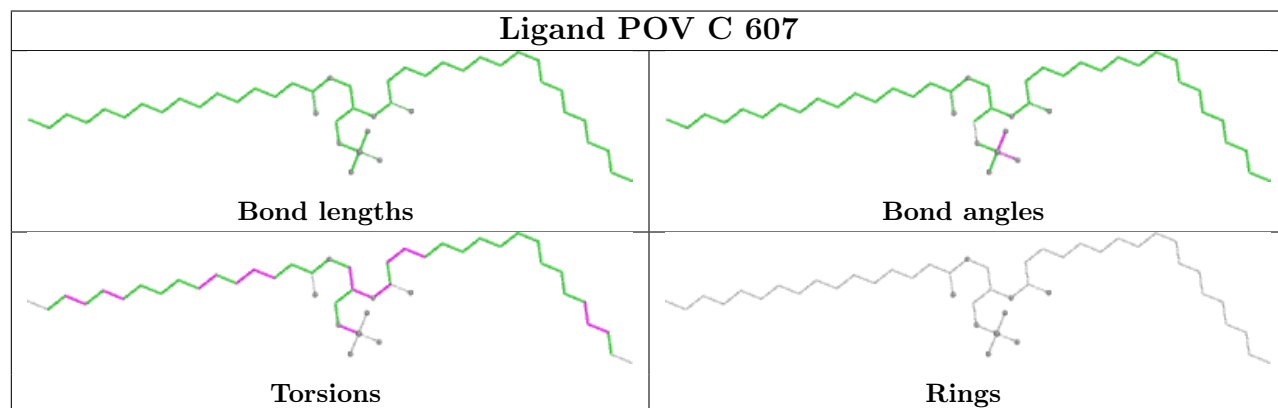
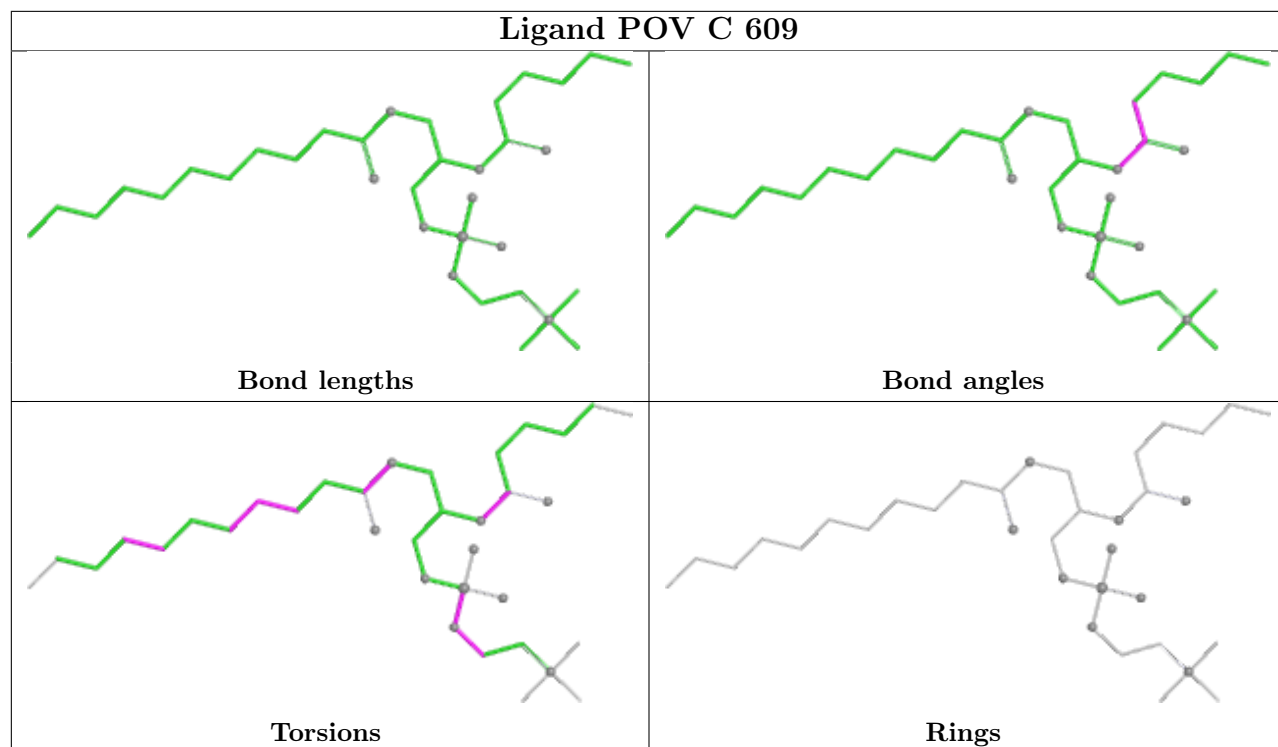
There are no ring outliers.

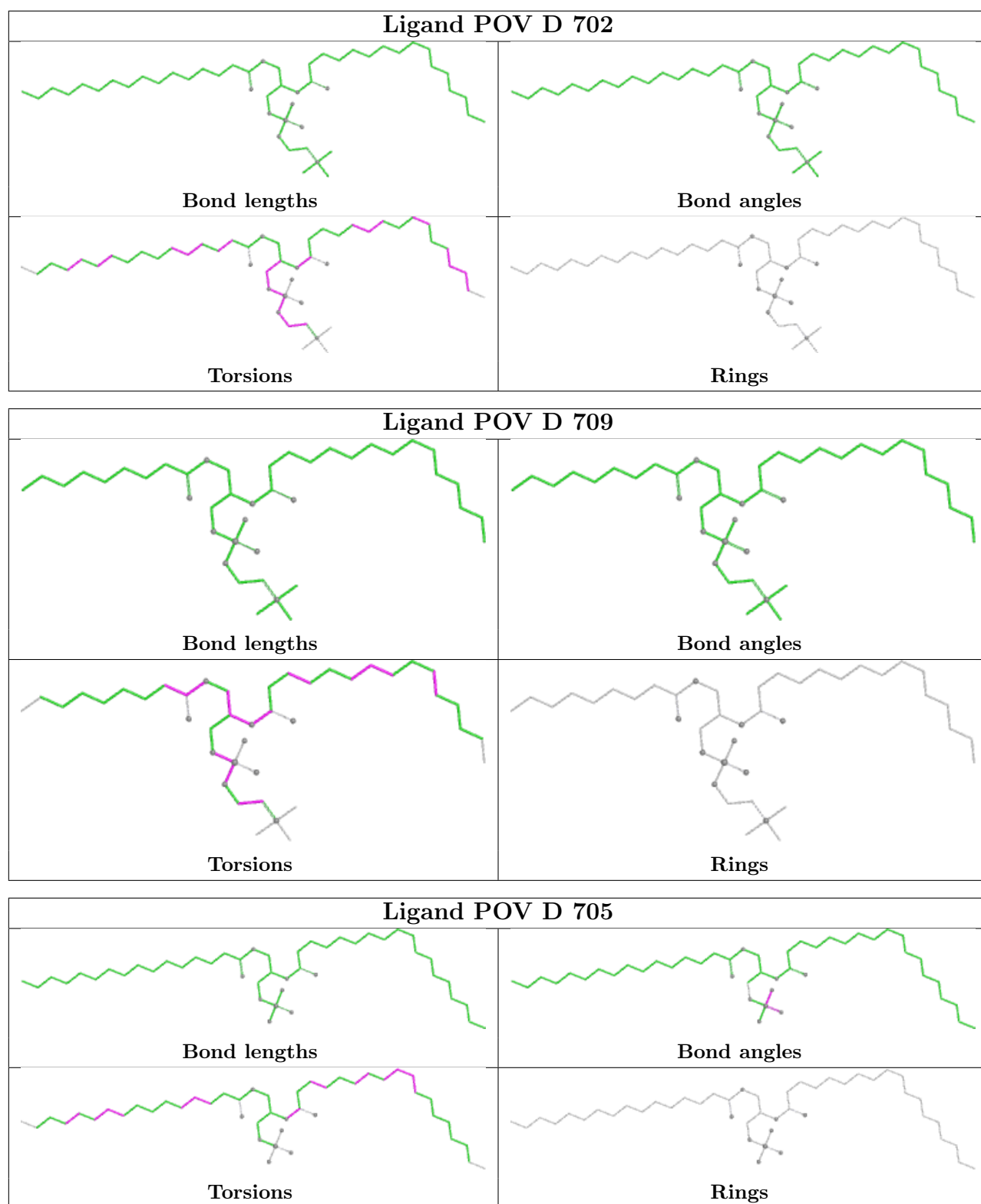
17 monomers are involved in 26 short contacts:

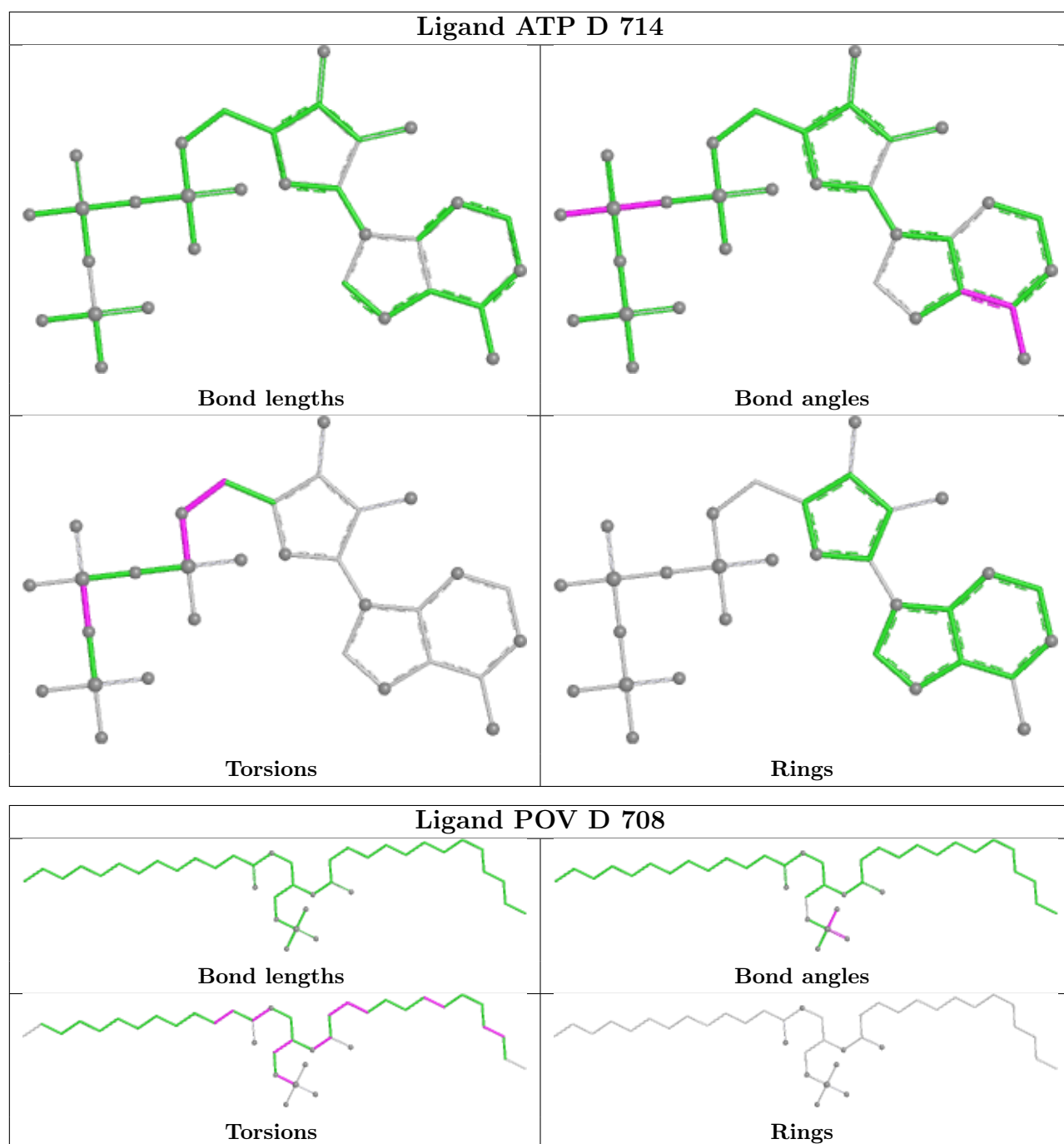
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	611	POV	1	0
3	C	609	POV	1	0
3	C	607	POV	2	0
3	D	702	POV	2	0
3	D	705	POV	2	0
4	D	714	ATP	2	0
3	D	708	POV	1	0
3	C	606	POV	3	0
3	D	703	POV	1	0
4	C	615	ATP	1	0
3	D	711	POV	1	0
5	D	715	HT1	2	0
3	C	608	POV	5	0
3	C	605	POV	1	0
3	C	604	POV	1	0
3	C	614	POV	1	0
3	D	701	POV	1	0

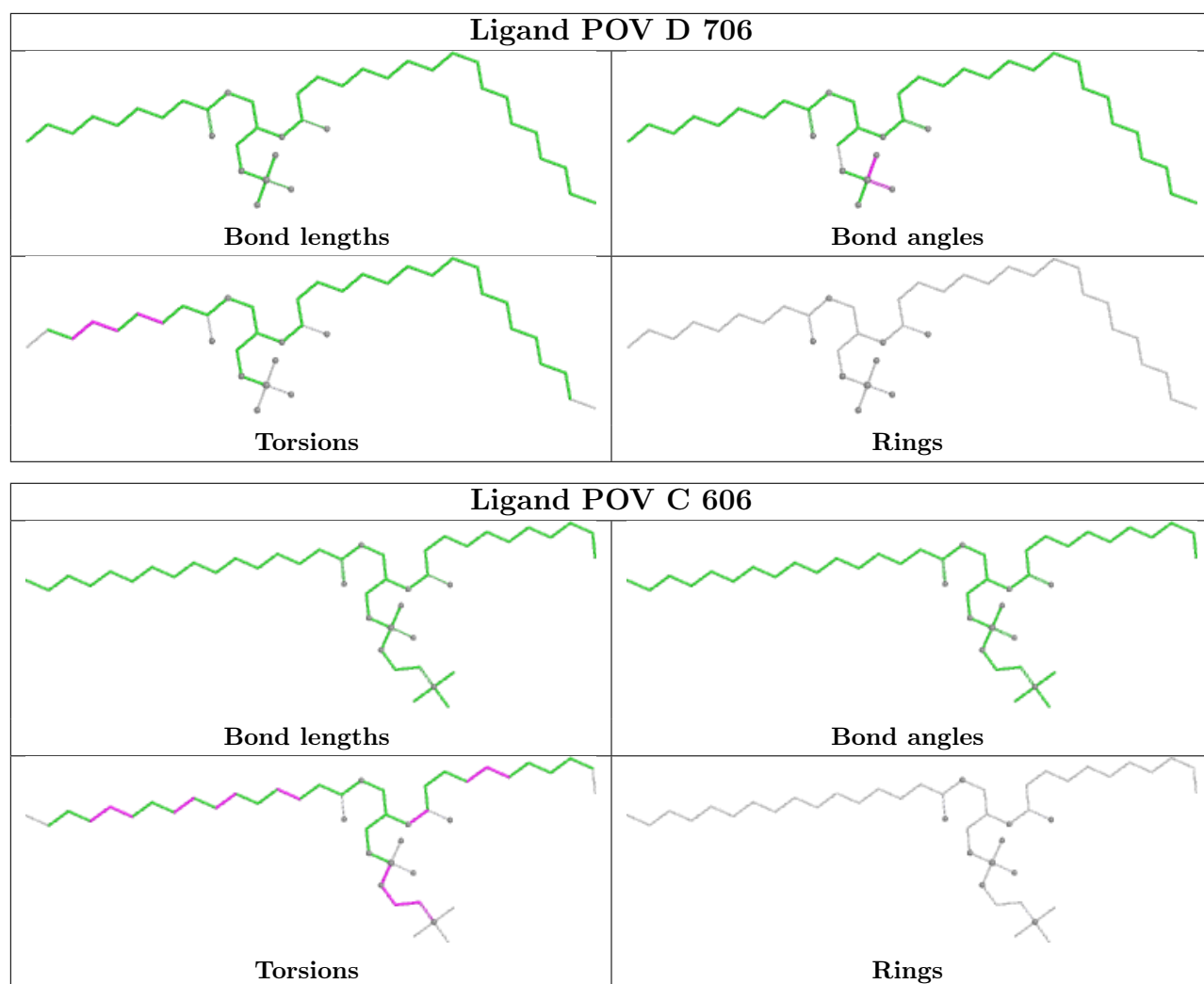
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



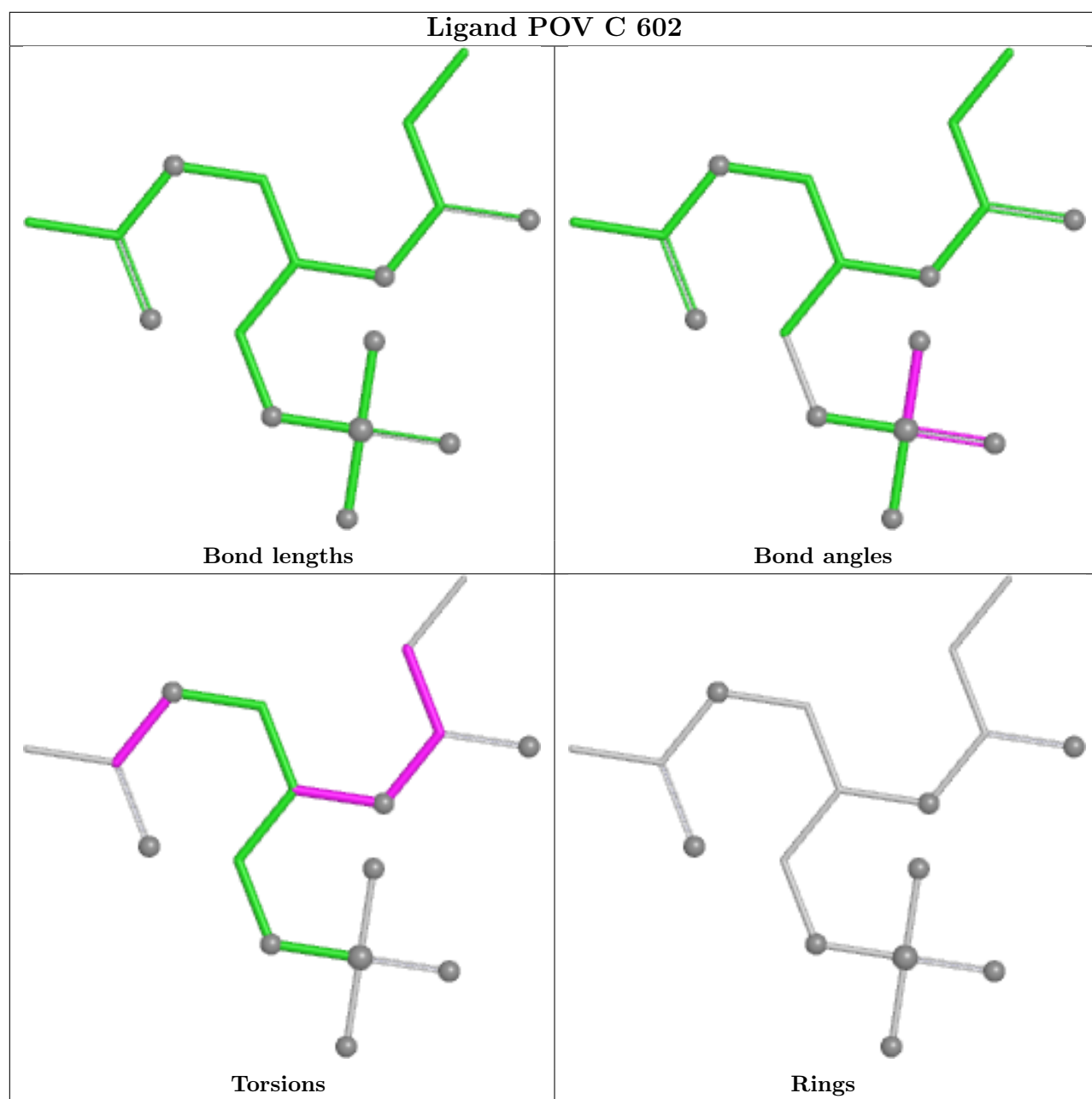


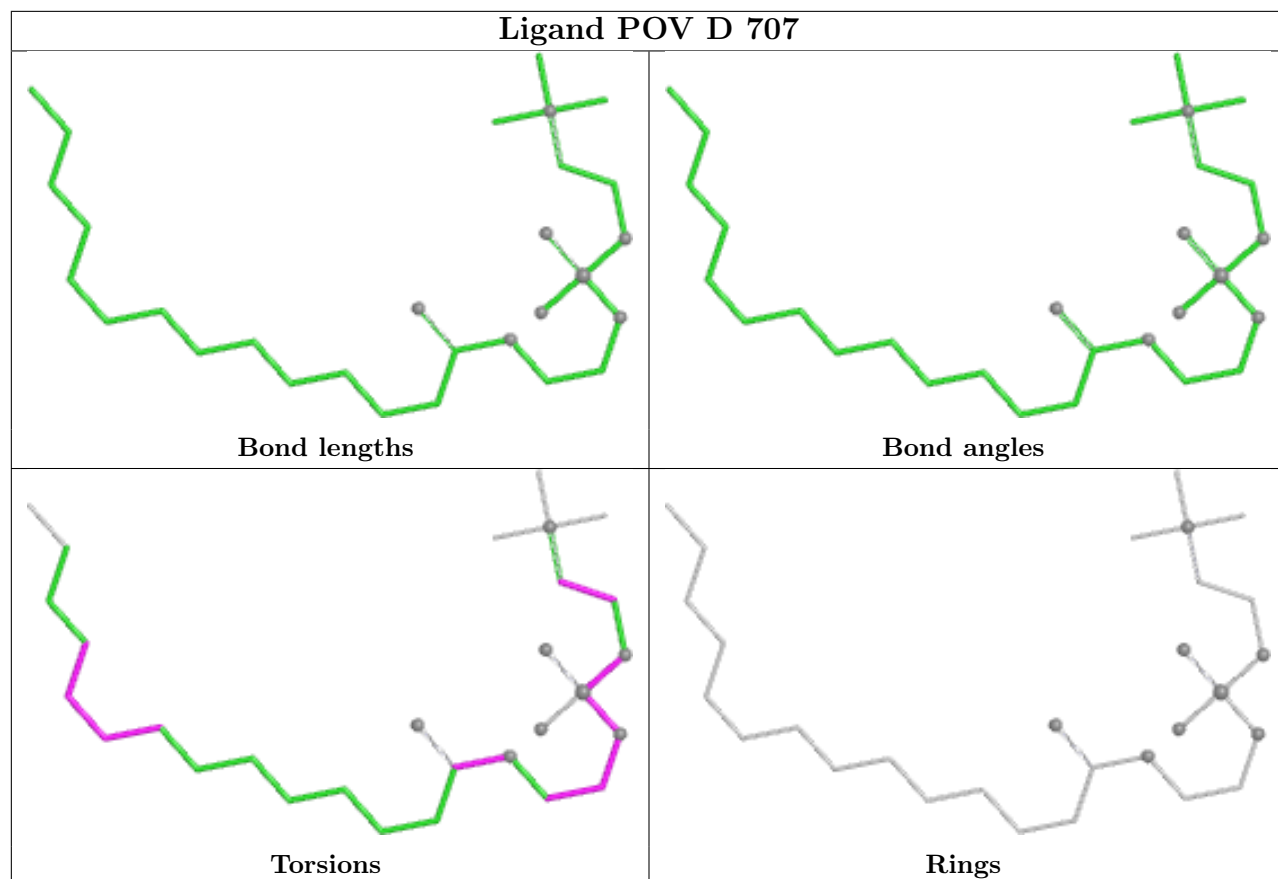


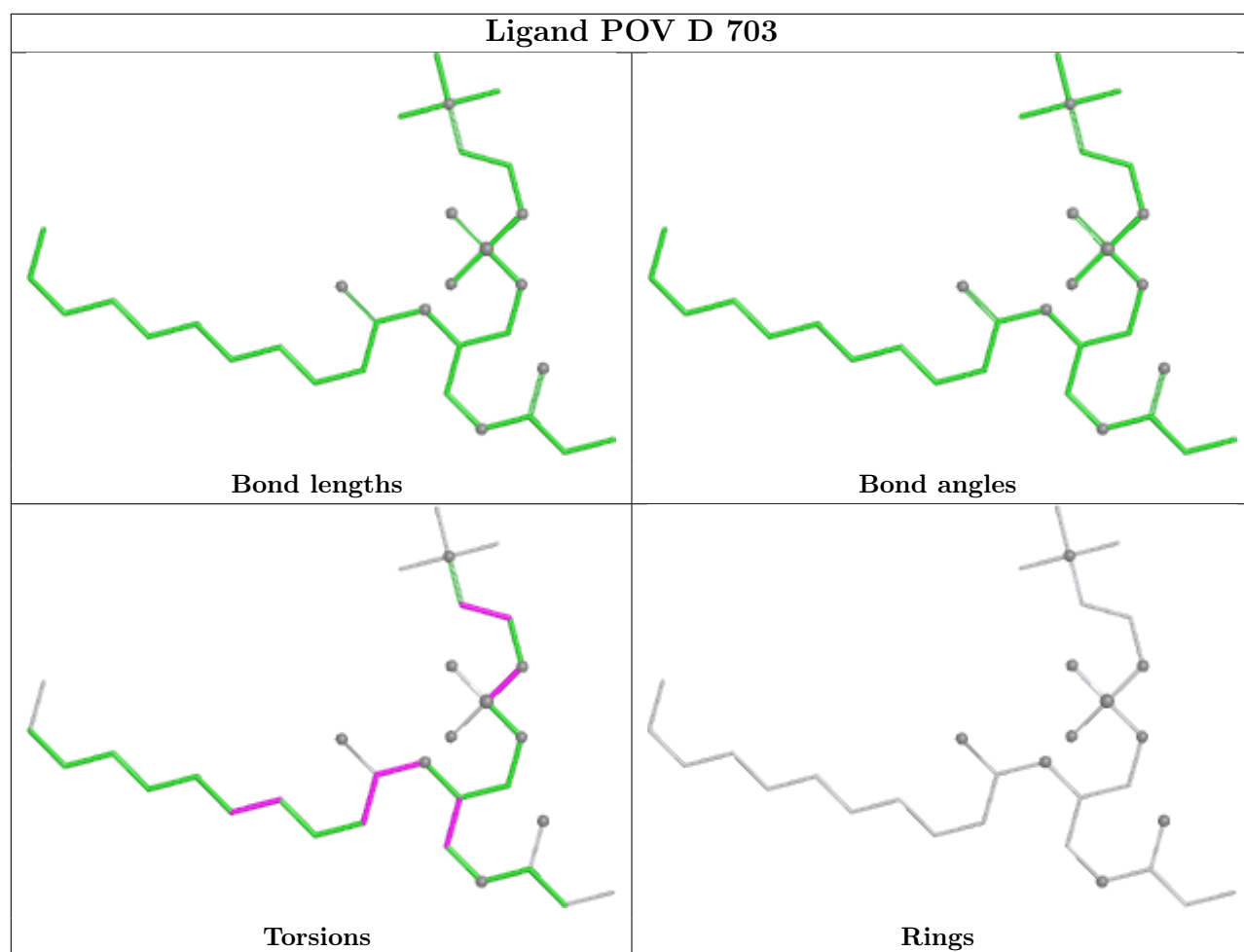


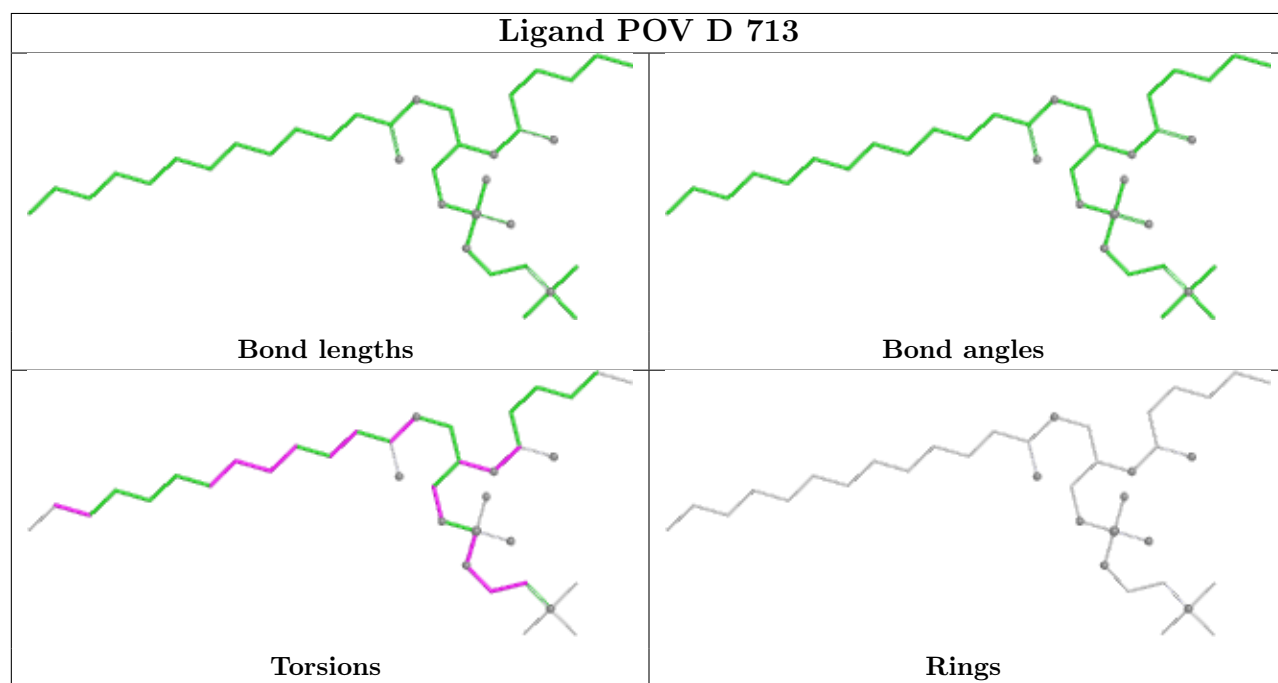
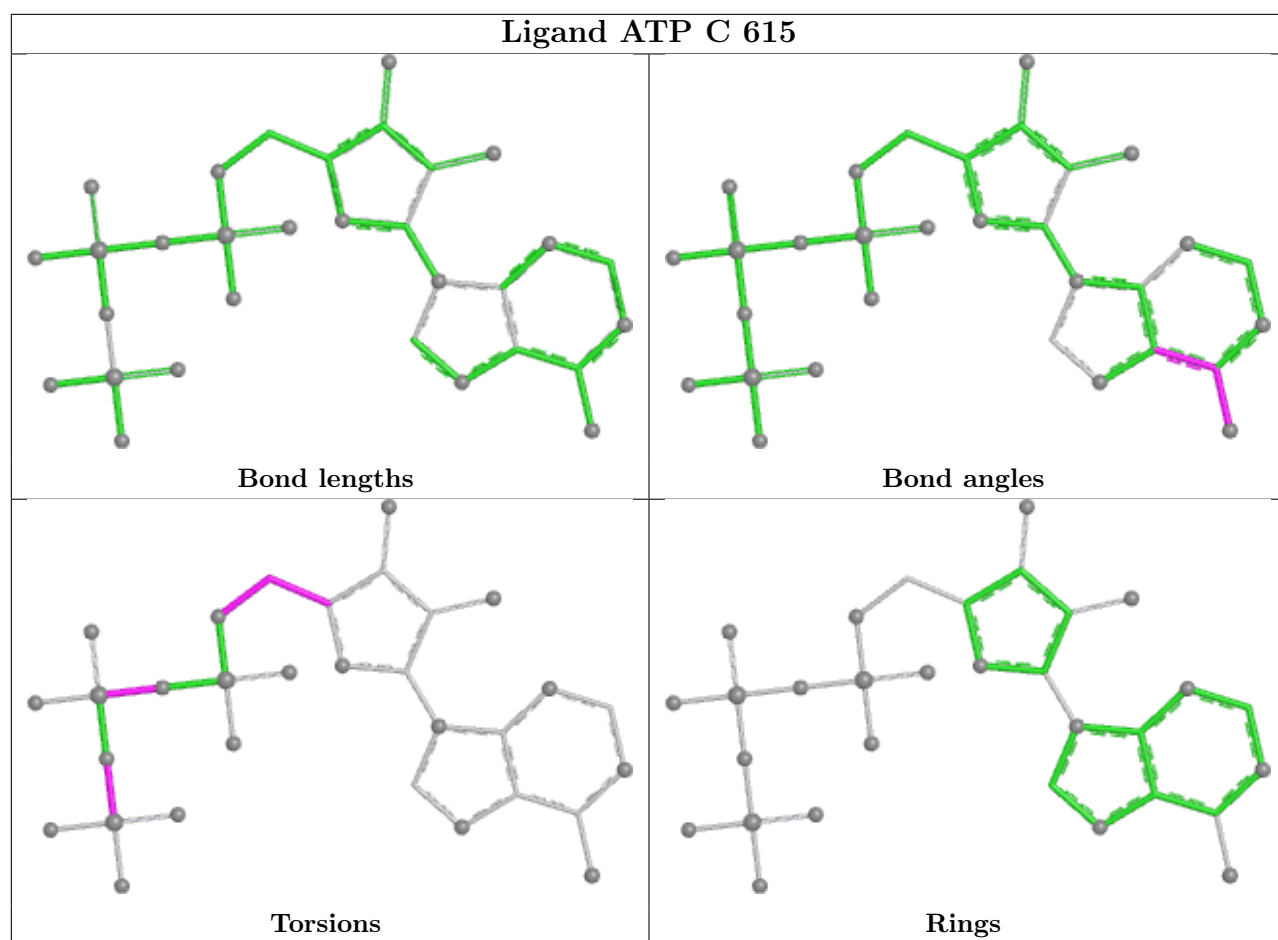


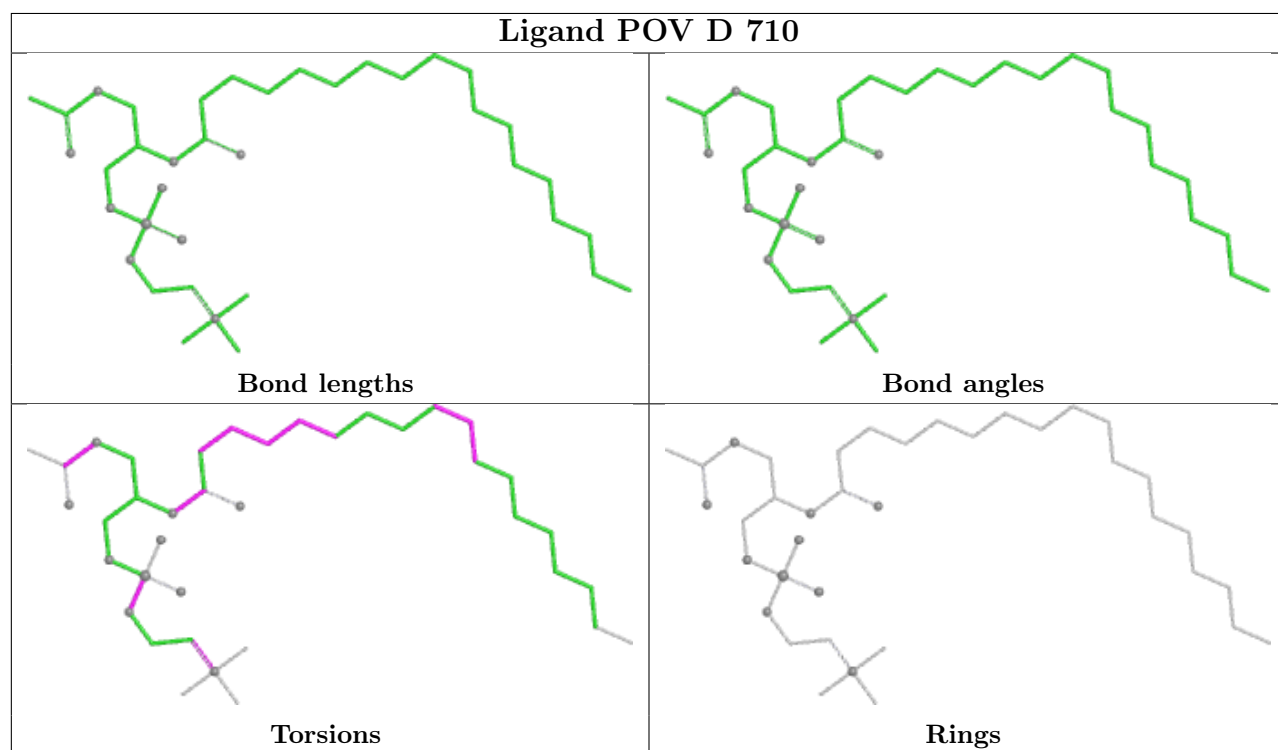
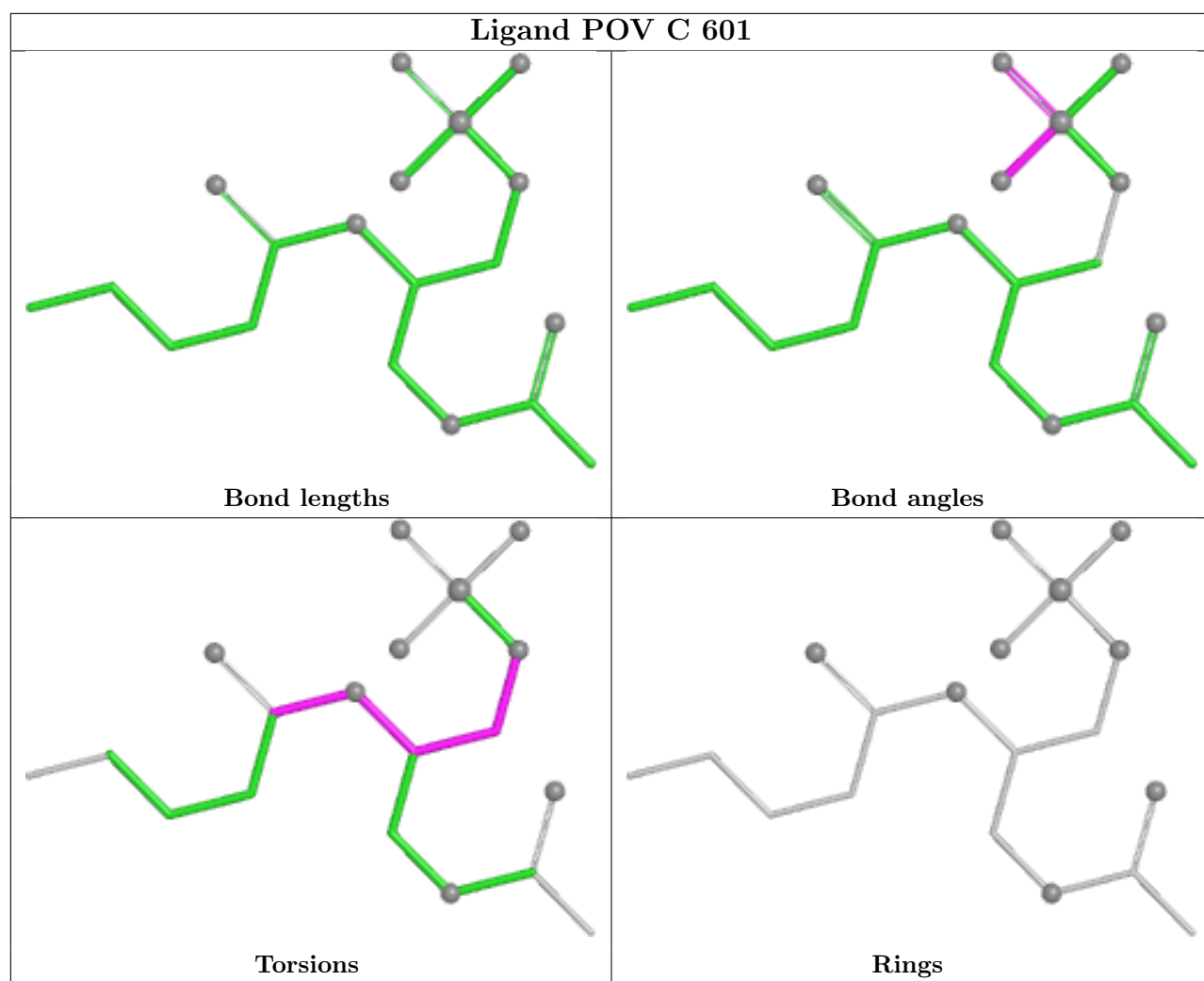


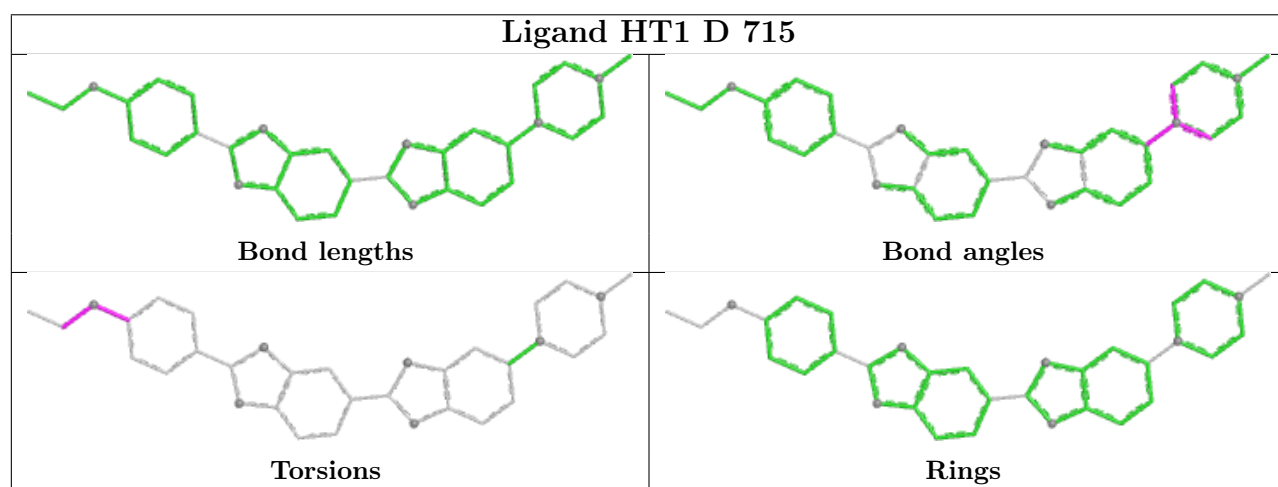
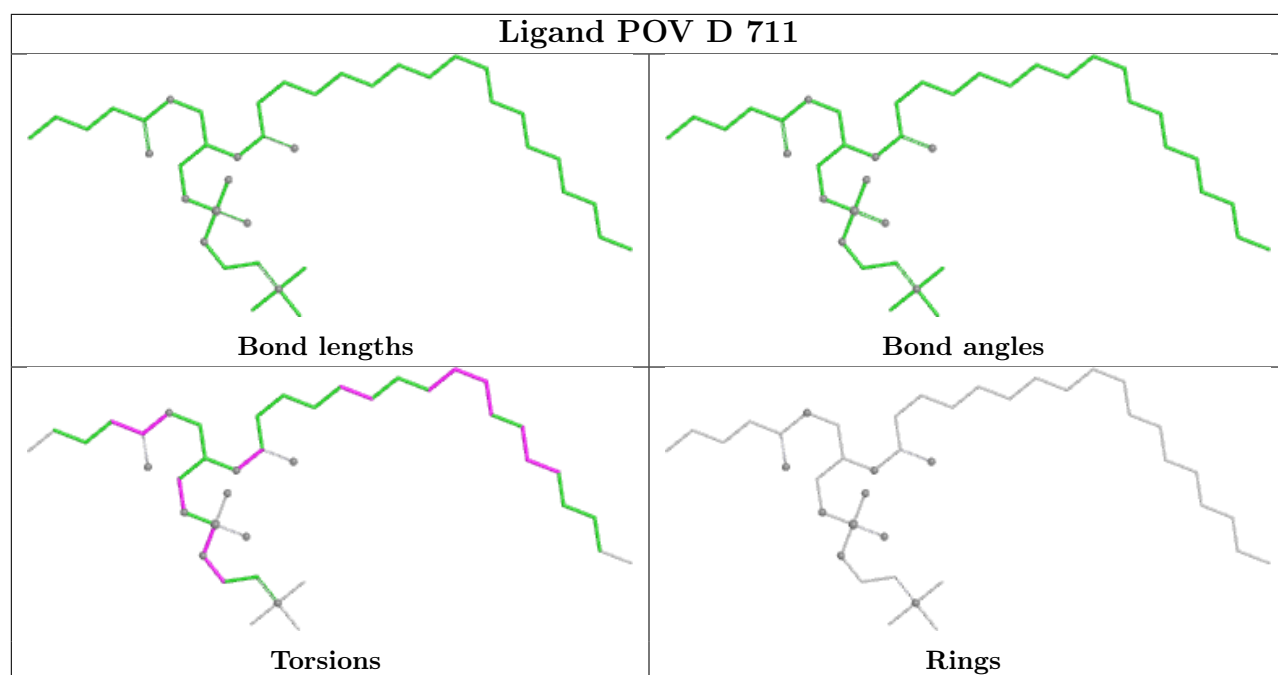


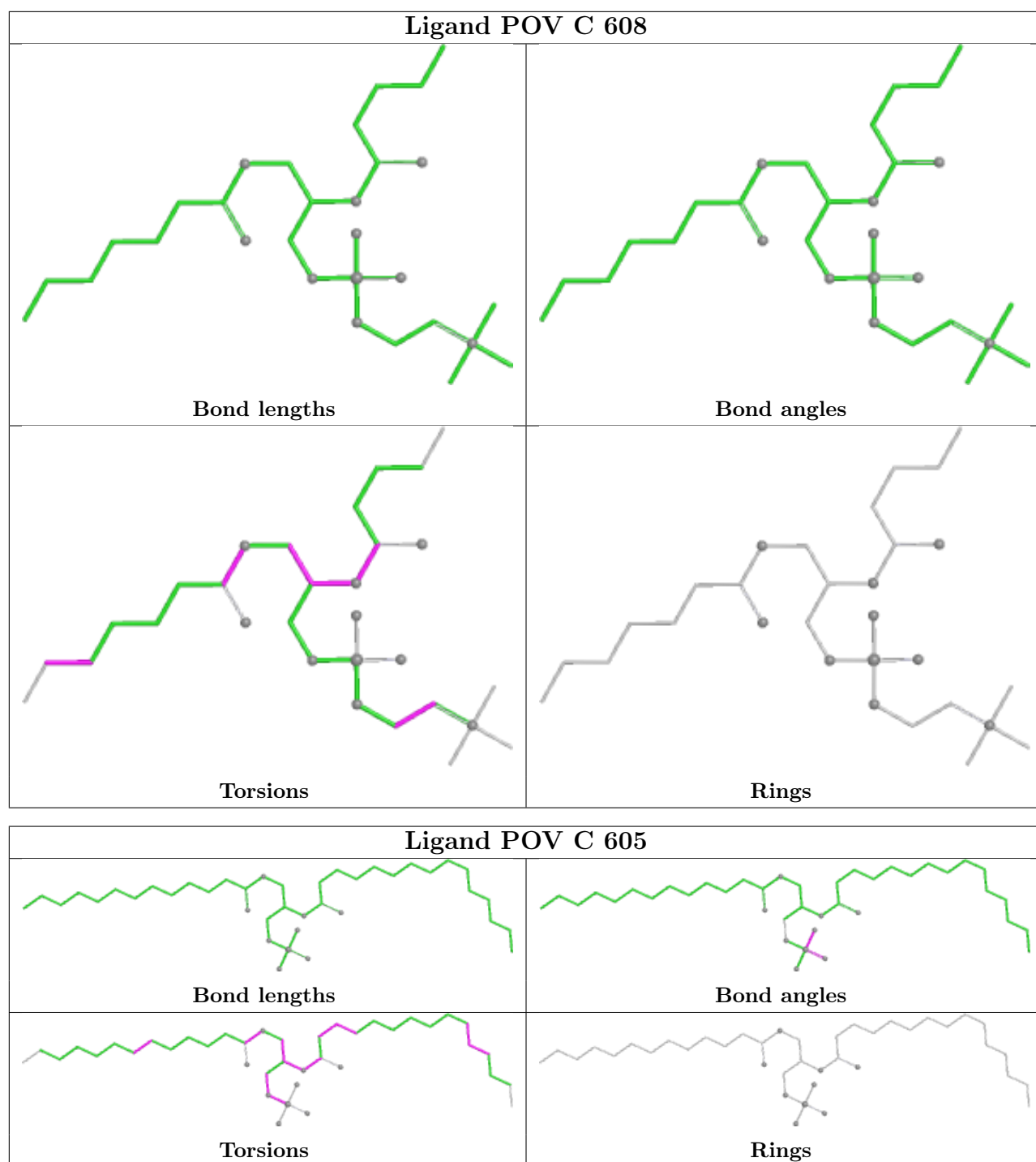


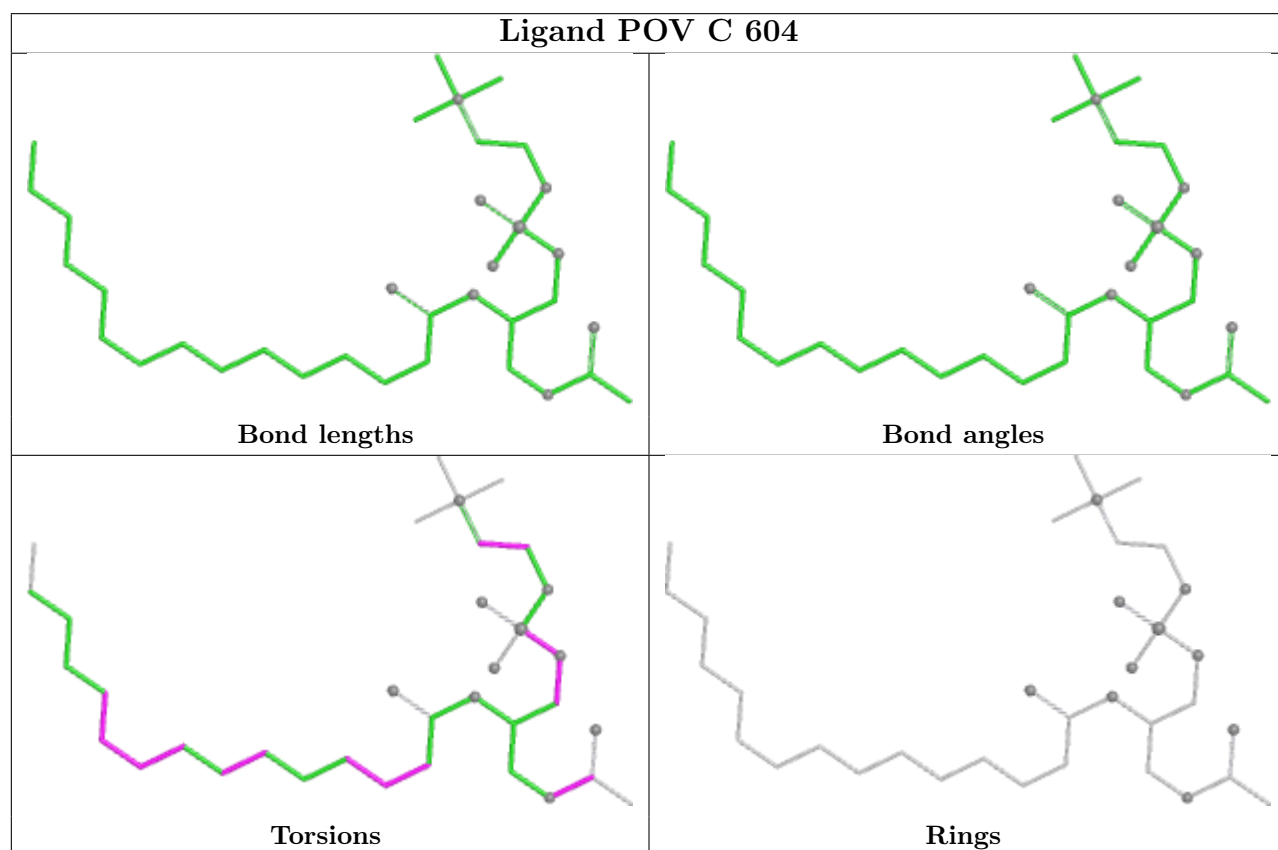
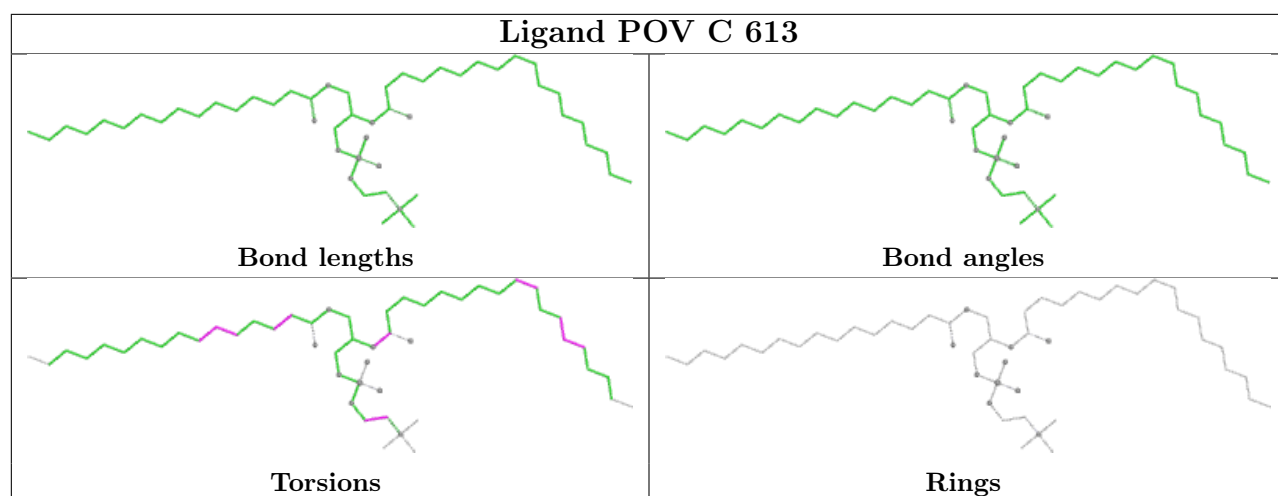




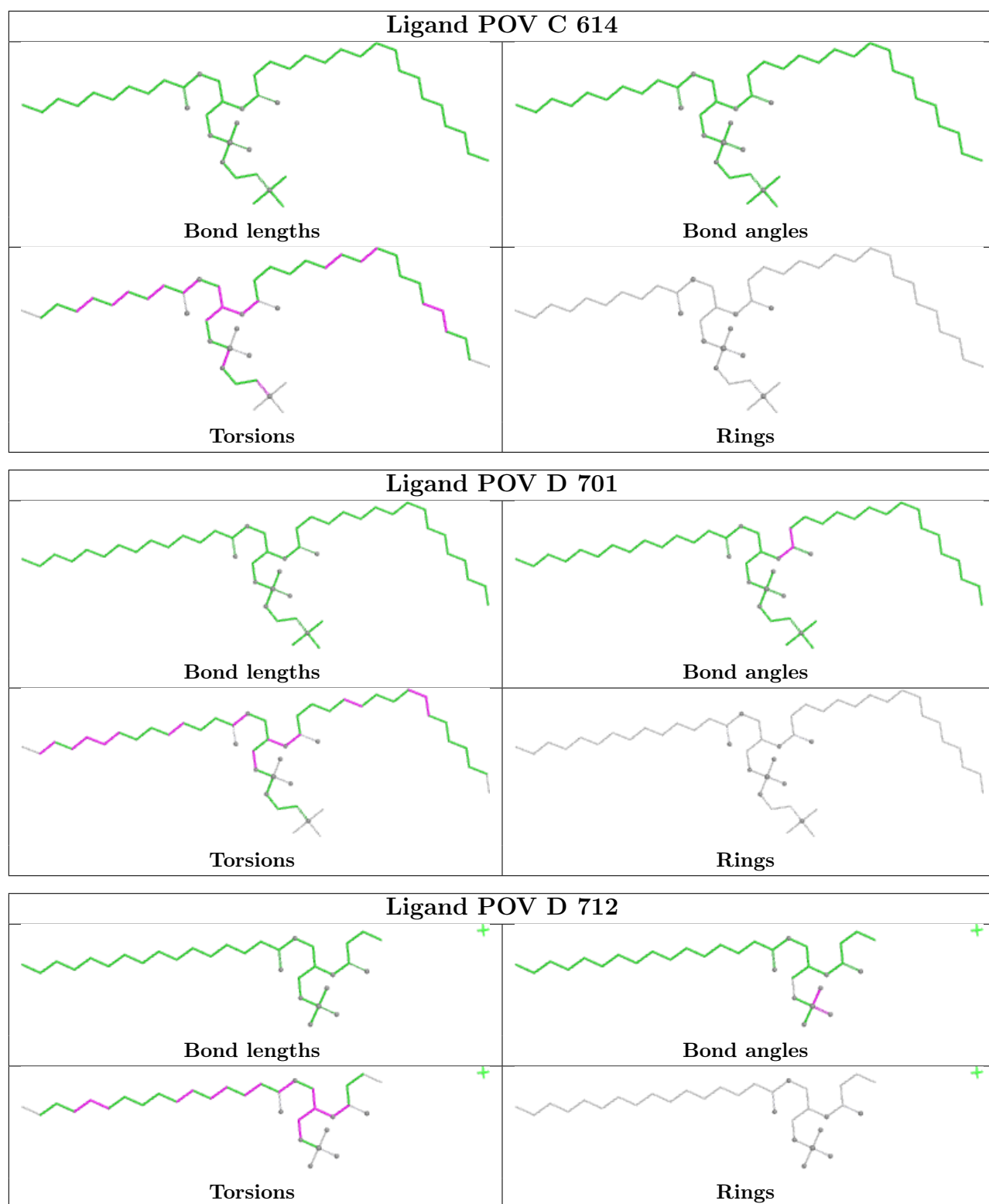


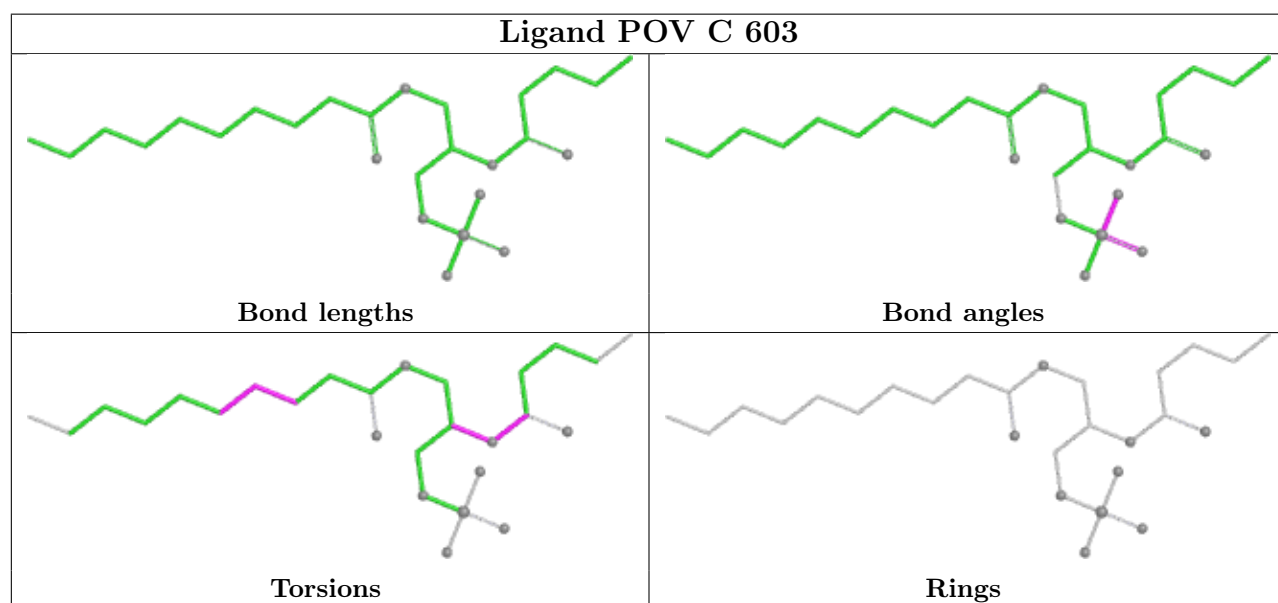
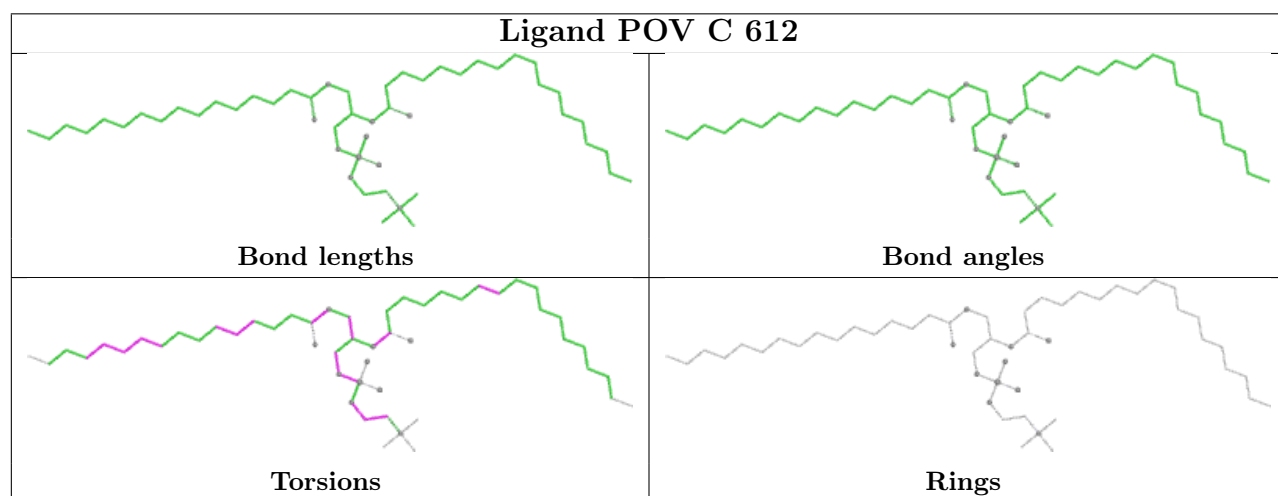
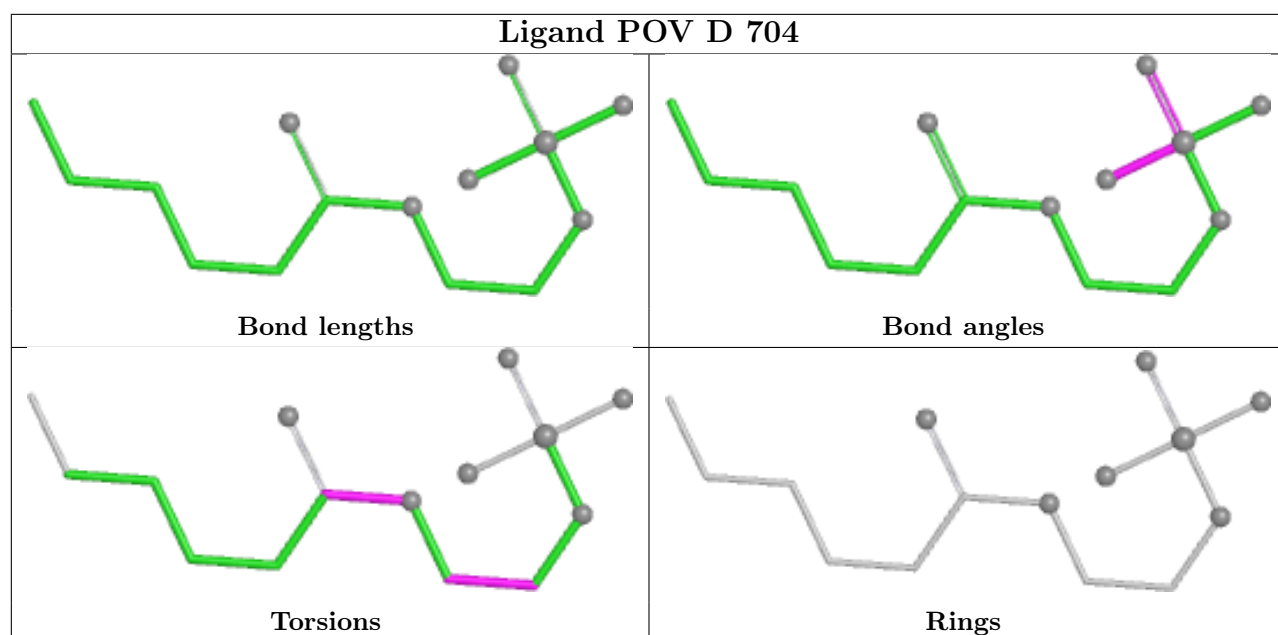












## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

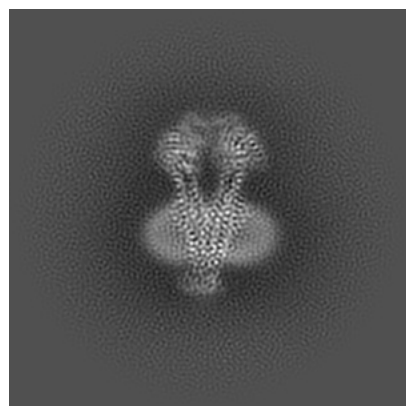
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-45939. These allow visual inspection of the internal detail of the map and identification of artifacts.

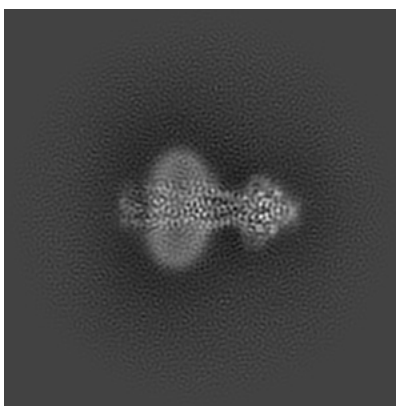
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

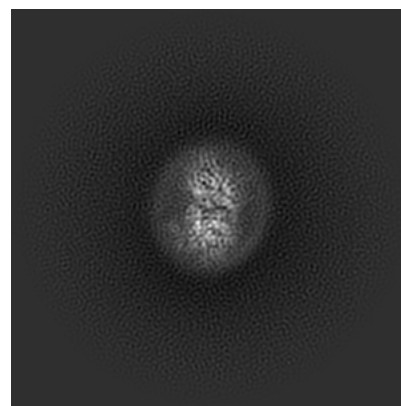
#### 6.1.1 Primary map



X

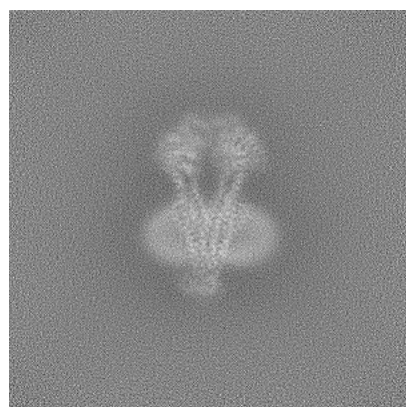


Y

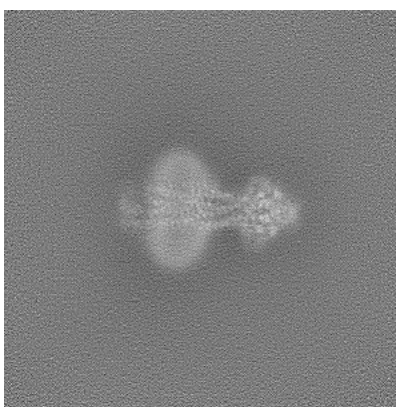


Z

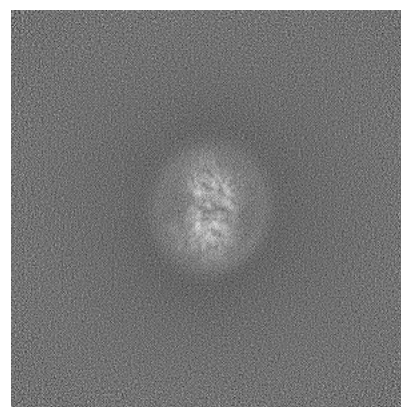
#### 6.1.2 Raw map



X



Y

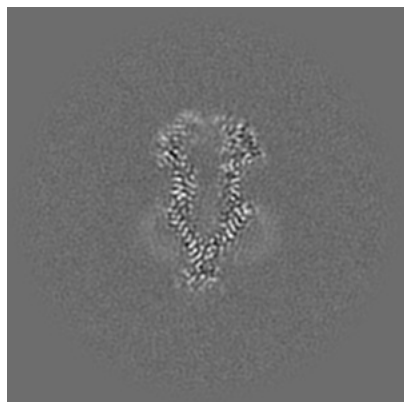


Z

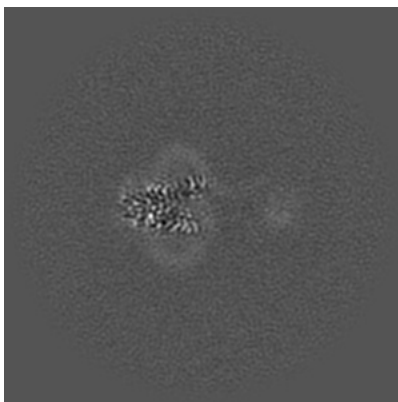
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

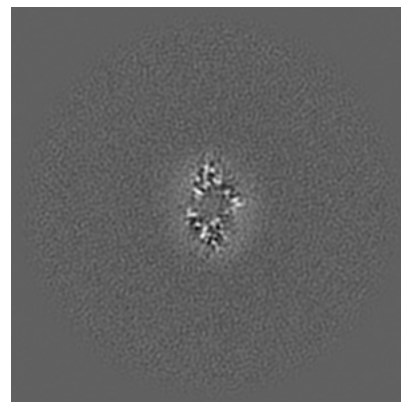
### 6.2.1 Primary map



X Index: 240

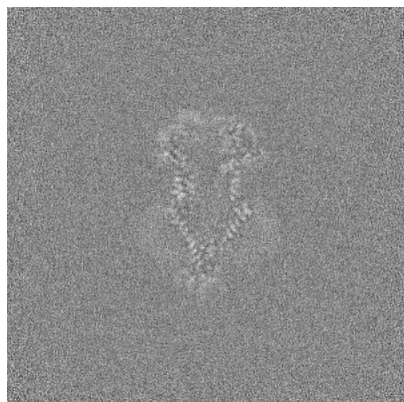


Y Index: 240

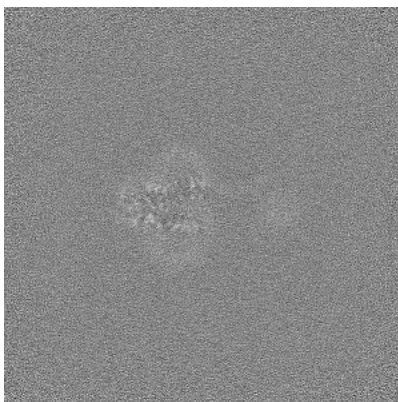


Z Index: 240

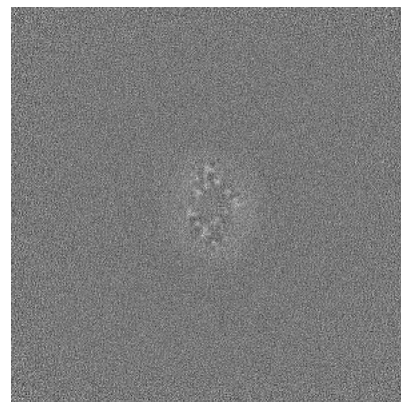
### 6.2.2 Raw map



X Index: 240



Y Index: 240



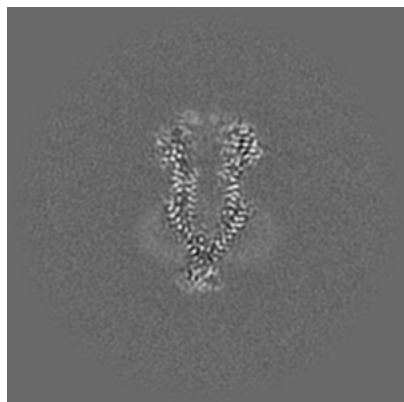
Z Index: 240

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

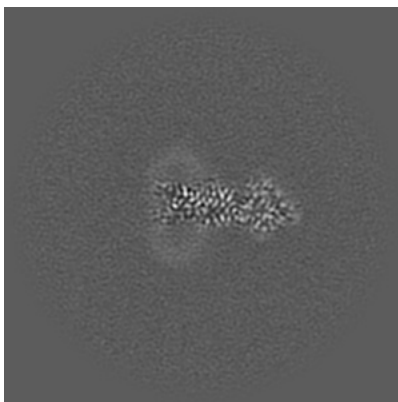


## 6.3 Largest variance slices [i](#)

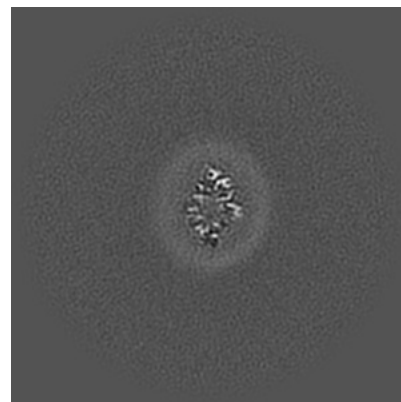
### 6.3.1 Primary map



X Index: 243

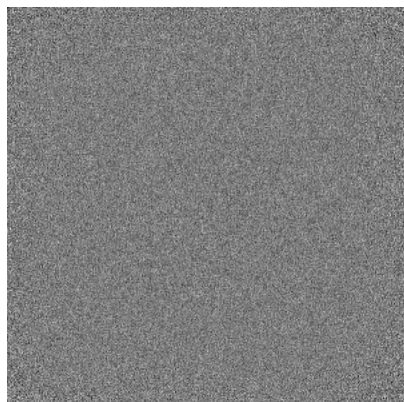


Y Index: 268

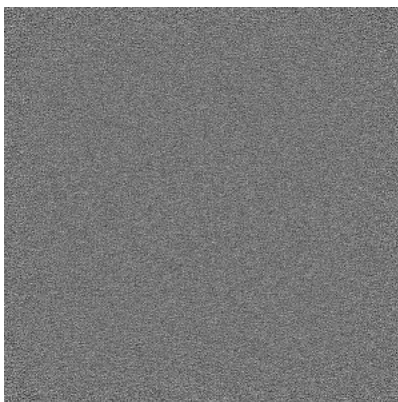


Z Index: 225

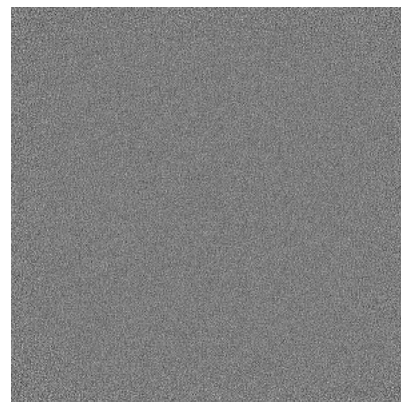
### 6.3.2 Raw map



X Index: 0



Y Index: 0

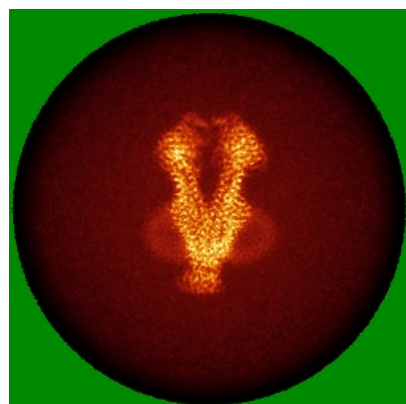


Z Index: 479

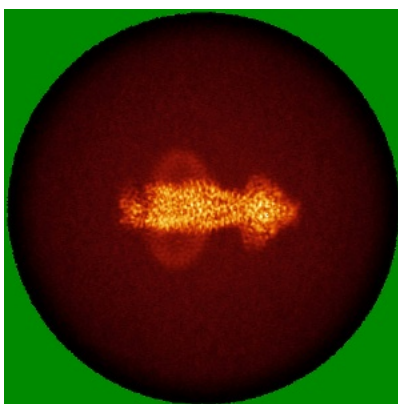
The images above show the largest variance slices of the map in three orthogonal directions.

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

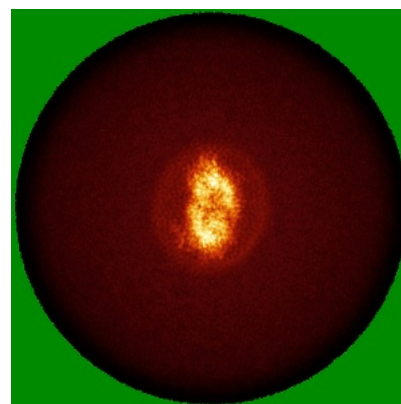
### 6.4.1 Primary map



X

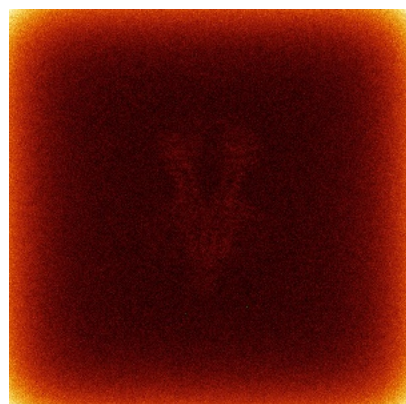


Y

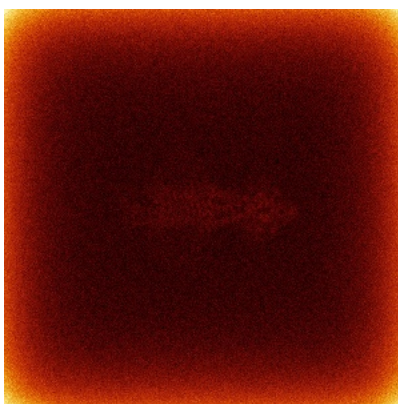


Z

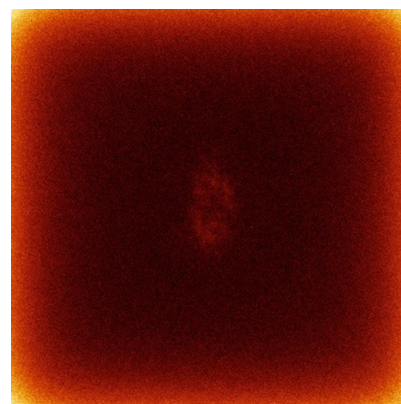
### 6.4.2 Raw map



X



Y

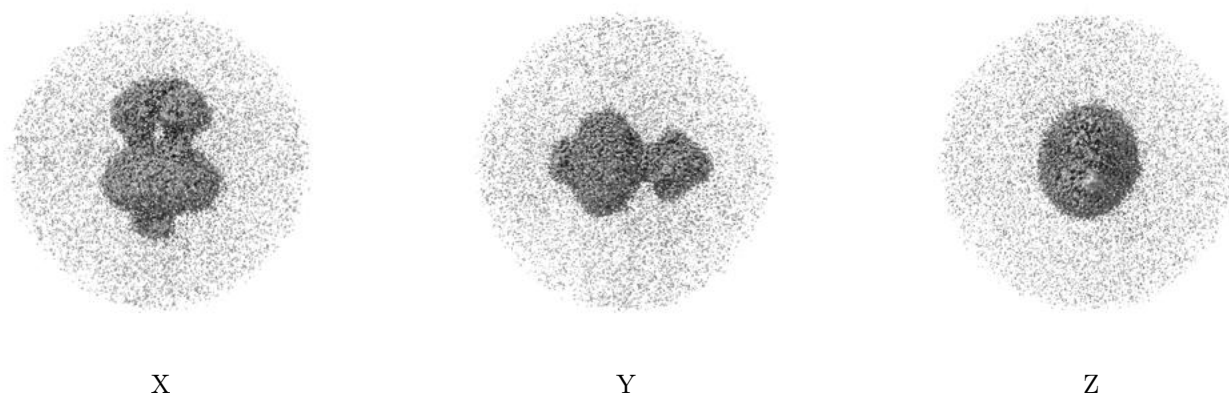


Z

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.

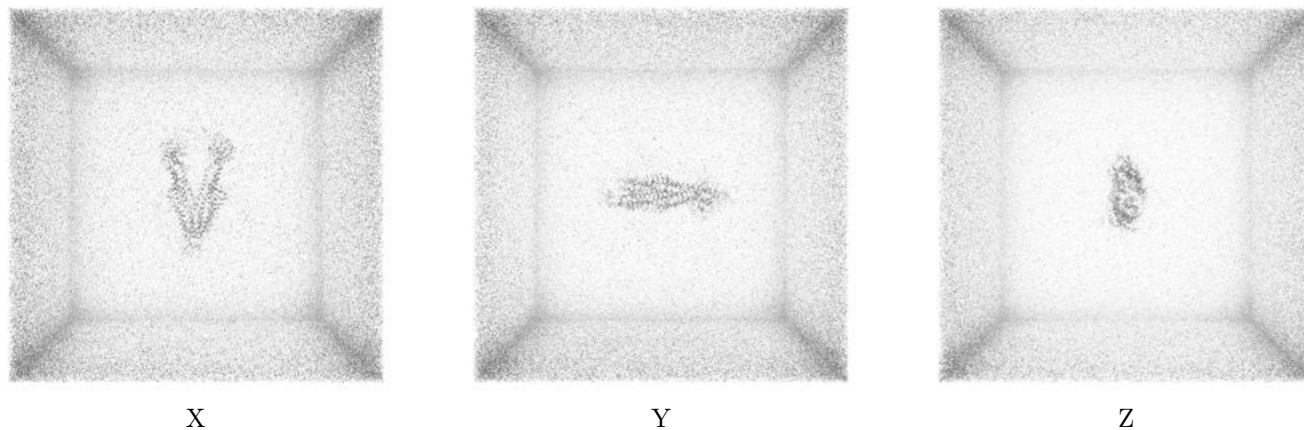
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.036. 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](#)

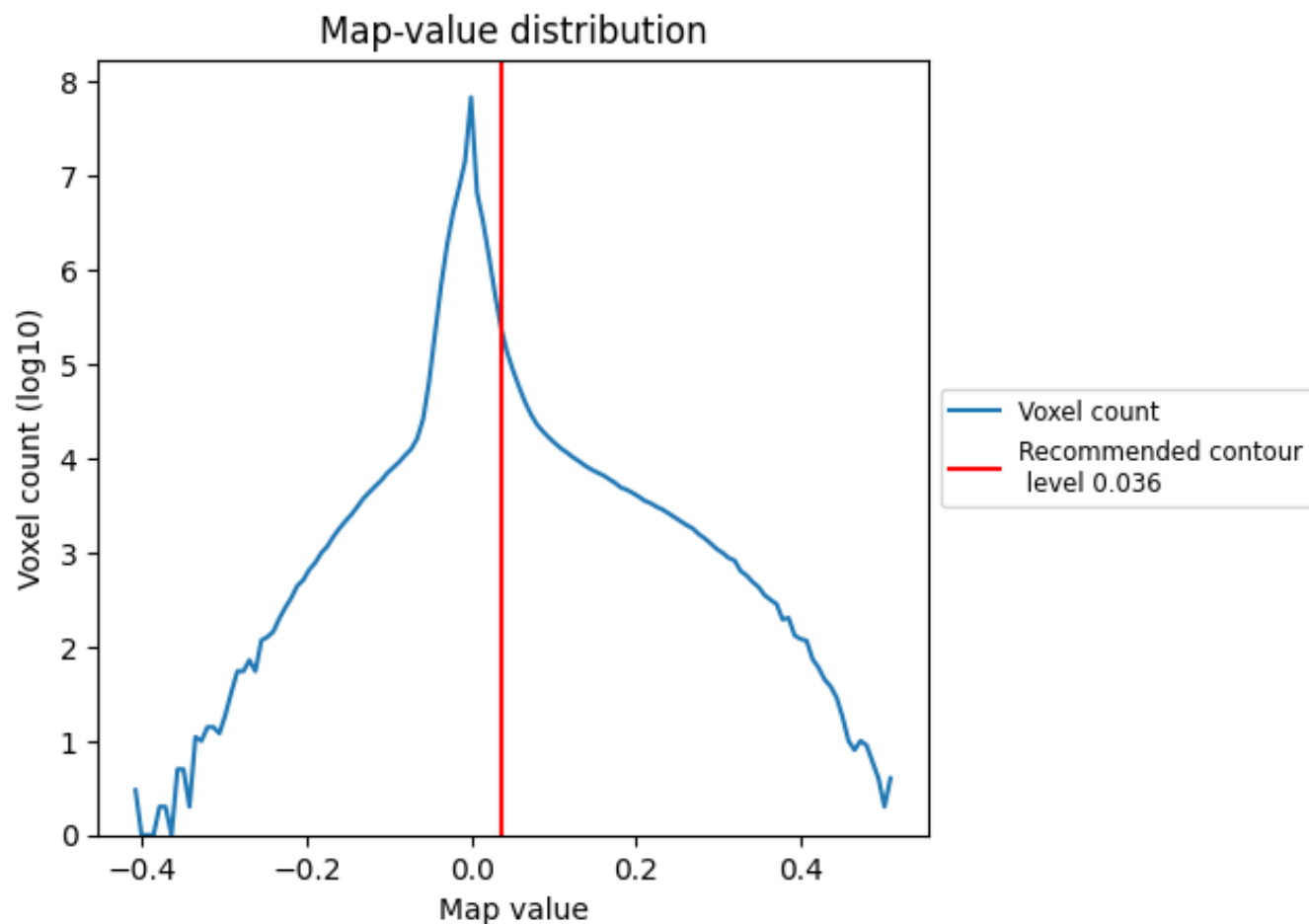
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

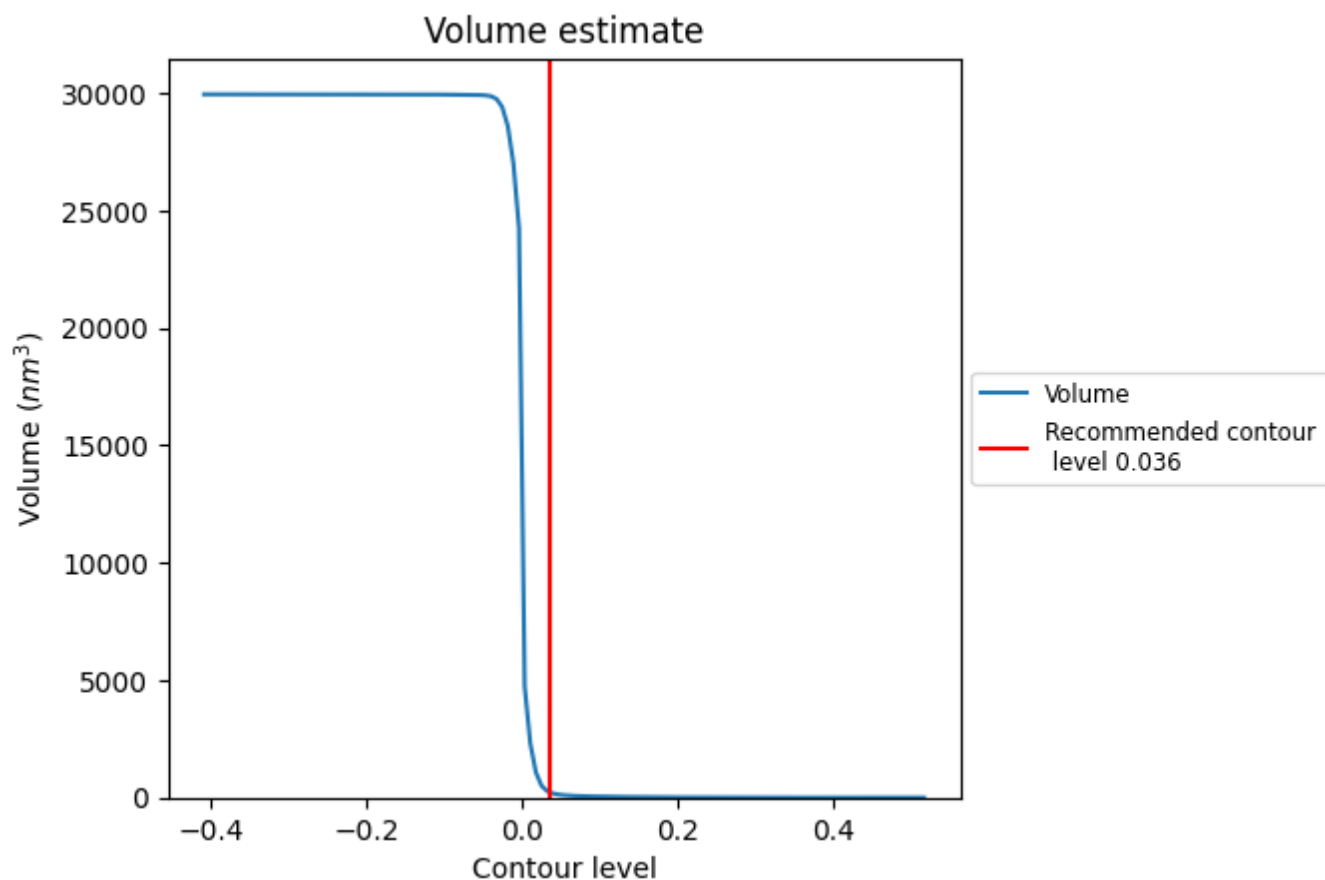
This section contains the results of statistical analysis of the map.

### 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.

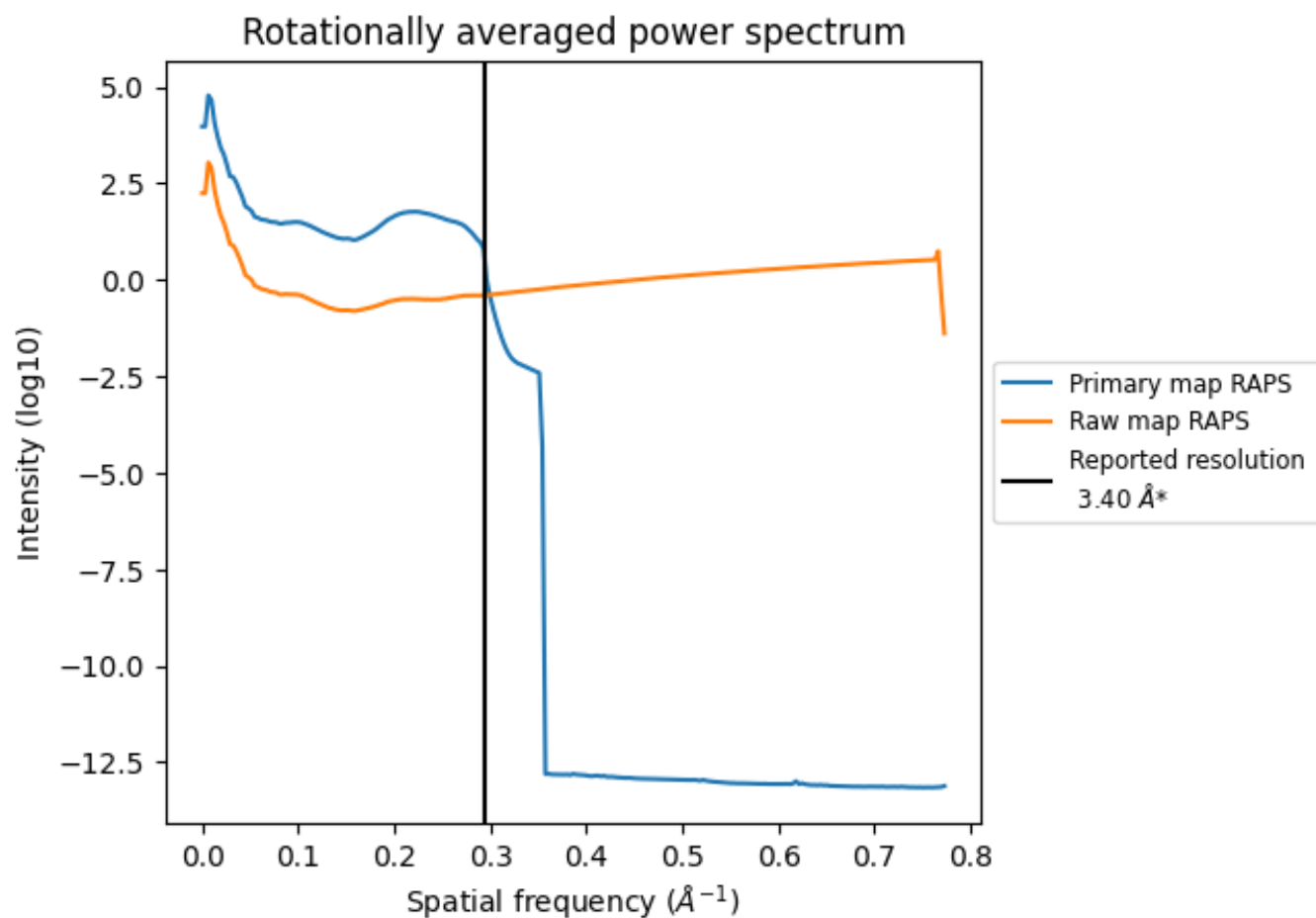
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 230 nm<sup>3</sup>; this corresponds to an approximate mass of 208 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 ⓘ

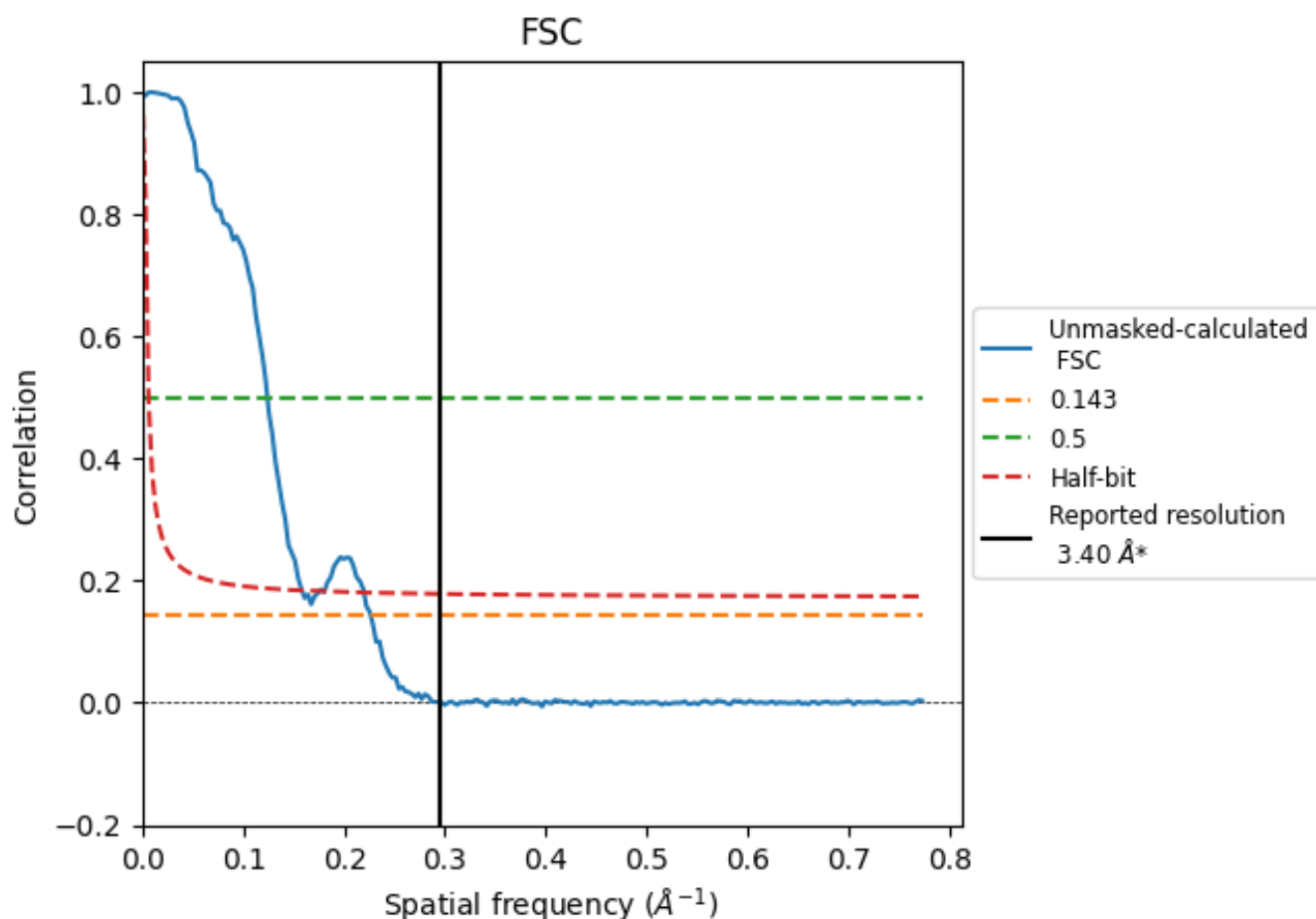


\*Reported resolution corresponds to spatial frequency of 0.294 Å<sup>-1</sup>

## 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 0.294  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

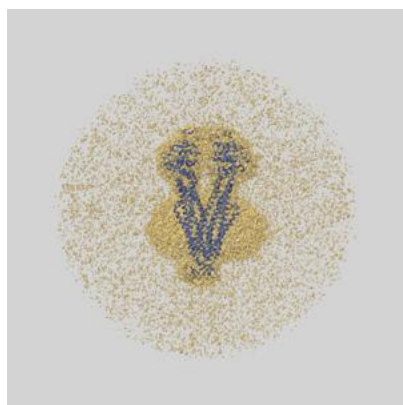
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.42	8.06	6.32

\*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 4.42 differs from the reported value 3.4 by more than 10 %

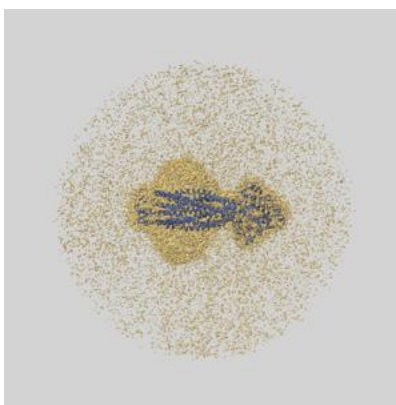
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-45939 and PDB model 9CUR. Per-residue inclusion information can be found in section [3](#) on page [8](#).

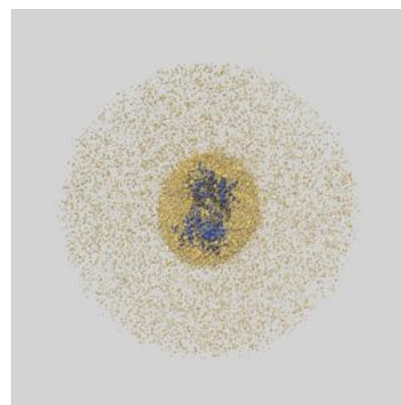
### 9.1 Map-model overlay [i](#)



X



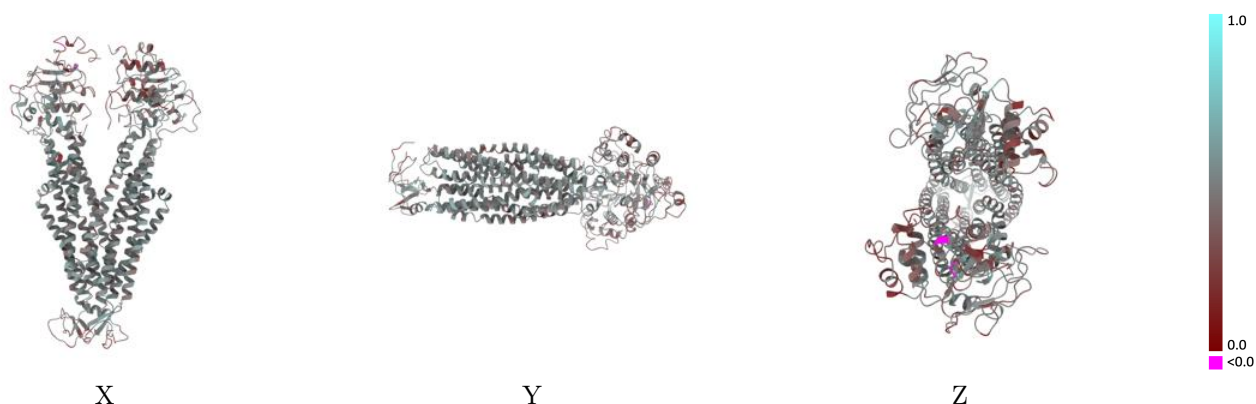
Y



Z

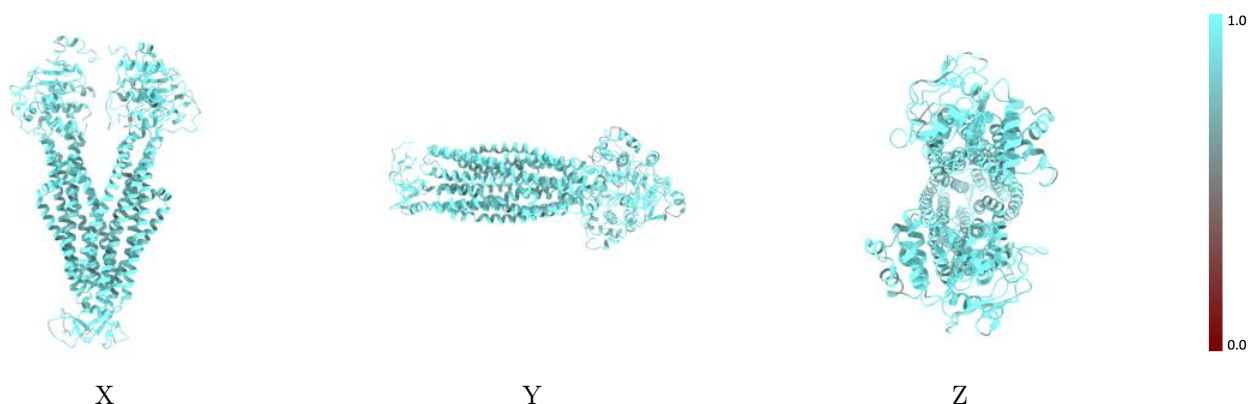
The images above show the 3D surface view of the map at the recommended contour level 0.036 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



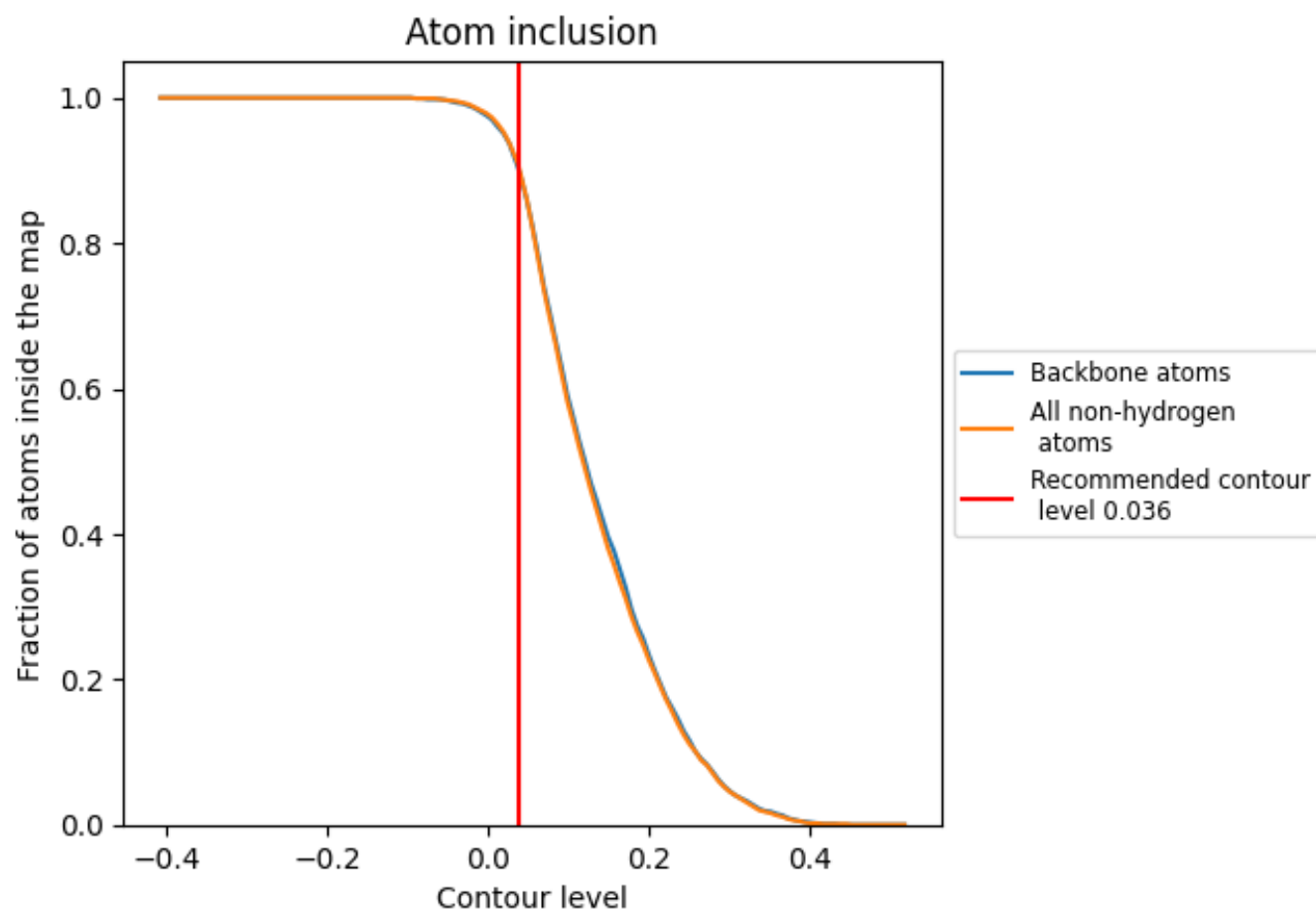
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.036).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 91% 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 (0.036) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.9100	<div></div> 0.4650
C	<div></div> 0.9140	<div></div> 0.4730
D	<div></div> 0.9090	<div></div> 0.4580

