



Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 03:33 AM UTC

PDB ID : 6WEL / pdb_00006wel
EMDB ID : EMD-21651
Title : Structure of cGMP-unbound F403V/V407A mutant TAX-4 reconstituted in lipid nanodiscs
Authors : Zheng, X.; Fu, Z.; Su, D.; Zhang, Y.; Li, M.; Pan, Y.; Li, H.; Li, S.; Grassucci, R.A.; Ren, Z.; Hu, Z.; Li, X.; Zhou, M.; Li, G.; Frank, J.; Yang, J.
Deposited on : 2020-04-02
Resolution : 2.50 Å (reported)
Based on initial model : 5H3O

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:

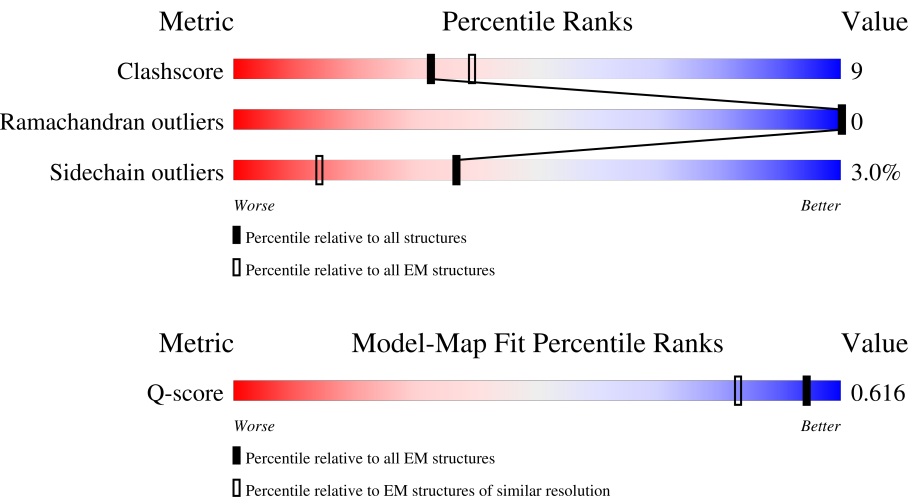
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	7115 (2.00 - 3.00)

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	733	53%16%30%
1	B	733	53%17%30%
1	C	733	53%16%30%

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Mol	Chain	Length	Quality of chain
1	D	733	 53% 16% 30%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 17725 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.

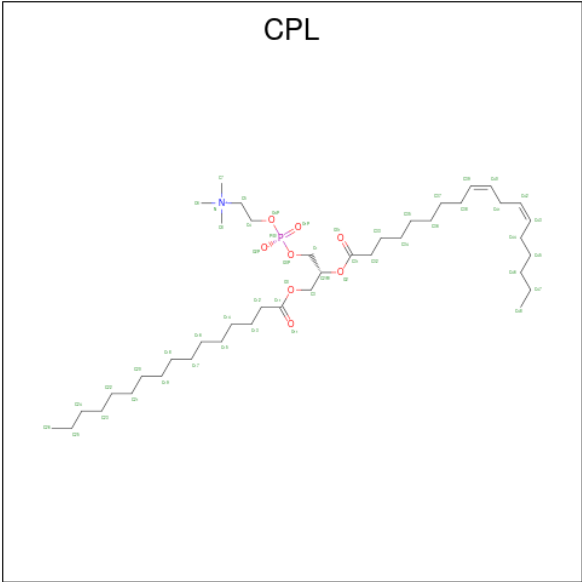
- Molecule 1 is a protein called Cyclic nucleotide-gated cation channel.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	513	Total	C	N	O	S	0	0
			4235	2751	715	745	24		
1	B	513	Total	C	N	O	S	0	0
			4235	2751	715	745	24		
1	C	513	Total	C	N	O	S	0	0
			4235	2751	715	745	24		
1	D	513	Total	C	N	O	S	0	0
			4235	2751	715	745	24		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	403	VAL	PHE	engineered mutation	UNP Q03611
A	407	ALA	VAL	engineered mutation	UNP Q03611
B	403	VAL	PHE	engineered mutation	UNP Q03611
B	407	ALA	VAL	engineered mutation	UNP Q03611
C	403	VAL	PHE	engineered mutation	UNP Q03611
C	407	ALA	VAL	engineered mutation	UNP Q03611
D	403	VAL	PHE	engineered mutation	UNP Q03611
D	407	ALA	VAL	engineered mutation	UNP Q03611

- Molecule 2 is 1-PALMITOYL-2-LINOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: CPL) (formula: C₄₂H₈₀NO₈P) (labeled as "Ligand of Interest" by depositor).



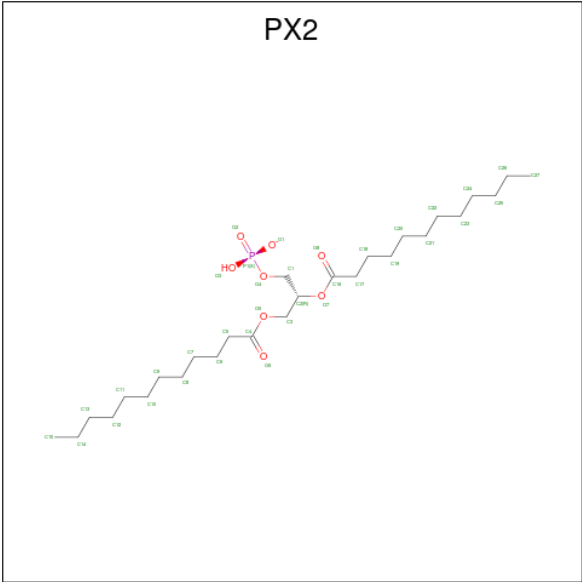
Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			49	39	1	8	1	
2	A	1	Total	C	O	P		0
			41	32	8	1		
2	A	1	Total	C				0
			9	9				
2	A	1	Total	C				0
			9	9				
2	A	1	Total	C				0
			12	12				
2	A	1	Total	C				0
			13	13				
2	A	1	Total	C				0
			15	15				
2	B	1	Total	C	N	O	P	0
			49	39	1	8	1	
2	B	1	Total	C	O	P		0
			41	32	8	1		
2	B	1	Total	C				0
			9	9				
2	B	1	Total	C				0
			9	9				
2	B	1	Total	C				0
			12	12				
2	B	1	Total	C				0
			13	13				
2	B	1	Total	C				0
			15	15				

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Mol	Chain	Residues	Atoms					AltConf
2	C	1	Total	C	N	O	P	0
			49	39	1	8	1	
2	C	1	Total	C	O	P		0
			41	32	8	1		
2	C	1	Total	C				0
			9	9				
2	C	1	Total	C				0
			9	9				
2	C	1	Total	C				0
			12	12				
2	C	1	Total	C				0
			13	13				
2	C	1	Total	C				0
			15	15				
2	D	1	Total	C	N	O	P	0
			49	39	1	8	1	
2	D	1	Total	C	O	P		0
			41	32	8	1		
2	D	1	Total	C				0
			9	9				
2	D	1	Total	C				0
			9	9				
2	D	1	Total	C				0
			12	12				
2	D	1	Total	C				0
			13	13				
2	D	1	Total	C				0
			15	15				

- Molecule 3 is 1,2-DILAULOYL-SN-GLYCERO-3-PHOSPHATE (CCD ID: PX2) (formula: $C_{27}H_{52}O_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	O	P	0
			23	14	8	1	
3	A	1	Total	C	O	P	0
			25	16	8	1	
3	B	1	Total	C	O	P	0
			23	14	8	1	
3	B	1	Total	C	O	P	0
			25	16	8	1	
3	C	1	Total	C	O	P	0
			23	14	8	1	
3	C	1	Total	C	O	P	0
			25	16	8	1	
3	D	1	Total	C	O	P	0
			23	14	8	1	
3	D	1	Total	C	O	P	0
			25	16	8	1	

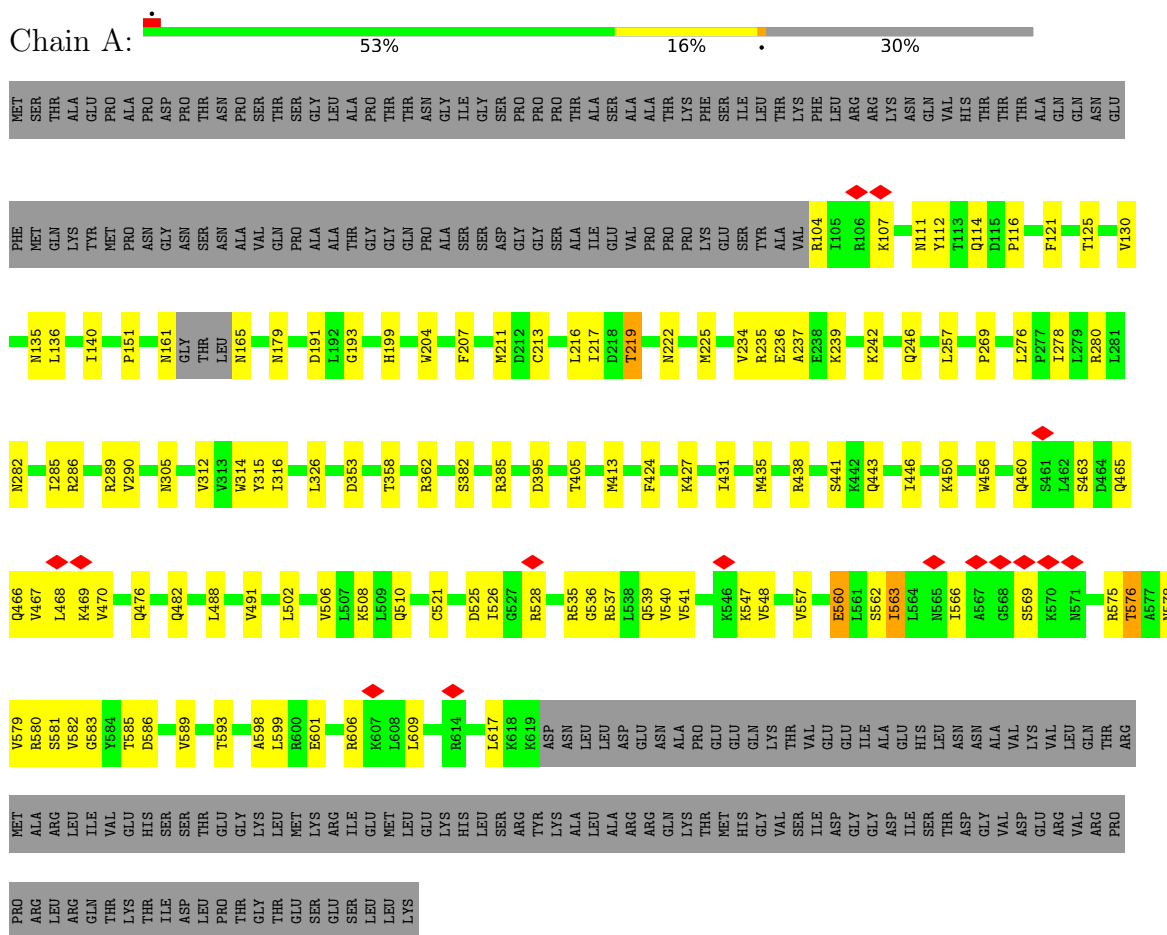
- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na) (labeled as "Ligand of Interest" by depositor).

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

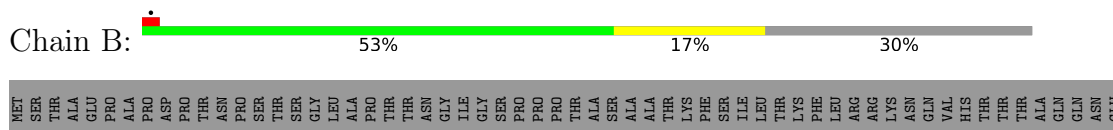
3 Residue-property plots

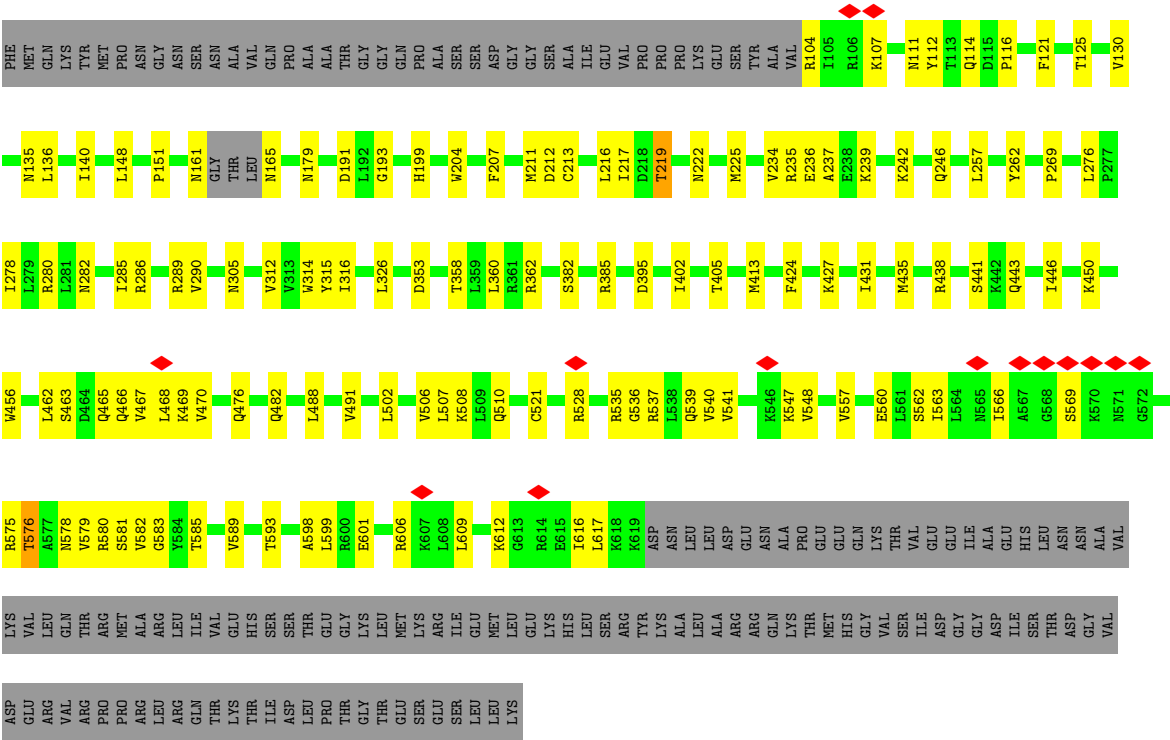
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Cyclic nucleotide-gated cation channel

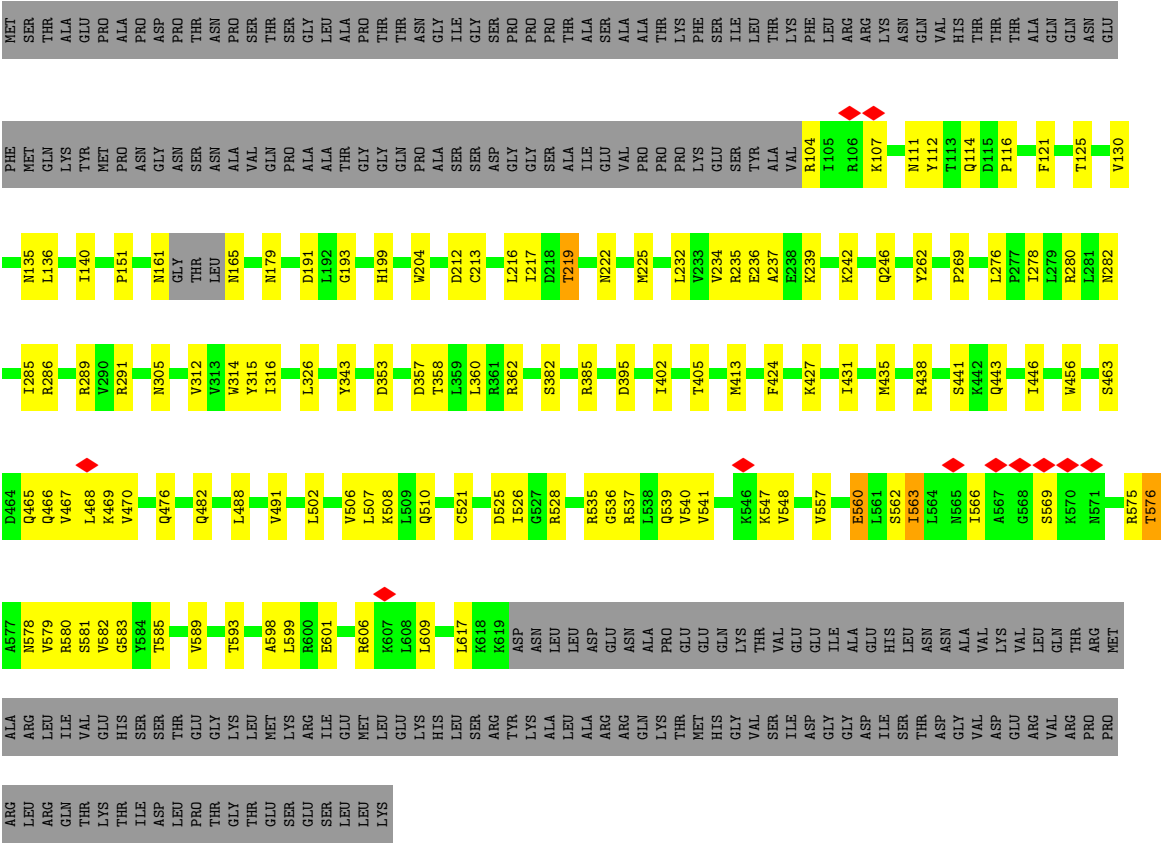


• Molecule 1: Cyclic nucleotide-gated cation channel

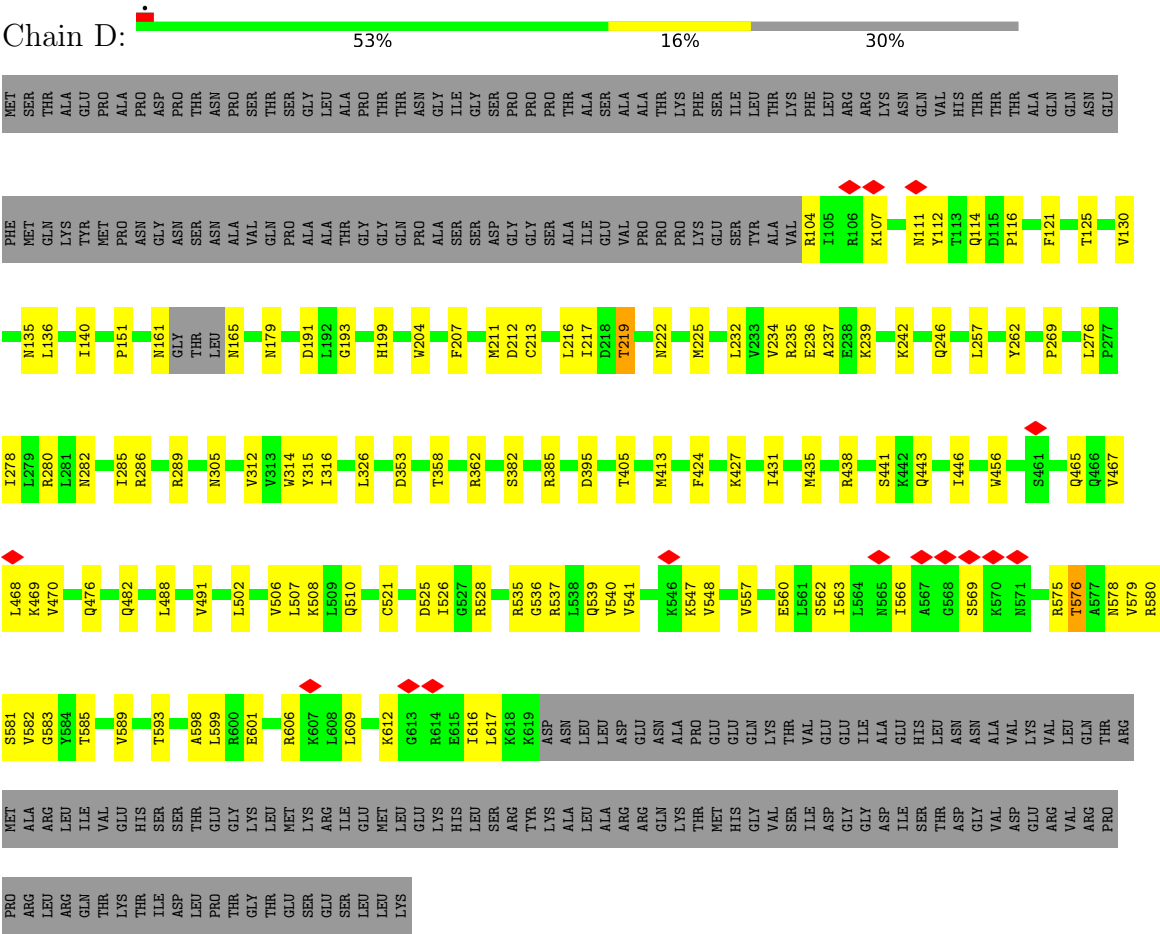




● Molecule 1: Cyclic nucleotide-gated cation channel



● Molecule 1: Cyclic nucleotide-gated cation channel



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	445131	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 ($e^-/\text{\AA}^2$)	56.45	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	3.554	Depositor
Minimum map value	-2.384	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.071	Depositor
Recommended contour level	0.21	Depositor
Map size ($\text{\AA}$)	313.75998, 313.75998, 313.75998	wwPDB
Map dimensions	296, 296, 296	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.06, 1.06, 1.06	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CPL, NA, PX2

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	0.52	6/4336 (0.1%)	0.49	1/5880 (0.0%)
1	B	0.52	6/4336 (0.1%)	0.49	1/5880 (0.0%)
1	C	0.52	5/4336 (0.1%)	0.49	1/5880 (0.0%)
1	D	0.52	6/4336 (0.1%)	0.49	1/5880 (0.0%)
All	All	0.52	23/17344 (0.1%)	0.49	4/23520 (0.0%)

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	234	VAL	C-O	-7.63	1.15	1.24
1	D	234	VAL	C-O	-7.61	1.15	1.24
1	B	237	ALA	C-O	-7.59	1.15	1.24
1	C	237	ALA	C-O	-7.58	1.15	1.24
1	D	237	ALA	C-O	-7.58	1.15	1.24
1	A	234	VAL	C-O	-7.58	1.15	1.24
1	C	234	VAL	C-O	-7.53	1.15	1.24
1	A	237	ALA	C-O	-7.52	1.15	1.24
1	C	237	ALA	C-N	-5.43	1.26	1.33
1	D	237	ALA	C-N	-5.42	1.27	1.33
1	B	237	ALA	C-N	-5.41	1.27	1.33
1	A	237	ALA	C-N	-5.40	1.27	1.33
1	D	257	LEU	CA-C	-5.33	1.46	1.52
1	D	235	ARG	CZ-NH1	-5.26	1.25	1.32
1	C	235	ARG	CZ-NH1	-5.25	1.25	1.32
1	A	235	ARG	CZ-NH1	-5.23	1.25	1.32
1	C	234	VAL	CA-CB	-5.19	1.47	1.54
1	B	234	VAL	CA-CB	-5.17	1.47	1.54
1	D	234	VAL	CA-CB	-5.17	1.47	1.54
1	B	235	ARG	CZ-NH1	-5.16	1.25	1.32
1	A	234	VAL	CA-CB	-5.14	1.47	1.54
1	B	257	LEU	C-O	-5.09	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	257	LEU	C-O	-5.01	1.17	1.24

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	563	ILE	N-CA-C	-5.18	107.36	113.42
1	B	563	ILE	N-CA-C	-5.15	107.40	113.42
1	D	563	ILE	N-CA-C	-5.14	107.41	113.42
1	A	563	ILE	N-CA-C	-5.11	107.44	113.42

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4235	0	4279	76	0
1	B	4235	0	4279	81	0
1	C	4235	0	4279	81	0
1	D	4235	0	4279	75	0
2	A	148	0	221	10	0
2	B	148	0	221	10	0
2	C	148	0	221	9	0
2	D	148	0	221	9	0
3	A	48	0	44	3	0
3	B	48	0	44	4	0
3	C	48	0	44	5	0
3	D	48	0	44	3	0
4	A	1	0	0	0	0
All	All	17725	0	18176	306	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 9.

All (306) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:179:ASN:ND2	1:B:353:ASP:O	2.11	0.83
1:D:179:ASN:ND2	1:D:353:ASP:O	2.11	0.83
1:A:179:ASN:ND2	1:A:353:ASP:O	2.11	0.82
1:C:179:ASN:ND2	1:C:353:ASP:O	2.11	0.82
1:B:305:ASN:HB3	1:B:413:MET:HG3	1.62	0.81
1:A:305:ASN:HB3	1:A:413:MET:HG3	1.62	0.80
1:C:305:ASN:HB3	1:C:413:MET:HG3	1.62	0.79
1:D:305:ASN:HB3	1:D:413:MET:HG3	1.62	0.79
1:C:385:ARG:NH2	3:C:803:PX2:O3	2.17	0.77
1:B:385:ARG:NH2	3:B:803:PX2:O3	2.17	0.77
1:A:385:ARG:NH2	3:A:803:PX2:O3	2.17	0.77
1:D:385:ARG:NH2	3:D:803:PX2:O3	2.17	0.76
1:C:236:GLU:OE1	1:C:239:LYS:HE3	1.87	0.75
1:D:236:GLU:OE1	1:D:239:LYS:HE3	1.87	0.75
1:C:413:MET:HE1	3:D:809:PX2:H35	1.67	0.75
1:A:236:GLU:OE1	1:A:239:LYS:HE3	1.87	0.74
1:B:236:GLU:OE1	1:B:239:LYS:HE3	1.87	0.74
1:D:191:ASP:O	1:D:193:GLY:N	2.22	0.73
1:C:191:ASP:O	1:C:193:GLY:N	2.22	0.72
1:A:191:ASP:O	1:A:193:GLY:N	2.22	0.72
1:B:191:ASP:O	1:B:193:GLY:N	2.22	0.71
1:C:125:THR:HG22	1:C:289:ARG:HD2	1.73	0.70
1:B:413:MET:HE1	3:C:809:PX2:H35	1.73	0.70
1:C:140:ILE:HD11	2:C:806:CPL:H202	1.74	0.70
1:D:140:ILE:HD11	2:D:806:CPL:H202	1.74	0.70
1:D:125:THR:HG22	1:D:289:ARG:HD2	1.73	0.70
1:A:140:ILE:HD11	2:A:806:CPL:H202	1.74	0.69
1:A:125:THR:HG22	1:A:289:ARG:HD2	1.73	0.69
1:B:140:ILE:HD11	2:B:806:CPL:H202	1.74	0.69
1:B:125:THR:HG22	1:B:289:ARG:HD2	1.73	0.69
3:A:809:PX2:H35	1:D:413:MET:HE1	1.75	0.69
1:A:112:TYR:OH	1:A:114:GLN:NE2	2.26	0.69
1:A:161:ASN:O	1:A:165:ASN:N	2.26	0.68
1:B:112:TYR:OH	1:B:114:GLN:NE2	2.26	0.68
1:C:135:ASN:OD1	1:C:280:ARG:NH1	2.27	0.68
1:C:161:ASN:O	1:C:165:ASN:N	2.26	0.68
1:C:112:TYR:OH	1:C:114:GLN:NE2	2.26	0.68
1:B:135:ASN:OD1	1:B:280:ARG:NH1	2.27	0.68
1:A:535:ARG:HD3	1:D:438:ARG:HH12	1.59	0.68
1:B:161:ASN:O	1:B:165:ASN:N	2.26	0.67
1:D:112:TYR:OH	1:D:114:GLN:NE2	2.26	0.67
1:D:161:ASN:O	1:D:165:ASN:N	2.26	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:ASN:OD1	1:A:280:ARG:NH1	2.27	0.67
1:D:135:ASN:OD1	1:D:280:ARG:NH1	2.27	0.67
1:C:547:LYS:HG3	1:C:548:VAL:N	2.12	0.65
1:B:547:LYS:HG3	1:B:548:VAL:N	2.12	0.65
1:A:547:LYS:HG3	1:A:548:VAL:N	2.12	0.64
1:D:547:LYS:HG3	1:D:548:VAL:N	2.12	0.64
1:A:413:MET:HE1	3:B:809:PX2:H35	1.80	0.64
1:C:438:ARG:HH12	1:D:535:ARG:HD3	1.63	0.63
1:B:326:LEU:HB2	2:B:806:CPL:H211	1.82	0.62
1:B:547:LYS:HG3	1:B:548:VAL:H	1.64	0.62
1:D:222:ASN:OD1	1:D:289:ARG:NH2	2.33	0.62
1:A:326:LEU:HB2	2:A:806:CPL:H211	1.82	0.61
1:B:441:SER:H	1:C:482:GLN:NE2	1.98	0.61
1:A:222:ASN:OD1	1:A:289:ARG:NH2	2.33	0.61
1:D:547:LYS:HG3	1:D:548:VAL:H	1.64	0.61
1:B:222:ASN:OD1	1:B:289:ARG:NH2	2.33	0.61
1:A:547:LYS:HG3	1:A:548:VAL:H	1.64	0.61
1:C:326:LEU:HB2	2:C:806:CPL:H211	1.82	0.61
1:C:222:ASN:OD1	1:C:289:ARG:NH2	2.33	0.61
1:C:547:LYS:HG3	1:C:548:VAL:H	1.64	0.61
1:D:326:LEU:HB2	2:D:806:CPL:H211	1.82	0.60
1:C:468:LEU:O	1:C:476:GLN:NE2	2.35	0.60
1:B:468:LEU:O	1:B:476:GLN:NE2	2.35	0.59
1:D:468:LEU:O	1:D:476:GLN:NE2	2.35	0.59
1:A:468:LEU:O	1:A:476:GLN:NE2	2.35	0.59
1:A:438:ARG:HH12	1:B:535:ARG:HD3	1.68	0.58
1:B:314:TRP:HB3	2:B:807:CPL:H172	1.85	0.57
1:C:314:TRP:HB3	2:C:807:CPL:H172	1.85	0.57
1:D:314:TRP:HB3	2:D:807:CPL:H172	1.85	0.57
1:A:314:TRP:HB3	2:A:807:CPL:H172	1.85	0.57
1:B:151:PRO:HD3	2:B:801:CPL:HC31	1.87	0.56
1:C:151:PRO:HD3	2:C:801:CPL:HC31	1.87	0.56
1:A:151:PRO:HD3	2:A:801:CPL:HC31	1.87	0.56
1:C:540:VAL:HG22	1:C:579:VAL:HG22	1.88	0.56
1:B:540:VAL:HG22	1:B:579:VAL:HG22	1.88	0.55
1:D:151:PRO:HD3	2:D:801:CPL:HC31	1.87	0.55
1:B:465:GLN:HA	1:B:468:LEU:HB3	1.89	0.55
1:D:540:VAL:HG22	1:D:579:VAL:HG22	1.88	0.55
1:C:465:GLN:HA	1:C:468:LEU:HB3	1.88	0.55
1:A:199:HIS:CD2	1:A:199:HIS:H	2.25	0.55
1:A:465:GLN:HA	1:A:468:LEU:HB3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:540:VAL:HG22	1:A:579:VAL:HG22	1.88	0.54
1:A:116:PRO:HB3	1:A:225:MET:HE3	1.90	0.54
1:C:116:PRO:HB3	1:C:225:MET:HE3	1.90	0.54
1:D:116:PRO:HB3	1:D:225:MET:HE3	1.90	0.54
1:B:107:LYS:O	1:B:111:ASN:ND2	2.32	0.54
1:B:116:PRO:HB3	1:B:225:MET:HE3	1.90	0.54
1:D:465:GLN:HA	1:D:468:LEU:HB3	1.89	0.54
1:D:199:HIS:H	1:D:199:HIS:CD2	2.25	0.53
1:B:547:LYS:O	1:B:548:VAL:HG23	2.09	0.53
1:A:104:ARG:N	1:A:107:LYS:HD3	2.25	0.52
1:A:315:TYR:CE1	2:A:807:CPL:H182	2.45	0.52
1:D:104:ARG:N	1:D:107:LYS:HD3	2.25	0.52
1:A:547:LYS:O	1:A:548:VAL:HG23	2.09	0.52
1:B:315:TYR:CE1	2:B:807:CPL:H182	2.45	0.52
1:C:199:HIS:CD2	1:C:199:HIS:H	2.25	0.52
1:A:482:GLN:NE2	1:D:441:SER:H	2.08	0.52
1:B:199:HIS:H	1:B:199:HIS:CD2	2.25	0.52
1:C:547:LYS:O	1:C:548:VAL:HG23	2.09	0.52
1:D:575:ARG:O	1:D:576:THR:HG22	2.10	0.52
1:B:575:ARG:O	1:B:576:THR:HG22	2.10	0.52
1:C:276:LEU:HG	1:C:278:ILE:HG22	1.92	0.52
1:C:104:ARG:N	1:C:107:LYS:HD3	2.25	0.52
1:B:566:ILE:HG21	1:B:617:LEU:HD22	1.92	0.52
1:C:566:ILE:HG21	1:C:617:LEU:HD22	1.92	0.52
1:C:575:ARG:O	1:C:576:THR:HG22	2.10	0.52
1:D:107:LYS:O	1:D:111:ASN:ND2	2.32	0.52
1:B:276:LEU:HG	1:B:278:ILE:HG22	1.92	0.51
1:C:536:GLY:HA3	1:C:585:THR:HG23	1.92	0.51
1:D:547:LYS:O	1:D:548:VAL:HG23	2.09	0.51
1:C:502:LEU:O	1:C:506:VAL:HG13	2.11	0.51
1:B:104:ARG:N	1:B:107:LYS:HD3	2.25	0.51
1:A:547:LYS:O	1:A:548:VAL:CG2	2.59	0.51
1:D:547:LYS:O	1:D:548:VAL:CG2	2.59	0.51
1:A:276:LEU:HG	1:A:278:ILE:HG22	1.92	0.51
1:A:315:TYR:HE1	2:A:807:CPL:H182	1.76	0.51
1:C:315:TYR:CE1	2:C:807:CPL:H182	2.45	0.51
1:D:315:TYR:CE1	2:D:807:CPL:H182	2.45	0.51
1:B:547:LYS:O	1:B:548:VAL:CG2	2.59	0.51
1:A:502:LEU:O	1:A:506:VAL:HG13	2.11	0.51
1:A:536:GLY:HA3	1:A:585:THR:HG23	1.92	0.51
1:B:502:LEU:O	1:B:506:VAL:HG13	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:547:LYS:O	1:C:548:VAL:CG2	2.59	0.50
1:A:566:ILE:HG21	1:A:617:LEU:HD22	1.92	0.50
1:A:575:ARG:O	1:A:576:THR:HG22	2.10	0.50
1:B:536:GLY:HA3	1:B:585:THR:HG23	1.92	0.50
1:C:315:TYR:HE1	2:C:807:CPL:H182	1.76	0.50
1:D:276:LEU:HG	1:D:278:ILE:HG22	1.92	0.50
1:A:441:SER:H	1:B:482:GLN:NE2	2.10	0.50
1:B:212:ASP:OD2	1:B:262:TYR:OH	2.27	0.50
1:D:566:ILE:HG21	1:D:617:LEU:HD22	1.92	0.50
1:D:536:GLY:HA3	1:D:585:THR:HG23	1.92	0.50
1:A:107:LYS:O	1:A:111:ASN:ND2	2.32	0.50
1:B:405:THR:HG23	3:B:809:PX2:H30	1.94	0.50
1:D:502:LEU:O	1:D:506:VAL:HG13	2.11	0.50
1:D:528:ARG:NH2	1:D:593:THR:OG1	2.45	0.50
1:B:315:TYR:HE1	2:B:807:CPL:H182	1.76	0.50
1:C:405:THR:HG23	3:C:809:PX2:H30	1.94	0.50
1:B:566:ILE:HB	1:B:569:SER:HB3	1.94	0.49
1:C:358:THR:O	1:C:362:ARG:HG3	2.12	0.49
1:C:541:VAL:HG11	1:C:580:ARG:CZ	2.42	0.49
1:D:315:TYR:HE1	2:D:807:CPL:H182	1.76	0.49
1:D:443:GLN:O	1:D:446:ILE:HG13	2.13	0.49
1:D:541:VAL:HG11	1:D:580:ARG:CZ	2.42	0.49
1:A:528:ARG:NH2	1:A:593:THR:OG1	2.45	0.49
1:C:107:LYS:O	1:C:111:ASN:ND2	2.32	0.49
1:C:528:ARG:NH2	1:C:593:THR:OG1	2.45	0.49
1:C:566:ILE:HB	1:C:569:SER:HB3	1.94	0.49
1:A:358:THR:O	1:A:362:ARG:HG3	2.12	0.49
1:C:491:VAL:HG22	1:C:557:VAL:HG21	1.94	0.49
1:B:528:ARG:NH2	1:B:593:THR:OG1	2.45	0.49
1:D:566:ILE:HB	1:D:569:SER:HB3	1.94	0.49
1:B:541:VAL:HG11	1:B:580:ARG:CZ	2.42	0.49
1:C:443:GLN:O	1:C:446:ILE:HG13	2.13	0.49
1:B:358:THR:O	1:B:362:ARG:HG3	2.12	0.48
1:D:491:VAL:HG22	1:D:557:VAL:HG21	1.94	0.48
1:A:541:VAL:HG11	1:A:580:ARG:CZ	2.42	0.48
1:D:358:THR:O	1:D:362:ARG:HG3	2.12	0.48
1:A:443:GLN:O	1:A:446:ILE:HG13	2.13	0.48
1:A:491:VAL:HG22	1:A:557:VAL:HG21	1.94	0.48
1:A:405:THR:HG23	3:A:809:PX2:H30	1.94	0.48
1:A:566:ILE:HB	1:A:569:SER:HB3	1.94	0.48
1:B:491:VAL:HG22	1:B:557:VAL:HG21	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:405:THR:HG23	3:D:809:PX2:H30	1.94	0.48
1:B:443:GLN:O	1:B:446:ILE:HG13	2.13	0.47
1:A:581:SER:OG	1:A:585:THR:OG1	2.30	0.47
1:C:282:ASN:O	1:C:285:ILE:HG12	2.14	0.47
1:D:282:ASN:O	1:D:285:ILE:HG12	2.14	0.47
1:A:282:ASN:O	1:A:285:ILE:HG12	2.14	0.47
1:C:212:ASP:OD2	1:C:262:TYR:OH	2.27	0.47
1:C:581:SER:OG	1:C:585:THR:OG1	2.30	0.47
1:A:216:LEU:O	1:A:219:THR:HG22	2.15	0.47
1:B:282:ASN:O	1:B:285:ILE:HG12	2.14	0.47
1:C:537:ARG:HD2	1:C:582:VAL:HG21	1.97	0.47
1:D:537:ARG:HD2	1:D:582:VAL:HG21	1.97	0.47
1:D:216:LEU:O	1:D:219:THR:HG22	2.15	0.47
1:D:562:SER:O	1:D:562:SER:OG	2.32	0.47
1:A:424:PHE:CE1	1:A:456:TRP:HB2	2.50	0.46
1:B:424:PHE:CE1	1:B:456:TRP:HB2	2.50	0.46
1:D:465:GLN:O	1:D:469:LYS:NZ	2.49	0.46
1:A:562:SER:O	1:A:562:SER:OG	2.32	0.46
1:B:216:LEU:O	1:B:219:THR:HG22	2.15	0.46
1:C:465:GLN:O	1:C:469:LYS:NZ	2.49	0.46
1:D:581:SER:OG	1:D:585:THR:OG1	2.30	0.46
1:C:242:LYS:HE3	1:C:242:LYS:HB2	1.78	0.46
1:D:424:PHE:CE1	1:D:456:TRP:HB2	2.50	0.46
1:A:537:ARG:HD2	1:A:582:VAL:HG21	1.97	0.46
1:C:424:PHE:CE1	1:C:456:TRP:HB2	2.50	0.46
1:B:537:ARG:HD2	1:B:582:VAL:HG21	1.97	0.46
1:D:539:GLN:HE21	1:D:580:ARG:HE	1.64	0.46
1:C:539:GLN:HE21	1:C:580:ARG:HE	1.64	0.46
1:B:465:GLN:O	1:B:469:LYS:NZ	2.49	0.45
1:C:441:SER:H	1:D:482:GLN:NE2	2.13	0.45
1:C:575:ARG:HD3	1:C:575:ARG:HA	1.77	0.45
1:A:465:GLN:O	1:A:469:LYS:NZ	2.49	0.45
1:C:216:LEU:O	1:C:219:THR:HG22	2.15	0.45
1:A:539:GLN:HE21	1:A:580:ARG:HE	1.64	0.45
1:B:539:GLN:HE21	1:B:580:ARG:HE	1.64	0.45
1:B:438:ARG:HH12	1:C:535:ARG:HD3	1.82	0.45
1:B:213:CYS:O	1:B:217:ILE:HG12	2.17	0.45
1:A:312:VAL:O	1:A:316:ILE:HG12	2.17	0.44
1:D:213:CYS:O	1:D:217:ILE:HG12	2.17	0.44
1:A:431:ILE:HG22	1:A:435:MET:HE2	1.98	0.44
1:B:191:ASP:HA	1:B:269:PRO:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:312:VAL:O	1:C:316:ILE:HG12	2.17	0.44
1:B:431:ILE:HG22	1:B:435:MET:HE2	1.98	0.44
1:B:441:SER:H	1:C:482:GLN:HE22	1.65	0.44
1:B:450:LYS:HE2	1:B:450:LYS:HB3	1.82	0.44
1:C:213:CYS:O	1:C:217:ILE:HG12	2.17	0.44
1:D:191:ASP:HA	1:D:269:PRO:HB3	2.00	0.44
1:D:431:ILE:HG22	1:D:435:MET:HE2	1.98	0.44
1:C:431:ILE:HG22	1:C:435:MET:HE2	1.98	0.44
1:D:312:VAL:O	1:D:316:ILE:HG12	2.17	0.44
1:A:213:CYS:O	1:A:217:ILE:HG12	2.17	0.44
1:A:521:CYS:HB2	1:A:575:ARG:HG3	2.00	0.44
1:C:562:SER:O	1:C:562:SER:OG	2.32	0.44
1:B:507:LEU:HA	1:B:507:LEU:HD23	1.84	0.44
1:B:312:VAL:O	1:B:316:ILE:HG12	2.17	0.43
1:C:581:SER:OG	1:C:583:GLY:O	2.35	0.43
1:D:242:LYS:HB2	1:D:242:LYS:HE3	1.78	0.43
1:C:219:THR:HB	1:C:286:ARG:HH22	1.84	0.43
1:C:507:LEU:HD23	1:C:507:LEU:HA	1.84	0.43
1:D:130:VAL:HG22	2:D:808:CPL:H202	2.01	0.43
1:C:242:LYS:O	1:C:246:GLN:HG2	2.18	0.43
1:D:581:SER:OG	1:D:583:GLY:O	2.35	0.43
1:B:562:SER:O	1:B:562:SER:OG	2.32	0.43
1:C:130:VAL:HG22	2:C:808:CPL:H202	2.01	0.43
1:C:191:ASP:HA	1:C:269:PRO:HB3	2.00	0.43
1:B:121:PHE:CZ	1:B:225:MET:HE1	2.54	0.43
1:B:581:SER:OG	1:B:583:GLY:O	2.35	0.43
1:C:121:PHE:CZ	1:C:225:MET:HE1	2.54	0.43
1:C:521:CYS:HB2	1:C:575:ARG:HG3	2.00	0.43
1:D:242:LYS:O	1:D:246:GLN:HG2	2.18	0.43
1:B:242:LYS:O	1:B:246:GLN:HG2	2.18	0.42
1:D:521:CYS:HB2	1:D:575:ARG:HG3	2.00	0.42
1:D:599:LEU:HG	1:D:606:ARG:HB2	2.01	0.42
1:B:219:THR:HB	1:B:286:ARG:HH22	1.84	0.42
1:B:581:SER:OG	1:B:585:THR:OG1	2.30	0.42
1:D:219:THR:HB	1:D:286:ARG:HH22	1.84	0.42
1:A:242:LYS:O	1:A:246:GLN:HG2	2.18	0.42
1:A:599:LEU:HG	1:A:606:ARG:HB2	2.01	0.42
1:A:130:VAL:HG22	2:A:808:CPL:H202	2.01	0.42
1:A:191:ASP:HA	1:A:269:PRO:HB3	2.00	0.42
1:B:462:LEU:HD12	1:B:462:LEU:HA	1.92	0.42
1:C:547:LYS:C	1:C:548:VAL:HG23	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:121:PHE:CZ	1:D:225:MET:HE1	2.54	0.42
1:A:121:PHE:CZ	1:A:225:MET:HE1	2.54	0.42
1:A:219:THR:HB	1:A:286:ARG:HH22	1.84	0.42
1:A:547:LYS:C	1:A:548:VAL:HG23	2.45	0.42
1:A:575:ARG:HD3	1:A:575:ARG:HA	1.77	0.42
1:B:521:CYS:HB2	1:B:575:ARG:HG3	2.00	0.42
2:A:806:CPL:H222	2:A:806:CPL:H191	1.77	0.42
1:C:232:LEU:HD23	1:C:232:LEU:HA	1.92	0.42
2:D:806:CPL:H222	2:D:806:CPL:H191	1.77	0.42
1:C:599:LEU:HG	1:C:606:ARG:HB2	2.01	0.42
1:B:547:LYS:C	1:B:548:VAL:HG23	2.45	0.42
1:C:343:TYR:OH	1:C:357:ASP:OD1	2.24	0.42
1:C:547:LYS:CG	1:C:548:VAL:N	2.83	0.42
1:D:212:ASP:OD2	1:D:262:TYR:OH	2.27	0.42
1:D:507:LEU:HA	1:D:507:LEU:HD23	1.85	0.42
1:A:508:LYS:NZ	1:A:598:ALA:HB2	2.35	0.41
1:B:599:LEU:HG	1:B:606:ARG:HB2	2.01	0.41
1:C:508:LYS:NZ	1:C:598:ALA:HB2	2.35	0.41
1:A:427:LYS:O	1:A:431:ILE:HG12	2.21	0.41
1:A:581:SER:OG	1:A:583:GLY:O	2.35	0.41
1:D:427:LYS:O	1:D:431:ILE:HG12	2.20	0.41
1:D:508:LYS:NZ	1:D:598:ALA:HB2	2.35	0.41
1:A:460:GLN:NE2	1:A:586:ASP:OD1	2.53	0.41
1:B:130:VAL:HG22	2:B:808:CPL:H202	2.01	0.41
1:B:508:LYS:NZ	1:B:598:ALA:HB2	2.35	0.41
1:D:547:LYS:C	1:D:548:VAL:HG23	2.45	0.41
1:D:207:PHE:O	1:D:211:MET:HG2	2.21	0.41
1:C:427:LYS:O	1:C:431:ILE:HG12	2.20	0.41
1:D:525:ASP:OD1	1:D:526:ILE:N	2.54	0.41
1:B:463:SER:O	1:B:466:GLN:NE2	2.54	0.41
1:B:290:VAL:HG11	2:B:807:CPL:H201	2.02	0.41
1:B:547:LYS:CG	1:B:548:VAL:N	2.83	0.41
1:C:525:ASP:OD1	1:C:526:ILE:N	2.54	0.41
1:A:207:PHE:O	1:A:211:MET:HG2	2.21	0.41
1:A:560:GLU:O	1:A:563:ILE:HG22	2.21	0.41
1:B:427:LYS:O	1:B:431:ILE:HG12	2.20	0.41
1:A:204:TRP:CZ3	2:A:801:CPL:H212	2.56	0.41
1:B:207:PHE:O	1:B:211:MET:HG2	2.21	0.41
1:C:560:GLU:O	1:C:563:ILE:HG22	2.21	0.40
1:B:204:TRP:CZ3	2:B:801:CPL:H212	2.56	0.40
1:C:204:TRP:CZ3	2:C:801:CPL:H212	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:463:SER:O	1:C:466:GLN:NE2	2.54	0.40
1:A:121:PHE:O	1:A:125:THR:HG23	2.22	0.40
1:A:463:SER:O	1:A:466:GLN:NE2	2.54	0.40
1:A:525:ASP:OD1	1:A:526:ILE:N	2.54	0.40
1:B:612:LYS:HE3	1:B:616:ILE:HD11	2.03	0.40
1:C:291:ARG:NH1	3:C:809:PX2:O1	2.50	0.40
1:D:204:TRP:CZ3	2:D:801:CPL:H212	2.56	0.40
1:D:575:ARG:HA	1:D:575:ARG:HD3	1.77	0.40
1:D:612:LYS:HE3	1:D:616:ILE:HD11	2.03	0.40
1:A:290:VAL:HG11	2:A:807:CPL:H201	2.02	0.40
1:C:360:LEU:HD22	2:C:802:CPL:H341	2.04	0.40
1:D:232:LEU:HD23	1:D:232:LEU:HA	1.92	0.40
1:A:450:LYS:HB3	1:A:450:LYS:HE2	1.82	0.40
1:B:121:PHE:O	1:B:125:THR:HG23	2.22	0.40
1:B:148:LEU:HD23	1:B:148:LEU:HA	1.94	0.40
1:B:360:LEU:HD22	2:B:802:CPL:H341	2.04	0.40
1:B:402:ILE:HG12	3:B:809:PX2:H14	2.04	0.40
1:C:402:ILE:HG12	3:C:809:PX2:H14	2.04	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	509/733 (69%)	489 (96%)	20 (4%)	0	100	100
1	B	509/733 (69%)	488 (96%)	21 (4%)	0	100	100
1	C	509/733 (69%)	489 (96%)	20 (4%)	0	100	100
1	D	509/733 (69%)	490 (96%)	19 (4%)	0	100	100
All	All	2036/2932 (69%)	1956 (96%)	80 (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	A	464/650 (71%)	450 (97%)	14 (3%)	36	64
1	B	464/650 (71%)	450 (97%)	14 (3%)	36	64
1	C	464/650 (71%)	450 (97%)	14 (3%)	36	64
1	D	464/650 (71%)	450 (97%)	14 (3%)	36	64
All	All	1856/2600 (71%)	1800 (97%)	56 (3%)	37	64

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	136	LEU
1	A	219	THR
1	A	382	SER
1	A	395	ASP
1	A	467	VAL
1	A	470	VAL
1	A	488	LEU
1	A	510	GLN
1	A	560	GLU
1	A	576	THR
1	A	578	ASN
1	A	589	VAL
1	A	601	GLU
1	A	609	LEU
1	B	136	LEU
1	B	219	THR
1	B	382	SER
1	B	395	ASP
1	B	467	VAL
1	B	470	VAL
1	B	488	LEU
1	B	510	GLN
1	B	560	GLU
1	B	576	THR

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Mol	Chain	Res	Type
1	B	578	ASN
1	B	589	VAL
1	B	601	GLU
1	B	609	LEU
1	C	136	LEU
1	C	219	THR
1	C	382	SER
1	C	395	ASP
1	C	467	VAL
1	C	470	VAL
1	C	488	LEU
1	C	510	GLN
1	C	560	GLU
1	C	576	THR
1	C	578	ASN
1	C	589	VAL
1	C	601	GLU
1	C	609	LEU
1	D	136	LEU
1	D	219	THR
1	D	382	SER
1	D	395	ASP
1	D	467	VAL
1	D	470	VAL
1	D	488	LEU
1	D	510	GLN
1	D	560	GLU
1	D	576	THR
1	D	578	ASN
1	D	589	VAL
1	D	601	GLU
1	D	609	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (55) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	114	GLN
1	A	120	ASN
1	A	154	GLN
1	A	179	ASN
1	A	199	HIS
1	A	230	GLN

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Mol	Chain	Res	Type
1	A	323	ASN
1	A	345	HIS
1	A	416	ASN
1	A	443	GLN
1	A	458	ASN
1	A	482	GLN
1	A	512	GLN
1	A	553	GLN
1	B	114	GLN
1	B	120	ASN
1	B	154	GLN
1	B	199	HIS
1	B	230	GLN
1	B	323	ASN
1	B	345	HIS
1	B	416	ASN
1	B	433	GLN
1	B	443	GLN
1	B	458	ASN
1	B	482	GLN
1	B	512	GLN
1	B	553	GLN
1	C	114	GLN
1	C	120	ASN
1	C	154	GLN
1	C	199	HIS
1	C	230	GLN
1	C	323	ASN
1	C	345	HIS
1	C	416	ASN
1	C	443	GLN
1	C	458	ASN
1	C	482	GLN
1	C	512	GLN
1	C	553	GLN
1	D	114	GLN
1	D	120	ASN
1	D	154	GLN
1	D	179	ASN
1	D	199	HIS
1	D	230	GLN
1	D	323	ASN

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Mol	Chain	Res	Type
1	D	345	HIS
1	D	416	ASN
1	D	443	GLN
1	D	458	ASN
1	D	482	GLN
1	D	512	GLN
1	D	553	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 37 ligands modelled in this entry, 1 is monoatomic - leaving 36 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	$\# Z > 2$
2	CPL	C	807	-	12,12,51	0.22	0	11,11,59	0.87	0
2	CPL	D	807	-	12,12,51	0.22	0	11,11,59	0.87	0
2	CPL	C	806	-	11,11,51	0.19	0	10,10,59	0.82	0
2	CPL	A	802	-	40,40,51	1.01	4 (10%)	43,45,59	1.30	2 (4%)
2	CPL	A	804	-	8,8,51	0.27	0	7,7,59	0.72	0
2	CPL	D	806	-	11,11,51	0.18	0	10,10,59	0.82	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PX2	A	803	-	22,22,35	1.22	3 (13%)	25,27,40	1.47	3 (12%)
2	CPL	D	808	-	14,14,51	0.24	0	13,13,59	0.84	0
2	CPL	A	806	-	11,11,51	0.18	0	10,10,59	0.83	0
2	CPL	C	808	-	14,14,51	0.24	0	13,13,59	0.84	0
2	CPL	C	804	-	8,8,51	0.27	0	7,7,59	0.71	0
2	CPL	D	805	-	8,8,51	0.28	0	7,7,59	0.78	0
2	CPL	B	807	-	12,12,51	0.22	0	11,11,59	0.87	0
2	CPL	C	801	-	48,48,51	1.02	4 (8%)	54,56,59	1.19	2 (3%)
3	PX2	D	803	-	22,22,35	1.22	3 (13%)	25,27,40	1.48	3 (12%)
3	PX2	C	803	-	22,22,35	1.23	3 (13%)	25,27,40	1.48	3 (12%)
2	CPL	D	804	-	8,8,51	0.27	0	7,7,59	0.71	0
2	CPL	C	805	-	8,8,51	0.28	0	7,7,59	0.78	0
3	PX2	B	803	-	22,22,35	1.23	3 (13%)	25,27,40	1.48	3 (12%)
3	PX2	D	809	-	24,24,35	1.16	4 (16%)	27,29,40	1.35	2 (7%)
2	CPL	A	808	-	14,14,51	0.24	0	13,13,59	0.84	0
2	CPL	D	801	-	48,48,51	1.03	4 (8%)	54,56,59	1.19	2 (3%)
3	PX2	A	809	-	24,24,35	1.16	4 (16%)	27,29,40	1.35	2 (7%)
2	CPL	A	805	-	8,8,51	0.28	0	7,7,59	0.78	0
2	CPL	B	802	-	40,40,51	1.00	4 (10%)	43,45,59	1.30	2 (4%)
2	CPL	B	808	-	14,14,51	0.24	0	13,13,59	0.84	0
2	CPL	B	806	-	11,11,51	0.18	0	10,10,59	0.82	0
2	CPL	A	807	-	12,12,51	0.23	0	11,11,59	0.87	0
2	CPL	B	801	-	48,48,51	1.03	4 (8%)	54,56,59	1.19	2 (3%)
3	PX2	B	809	-	24,24,35	1.15	4 (16%)	27,29,40	1.35	2 (7%)
2	CPL	B	804	-	8,8,51	0.26	0	7,7,59	0.71	0
2	CPL	B	805	-	8,8,51	0.28	0	7,7,59	0.78	0
2	CPL	D	802	-	40,40,51	1.00	4 (10%)	43,45,59	1.30	2 (4%)
3	PX2	C	809	-	24,24,35	1.16	4 (16%)	27,29,40	1.35	2 (7%)
2	CPL	A	801	-	48,48,51	1.02	4 (8%)	54,56,59	1.19	2 (3%)
2	CPL	C	802	-	40,40,51	1.00	4 (10%)	43,45,59	1.30	2 (4%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CPL	C	807	-	-	4/10/10/55	-
2	CPL	D	807	-	-	4/10/10/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CPL	C	806	-	-	3/9/9/55	-
2	CPL	A	802	-	-	23/44/44/55	-
2	CPL	A	804	-	-	1/6/6/55	-
2	CPL	D	806	-	-	2/9/9/55	-
3	PX2	A	803	-	-	10/24/24/37	-
2	CPL	D	808	-	-	7/12/12/55	-
2	CPL	A	806	-	-	2/9/9/55	-
2	CPL	C	808	-	-	7/12/12/55	-
2	CPL	C	804	-	-	1/6/6/55	-
2	CPL	D	805	-	-	4/6/6/55	-
2	CPL	B	807	-	-	4/10/10/55	-
2	CPL	C	801	-	-	20/52/52/55	-
3	PX2	D	803	-	-	10/24/24/37	-
3	PX2	C	803	-	-	10/24/24/37	-
2	CPL	D	804	-	-	1/6/6/55	-
2	CPL	C	805	-	-	4/6/6/55	-
3	PX2	B	803	-	-	10/24/24/37	-
3	PX2	D	809	-	-	12/26/26/37	-
2	CPL	A	808	-	-	7/12/12/55	-
2	CPL	D	801	-	-	20/52/52/55	-
3	PX2	A	809	-	-	12/26/26/37	-
2	CPL	A	805	-	-	4/6/6/55	-
2	CPL	B	802	-	-	23/44/44/55	-
2	CPL	B	808	-	-	7/12/12/55	-
2	CPL	B	806	-	-	2/9/9/55	-
2	CPL	A	807	-	-	4/10/10/55	-
2	CPL	B	801	-	-	20/52/52/55	-
3	PX2	B	809	-	-	12/26/26/37	-
2	CPL	B	804	-	-	1/6/6/55	-
2	CPL	B	805	-	-	4/6/6/55	-
2	CPL	D	802	-	-	23/44/44/55	-
3	PX2	C	809	-	-	12/26/26/37	-
2	CPL	A	801	-	-	20/52/52/55	-
2	CPL	C	802	-	-	23/44/44/55	-

All (60) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	802	CPL	O2-C2	-2.71	1.40	1.46
2	B	802	CPL	O2-C2	-2.71	1.40	1.46
2	D	802	CPL	O2-C2	-2.70	1.40	1.46
2	C	802	CPL	O2-C2	-2.69	1.40	1.46
2	A	802	CPL	O3-C11	2.56	1.40	1.33
2	D	802	CPL	O3-C11	2.54	1.40	1.33
2	C	802	CPL	O3-C11	2.53	1.40	1.33
3	C	803	PX2	O5-C3	-2.53	1.39	1.45
2	B	802	CPL	O3-C11	2.52	1.40	1.33
3	A	803	PX2	O5-C3	-2.52	1.39	1.45
3	B	803	PX2	O5-C3	-2.51	1.39	1.45
3	D	803	PX2	O5-C3	-2.50	1.39	1.45
3	C	803	PX2	O7-C2	-2.46	1.40	1.46
3	B	803	PX2	O7-C2	-2.44	1.40	1.46
3	D	803	PX2	O7-C2	-2.43	1.40	1.46
2	C	802	CPL	O2-C31	2.42	1.41	1.34
2	D	802	CPL	O2-C31	2.42	1.41	1.34
2	A	802	CPL	O2-C31	2.42	1.41	1.34
2	B	802	CPL	O2-C31	2.41	1.41	1.34
2	B	801	CPL	O2-C2	-2.41	1.40	1.46
3	A	803	PX2	O7-C2	-2.41	1.40	1.46
2	C	801	CPL	O2-C31	2.41	1.41	1.34
2	D	801	CPL	O2-C31	2.41	1.41	1.34
2	A	801	CPL	O2-C31	2.40	1.41	1.34
2	C	801	CPL	O2-C2	-2.40	1.41	1.46
2	D	801	CPL	O2-C2	-2.40	1.41	1.46
2	B	801	CPL	O2-C31	2.39	1.41	1.34
2	A	801	CPL	O2-C2	-2.38	1.41	1.46
3	A	809	PX2	O7-C2	-2.34	1.41	1.46
3	D	809	PX2	O7-C2	-2.32	1.41	1.46
3	B	803	PX2	O7-C16	2.32	1.40	1.34
3	B	809	PX2	O7-C2	-2.30	1.41	1.46
3	A	803	PX2	O7-C16	2.29	1.40	1.34
3	C	809	PX2	O7-C2	-2.29	1.41	1.46
3	D	803	PX2	O7-C16	2.29	1.40	1.34
2	B	801	CPL	O3-C3	-2.28	1.40	1.45
3	C	803	PX2	O7-C16	2.28	1.40	1.34
3	A	809	PX2	O5-C4	2.26	1.40	1.33
2	A	801	CPL	O3-C3	-2.26	1.40	1.45
3	C	809	PX2	O5-C4	2.26	1.39	1.33
3	D	809	PX2	O5-C4	2.26	1.39	1.33
2	D	801	CPL	O3-C3	-2.25	1.40	1.45
3	B	809	PX2	O5-C4	2.25	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	801	CPL	O3-C3	-2.24	1.40	1.45
3	C	809	PX2	O5-C3	-2.22	1.40	1.45
2	A	802	CPL	O3-C3	-2.21	1.40	1.45
3	B	809	PX2	O5-C3	-2.19	1.40	1.45
2	B	801	CPL	O3-C11	2.19	1.39	1.33
3	D	809	PX2	O5-C3	-2.19	1.40	1.45
2	C	802	CPL	O3-C3	-2.18	1.40	1.45
2	D	802	CPL	O3-C3	-2.17	1.40	1.45
3	A	809	PX2	O5-C3	-2.17	1.40	1.45
3	A	809	PX2	O7-C16	2.17	1.40	1.34
2	A	801	CPL	O3-C11	2.15	1.39	1.33
2	D	801	CPL	O3-C11	2.15	1.39	1.33
3	C	809	PX2	O7-C16	2.15	1.40	1.34
3	D	809	PX2	O7-C16	2.15	1.40	1.34
3	B	809	PX2	O7-C16	2.14	1.40	1.34
2	B	802	CPL	O3-C3	-2.13	1.40	1.45
2	C	801	CPL	O3-C11	2.12	1.39	1.33

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	802	CPL	O2-C31-C32	4.76	121.78	111.48
2	A	802	CPL	O2-C31-C32	4.76	121.77	111.48
2	D	802	CPL	O2-C31-C32	4.75	121.76	111.48
2	C	802	CPL	O2-C31-C32	4.74	121.74	111.48
2	B	801	CPL	O2-C31-C32	4.65	121.55	111.48
2	D	801	CPL	O2-C31-C32	4.64	121.52	111.48
2	A	801	CPL	O2-C31-C32	4.63	121.49	111.48
2	C	801	CPL	O2-C31-C32	4.62	121.47	111.48
3	C	803	PX2	O7-C16-C17	4.42	121.05	111.48
3	B	803	PX2	O7-C16-C17	4.42	121.03	111.48
3	D	803	PX2	O7-C16-C17	4.41	121.01	111.48
3	A	803	PX2	O7-C16-C17	4.39	120.98	111.48
3	A	809	PX2	O7-C16-C17	3.83	119.77	111.48
3	D	809	PX2	O7-C16-C17	3.83	119.76	111.48
3	C	809	PX2	O7-C16-C17	3.81	119.72	111.48
3	B	809	PX2	O7-C16-C17	3.80	119.71	111.48
2	C	801	CPL	O3-C11-C12	3.35	122.06	111.83
2	A	801	CPL	O3-C11-C12	3.35	122.04	111.83
2	B	801	CPL	O3-C11-C12	3.34	122.02	111.83
2	D	801	CPL	O3-C11-C12	3.34	122.02	111.83
3	B	809	PX2	O5-C4-C5	3.16	121.47	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	809	PX2	O5-C4-C5	3.16	121.46	111.83
3	A	809	PX2	O5-C4-C5	3.14	121.42	111.83
3	D	809	PX2	O5-C4-C5	3.14	121.42	111.83
2	B	802	CPL	O3-C11-C12	3.01	121.01	111.83
2	D	802	CPL	O3-C11-C12	3.01	121.00	111.83
2	A	802	CPL	O3-C11-C12	3.00	120.98	111.83
2	C	802	CPL	O3-C11-C12	2.99	120.96	111.83
3	B	803	PX2	O5-C4-C5	2.85	120.51	111.83
3	D	803	PX2	O5-C4-C5	2.83	120.47	111.83
3	A	803	PX2	O5-C4-C5	2.83	120.46	111.83
3	C	803	PX2	O5-C4-C5	2.83	120.46	111.83
3	D	803	PX2	C3-C2-C1	-2.23	106.59	111.78
3	C	803	PX2	C3-C2-C1	-2.23	106.60	111.78
3	B	803	PX2	C3-C2-C1	-2.22	106.61	111.78
3	A	803	PX2	C3-C2-C1	-2.21	106.64	111.78

There are no chirality outliers.

All (333) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	CPL	O4P-C4-C5-N
2	A	801	CPL	C32-C31-O2-C2
2	A	801	CPL	C1-O3P-P-O1P
2	A	801	CPL	C1-O3P-P-O2P
2	A	801	CPL	C1-O3P-P-O4P
2	A	801	CPL	C4-O4P-P-O1P
2	A	801	CPL	C4-O4P-P-O3P
2	A	802	CPL	O31-C31-O2-C2
2	A	802	CPL	C4-O4P-P-O1P
2	A	802	CPL	C4-O4P-P-O2P
2	A	802	CPL	C4-O4P-P-O3P
2	B	801	CPL	O4P-C4-C5-N
2	B	801	CPL	C32-C31-O2-C2
2	B	801	CPL	C1-O3P-P-O1P
2	B	801	CPL	C1-O3P-P-O2P
2	B	801	CPL	C1-O3P-P-O4P
2	B	801	CPL	C4-O4P-P-O1P
2	B	801	CPL	C4-O4P-P-O3P
2	B	802	CPL	O31-C31-O2-C2
2	B	802	CPL	C4-O4P-P-O1P
2	B	802	CPL	C4-O4P-P-O2P
2	B	802	CPL	C4-O4P-P-O3P

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Mol	Chain	Res	Type	Atoms
2	C	801	CPL	O4P-C4-C5-N
2	C	801	CPL	C32-C31-O2-C2
2	C	801	CPL	C1-O3P-P-O1P
2	C	801	CPL	C1-O3P-P-O2P
2	C	801	CPL	C1-O3P-P-O4P
2	C	801	CPL	C4-O4P-P-O1P
2	C	801	CPL	C4-O4P-P-O3P
2	C	802	CPL	O31-C31-O2-C2
2	C	802	CPL	C4-O4P-P-O1P
2	C	802	CPL	C4-O4P-P-O2P
2	C	802	CPL	C4-O4P-P-O3P
2	D	801	CPL	O4P-C4-C5-N
2	D	801	CPL	C32-C31-O2-C2
2	D	801	CPL	C1-O3P-P-O1P
2	D	801	CPL	C1-O3P-P-O2P
2	D	801	CPL	C1-O3P-P-O4P
2	D	801	CPL	C4-O4P-P-O1P
2	D	801	CPL	C4-O4P-P-O3P
2	D	802	CPL	O31-C31-O2-C2
2	D	802	CPL	C4-O4P-P-O1P
2	D	802	CPL	C4-O4P-P-O2P
2	D	802	CPL	C4-O4P-P-O3P
2	A	801	CPL	O31-C31-O2-C2
2	B	801	CPL	O31-C31-O2-C2
2	C	801	CPL	O31-C31-O2-C2
2	D	801	CPL	O31-C31-O2-C2
2	A	802	CPL	C32-C31-O2-C2
2	B	802	CPL	C32-C31-O2-C2
2	C	802	CPL	C32-C31-O2-C2
2	D	802	CPL	C32-C31-O2-C2
3	A	803	PX2	C17-C16-O7-C2
3	B	803	PX2	C17-C16-O7-C2
3	C	803	PX2	C17-C16-O7-C2
3	D	803	PX2	C17-C16-O7-C2
3	A	803	PX2	O8-C16-O7-C2
3	B	803	PX2	O8-C16-O7-C2
3	C	803	PX2	O8-C16-O7-C2
3	D	803	PX2	O8-C16-O7-C2
2	A	802	CPL	C12-C11-O3-C3
2	B	802	CPL	C12-C11-O3-C3
2	C	802	CPL	C12-C11-O3-C3
2	D	802	CPL	C12-C11-O3-C3

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Mol	Chain	Res	Type	Atoms
2	A	802	CPL	O11-C11-O3-C3
2	C	802	CPL	O11-C11-O3-C3
2	B	802	CPL	O11-C11-O3-C3
2	D	802	CPL	O11-C11-O3-C3
3	A	809	PX2	C5-C4-O5-C3
3	B	809	PX2	C5-C4-O5-C3
3	C	809	PX2	C5-C4-O5-C3
3	D	809	PX2	C5-C4-O5-C3
2	A	802	CPL	C11-C12-C13-C14
2	B	802	CPL	C11-C12-C13-C14
2	C	802	CPL	C11-C12-C13-C14
2	D	802	CPL	C11-C12-C13-C14
2	A	806	CPL	C19-C20-C21-C22
2	B	806	CPL	C19-C20-C21-C22
2	C	806	CPL	C19-C20-C21-C22
2	D	806	CPL	C19-C20-C21-C22
3	A	809	PX2	C4-C5-C6-C7
3	B	809	PX2	C4-C5-C6-C7
3	C	809	PX2	C4-C5-C6-C7
3	D	809	PX2	C4-C5-C6-C7
3	A	809	PX2	O6-C4-O5-C3
3	B	809	PX2	O6-C4-O5-C3
3	C	809	PX2	O6-C4-O5-C3
3	D	809	PX2	O6-C4-O5-C3
3	A	809	PX2	O8-C16-O7-C2
3	B	809	PX2	O8-C16-O7-C2
3	C	809	PX2	O8-C16-O7-C2
3	D	809	PX2	O8-C16-O7-C2
3	A	809	PX2	C17-C16-O7-C2
3	B	809	PX2	C17-C16-O7-C2
3	C	809	PX2	C17-C16-O7-C2
3	D	809	PX2	C17-C16-O7-C2
2	A	801	CPL	C1-C2-O2-C31
2	B	801	CPL	C1-C2-O2-C31
2	C	801	CPL	C1-C2-O2-C31
2	D	801	CPL	C1-C2-O2-C31
2	A	808	CPL	C13-C14-C15-C16
2	B	808	CPL	C13-C14-C15-C16
2	C	808	CPL	C13-C14-C15-C16
2	D	808	CPL	C13-C14-C15-C16
3	A	803	PX2	C5-C6-C7-C8
3	B	803	PX2	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
3	C	803	PX2	C5-C6-C7-C8
3	D	803	PX2	C5-C6-C7-C8
2	A	808	CPL	C17-C18-C19-C20
2	B	808	CPL	C17-C18-C19-C20
2	C	808	CPL	C17-C18-C19-C20
2	D	808	CPL	C17-C18-C19-C20
2	A	801	CPL	C31-C32-C33-C34
2	B	801	CPL	C31-C32-C33-C34
2	C	801	CPL	C31-C32-C33-C34
2	D	801	CPL	C31-C32-C33-C34
2	A	802	CPL	C19-C20-C21-C22
2	C	802	CPL	C19-C20-C21-C22
2	D	802	CPL	C19-C20-C21-C22
2	B	802	CPL	C19-C20-C21-C22
2	A	802	CPL	C34-C35-C36-C37
2	B	802	CPL	C34-C35-C36-C37
2	C	802	CPL	C34-C35-C36-C37
2	D	802	CPL	C34-C35-C36-C37
2	A	802	CPL	C15-C16-C17-C18
2	B	802	CPL	C15-C16-C17-C18
2	C	802	CPL	C15-C16-C17-C18
2	D	802	CPL	C15-C16-C17-C18
2	A	802	CPL	C32-C33-C34-C35
2	C	802	CPL	C32-C33-C34-C35
2	D	802	CPL	C32-C33-C34-C35
2	B	802	CPL	C32-C33-C34-C35
2	A	802	CPL	C31-C32-C33-C34
2	B	802	CPL	C31-C32-C33-C34
2	C	802	CPL	C31-C32-C33-C34
2	D	802	CPL	C31-C32-C33-C34
2	A	807	CPL	C19-C20-C21-C22
2	B	807	CPL	C19-C20-C21-C22
2	C	807	CPL	C19-C20-C21-C22
2	D	807	CPL	C19-C20-C21-C22
2	A	802	CPL	C36-C37-C38-C39
2	B	802	CPL	C36-C37-C38-C39
2	C	802	CPL	C36-C37-C38-C39
2	D	802	CPL	C36-C37-C38-C39
2	A	807	CPL	C12-C13-C14-C15
2	B	807	CPL	C12-C13-C14-C15
2	C	807	CPL	C12-C13-C14-C15
2	D	807	CPL	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
2	A	802	CPL	C18-C19-C20-C21
2	B	802	CPL	C18-C19-C20-C21
2	C	802	CPL	C18-C19-C20-C21
2	D	802	CPL	C18-C19-C20-C21
2	A	801	CPL	C21-C22-C23-C24
2	B	801	CPL	C21-C22-C23-C24
2	C	801	CPL	C21-C22-C23-C24
2	D	801	CPL	C21-C22-C23-C24
2	B	806	CPL	C17-C18-C19-C20
2	D	806	CPL	C17-C18-C19-C20
2	A	806	CPL	C17-C18-C19-C20
2	C	806	CPL	C17-C18-C19-C20
3	A	809	PX2	O4-C1-C2-C3
3	B	809	PX2	O4-C1-C2-C3
3	C	809	PX2	O4-C1-C2-C3
3	D	809	PX2	O4-C1-C2-C3
2	B	808	CPL	C14-C15-C16-C17
2	C	808	CPL	C14-C15-C16-C17
2	A	808	CPL	C14-C15-C16-C17
2	D	808	CPL	C14-C15-C16-C17
3	A	803	PX2	C5-C4-O5-C3
3	B	803	PX2	C5-C4-O5-C3
3	C	803	PX2	C5-C4-O5-C3
3	D	803	PX2	C5-C4-O5-C3
2	A	802	CPL	C12-C13-C14-C15
2	B	801	CPL	C18-C19-C20-C21
2	C	801	CPL	C18-C19-C20-C21
2	D	801	CPL	C18-C19-C20-C21
2	A	801	CPL	C18-C19-C20-C21
2	B	802	CPL	C12-C13-C14-C15
2	C	802	CPL	C12-C13-C14-C15
2	D	802	CPL	C12-C13-C14-C15
2	B	801	CPL	C12-C13-C14-C15
2	A	801	CPL	C12-C13-C14-C15
2	C	801	CPL	C12-C13-C14-C15
2	D	801	CPL	C12-C13-C14-C15
3	A	809	PX2	C3-C2-O7-C16
3	B	809	PX2	C3-C2-O7-C16
3	C	809	PX2	C3-C2-O7-C16
3	D	809	PX2	C3-C2-O7-C16
2	A	808	CPL	C11-C12-C13-C14
2	B	808	CPL	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
2	C	808	CPL	C11-C12-C13-C14
2	D	808	CPL	C11-C12-C13-C14
2	A	805	CPL	C12-C13-C14-C15
2	B	805	CPL	C12-C13-C14-C15
2	C	805	CPL	C12-C13-C14-C15
2	D	805	CPL	C12-C13-C14-C15
3	A	803	PX2	C2-C1-O4-P1
3	B	803	PX2	C2-C1-O4-P1
3	C	803	PX2	C2-C1-O4-P1
3	D	803	PX2	C2-C1-O4-P1
3	A	803	PX2	O6-C4-O5-C3
3	B	803	PX2	O6-C4-O5-C3
3	D	803	PX2	O6-C4-O5-C3
3	C	803	PX2	O6-C4-O5-C3
2	C	808	CPL	C12-C13-C14-C15
2	A	802	CPL	C1-C2-C3-O3
2	B	802	CPL	C1-C2-C3-O3
2	C	802	CPL	C1-C2-C3-O3
2	D	802	CPL	C1-C2-C3-O3
3	A	809	PX2	C5-C6-C7-C8
2	D	808	CPL	C12-C13-C14-C15
3	B	809	PX2	C5-C6-C7-C8
3	C	809	PX2	C5-C6-C7-C8
3	D	809	PX2	C5-C6-C7-C8
2	A	808	CPL	C12-C13-C14-C15
2	B	808	CPL	C12-C13-C14-C15
2	B	804	CPL	C15-C16-C17-C18
2	C	804	CPL	C15-C16-C17-C18
2	D	804	CPL	C15-C16-C17-C18
2	A	804	CPL	C15-C16-C17-C18
3	A	803	PX2	O7-C2-C3-O5
3	B	803	PX2	O7-C2-C3-O5
3	C	803	PX2	O7-C2-C3-O5
3	D	803	PX2	O7-C2-C3-O5
2	A	801	CPL	C39-C40-C41-C42
2	B	801	CPL	C39-C40-C41-C42
2	C	801	CPL	C39-C40-C41-C42
2	D	801	CPL	C39-C40-C41-C42
2	A	802	CPL	C35-C36-C37-C38
2	A	805	CPL	C13-C14-C15-C16
2	B	802	CPL	C35-C36-C37-C38
2	B	805	CPL	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
2	C	802	CPL	C35-C36-C37-C38
2	C	805	CPL	C13-C14-C15-C16
2	D	802	CPL	C35-C36-C37-C38
2	D	805	CPL	C13-C14-C15-C16
2	C	801	CPL	C15-C16-C17-C18
2	A	801	CPL	C15-C16-C17-C18
2	B	801	CPL	C15-C16-C17-C18
2	D	801	CPL	C15-C16-C17-C18
2	A	808	CPL	C22-C23-C24-C25
2	B	808	CPL	C22-C23-C24-C25
2	C	808	CPL	C22-C23-C24-C25
2	D	808	CPL	C22-C23-C24-C25
2	A	801	CPL	C12-C11-O3-C3
2	B	801	CPL	C12-C11-O3-C3
2	C	801	CPL	C12-C11-O3-C3
2	D	801	CPL	C12-C11-O3-C3
3	A	809	PX2	C1-C2-C3-O5
3	B	809	PX2	C1-C2-C3-O5
3	C	809	PX2	C1-C2-C3-O5
3	D	809	PX2	C1-C2-C3-O5
2	A	802	CPL	O2-C2-C3-O3
2	B	802	CPL	O2-C2-C3-O3
2	C	802	CPL	O2-C2-C3-O3
2	D	802	CPL	O2-C2-C3-O3
2	C	801	CPL	O11-C11-O3-C3
2	A	802	CPL	C21-C22-C23-C24
2	B	802	CPL	C21-C22-C23-C24
2	C	802	CPL	C21-C22-C23-C24
2	D	802	CPL	C21-C22-C23-C24
2	D	801	CPL	O11-C11-O3-C3
2	A	801	CPL	O11-C11-O3-C3
2	B	801	CPL	O11-C11-O3-C3
3	A	809	PX2	O4-C1-C2-O7
3	B	809	PX2	O4-C1-C2-O7
3	C	809	PX2	O4-C1-C2-O7
3	D	809	PX2	O4-C1-C2-O7
3	A	809	PX2	O7-C2-C3-O5
3	B	809	PX2	O7-C2-C3-O5
3	C	809	PX2	O7-C2-C3-O5
3	D	809	PX2	O7-C2-C3-O5
2	A	802	CPL	C33-C34-C35-C36
2	B	802	CPL	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
2	D	802	CPL	C33-C34-C35-C36
2	C	802	CPL	C33-C34-C35-C36
3	A	803	PX2	C6-C7-C8-C9
2	A	805	CPL	C14-C15-C16-C17
2	B	805	CPL	C14-C15-C16-C17
3	B	803	PX2	C6-C7-C8-C9
3	C	803	PX2	C6-C7-C8-C9
3	D	803	PX2	C6-C7-C8-C9
2	C	805	CPL	C14-C15-C16-C17
2	D	805	CPL	C14-C15-C16-C17
2	B	808	CPL	C19-C20-C21-C22
2	A	808	CPL	C19-C20-C21-C22
2	D	808	CPL	C19-C20-C21-C22
3	B	803	PX2	O7-C16-C17-C18
2	C	808	CPL	C19-C20-C21-C22
2	C	805	CPL	C17-C18-C19-C20
2	D	805	CPL	C17-C18-C19-C20
2	A	805	CPL	C17-C18-C19-C20
2	B	805	CPL	C17-C18-C19-C20
3	A	803	PX2	O7-C16-C17-C18
3	C	803	PX2	O7-C16-C17-C18
3	D	803	PX2	O7-C16-C17-C18
3	A	803	PX2	C1-C2-C3-O5
3	B	803	PX2	C1-C2-C3-O5
3	C	803	PX2	C1-C2-C3-O5
3	D	803	PX2	C1-C2-C3-O5
2	A	801	CPL	C40-C41-C42-C43
2	B	801	CPL	C40-C41-C42-C43
2	C	801	CPL	C40-C41-C42-C43
2	D	801	CPL	C40-C41-C42-C43
2	C	807	CPL	C14-C15-C16-C17
2	D	807	CPL	C14-C15-C16-C17
2	A	807	CPL	C14-C15-C16-C17
2	B	807	CPL	C14-C15-C16-C17
2	D	802	CPL	C14-C15-C16-C17
2	A	802	CPL	C14-C15-C16-C17
2	C	802	CPL	C14-C15-C16-C17
2	B	802	CPL	C14-C15-C16-C17
2	A	801	CPL	C37-C38-C39-C40
2	B	801	CPL	C37-C38-C39-C40
2	C	801	CPL	C37-C38-C39-C40
2	D	801	CPL	C37-C38-C39-C40

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Mol	Chain	Res	Type	Atoms
2	A	802	CPL	C20-C21-C22-C23
2	C	802	CPL	C20-C21-C22-C23
2	B	802	CPL	C20-C21-C22-C23
2	D	802	CPL	C20-C21-C22-C23
2	A	801	CPL	C14-C15-C16-C17
2	B	801	CPL	C14-C15-C16-C17
2	D	801	CPL	C14-C15-C16-C17
2	C	801	CPL	C14-C15-C16-C17
2	C	807	CPL	C21-C22-C23-C24
2	A	807	CPL	C21-C22-C23-C24
2	D	807	CPL	C21-C22-C23-C24
2	B	807	CPL	C21-C22-C23-C24
3	B	809	PX2	C17-C18-C19-C20
3	A	809	PX2	C17-C18-C19-C20
3	D	809	PX2	C17-C18-C19-C20
3	C	809	PX2	C17-C18-C19-C20
2	C	806	CPL	C12-C13-C14-C15

There are no ring outliers.

26 monomers are involved in 53 short contacts:

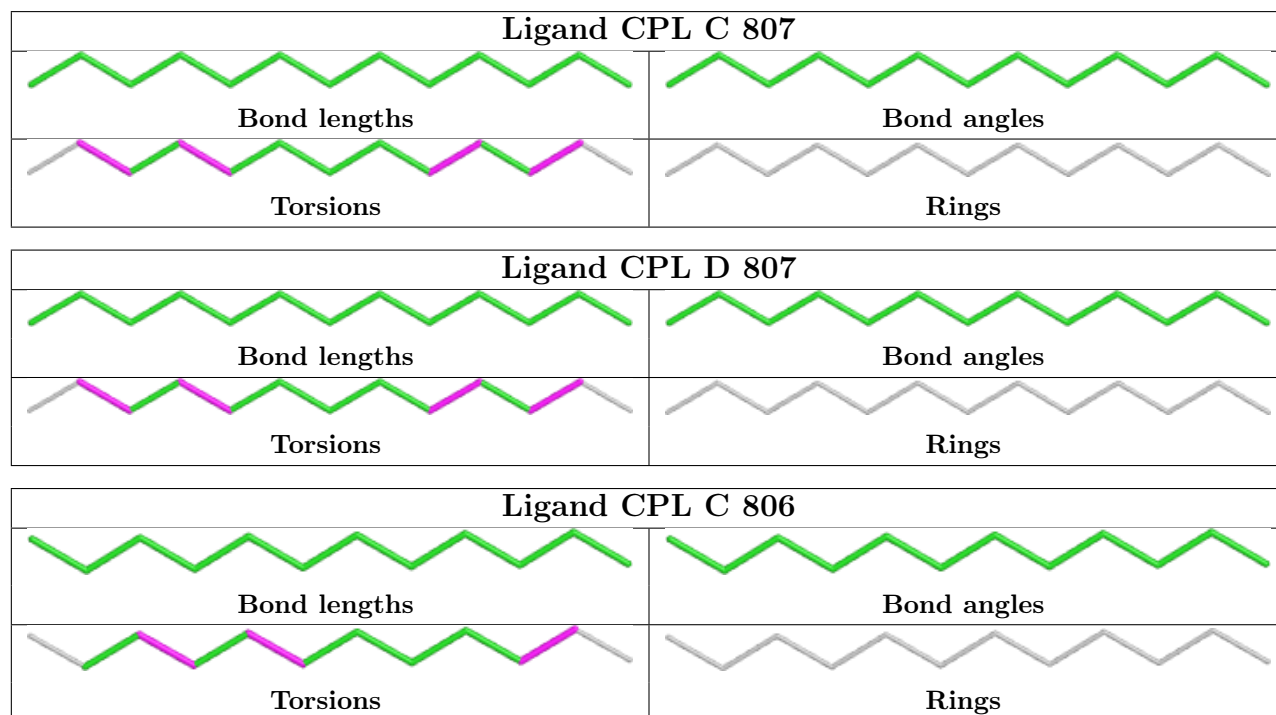
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	807	CPL	3	0
2	D	807	CPL	3	0
2	C	806	CPL	2	0
2	D	806	CPL	3	0
3	A	803	PX2	1	0
2	D	808	CPL	1	0
2	A	806	CPL	3	0
2	C	808	CPL	1	0
2	B	807	CPL	4	0
2	C	801	CPL	2	0
3	D	803	PX2	1	0
3	C	803	PX2	1	0
3	B	803	PX2	1	0
3	D	809	PX2	2	0
2	A	808	CPL	1	0
2	D	801	CPL	2	0
3	A	809	PX2	2	0
2	B	802	CPL	1	0
2	B	808	CPL	1	0
2	B	806	CPL	2	0

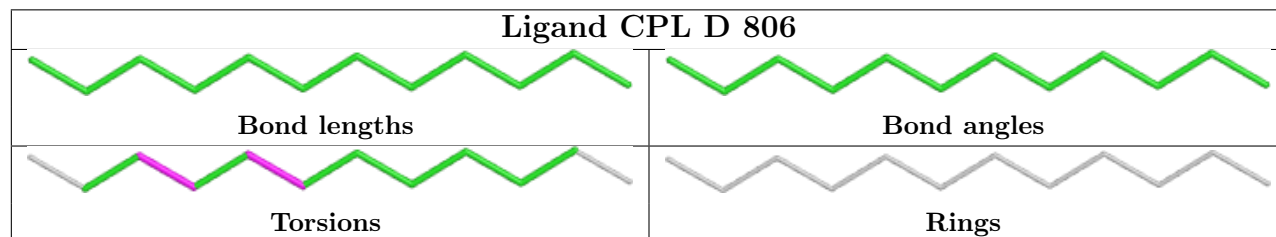
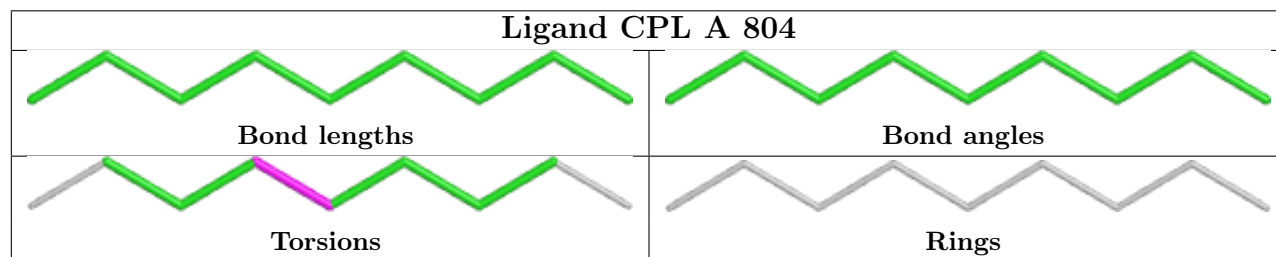
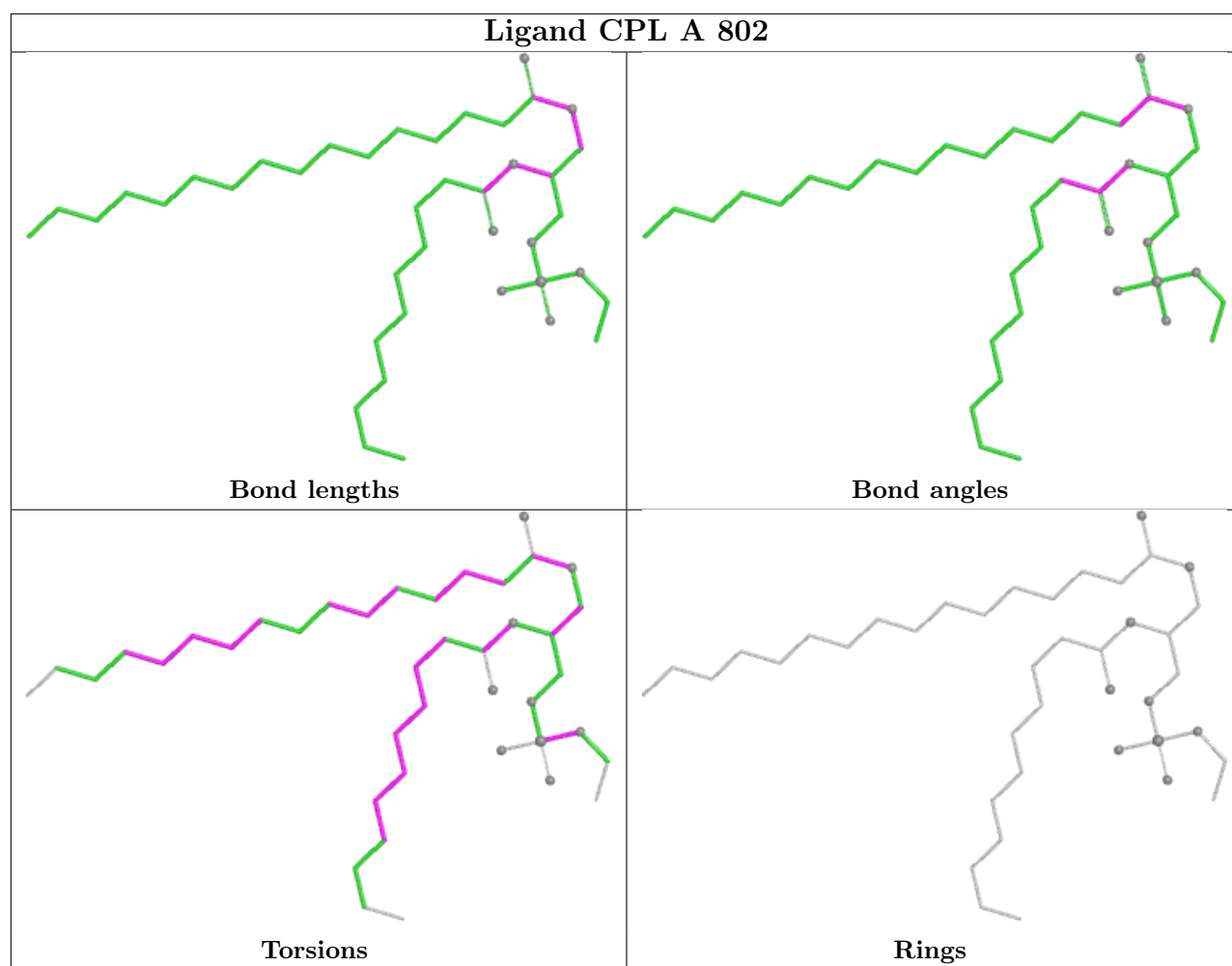
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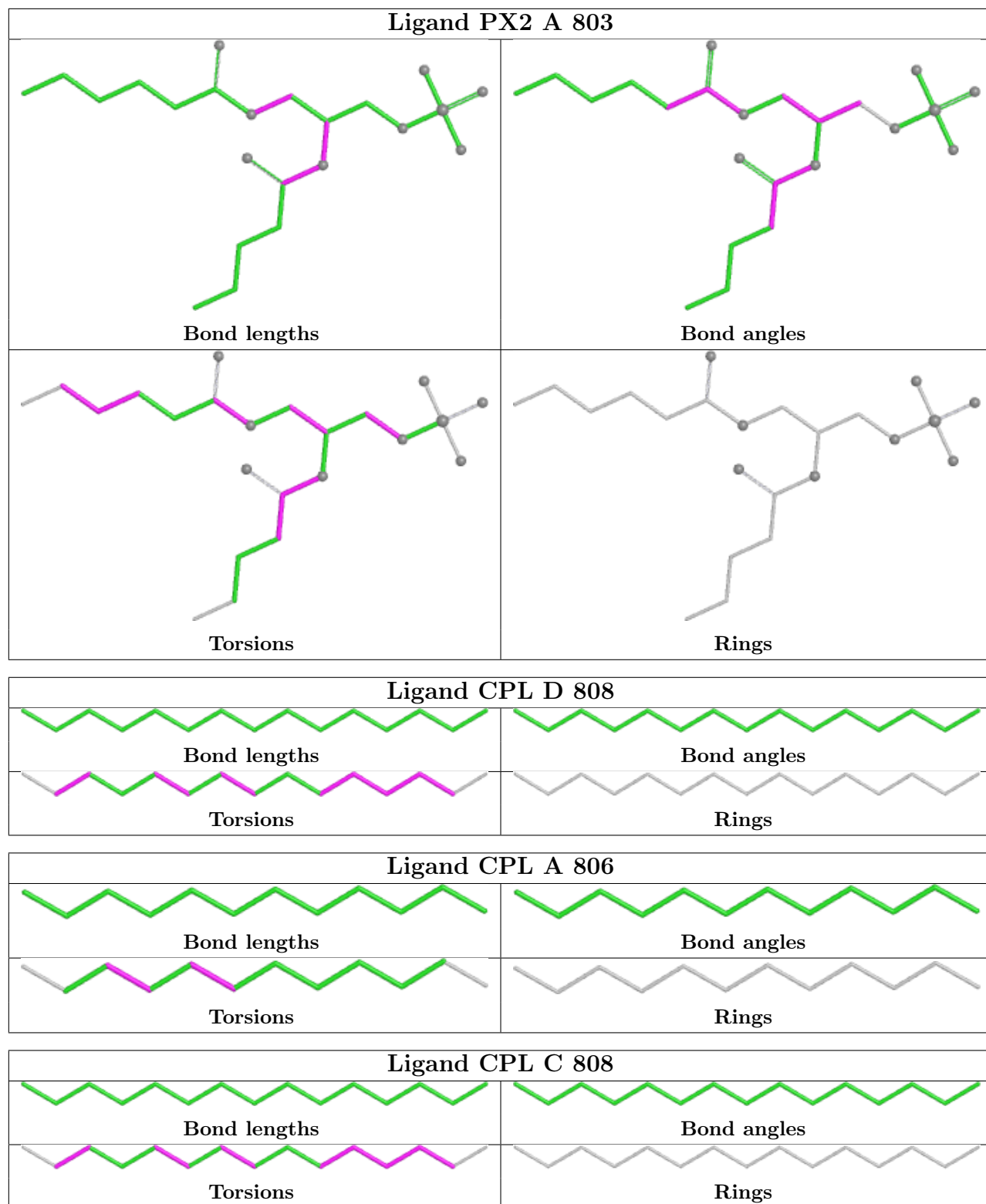
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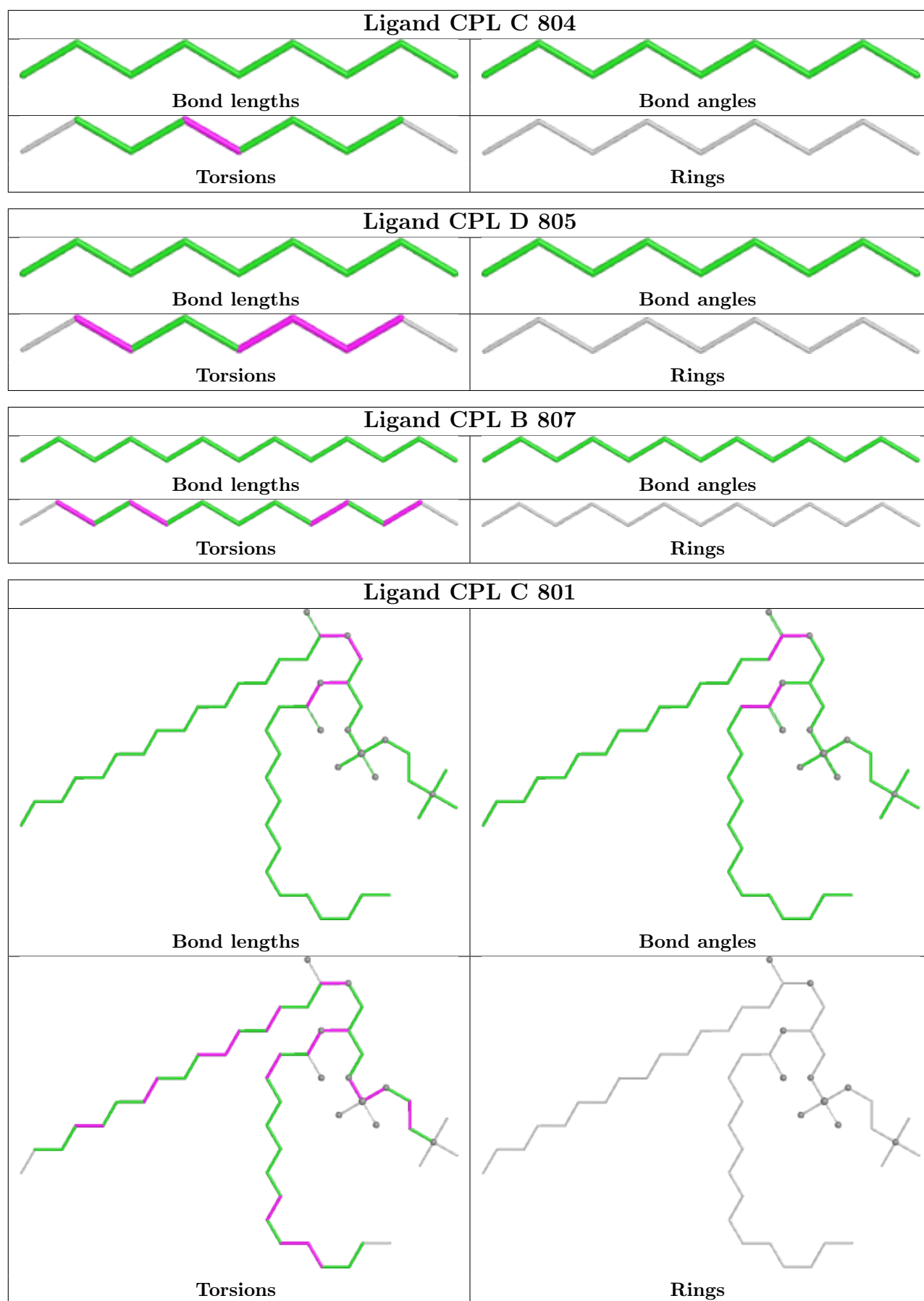
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	807	CPL	4	0
2	B	801	CPL	2	0
3	B	809	PX2	3	0
3	C	809	PX2	4	0
2	A	801	CPL	2	0
2	C	802	CPL	1	0

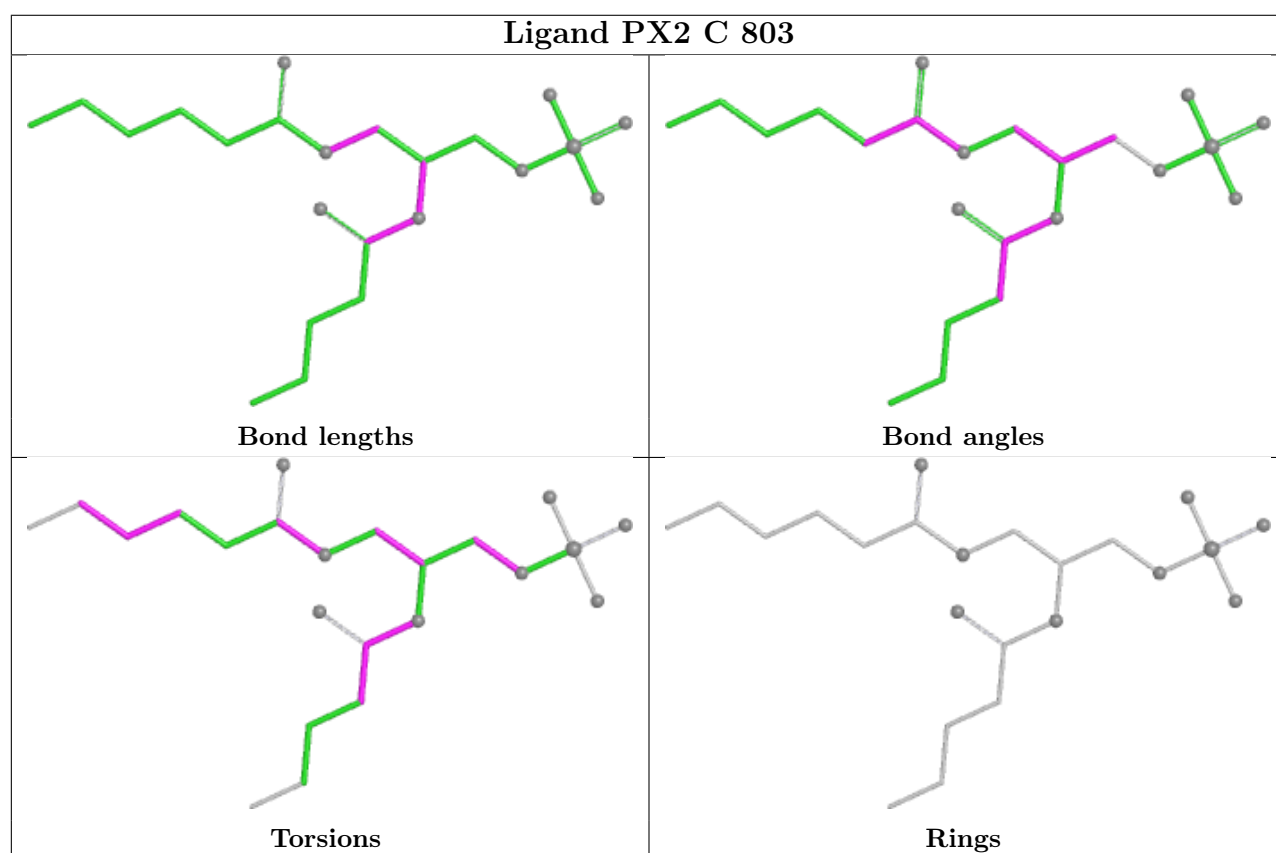
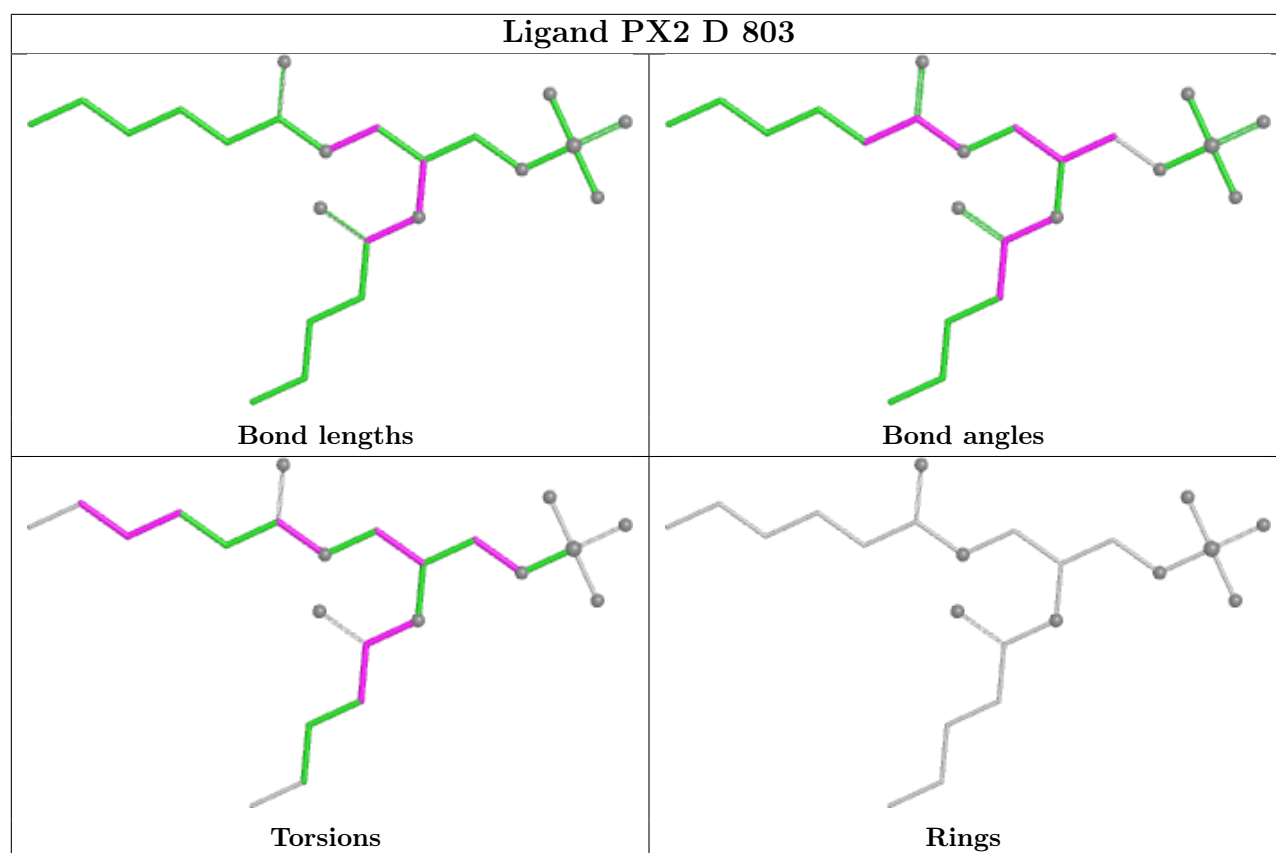
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

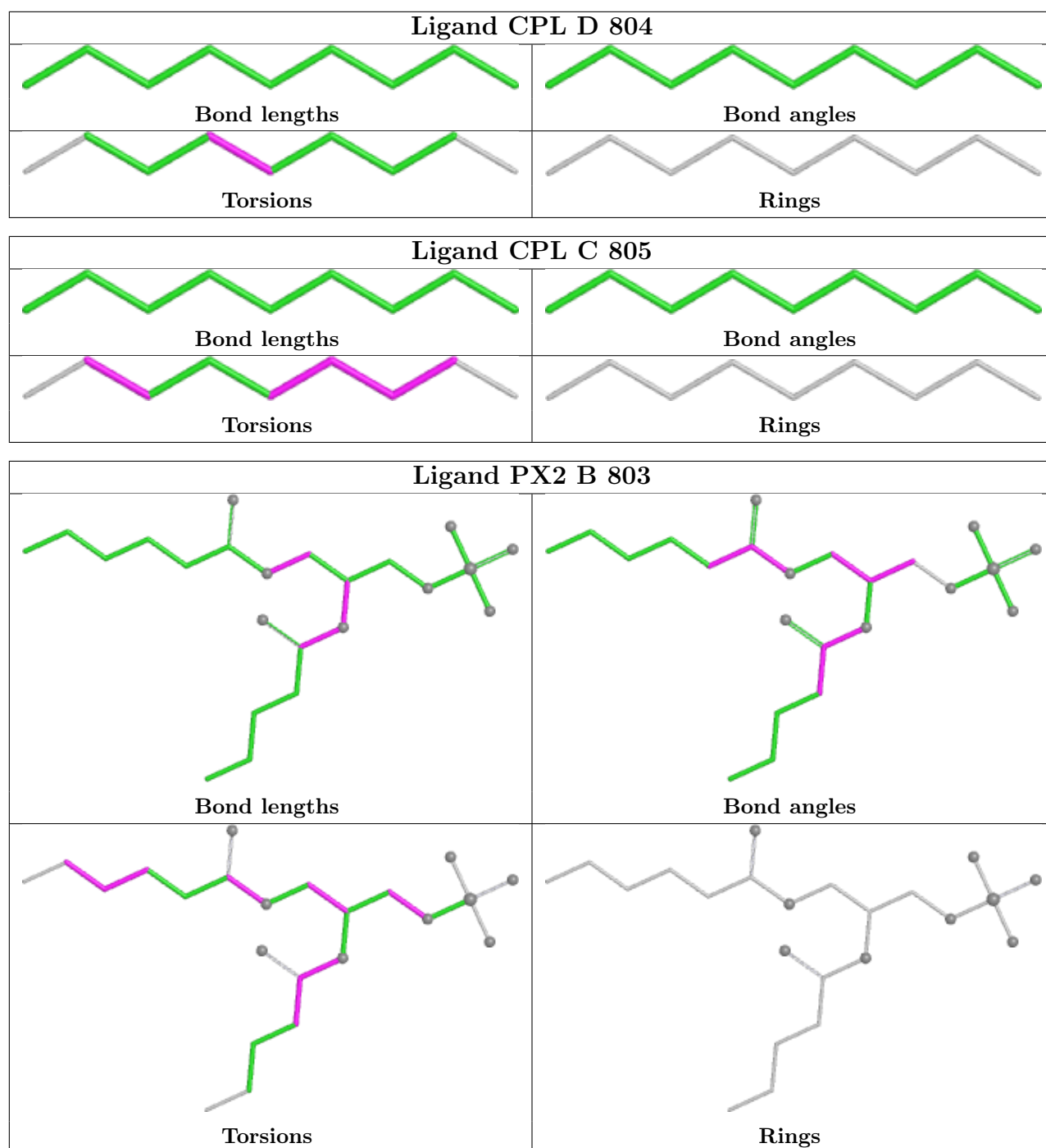


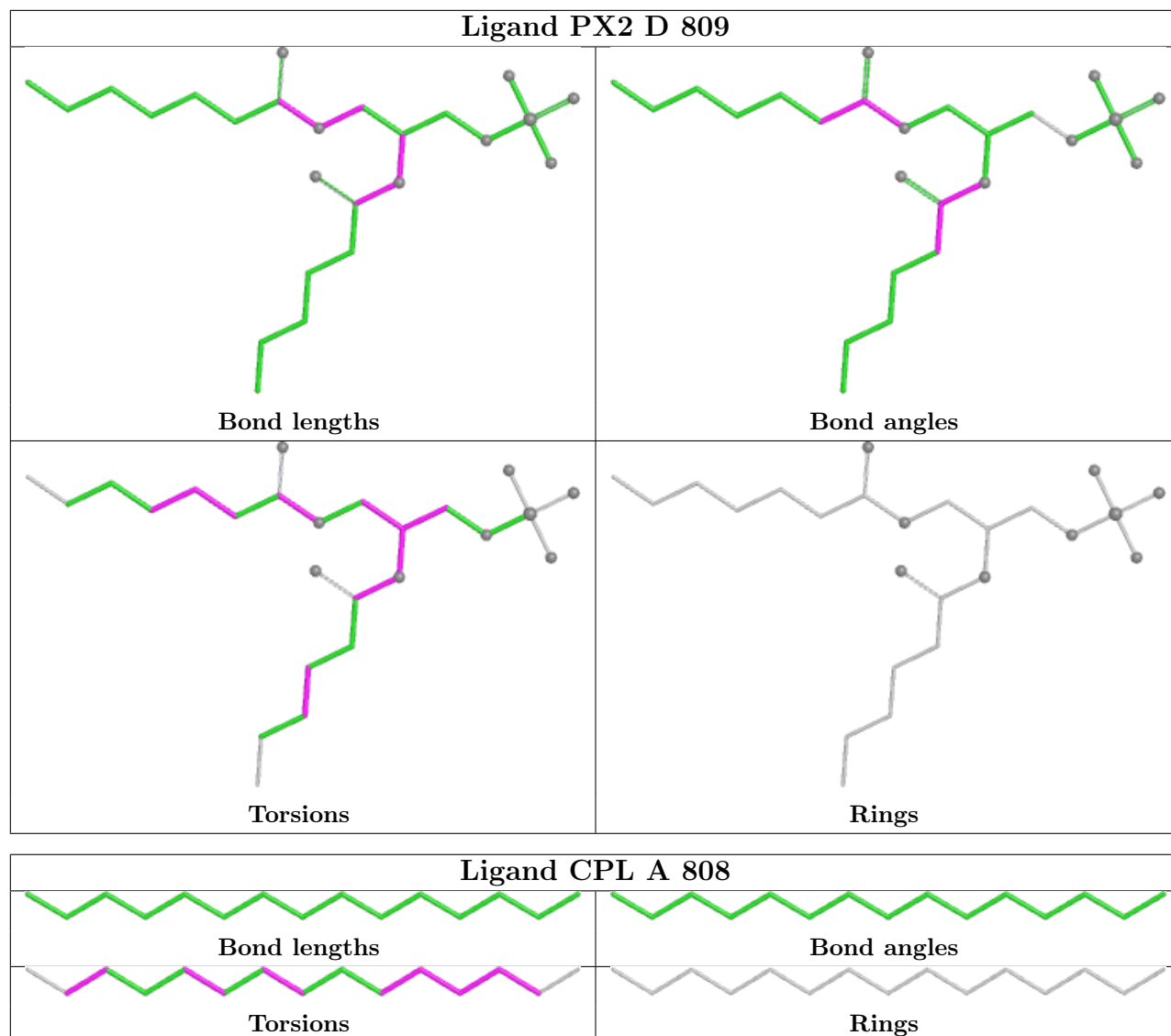


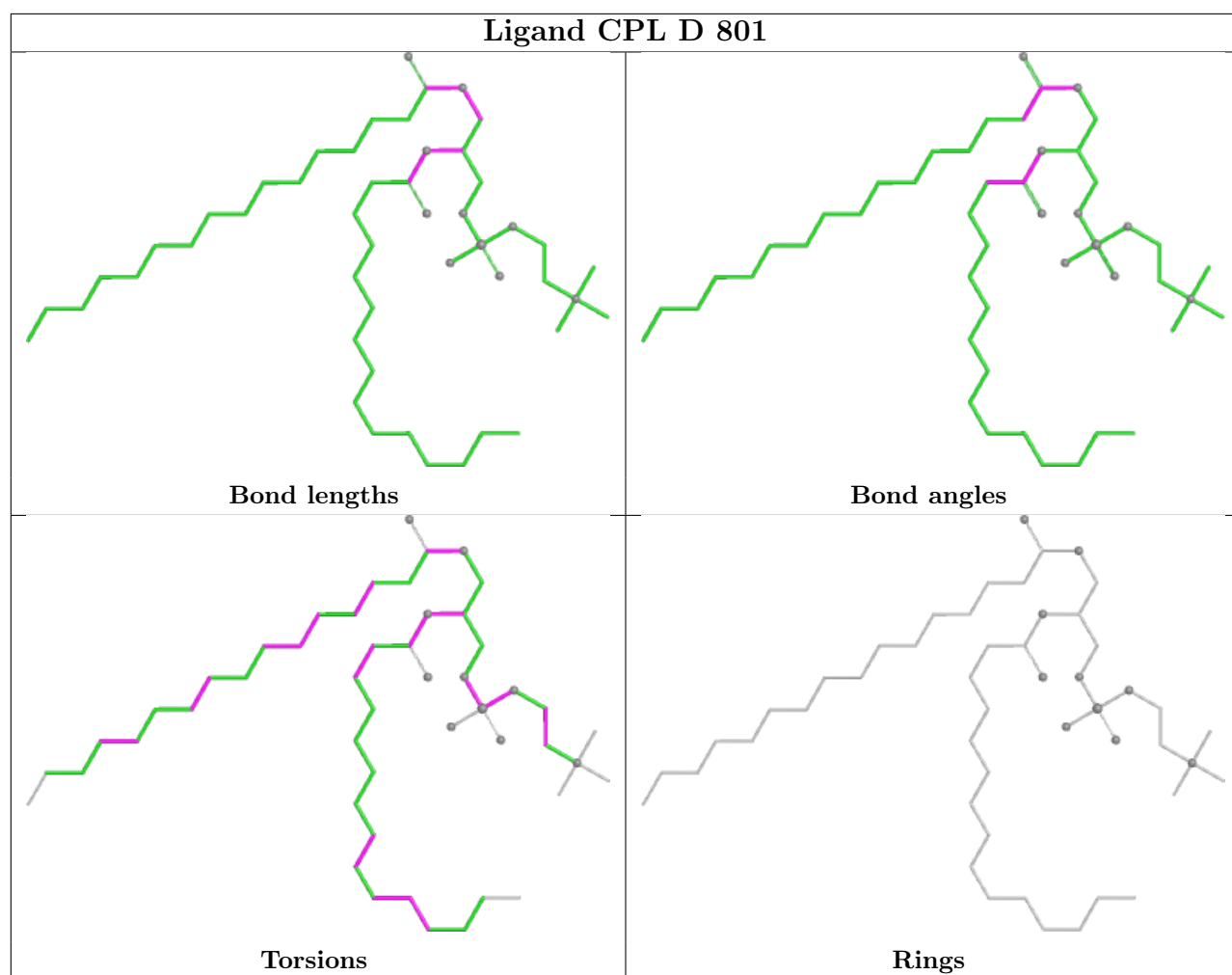


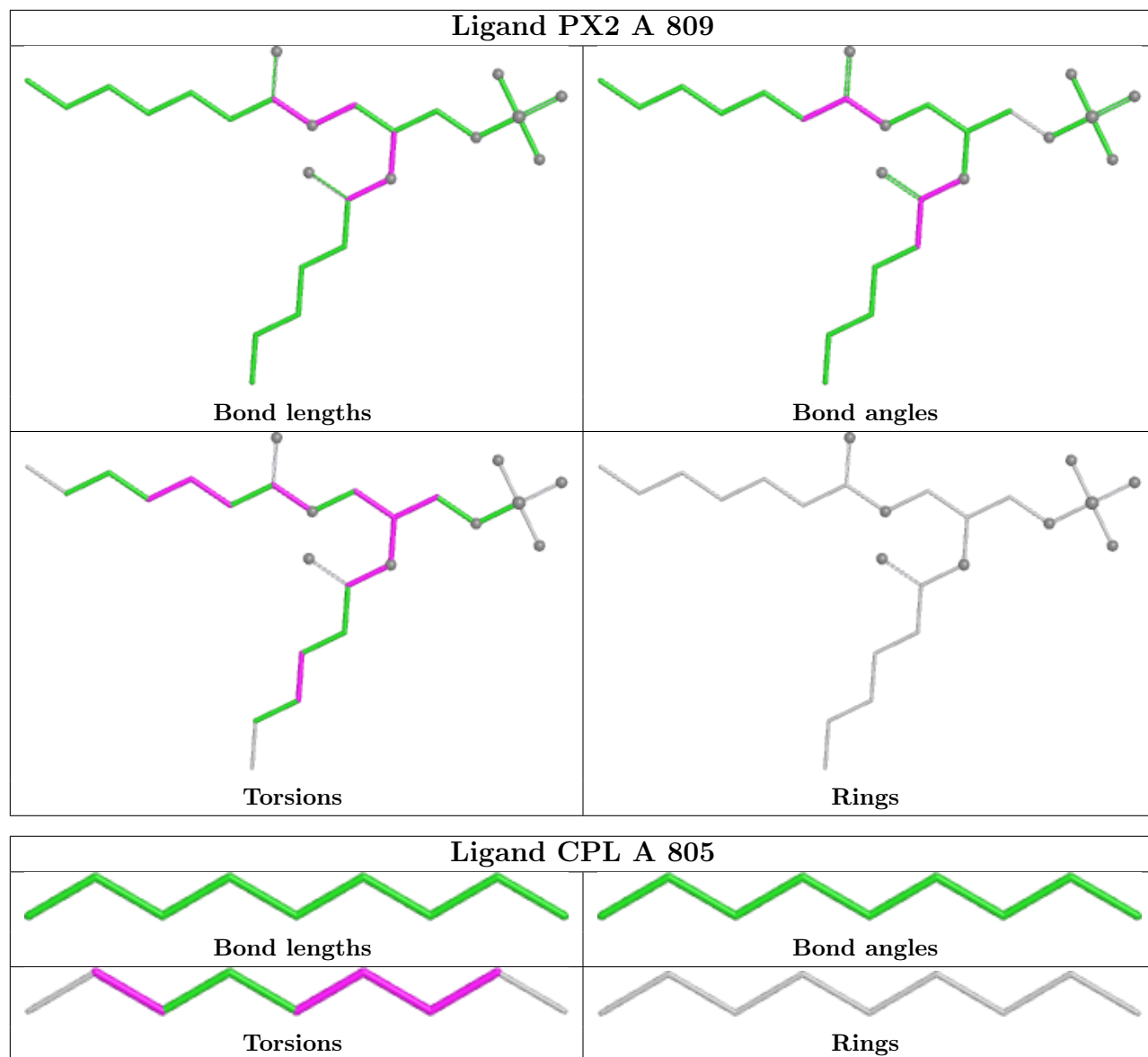


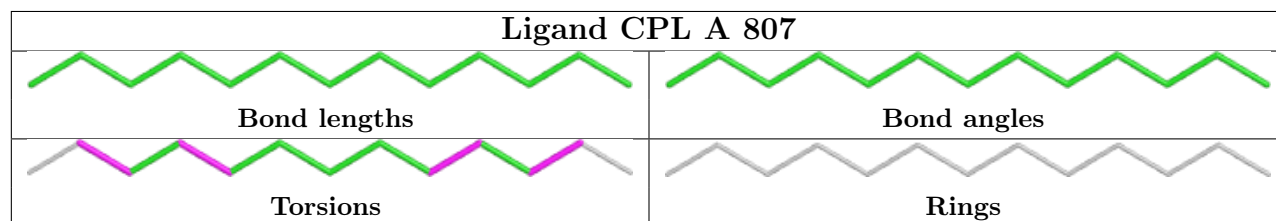
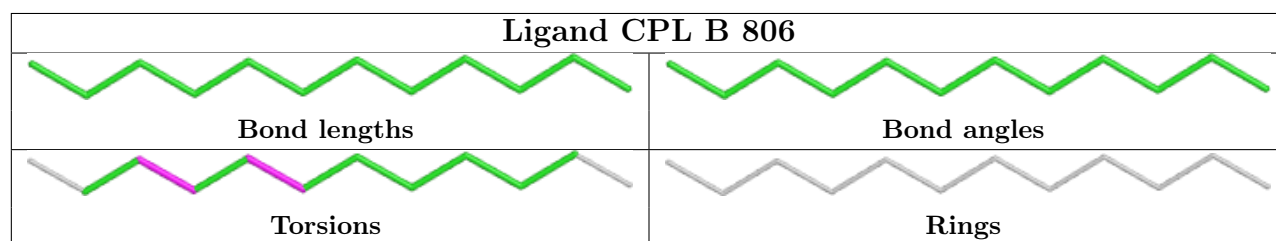
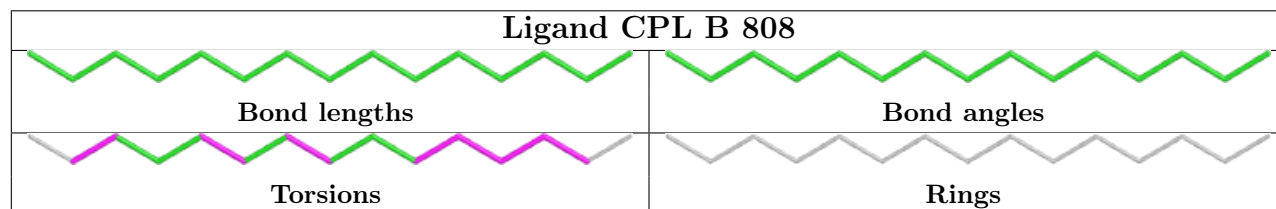
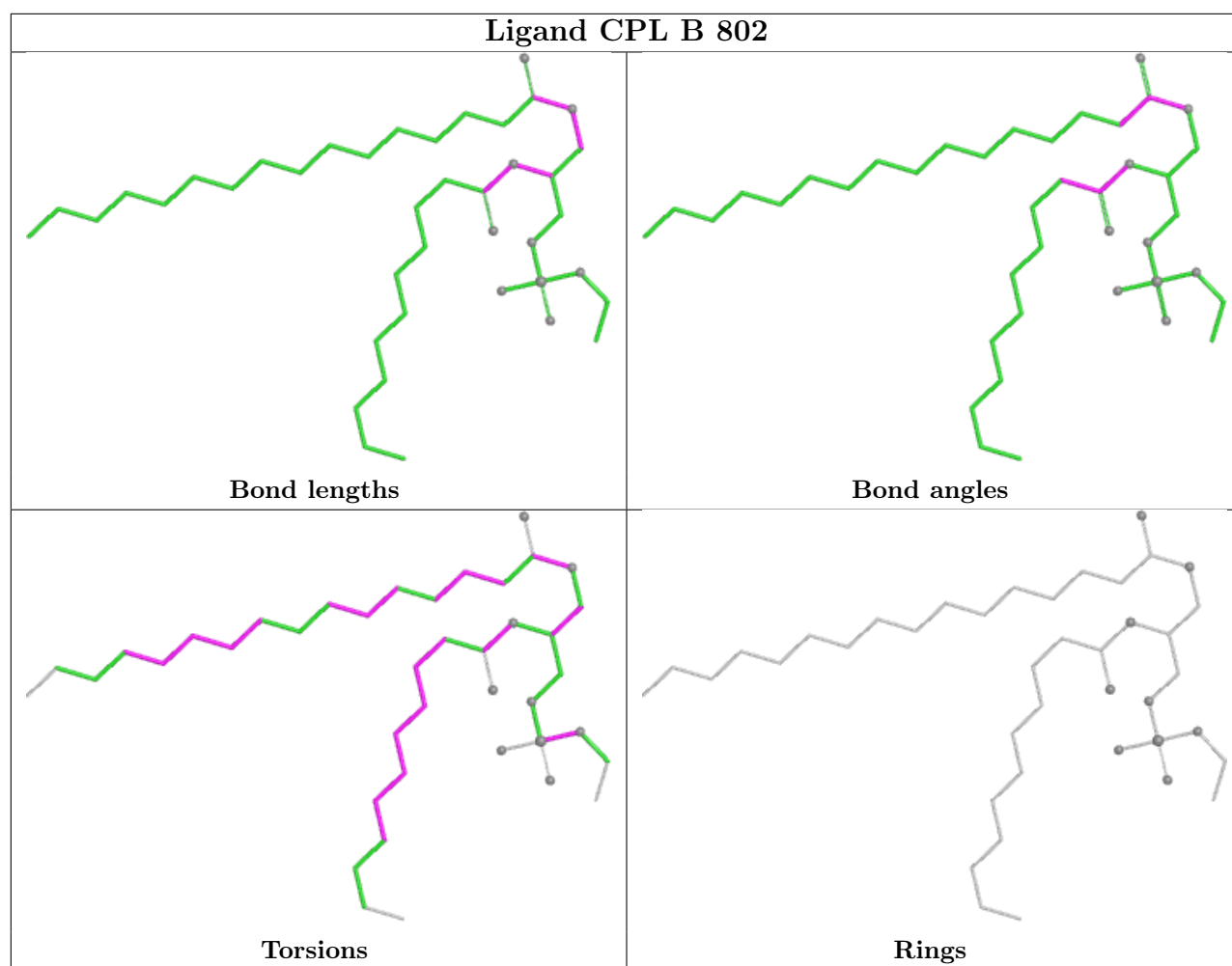


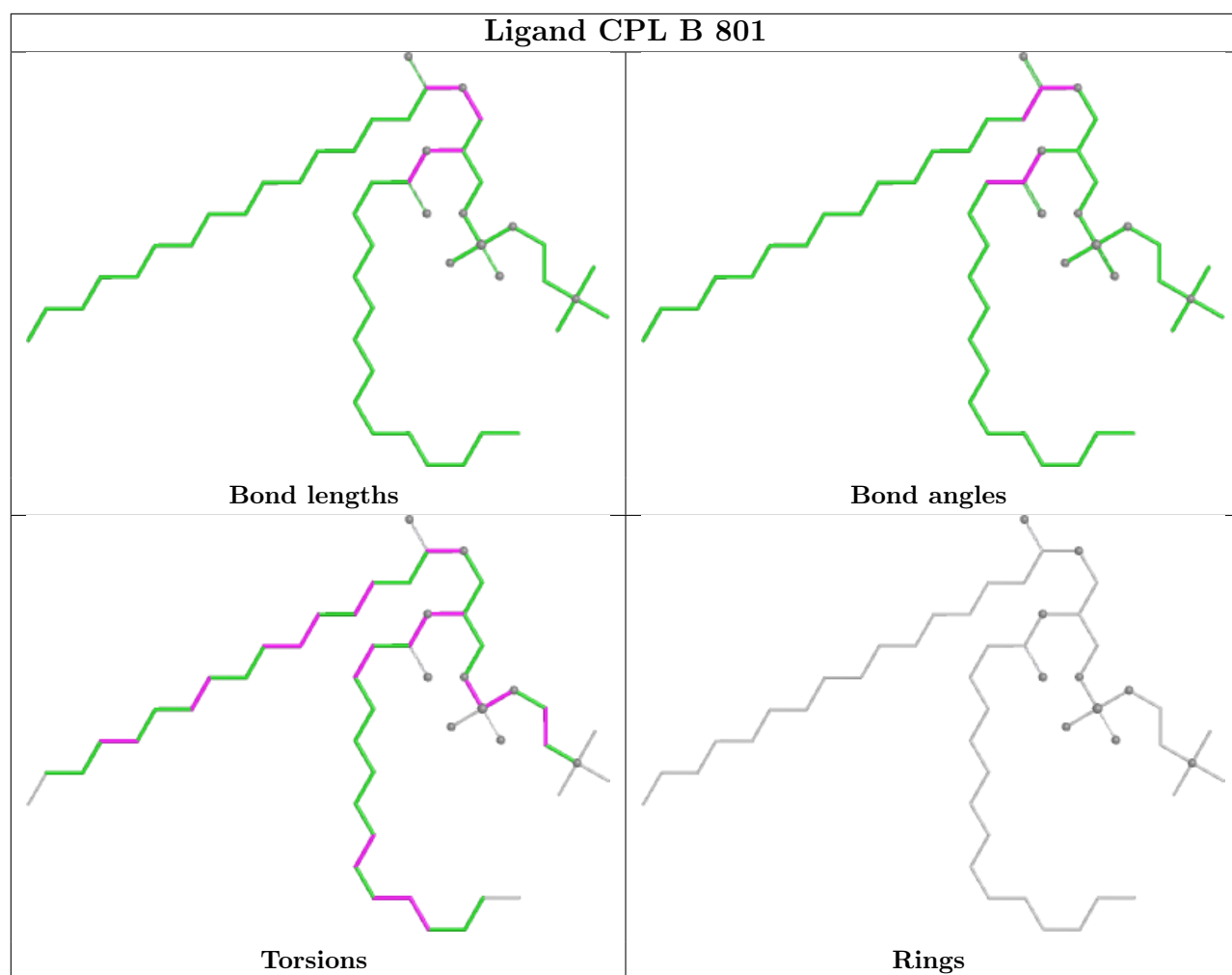


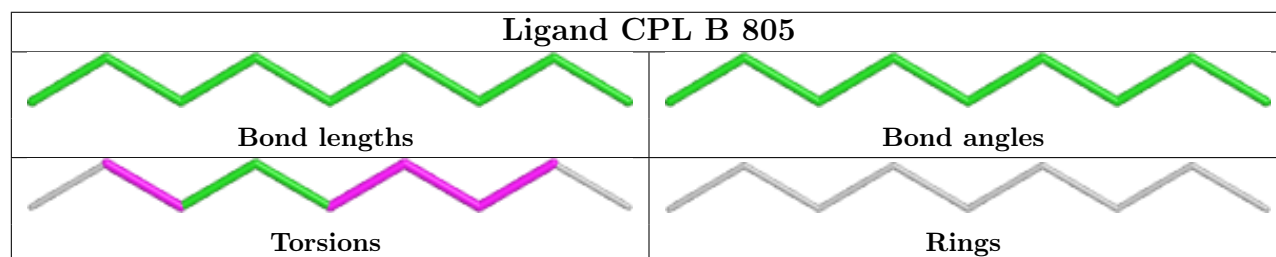
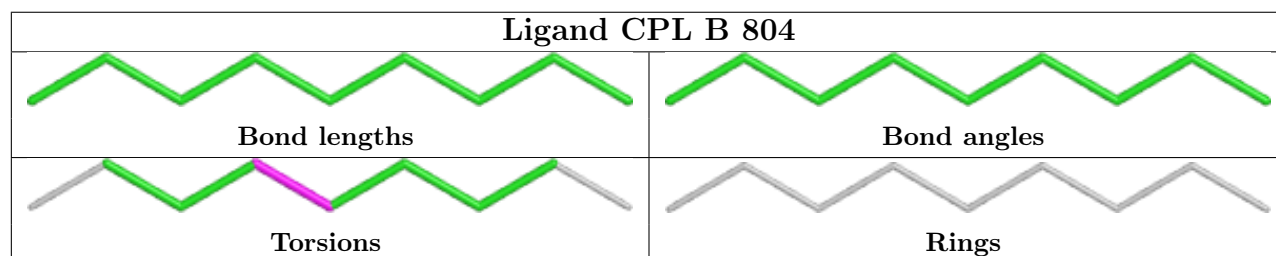
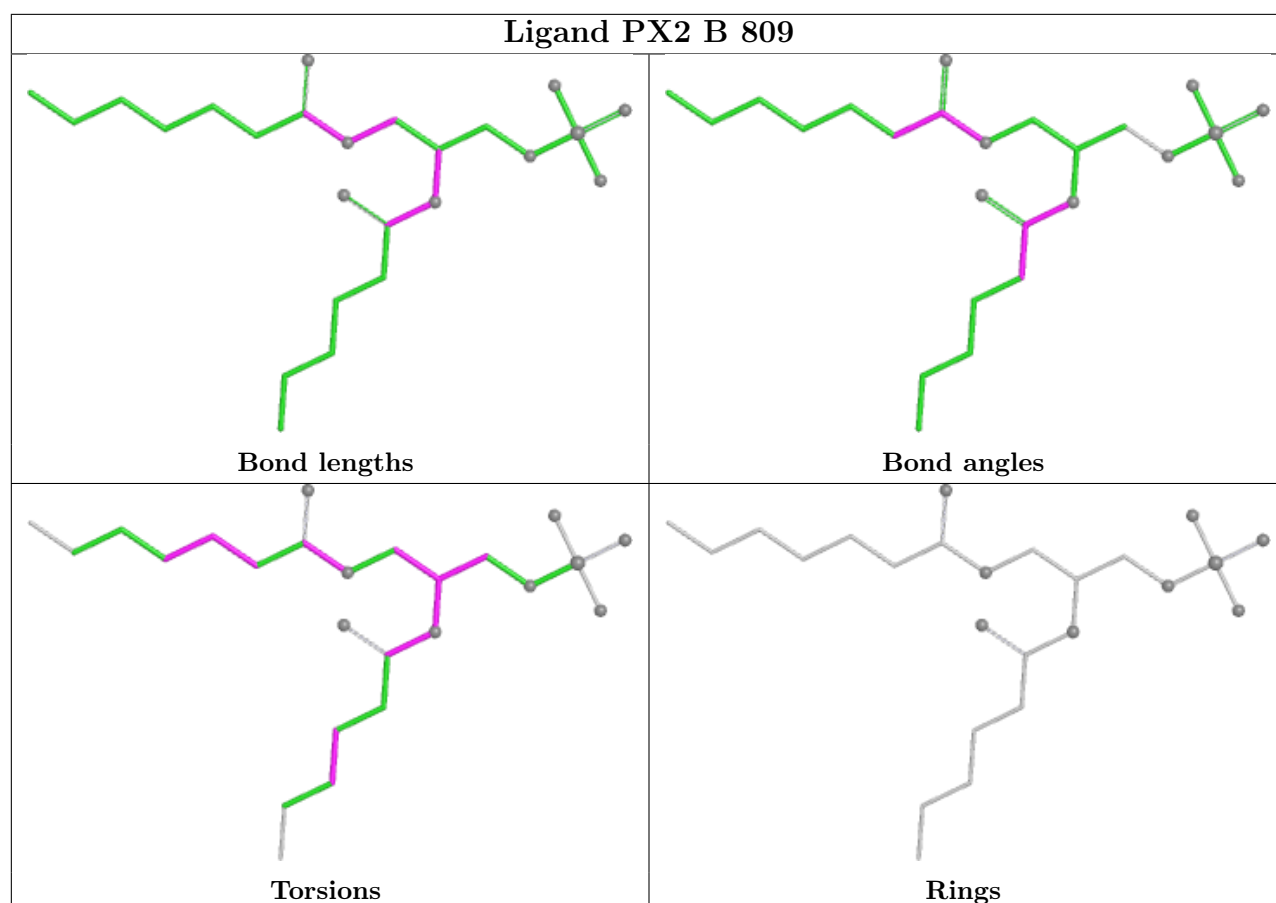


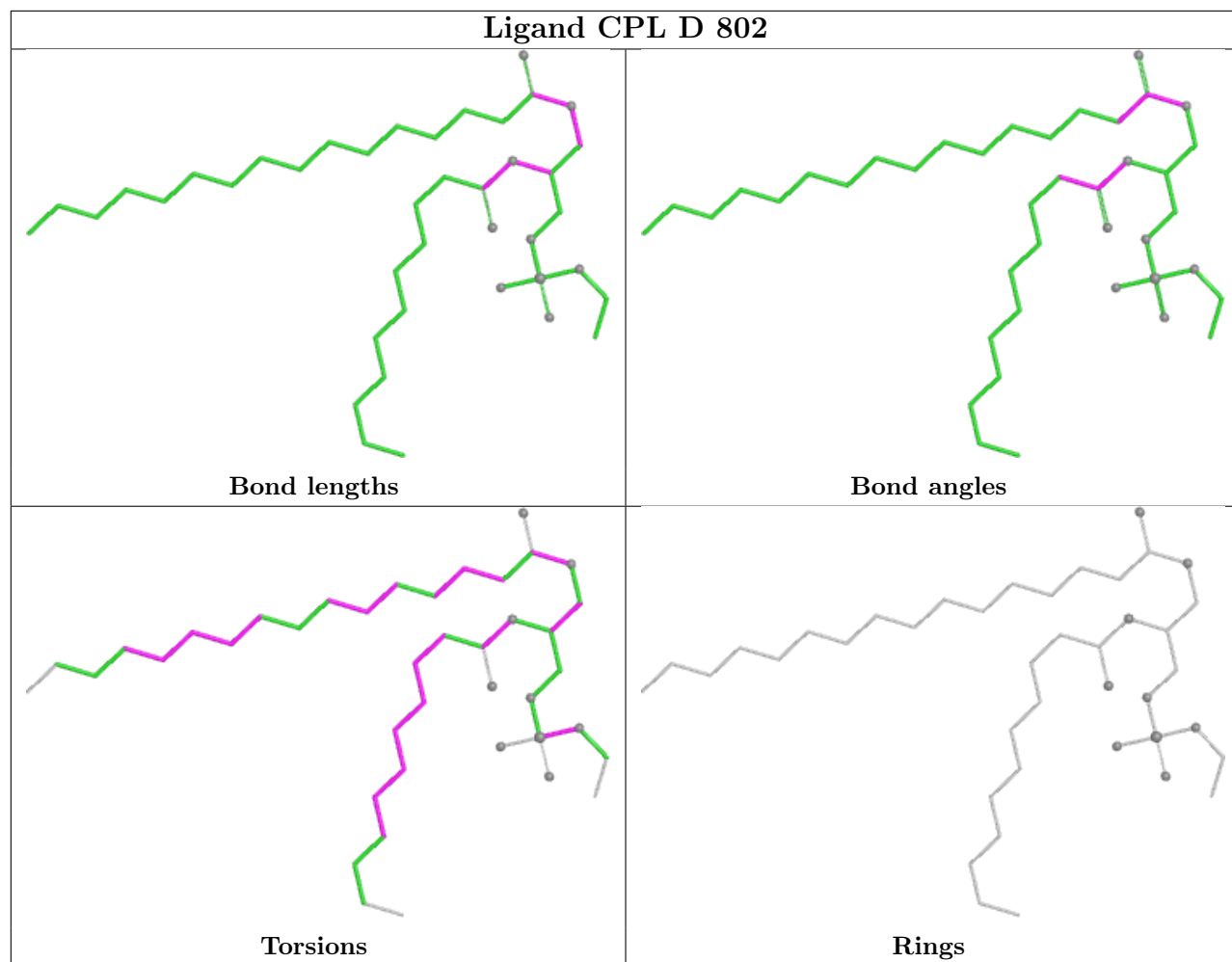


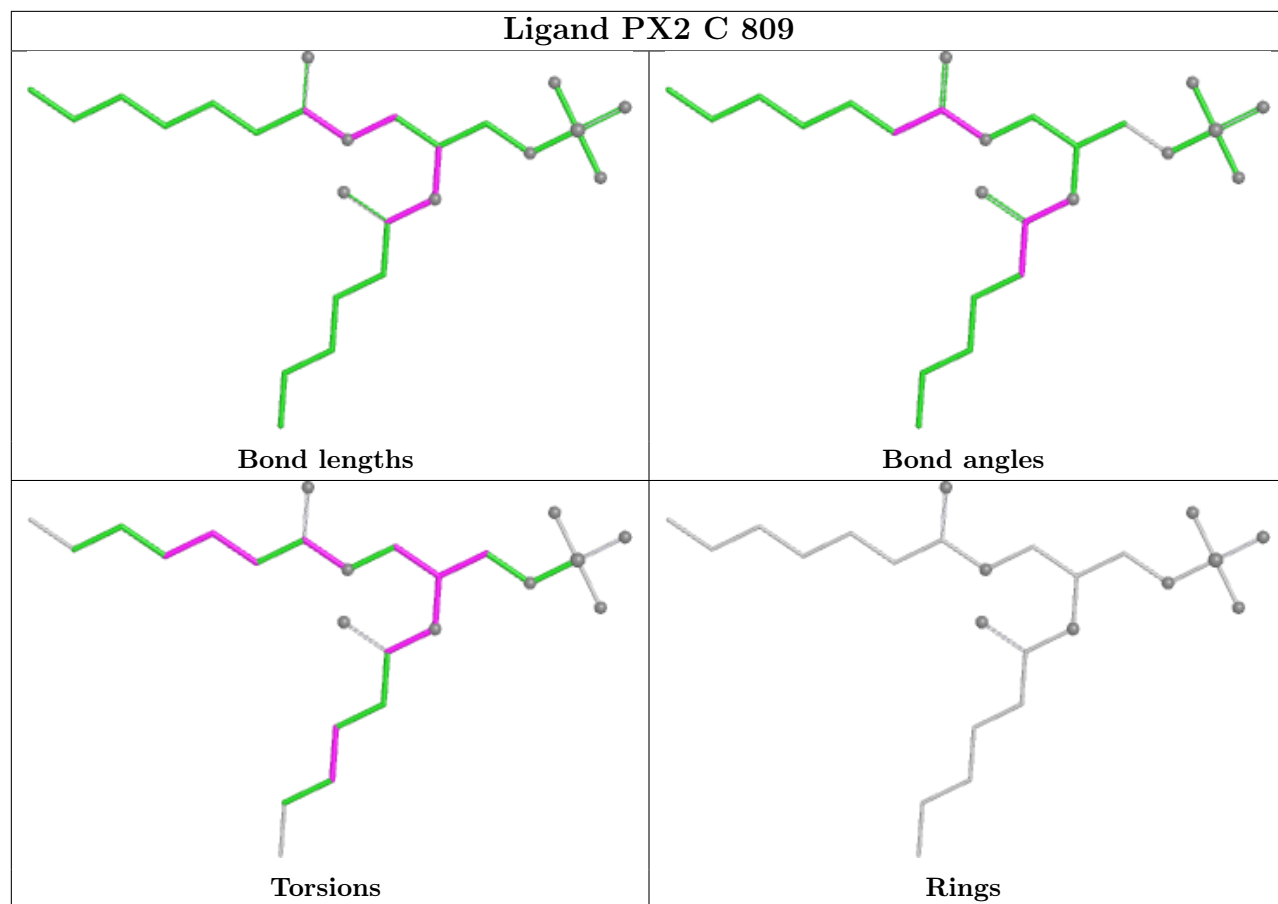


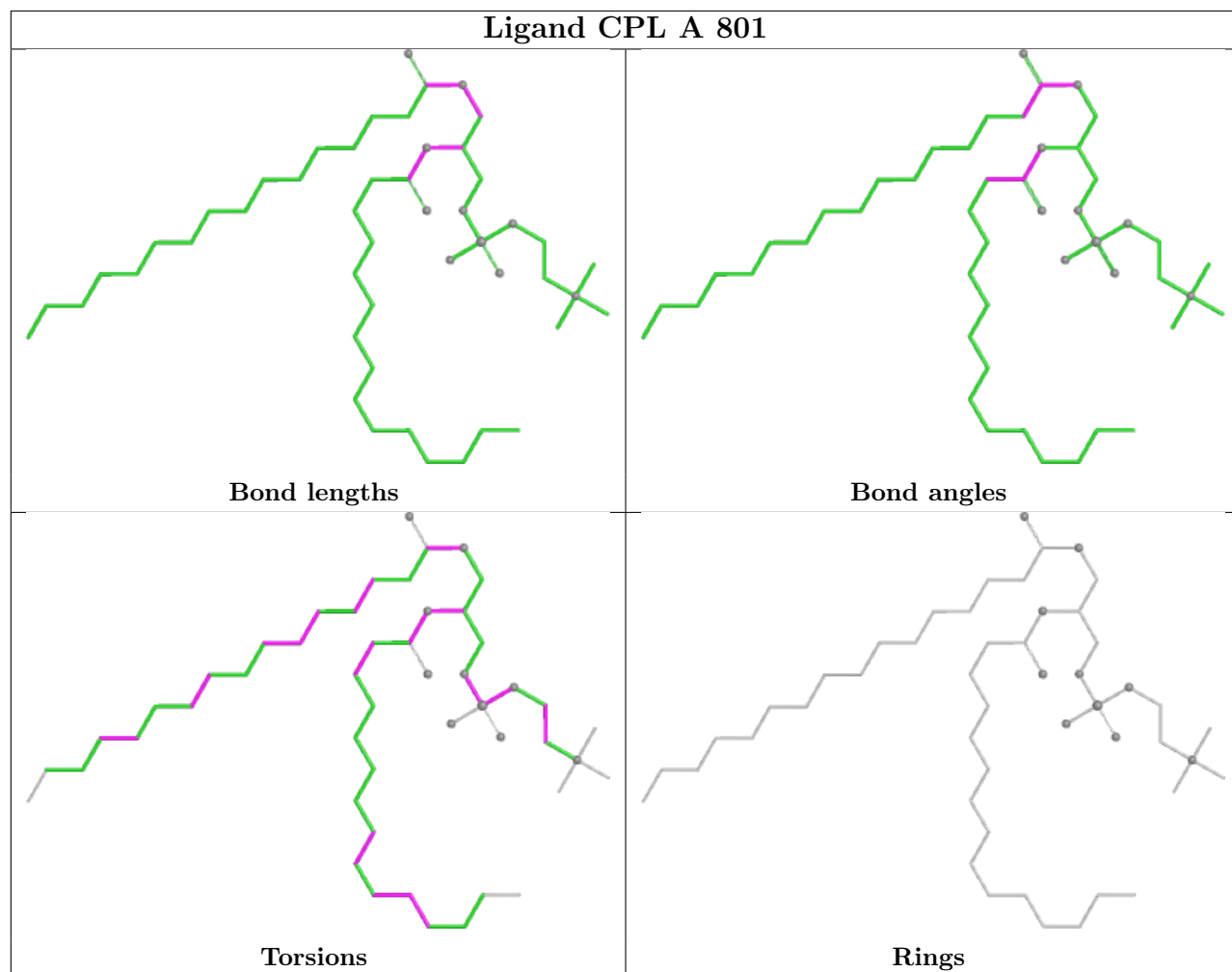


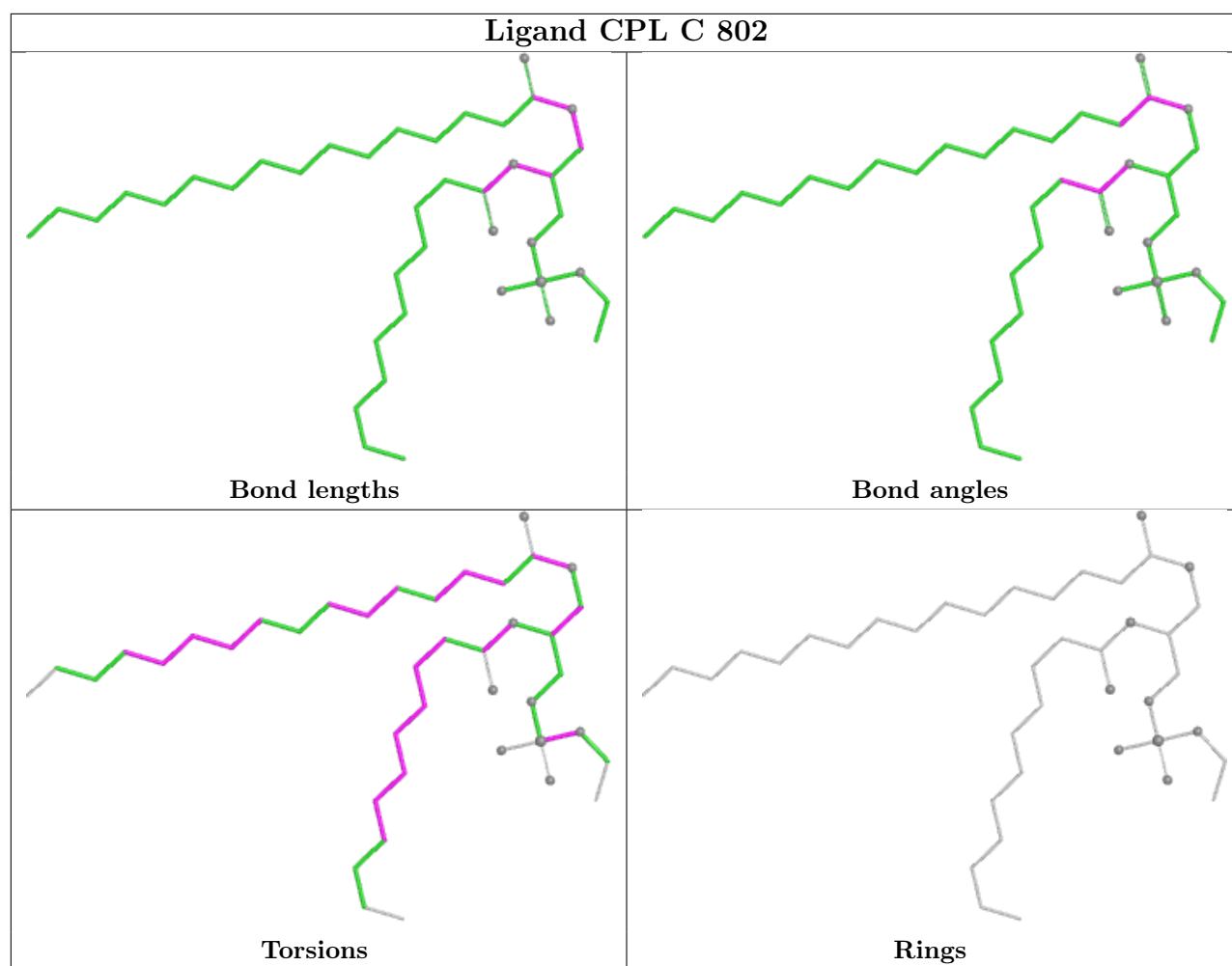












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

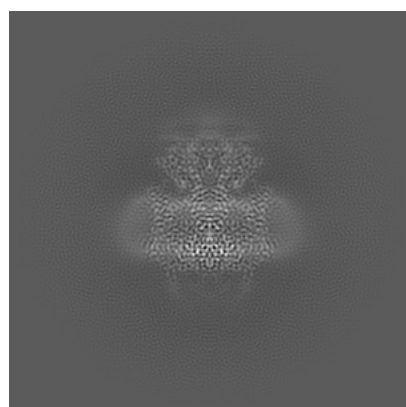
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21651. These allow visual inspection of the internal detail of the map and identification of artifacts.

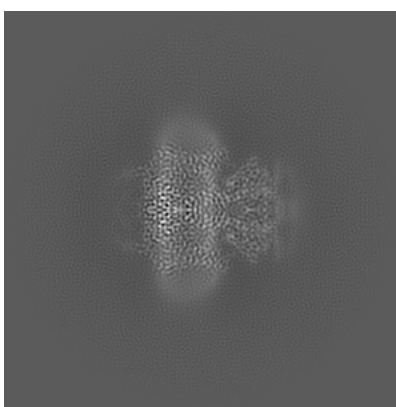
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

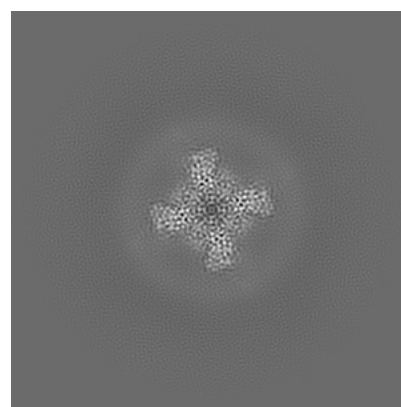
6.1.1 Primary map



X



Y

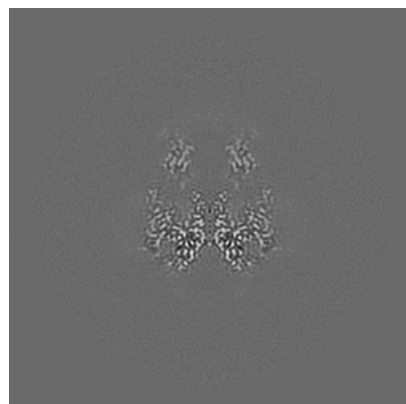


Z

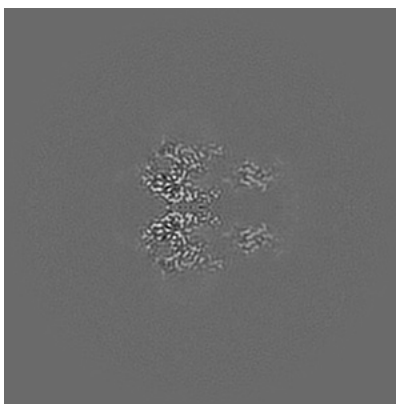
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

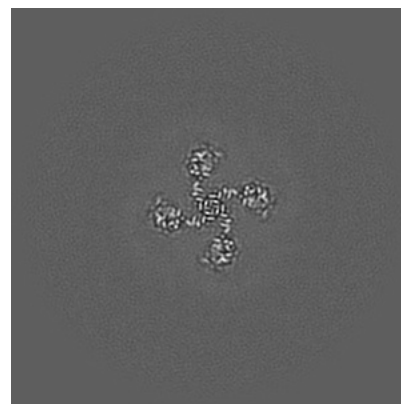
6.2.1 Primary map



X Index: 148



Y Index: 148

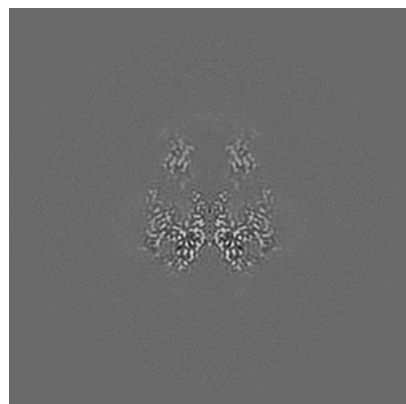


Z Index: 148

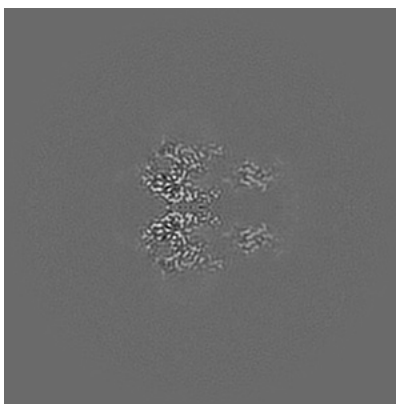
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

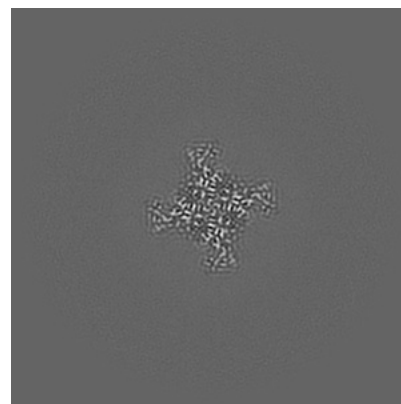
6.3.1 Primary map



X Index: 148



Y Index: 148

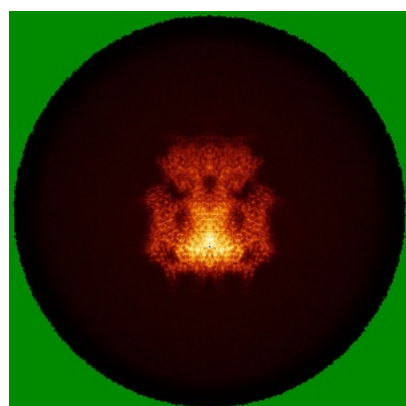


Z Index: 122

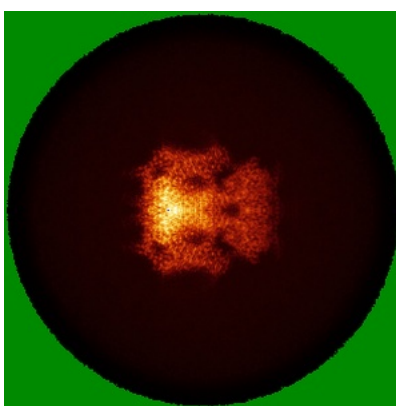
The images above show the largest variance slices of the map in three orthogonal directions.

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

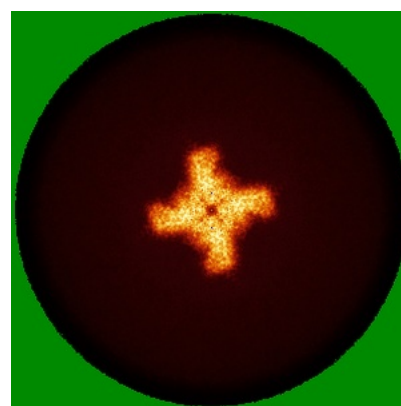
6.4.1 Primary map



X



Y



Z

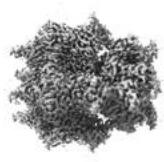
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.21. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

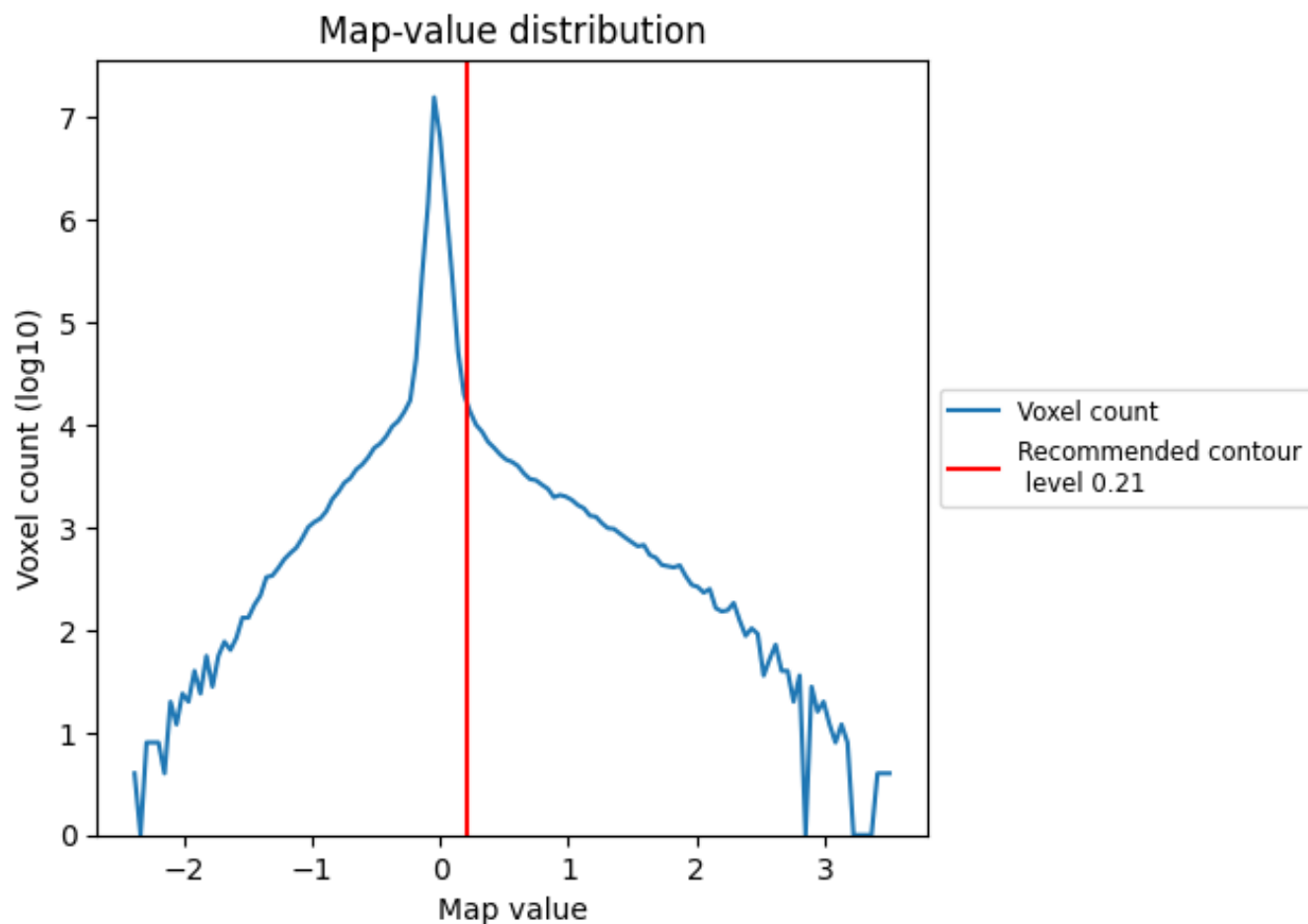
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

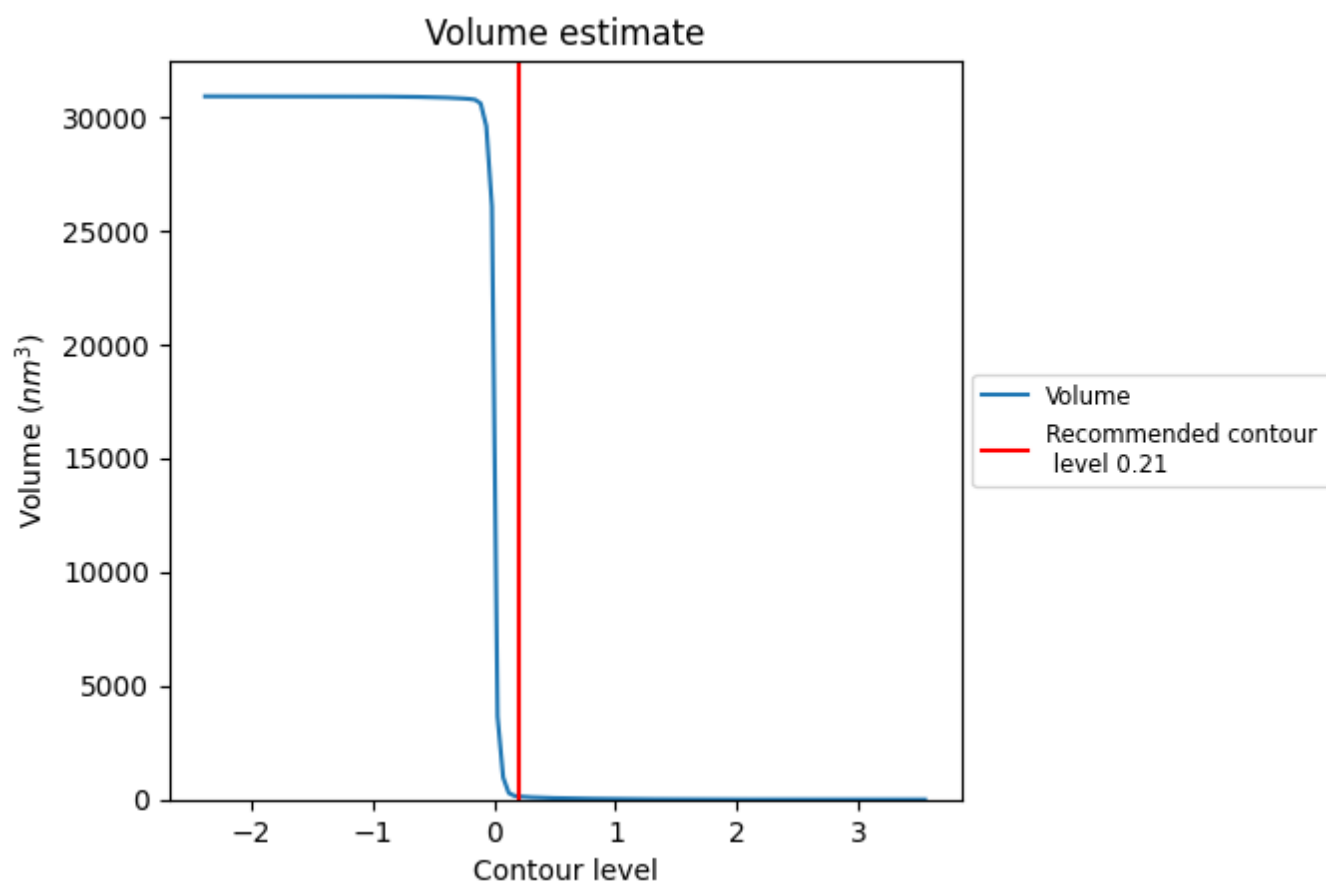
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

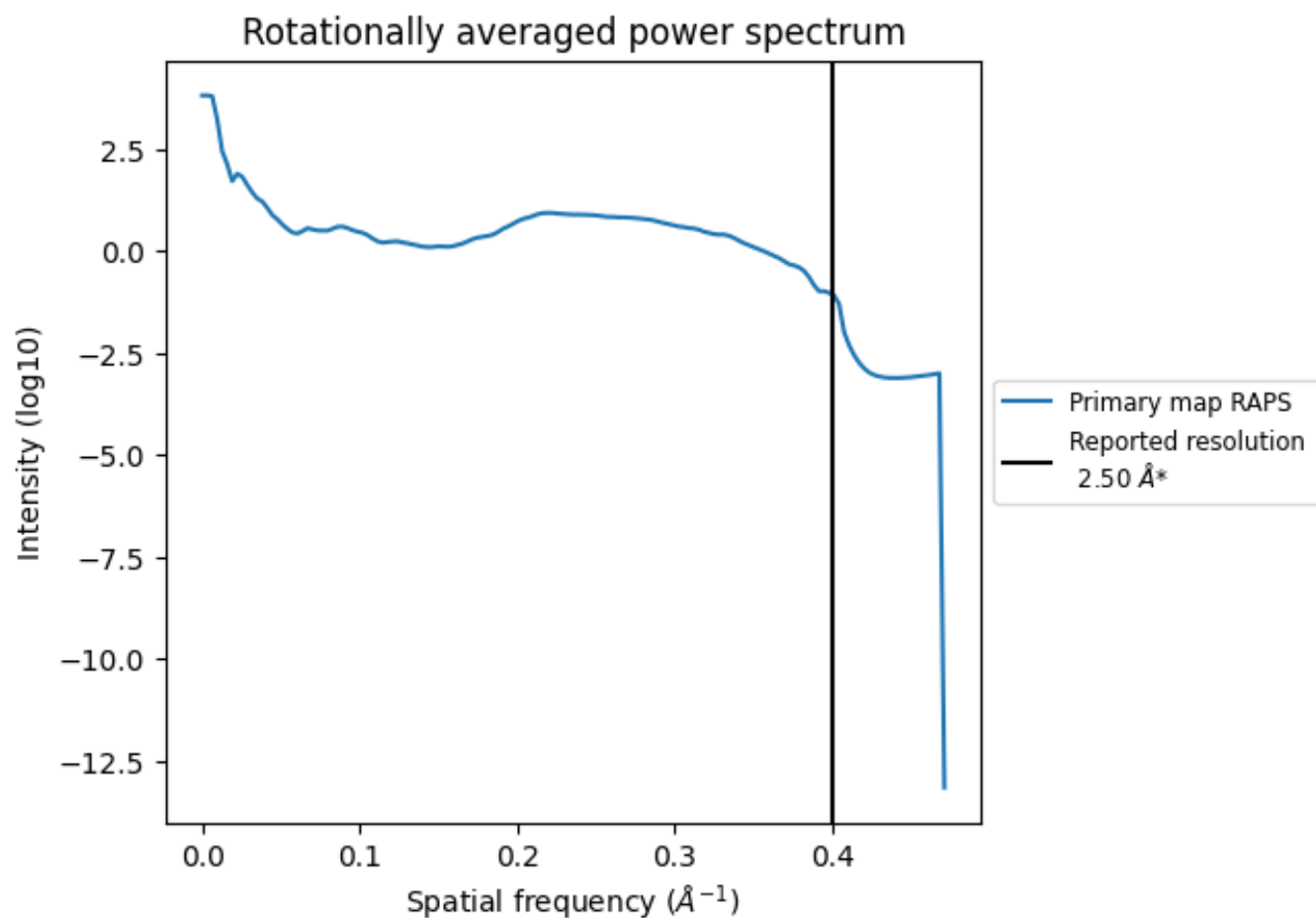
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 135 nm³; this corresponds to an approximate mass of 122 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 0.400 Å⁻¹

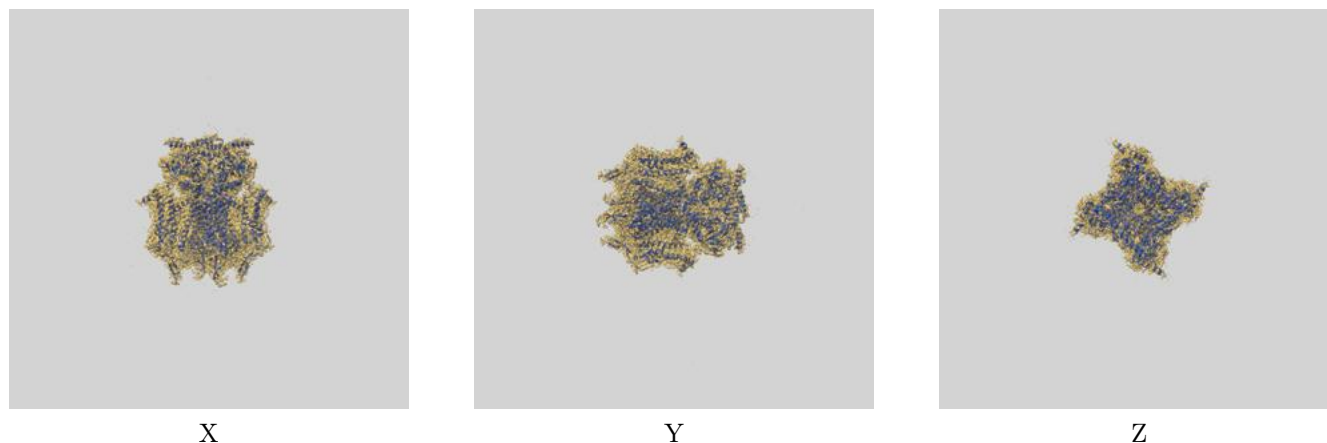
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

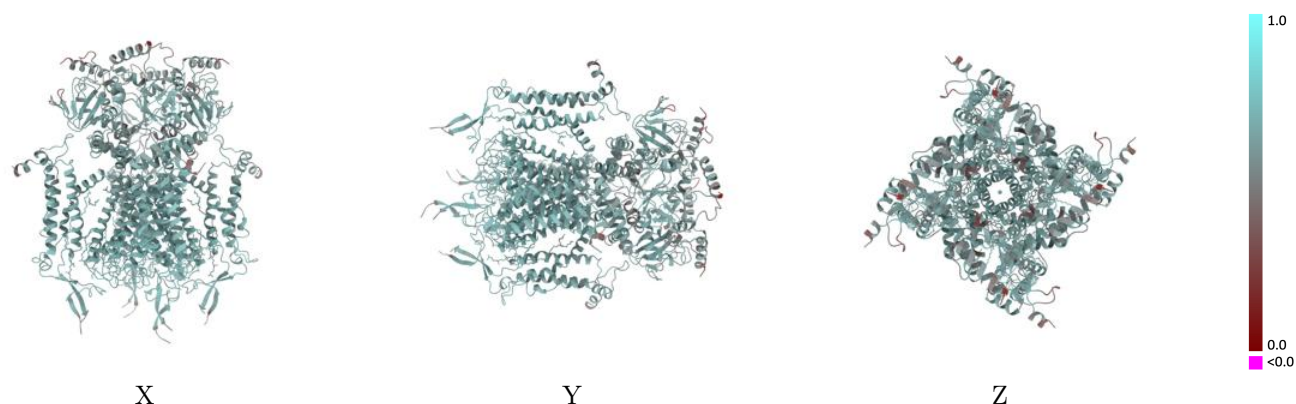
This section contains information regarding the fit between EMDB map EMD-21651 and PDB model 6WEL. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

9.1 Map-model overlay [i](#)



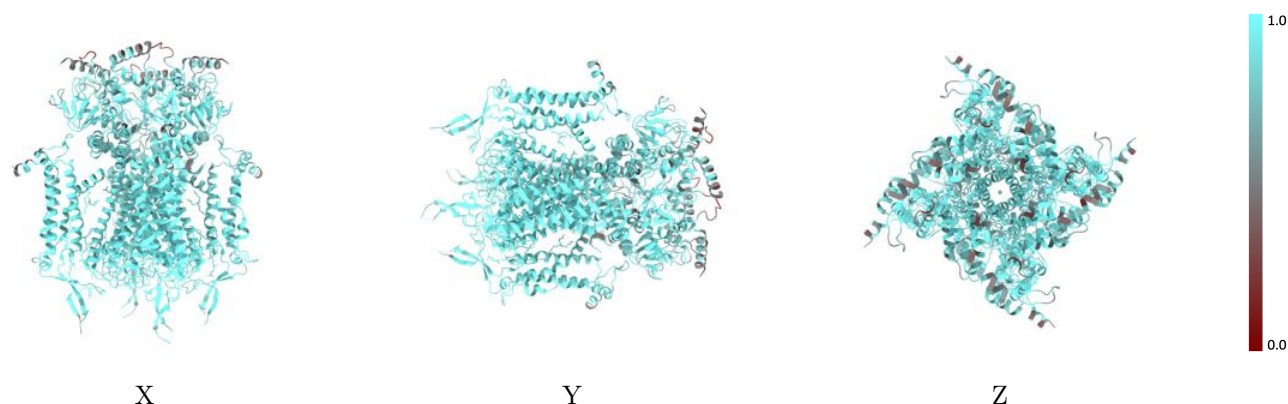
The images above show the 3D surface view of the map at the recommended contour level 0.21 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



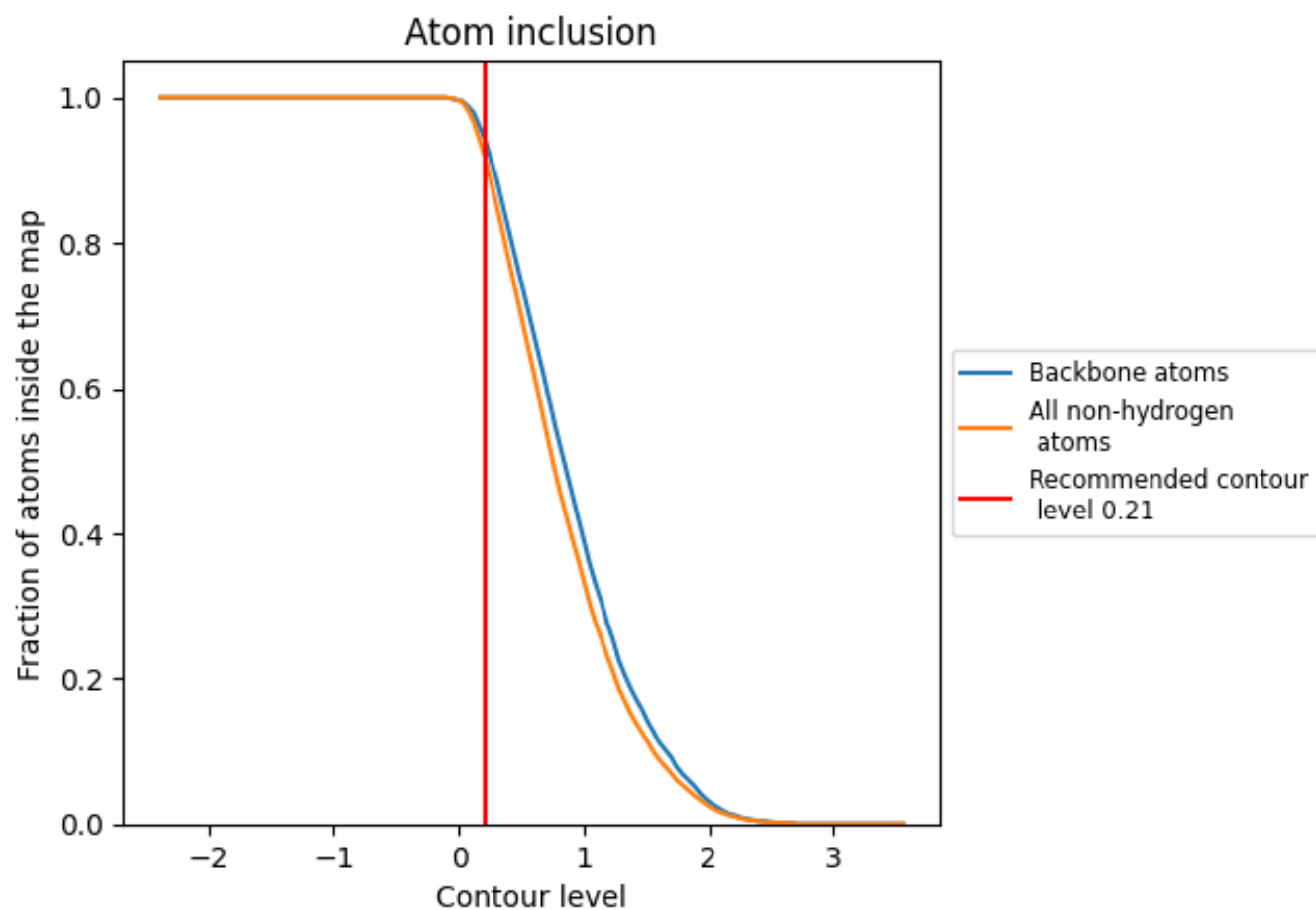
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.21).

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 92% 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 (0.21) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9190	0.6160
A	0.9200	0.6180
B	0.9150	0.6140
C	0.9200	0.6170
D	0.9190	0.6150

