



## Full wwPDB EM Validation Report ⓘ

Nov 21, 2022 – 09:48 AM EST

PDB ID : 7N17  
EMDB ID : EMD-24115  
Title : Structure of TAX-4\_R421W apo open state  
Authors : Zheng, X.; Li, H.; Hu, Z.; Su, D.; Yang, J.  
Deposited on : 2021-05-27  
Resolution : 3.10 Å (reported)  
Based on initial model : 6WEK

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:

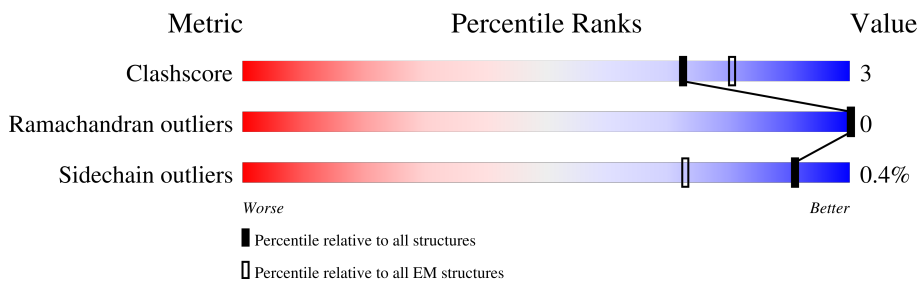
EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.3

# 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 3.10 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	A	738	
1	B	738	
1	C	738	
1	D	738	

## 2 Entry composition i

There are 2 unique types of molecules in this entry. The entry contains 17596 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
			Total	C	N	O	S		
1	A	517	4270	2779	717	750	24	0	0
1	B	517	4270	2779	717	750	24	0	0
1	C	517	4270	2779	717	750	24	0	0
1	D	517	4270	2779	717	750	24	0	0

There are 24 discrepancies between the modelled and reference sequences:

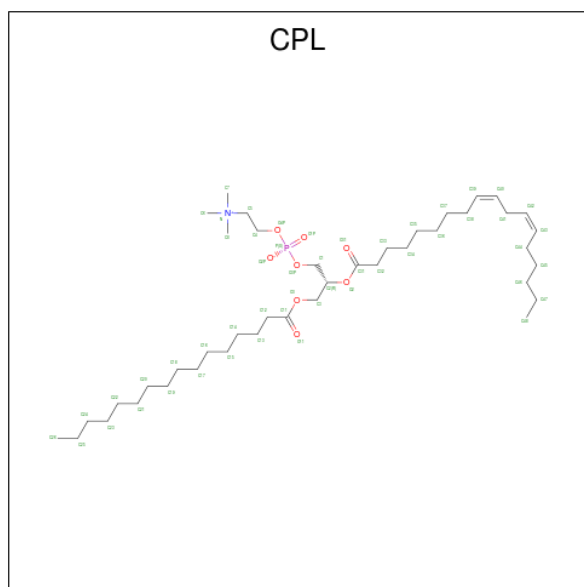
Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	expression tag	UNP Q03611
A	-3	GLY	-	expression tag	UNP Q03611
A	-2	GLY	-	expression tag	UNP Q03611
A	-1	GLY	-	expression tag	UNP Q03611
A	0	SER	-	expression tag	UNP Q03611
A	421	TRP	ARG	engineered mutation	UNP Q03611
B	-4	GLY	-	expression tag	UNP Q03611
B	-3	GLY	-	expression tag	UNP Q03611
B	-2	GLY	-	expression tag	UNP Q03611
B	-1	GLY	-	expression tag	UNP Q03611
B	0	SER	-	expression tag	UNP Q03611
B	421	TRP	ARG	engineered mutation	UNP Q03611
C	-4	GLY	-	expression tag	UNP Q03611
C	-3	GLY	-	expression tag	UNP Q03611
C	-2	GLY	-	expression tag	UNP Q03611
C	-1	GLY	-	expression tag	UNP Q03611
C	0	SER	-	expression tag	UNP Q03611
C	421	TRP	ARG	engineered mutation	UNP Q03611
D	-4	GLY	-	expression tag	UNP Q03611
D	-3	GLY	-	expression tag	UNP Q03611
D	-2	GLY	-	expression tag	UNP Q03611
D	-1	GLY	-	expression tag	UNP Q03611

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Chain	Residue	Modelled	Actual	Comment	Reference
D	0	SER	-	expression tag	UNP Q03611
D	421	TRP	ARG	engineered mutation	UNP Q03611

- Molecule 2 is 1-PALMITOYL-2-LINOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: CPL) (formula: C<sub>42</sub>H<sub>80</sub>NO<sub>8</sub>P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
2	A	1	Total 129	C 101	N 1	O 24	P 3	0
2	A	1	Total 129	C 101	N 1	O 24	P 3	0
2	A	1	Total 129	C 101	N 1	O 24	P 3	0
2	A	1	Total 129	C 101	N 1	O 24	P 3	0
2	A	1	Total 129	C 101	N 1	O 24	P 3	0
2	A	1	Total 129	C 101	N 1	O 24	P 3	0
2	B	1	Total 129	C 101	N 1	O 24	P 3	0
2	B	1	Total 129	C 101	N 1	O 24	P 3	0
2	B	1	Total 129	C 101	N 1	O 24	P 3	0

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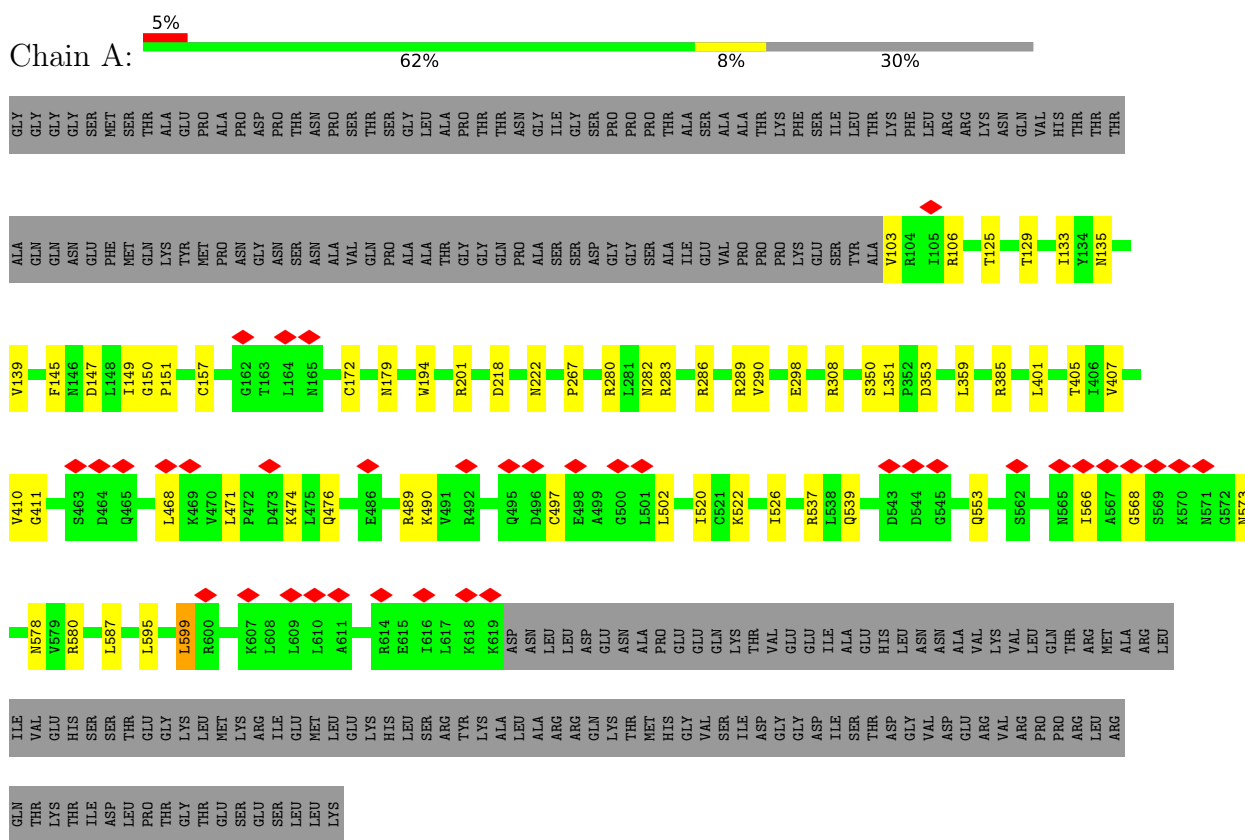
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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
2	B	1	Total 129	C 101	N 1	O 24	P 3	0
2	B	1	Total 129	C 101	N 1	O 24	P 3	0
2	B	1	Total 129	C 101	N 1	O 24	P 3	0
2	C	1	Total 129	C 101	N 1	O 24	P 3	0
2	C	1	Total 129	C 101	N 1	O 24	P 3	0
2	C	1	Total 129	C 101	N 1	O 24	P 3	0
2	C	1	Total 129	C 101	N 1	O 24	P 3	0
2	C	1	Total 129	C 101	N 1	O 24	P 3	0
2	C	1	Total 129	C 101	N 1	O 24	P 3	0
2	D	1	Total 129	C 101	N 1	O 24	P 3	0
2	D	1	Total 129	C 101	N 1	O 24	P 3	0
2	D	1	Total 129	C 101	N 1	O 24	P 3	0
2	D	1	Total 129	C 101	N 1	O 24	P 3	0
2	D	1	Total 129	C 101	N 1	O 24	P 3	0
2	D	1	Total 129	C 101	N 1	O 24	P 3	0

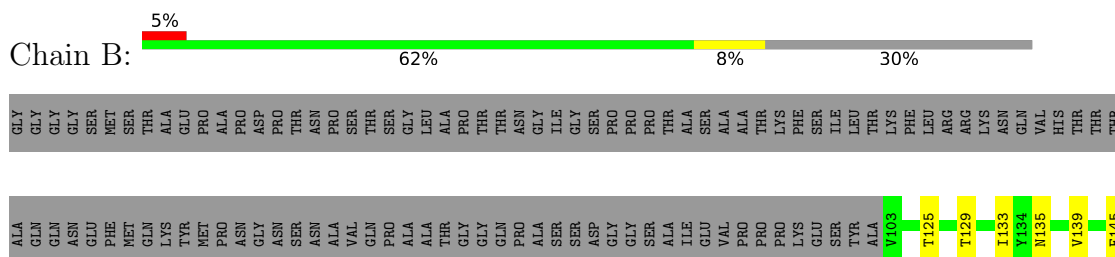
### 3 Residue-property plots

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.

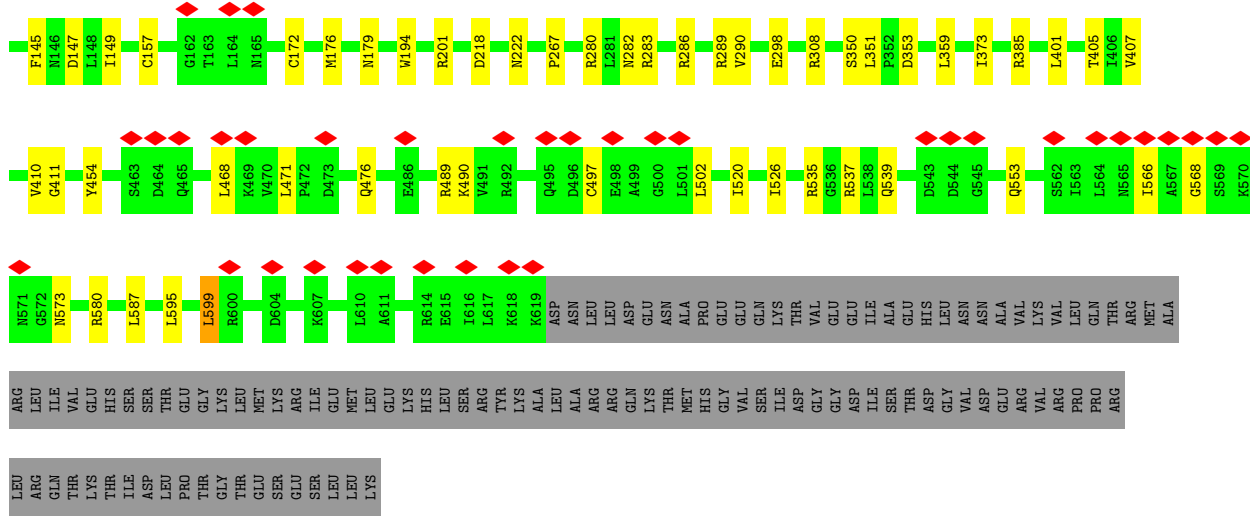
- Molecule 1: Cyclic nucleotide-gated cation channel



- Molecule 1: Cyclic nucleotide-gated cation channel









## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	100919	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 ( $e^-/\text{\AA}^2$ )	58	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.500	Depositor
Minimum map value	-2.470	Depositor
Average map value	0.006	Depositor
Map value standard deviation	0.100	Depositor
Recommended contour level	0.33	Depositor
Map size ( $\text{\AA}$ )	245.68, 245.68, 245.68	wwPDB
Map dimensions	296, 296, 296	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.83, 0.83, 0.83	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: CPL

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	0.45	1/4375 (0.0%)	0.65	3/5937 (0.1%)
1	B	0.45	1/4375 (0.0%)	0.65	3/5937 (0.1%)
1	C	0.45	1/4375 (0.0%)	0.65	3/5937 (0.1%)
1	D	0.45	1/4375 (0.0%)	0.65	3/5937 (0.1%)
All	All	0.45	4/17500 (0.0%)	0.65	12/23748 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	139	VAL	CB-CG2	-5.05	1.42	1.52
1	B	139	VAL	CB-CG2	-5.02	1.42	1.52
1	C	139	VAL	CB-CG2	-5.02	1.42	1.52
1	D	139	VAL	CB-CG2	-5.02	1.42	1.52

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	599	LEU	CA-CB-CG	6.12	129.37	115.30
1	C	599	LEU	CA-CB-CG	6.12	129.37	115.30
1	B	599	LEU	CA-CB-CG	6.11	129.35	115.30
1	A	599	LEU	CA-CB-CG	6.11	129.34	115.30
1	B	468	LEU	CA-CB-CG	5.59	128.15	115.30
1	A	468	LEU	CA-CB-CG	5.57	128.12	115.30
1	D	468	LEU	CA-CB-CG	5.57	128.11	115.30
1	C	468	LEU	CA-CB-CG	5.56	128.10	115.30
1	C	502	LEU	CA-CB-CG	5.42	127.76	115.30
1	A	502	LEU	CA-CB-CG	5.41	127.75	115.30
1	D	502	LEU	CA-CB-CG	5.41	127.75	115.30
1	B	502	LEU	CA-CB-CG	5.40	127.71	115.30

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	4270	0	4311	34	0
1	B	4270	0	4311	33	0
1	C	4270	0	4311	31	0
1	D	4270	0	4311	32	0
2	A	129	0	167	2	0
2	B	129	0	167	2	0
2	C	129	0	167	2	0
2	D	129	0	167	2	0
All	All	17596	0	17912	122	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (122) 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:179:ASN:HD21	1:D:353:ASP:HA	1.66	0.61
1:B:179:ASN:HD21	1:B:353:ASP:HA	1.66	0.61
1:A:179:ASN:HD21	1:A:353:ASP:HA	1.66	0.60
1:C:179:ASN:HD21	1:C:353:ASP:HA	1.66	0.60
1:D:129:THR:HG23	1:D:290:VAL:HG13	1.86	0.57
1:A:129:THR:HG23	1:A:290:VAL:HG13	1.86	0.56
1:B:129:THR:HG23	1:B:290:VAL:HG13	1.86	0.56
1:C:129:THR:HG23	1:C:290:VAL:HG13	1.86	0.55
1:A:135:ASN:OD1	1:A:280:ARG:NH1	2.41	0.54
1:B:135:ASN:OD1	1:B:280:ARG:NH1	2.41	0.54
1:D:135:ASN:OD1	1:D:280:ARG:NH1	2.41	0.54
1:C:135:ASN:OD1	1:C:280:ARG:NH1	2.41	0.54
1:D:157:CYS:N	1:D:172:CYS:SG	2.82	0.53
1:B:157:CYS:N	1:B:172:CYS:SG	2.82	0.53
1:C:157:CYS:N	1:C:172:CYS:SG	2.82	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:CYS:N	1:A:172:CYS:SG	2.82	0.52
1:B:385:ARG:NH2	2:B:1801:CPL:O1P	2.40	0.52
1:B:411:GLY:HA2	1:C:405:THR:HG22	1.92	0.51
1:C:385:ARG:NH2	2:C:1801:CPL:O1P	2.40	0.51
1:A:526:ILE:HG13	1:A:573:ASN:HB3	1.93	0.51
1:B:526:ILE:HG13	1:B:573:ASN:HB3	1.93	0.50
1:D:471:LEU:O	1:D:476:GLN:NE2	2.45	0.50
1:D:526:ILE:HG13	1:D:573:ASN:HB3	1.93	0.50
1:C:471:LEU:O	1:C:476:GLN:NE2	2.45	0.50
1:C:411:GLY:HA2	1:D:405:THR:HG22	1.94	0.50
1:B:537:ARG:NH2	1:B:553:GLN:OE1	2.45	0.50
1:C:526:ILE:HG13	1:C:573:ASN:HB3	1.93	0.50
1:D:537:ARG:NH2	1:D:553:GLN:OE1	2.45	0.50
1:A:471:LEU:O	1:A:476:GLN:NE2	2.45	0.50
1:A:537:ARG:NH2	1:A:553:GLN:OE1	2.45	0.50
1:B:222:ASN:OD1	1:B:289:ARG:NH2	2.45	0.50
1:D:222:ASN:OD1	1:D:289:ARG:NH2	2.45	0.50
1:A:405:THR:HG22	1:D:411:GLY:HA2	1.93	0.50
1:B:471:LEU:O	1:B:476:GLN:NE2	2.45	0.49
1:C:222:ASN:OD1	1:C:289:ARG:NH2	2.45	0.49
1:A:222:ASN:OD1	1:A:289:ARG:NH2	2.45	0.49
1:C:537:ARG:NH2	1:C:553:GLN:OE1	2.45	0.49
1:A:411:GLY:HA2	1:B:405:THR:HG22	1.94	0.48
1:D:385:ARG:NH2	2:D:1801:CPL:O1P	2.41	0.48
1:D:298:GLU:OE1	1:D:308:ARG:NH1	2.47	0.48
1:C:298:GLU:OE1	1:C:308:ARG:NH1	2.47	0.48
1:C:410:VAL:HG11	1:D:401:LEU:HD22	1.96	0.47
1:A:298:GLU:OE1	1:A:308:ARG:NH1	2.47	0.47
1:A:133:ILE:HD11	2:A:803:CPL:H172	1.97	0.47
1:B:298:GLU:OE1	1:B:308:ARG:NH1	2.47	0.47
1:B:218:ASP:OD1	1:B:289:ARG:NH1	2.48	0.47
1:B:218:ASP:OD2	1:B:286:ARG:NH2	2.48	0.47
1:D:218:ASP:OD2	1:D:286:ARG:NH2	2.48	0.47
1:D:194:TRP:NE1	1:D:267:PRO:O	2.44	0.47
1:A:218:ASP:OD1	1:A:289:ARG:NH1	2.48	0.46
1:D:218:ASP:OD1	1:D:289:ARG:NH1	2.48	0.46
1:B:566:ILE:HG22	1:B:568:GLY:H	1.80	0.46
1:C:539:GLN:OE1	1:C:580:ARG:NH1	2.48	0.46
1:A:282:ASN:OD1	1:A:283:ARG:NH1	2.45	0.46
1:A:566:ILE:HG22	1:A:568:GLY:H	1.80	0.46
1:B:133:ILE:HD11	2:B:1804:CPL:H172	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:539:GLN:OE1	1:B:580:ARG:NH1	2.48	0.46
1:D:566:ILE:HG22	1:D:568:GLY:H	1.81	0.46
1:C:218:ASP:OD2	1:C:286:ARG:NH2	2.48	0.46
1:A:401:LEU:HD22	1:D:410:VAL:HG11	1.98	0.46
1:A:218:ASP:OD2	1:A:286:ARG:NH2	2.48	0.46
1:D:133:ILE:HD11	2:D:1804:CPL:H172	1.97	0.46
1:D:539:GLN:OE1	1:D:580:ARG:NH1	2.48	0.46
1:C:218:ASP:OD1	1:C:289:ARG:NH1	2.48	0.46
1:B:410:VAL:HG11	1:C:401:LEU:HD22	1.97	0.46
1:C:145:PHE:HB3	1:C:359:LEU:HD11	1.98	0.45
1:C:566:ILE:HG22	1:C:568:GLY:H	1.81	0.45
1:D:282:ASN:OD1	1:D:283:ARG:NH1	2.45	0.45
1:A:539:GLN:OE1	1:A:580:ARG:NH1	2.48	0.45
1:C:133:ILE:HD11	2:C:1804:CPL:H172	1.97	0.45
1:D:145:PHE:HB3	1:D:359:LEU:HD11	1.98	0.45
1:A:595:LEU:HD12	1:A:599:LEU:HG	1.99	0.45
1:A:145:PHE:HB3	1:A:359:LEU:HD11	1.98	0.45
1:C:282:ASN:OD1	1:C:283:ARG:NH1	2.45	0.45
1:B:145:PHE:HB3	1:B:359:LEU:HD11	1.98	0.45
1:B:595:LEU:HD12	1:B:599:LEU:HG	1.99	0.45
1:B:125:THR:HG22	1:B:289:ARG:HD2	1.99	0.44
1:C:125:THR:HG22	1:C:289:ARG:HD2	1.99	0.44
1:D:595:LEU:HD12	1:D:599:LEU:HG	1.99	0.44
1:C:350:SER:OG	1:C:351:LEU:N	2.51	0.44
1:A:350:SER:OG	1:A:351:LEU:N	2.51	0.44
1:C:595:LEU:HD12	1:C:599:LEU:HG	1.99	0.44
1:D:125:THR:HG22	1:D:289:ARG:HD2	1.99	0.43
1:D:350:SER:OG	1:D:351:LEU:N	2.51	0.43
1:B:350:SER:OG	1:B:351:LEU:N	2.51	0.43
1:A:125:THR:HG22	1:A:289:ARG:HD2	1.99	0.43
1:B:194:TRP:NE1	1:B:267:PRO:O	2.44	0.43
1:A:289:ARG:HA	1:A:289:ARG:HD3	1.81	0.43
1:B:282:ASN:OD1	1:B:283:ARG:NH1	2.45	0.43
1:C:157:CYS:HB2	1:C:176:MET:HE1	2.01	0.42
1:A:489:ARG:HG3	1:A:490:LYS:HG3	2.02	0.42
1:A:520:ILE:HD13	1:A:587:LEU:HD11	2.01	0.42
1:B:489:ARG:HG3	1:B:490:LYS:HG3	2.02	0.42
1:C:149:ILE:O	1:C:201:ARG:NE	2.53	0.42
1:A:149:ILE:O	1:A:201:ARG:NE	2.53	0.42
1:C:194:TRP:NE1	1:C:267:PRO:O	2.44	0.42
1:D:520:ILE:HD13	1:D:587:LEU:HD11	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:385:ARG:NH2	2:A:806:CPL:O1P	2.47	0.41
1:B:520:ILE:HD13	1:B:587:LEU:HD11	2.02	0.41
1:A:147:ASP:HB2	1:A:359:LEU:HD22	2.02	0.41
1:C:520:ILE:HD13	1:C:587:LEU:HD11	2.02	0.41
1:A:194:TRP:NE1	1:A:267:PRO:O	2.44	0.41
1:C:147:ASP:HB2	1:C:359:LEU:HD22	2.02	0.41
1:C:489:ARG:HG3	1:C:490:LYS:HG3	2.02	0.41
1:D:147:ASP:HB2	1:D:359:LEU:HD22	2.03	0.41
1:B:157:CYS:HB2	1:B:176:MET:HE1	2.03	0.41
1:B:242:LYS:HE3	1:B:242:LYS:HB2	1.95	0.41
1:D:373:ILE:HD13	1:D:373:ILE:HA	1.97	0.41
1:D:149:ILE:O	1:D:201:ARG:NE	2.53	0.41
1:D:489:ARG:HG3	1:D:490:LYS:HG3	2.02	0.41
1:A:410:VAL:HG11	1:B:401:LEU:HD22	2.02	0.41
1:B:446:ILE:HA	1:B:449:ILE:HG12	2.03	0.41
1:D:157:CYS:HB2	1:D:176:MET:HE1	2.02	0.41
1:A:150:GLY:HA2	1:A:151:PRO:HD3	1.96	0.40
1:B:147:ASP:HB2	1:B:359:LEU:HD22	2.03	0.40
1:B:149:ILE:O	1:B:201:ARG:NE	2.53	0.40
1:D:454:TYR:OH	1:D:535:ARG:NH1	2.50	0.40
1:A:474:LYS:HE2	1:A:474:LYS:HB2	1.89	0.40
1:A:522:LYS:HA	1:A:578:ASN:HD22	1.87	0.40
1:B:522:LYS:HA	1:B:578:ASN:HD22	1.87	0.40
1:A:103:VAL:HG12	1:A:106:ARG:HH22	1.87	0.40
1:C:522:LYS:HA	1:C:578:ASN:HD22	1.87	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	515/738 (70%)	500 (97%)	15 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	515/738 (70%)	500 (97%)	15 (3%)	0	100	100
1	C	515/738 (70%)	500 (97%)	15 (3%)	0	100	100
1	D	515/738 (70%)	500 (97%)	15 (3%)	0	100	100
All	All	2060/2952 (70%)	2000 (97%)	60 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	468/652 (72%)	466 (100%)	2 (0%)	91	96
1	B	468/652 (72%)	466 (100%)	2 (0%)	91	96
1	C	468/652 (72%)	466 (100%)	2 (0%)	91	96
1	D	468/652 (72%)	466 (100%)	2 (0%)	91	96
All	All	1872/2608 (72%)	1864 (100%)	8 (0%)	91	96

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

Mol	Chain	Res	Type
1	A	407	VAL
1	A	497	CYS
1	B	407	VAL
1	B	497	CYS
1	C	407	VAL
1	C	497	CYS
1	D	407	VAL
1	D	497	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	179	ASN
1	A	246	GLN
1	A	426	ASN
1	A	476	GLN
1	A	578	ASN
1	B	179	ASN
1	B	246	GLN
1	B	426	ASN
1	B	476	GLN
1	B	578	ASN
1	C	179	ASN
1	C	246	GLN
1	C	426	ASN
1	C	476	GLN
1	C	578	ASN
1	D	179	ASN
1	D	246	GLN
1	D	426	ASN
1	D	476	GLN
1	D	578	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

24 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond



length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	CPL	B	1803	-	7,7,51	0.26	0	6,6,59	0.75	0
2	CPL	B	1805	-	11,11,51	0.25	0	10,10,59	0.84	0
2	CPL	D	1802	-	37,37,51	1.11	4 (10%)	43,45,59	1.02	2 (4%)
2	CPL	C	1801	-	21,21,51	1.31	3 (14%)	24,26,59	1.34	2 (8%)
2	CPL	C	1806	-	35,35,51	1.07	5 (14%)	39,40,59	1.17	2 (5%)
2	CPL	C	1804	-	12,12,51	0.24	0	11,11,59	0.83	0
2	CPL	B	1806	-	35,35,51	1.07	5 (14%)	39,40,59	1.17	2 (5%)
2	CPL	C	1802	-	37,37,51	1.11	4 (10%)	43,45,59	1.01	2 (4%)
2	CPL	D	1805	-	11,11,51	0.25	0	10,10,59	0.84	0
2	CPL	A	804	-	11,11,51	0.25	0	10,10,59	0.84	0
2	CPL	D	1803	-	7,7,51	0.26	0	6,6,59	0.75	0
2	CPL	B	1802	-	37,37,51	1.11	4 (10%)	43,45,59	1.02	2 (4%)
2	CPL	A	802	-	7,7,51	0.26	0	6,6,59	0.75	0
2	CPL	A	805	-	35,35,51	1.07	5 (14%)	39,40,59	1.17	2 (5%)
2	CPL	D	1801	-	21,21,51	1.32	3 (14%)	24,26,59	1.34	2 (8%)
2	CPL	C	1805	-	11,11,51	0.24	0	10,10,59	0.84	0
2	CPL	D	1806	-	35,35,51	1.07	5 (14%)	39,40,59	1.17	2 (5%)
2	CPL	A	803	-	12,12,51	0.24	0	11,11,59	0.83	0
2	CPL	B	1804	-	12,12,51	0.24	0	11,11,59	0.83	0
2	CPL	D	1804	-	12,12,51	0.24	0	11,11,59	0.83	0
2	CPL	A	801	-	37,37,51	1.11	4 (10%)	43,45,59	1.01	2 (4%)
2	CPL	B	1801	-	21,21,51	1.31	3 (14%)	24,26,59	1.34	2 (8%)
2	CPL	C	1803	-	7,7,51	0.27	0	6,6,59	0.75	0
2	CPL	A	806	-	21,21,51	1.31	3 (14%)	24,26,59	1.34	2 (8%)

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	B	1803	-	-	2/5/5/55	-
2	CPL	B	1805	-	-	4/9/9/55	-
2	CPL	D	1802	-	-	20/41/41/55	-
2	CPL	C	1801	-	-	11/25/25/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CPL	C	1806	-	-	17/37/37/55	-
2	CPL	C	1804	-	-	8/10/10/55	-
2	CPL	B	1806	-	-	17/37/37/55	-
2	CPL	C	1802	-	-	20/41/41/55	-
2	CPL	D	1805	-	-	4/9/9/55	-
2	CPL	A	804	-	-	4/9/9/55	-
2	CPL	D	1803	-	-	2/5/5/55	-
2	CPL	B	1802	-	-	20/41/41/55	-
2	CPL	A	802	-	-	2/5/5/55	-
2	CPL	A	805	-	-	17/37/37/55	-
2	CPL	D	1801	-	-	11/25/25/55	-
2	CPL	C	1805	-	-	4/9/9/55	-
2	CPL	D	1806	-	-	17/37/37/55	-
2	CPL	A	803	-	-	8/10/10/55	-
2	CPL	B	1804	-	-	8/10/10/55	-
2	CPL	D	1804	-	-	8/10/10/55	-
2	CPL	A	801	-	-	20/41/41/55	-
2	CPL	B	1801	-	-	11/25/25/55	-
2	CPL	C	1803	-	-	2/5/5/55	-
2	CPL	A	806	-	-	11/25/25/55	-

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1806	CPL	P-O4P	2.66	1.65	1.54
2	A	805	CPL	P-O4P	2.65	1.65	1.54
2	D	1806	CPL	P-O4P	2.64	1.65	1.54
2	C	1806	CPL	P-O4P	2.64	1.65	1.54
2	C	1806	CPL	O2-C2	-2.62	1.40	1.46
2	A	805	CPL	O2-C2	-2.61	1.40	1.46
2	D	1806	CPL	O2-C2	-2.60	1.40	1.46
2	B	1806	CPL	O2-C2	-2.59	1.40	1.46
2	B	1801	CPL	O2-C2	-2.56	1.40	1.46
2	C	1801	CPL	O2-C2	-2.56	1.40	1.46
2	D	1802	CPL	O2-C2	-2.56	1.40	1.46
2	D	1801	CPL	O2-C2	-2.55	1.40	1.46
2	C	1802	CPL	O2-C2	-2.55	1.40	1.46
2	A	801	CPL	O2-C2	-2.54	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1802	CPL	O2-C2	-2.53	1.40	1.46
2	A	806	CPL	O2-C2	-2.52	1.40	1.46
2	C	1806	CPL	O3-C11	2.41	1.40	1.33
2	A	805	CPL	O3-C11	2.40	1.40	1.33
2	B	1806	CPL	O3-C11	2.39	1.40	1.33
2	D	1801	CPL	O3-C11	2.38	1.40	1.33
2	D	1806	CPL	O3-C11	2.37	1.40	1.33
2	C	1801	CPL	O3-C11	2.37	1.40	1.33
2	B	1801	CPL	O3-C11	2.37	1.40	1.33
2	A	806	CPL	O3-C11	2.36	1.40	1.33
2	B	1802	CPL	O3-C11	2.33	1.40	1.33
2	C	1802	CPL	O3-C11	2.33	1.40	1.33
2	A	801	CPL	O3-C11	2.32	1.40	1.33
2	D	1801	CPL	O2-C31	2.31	1.40	1.34
2	B	1801	CPL	O2-C31	2.30	1.40	1.34
2	A	806	CPL	O2-C31	2.30	1.40	1.34
2	D	1802	CPL	O3-C11	2.30	1.40	1.33
2	C	1801	CPL	O2-C31	2.28	1.40	1.34
2	B	1802	CPL	O3-C3	-2.21	1.40	1.45
2	C	1802	CPL	O2-C31	2.21	1.40	1.34
2	C	1806	CPL	O3-C3	-2.20	1.40	1.45
2	D	1802	CPL	O3-C3	-2.20	1.40	1.45
2	A	801	CPL	O3-C3	-2.19	1.40	1.45
2	A	801	CPL	O2-C31	2.19	1.40	1.34
2	C	1802	CPL	O3-C3	-2.19	1.40	1.45
2	A	805	CPL	O3-C3	-2.19	1.40	1.45
2	D	1802	CPL	O2-C31	2.19	1.40	1.34
2	B	1806	CPL	O3-C3	-2.18	1.40	1.45
2	D	1806	CPL	O3-C3	-2.18	1.40	1.45
2	B	1802	CPL	O2-C31	2.17	1.40	1.34
2	B	1806	CPL	O2-C31	2.17	1.40	1.34
2	D	1806	CPL	O2-C31	2.16	1.40	1.34
2	C	1806	CPL	O2-C31	2.16	1.40	1.34
2	A	805	CPL	O2-C31	2.15	1.40	1.34

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	806	CPL	O2-C31-C32	4.84	121.93	111.50
2	C	1801	CPL	O2-C31-C32	4.83	121.92	111.50
2	B	1801	CPL	O2-C31-C32	4.83	121.92	111.50
2	D	1801	CPL	O2-C31-C32	4.81	121.87	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1806	CPL	O2-C31-C32	3.68	119.44	111.50
2	A	805	CPL	O2-C31-C32	3.68	119.43	111.50
2	D	1802	CPL	O2-C31-C32	3.68	119.42	111.50
2	C	1806	CPL	O2-C31-C32	3.67	119.41	111.50
2	B	1806	CPL	O2-C31-C32	3.66	119.39	111.50
2	A	801	CPL	O2-C31-C32	3.66	119.38	111.50
2	B	1802	CPL	O2-C31-C32	3.65	119.38	111.50
2	C	1802	CPL	O2-C31-C32	3.64	119.35	111.50
2	C	1806	CPL	O3-C11-C12	2.76	120.56	111.91
2	B	1806	CPL	O3-C11-C12	2.75	120.54	111.91
2	A	805	CPL	O3-C11-C12	2.75	120.54	111.91
2	D	1806	CPL	O3-C11-C12	2.75	120.53	111.91
2	D	1802	CPL	O3-C11-C12	2.66	120.26	111.91
2	B	1802	CPL	O3-C11-C12	2.66	120.26	111.91
2	A	801	CPL	O3-C11-C12	2.66	120.24	111.91
2	C	1802	CPL	O3-C11-C12	2.65	120.21	111.91
2	D	1801	CPL	O3-C11-C12	2.55	119.90	111.91
2	A	806	CPL	O3-C11-C12	2.54	119.89	111.91
2	C	1801	CPL	O3-C11-C12	2.54	119.89	111.91
2	B	1801	CPL	O3-C11-C12	2.54	119.88	111.91

There are no chirality outliers.

All (248) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	CPL	O4P-C4-C5-N
2	A	801	CPL	C4-O4P-P-O1P
2	A	806	CPL	C32-C31-O2-C2
2	A	806	CPL	O31-C31-O2-C2
2	A	806	CPL	C4-O4P-P-O1P
2	A	806	CPL	C4-O4P-P-O2P
2	A	806	CPL	C4-O4P-P-O3P
2	B	1801	CPL	C32-C31-O2-C2
2	B	1801	CPL	O31-C31-O2-C2
2	B	1801	CPL	C4-O4P-P-O1P
2	B	1801	CPL	C4-O4P-P-O2P
2	B	1801	CPL	C4-O4P-P-O3P
2	B	1802	CPL	O4P-C4-C5-N
2	B	1802	CPL	C4-O4P-P-O1P
2	C	1801	CPL	C32-C31-O2-C2
2	C	1801	CPL	O31-C31-O2-C2
2	C	1801	CPL	C4-O4P-P-O1P

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Mol	Chain	Res	Type	Atoms
2	C	1801	CPL	C4-O4P-P-O2P
2	C	1801	CPL	C4-O4P-P-O3P
2	C	1802	CPL	O4P-C4-C5-N
2	C	1802	CPL	C4-O4P-P-O1P
2	D	1801	CPL	C32-C31-O2-C2
2	D	1801	CPL	O31-C31-O2-C2
2	D	1801	CPL	C4-O4P-P-O1P
2	D	1801	CPL	C4-O4P-P-O2P
2	D	1801	CPL	C4-O4P-P-O3P
2	D	1802	CPL	O4P-C4-C5-N
2	D	1802	CPL	C4-O4P-P-O1P
2	A	805	CPL	C11-C12-C13-C14
2	B	1806	CPL	C11-C12-C13-C14
2	C	1806	CPL	C11-C12-C13-C14
2	D	1806	CPL	C11-C12-C13-C14
2	A	801	CPL	C31-C32-C33-C34
2	A	805	CPL	C31-C32-C33-C34
2	B	1802	CPL	C31-C32-C33-C34
2	B	1806	CPL	C31-C32-C33-C34
2	C	1802	CPL	C31-C32-C33-C34
2	C	1806	CPL	C31-C32-C33-C34
2	D	1802	CPL	C31-C32-C33-C34
2	D	1806	CPL	C31-C32-C33-C34
2	A	806	CPL	C1-O3P-P-O4P
2	B	1801	CPL	C1-O3P-P-O4P
2	C	1801	CPL	C1-O3P-P-O4P
2	D	1801	CPL	C1-O3P-P-O4P
2	A	803	CPL	C13-C14-C15-C16
2	B	1804	CPL	C13-C14-C15-C16
2	C	1804	CPL	C13-C14-C15-C16
2	D	1804	CPL	C13-C14-C15-C16
2	A	805	CPL	C12-C11-O3-C3
2	B	1806	CPL	C12-C11-O3-C3
2	C	1806	CPL	C12-C11-O3-C3
2	D	1806	CPL	C12-C11-O3-C3
2	A	805	CPL	C18-C19-C20-C21
2	B	1804	CPL	C14-C15-C16-C17
2	B	1806	CPL	C18-C19-C20-C21
2	C	1806	CPL	C18-C19-C20-C21
2	D	1806	CPL	C18-C19-C20-C21
2	A	803	CPL	C14-C15-C16-C17
2	A	804	CPL	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
2	B	1805	CPL	C18-C19-C20-C21
2	C	1804	CPL	C14-C15-C16-C17
2	C	1805	CPL	C18-C19-C20-C21
2	D	1804	CPL	C14-C15-C16-C17
2	D	1805	CPL	C18-C19-C20-C21
2	A	805	CPL	C32-C31-O2-C2
2	B	1806	CPL	C32-C31-O2-C2
2	C	1806	CPL	C32-C31-O2-C2
2	D	1806	CPL	C32-C31-O2-C2
2	A	803	CPL	C18-C19-C20-C21
2	B	1804	CPL	C18-C19-C20-C21
2	D	1804	CPL	C18-C19-C20-C21
2	C	1804	CPL	C18-C19-C20-C21
2	A	801	CPL	C19-C20-C21-C22
2	B	1802	CPL	C19-C20-C21-C22
2	C	1802	CPL	C19-C20-C21-C22
2	D	1802	CPL	C19-C20-C21-C22
2	A	805	CPL	O31-C31-O2-C2
2	B	1806	CPL	O31-C31-O2-C2
2	C	1806	CPL	O31-C31-O2-C2
2	D	1806	CPL	O31-C31-O2-C2
2	B	1804	CPL	C15-C16-C17-C18
2	D	1804	CPL	C15-C16-C17-C18
2	A	805	CPL	O11-C11-O3-C3
2	B	1806	CPL	O11-C11-O3-C3
2	C	1806	CPL	O11-C11-O3-C3
2	D	1806	CPL	O11-C11-O3-C3
2	A	803	CPL	C15-C16-C17-C18
2	C	1804	CPL	C15-C16-C17-C18
2	A	805	CPL	C15-C16-C17-C18
2	B	1806	CPL	C15-C16-C17-C18
2	C	1806	CPL	C15-C16-C17-C18
2	D	1806	CPL	C15-C16-C17-C18
2	A	801	CPL	C32-C31-O2-C2
2	B	1802	CPL	C32-C31-O2-C2
2	C	1802	CPL	C32-C31-O2-C2
2	D	1802	CPL	C32-C31-O2-C2
2	A	801	CPL	C17-C18-C19-C20
2	C	1802	CPL	C17-C18-C19-C20
2	B	1802	CPL	C17-C18-C19-C20
2	D	1802	CPL	C17-C18-C19-C20
2	A	801	CPL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
2	B	1802	CPL	O2-C2-C3-O3
2	C	1802	CPL	O2-C2-C3-O3
2	D	1802	CPL	O2-C2-C3-O3
2	A	804	CPL	C13-C14-C15-C16
2	C	1805	CPL	C13-C14-C15-C16
2	D	1805	CPL	C13-C14-C15-C16
2	B	1805	CPL	C13-C14-C15-C16
2	A	805	CPL	O3P-C1-C2-C3
2	B	1806	CPL	O3P-C1-C2-C3
2	C	1806	CPL	O3P-C1-C2-C3
2	D	1806	CPL	O3P-C1-C2-C3
2	A	801	CPL	C1-C2-C3-O3
2	A	805	CPL	C19-C20-C21-C22
2	B	1802	CPL	C1-C2-C3-O3
2	B	1806	CPL	C19-C20-C21-C22
2	C	1802	CPL	C1-C2-C3-O3
2	C	1806	CPL	C19-C20-C21-C22
2	D	1802	CPL	C1-C2-C3-O3
2	D	1806	CPL	C19-C20-C21-C22
2	A	804	CPL	C12-C13-C14-C15
2	B	1805	CPL	C12-C13-C14-C15
2	C	1805	CPL	C12-C13-C14-C15
2	D	1805	CPL	C12-C13-C14-C15
2	A	801	CPL	C18-C19-C20-C21
2	B	1802	CPL	C18-C19-C20-C21
2	C	1802	CPL	C18-C19-C20-C21
2	D	1802	CPL	C18-C19-C20-C21
2	A	801	CPL	O31-C31-O2-C2
2	B	1802	CPL	O31-C31-O2-C2
2	C	1802	CPL	O31-C31-O2-C2
2	D	1802	CPL	O31-C31-O2-C2
2	A	802	CPL	C16-C17-C18-C19
2	B	1803	CPL	C16-C17-C18-C19
2	C	1803	CPL	C16-C17-C18-C19
2	D	1803	CPL	C16-C17-C18-C19
2	A	802	CPL	C14-C15-C16-C17
2	B	1803	CPL	C14-C15-C16-C17
2	C	1803	CPL	C14-C15-C16-C17
2	D	1803	CPL	C14-C15-C16-C17
2	A	806	CPL	C1-C2-C3-O3
2	B	1801	CPL	C1-C2-C3-O3
2	C	1801	CPL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
2	D	1801	CPL	C1-C2-C3-O3
2	A	801	CPL	C4-O4P-P-O3P
2	B	1802	CPL	C4-O4P-P-O3P
2	C	1802	CPL	C4-O4P-P-O3P
2	D	1802	CPL	C4-O4P-P-O3P
2	A	803	CPL	C12-C13-C14-C15
2	B	1804	CPL	C12-C13-C14-C15
2	C	1804	CPL	C12-C13-C14-C15
2	D	1804	CPL	C12-C13-C14-C15
2	A	803	CPL	C21-C22-C23-C24
2	C	1804	CPL	C21-C22-C23-C24
2	D	1804	CPL	C21-C22-C23-C24
2	B	1804	CPL	C21-C22-C23-C24
2	B	1802	CPL	C32-C33-C34-C35
2	A	801	CPL	C32-C33-C34-C35
2	C	1802	CPL	C32-C33-C34-C35
2	D	1802	CPL	C32-C33-C34-C35
2	A	804	CPL	C17-C18-C19-C20
2	D	1805	CPL	C17-C18-C19-C20
2	B	1805	CPL	C17-C18-C19-C20
2	C	1805	CPL	C17-C18-C19-C20
2	A	806	CPL	C1-O3P-P-O2P
2	B	1801	CPL	C1-O3P-P-O2P
2	C	1801	CPL	C1-O3P-P-O2P
2	D	1801	CPL	C1-O3P-P-O2P
2	A	803	CPL	C20-C21-C22-C23
2	B	1804	CPL	C20-C21-C22-C23
2	D	1804	CPL	C20-C21-C22-C23
2	C	1804	CPL	C20-C21-C22-C23
2	A	801	CPL	O11-C11-O3-C3
2	B	1802	CPL	O11-C11-O3-C3
2	C	1802	CPL	O11-C11-O3-C3
2	D	1802	CPL	O11-C11-O3-C3
2	A	805	CPL	O3P-C1-C2-O2
2	B	1806	CPL	O3P-C1-C2-O2
2	C	1806	CPL	O3P-C1-C2-O2
2	D	1806	CPL	O3P-C1-C2-O2
2	A	801	CPL	C12-C11-O3-C3
2	B	1802	CPL	C12-C11-O3-C3
2	C	1802	CPL	C12-C11-O3-C3
2	D	1802	CPL	C12-C11-O3-C3
2	A	805	CPL	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
2	C	1806	CPL	C21-C22-C23-C24
2	B	1806	CPL	C21-C22-C23-C24
2	D	1806	CPL	C21-C22-C23-C24
2	A	801	CPL	C2-C1-O3P-P
2	B	1802	CPL	C2-C1-O3P-P
2	C	1802	CPL	C2-C1-O3P-P
2	D	1802	CPL	C2-C1-O3P-P
2	D	1802	CPL	C14-C15-C16-C17
2	A	801	CPL	C14-C15-C16-C17
2	C	1802	CPL	C14-C15-C16-C17
2	B	1802	CPL	C14-C15-C16-C17
2	B	1806	CPL	C13-C14-C15-C16
2	C	1806	CPL	C13-C14-C15-C16
2	A	805	CPL	C13-C14-C15-C16
2	D	1806	CPL	C13-C14-C15-C16
2	A	805	CPL	C17-C18-C19-C20
2	B	1806	CPL	C17-C18-C19-C20
2	C	1806	CPL	C17-C18-C19-C20
2	D	1806	CPL	C17-C18-C19-C20
2	A	806	CPL	O2-C2-C3-O3
2	B	1801	CPL	O2-C2-C3-O3
2	C	1801	CPL	O2-C2-C3-O3
2	D	1801	CPL	O2-C2-C3-O3
2	B	1806	CPL	C22-C23-C24-C25
2	D	1806	CPL	C22-C23-C24-C25
2	A	805	CPL	C22-C23-C24-C25
2	C	1806	CPL	C22-C23-C24-C25
2	A	806	CPL	O3-C11-C12-C13
2	B	1801	CPL	O3-C11-C12-C13
2	C	1801	CPL	O3-C11-C12-C13
2	D	1801	CPL	O3-C11-C12-C13
2	B	1806	CPL	C23-C24-C25-C26
2	A	805	CPL	C23-C24-C25-C26
2	A	801	CPL	C20-C21-C22-C23
2	B	1802	CPL	C20-C21-C22-C23
2	C	1802	CPL	C20-C21-C22-C23
2	C	1806	CPL	C23-C24-C25-C26
2	D	1802	CPL	C20-C21-C22-C23
2	D	1806	CPL	C23-C24-C25-C26
2	B	1804	CPL	C19-C20-C21-C22
2	A	803	CPL	C19-C20-C21-C22
2	D	1804	CPL	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
2	C	1804	CPL	C19-C20-C21-C22
2	A	801	CPL	C1-O3P-P-O1P
2	B	1802	CPL	C1-O3P-P-O1P
2	C	1802	CPL	C1-O3P-P-O1P
2	D	1802	CPL	C1-O3P-P-O1P
2	A	801	CPL	C33-C34-C35-C36
2	C	1802	CPL	C33-C34-C35-C36
2	D	1802	CPL	C33-C34-C35-C36
2	B	1802	CPL	C33-C34-C35-C36
2	A	801	CPL	C5-C4-O4P-P
2	B	1802	CPL	C5-C4-O4P-P
2	C	1802	CPL	C5-C4-O4P-P
2	D	1802	CPL	C5-C4-O4P-P
2	A	806	CPL	O11-C11-C12-C13
2	B	1801	CPL	O11-C11-C12-C13
2	C	1801	CPL	O11-C11-C12-C13
2	D	1801	CPL	O11-C11-C12-C13
2	A	805	CPL	O3-C11-C12-C13
2	B	1806	CPL	O3-C11-C12-C13
2	C	1806	CPL	O3-C11-C12-C13
2	D	1806	CPL	O3-C11-C12-C13

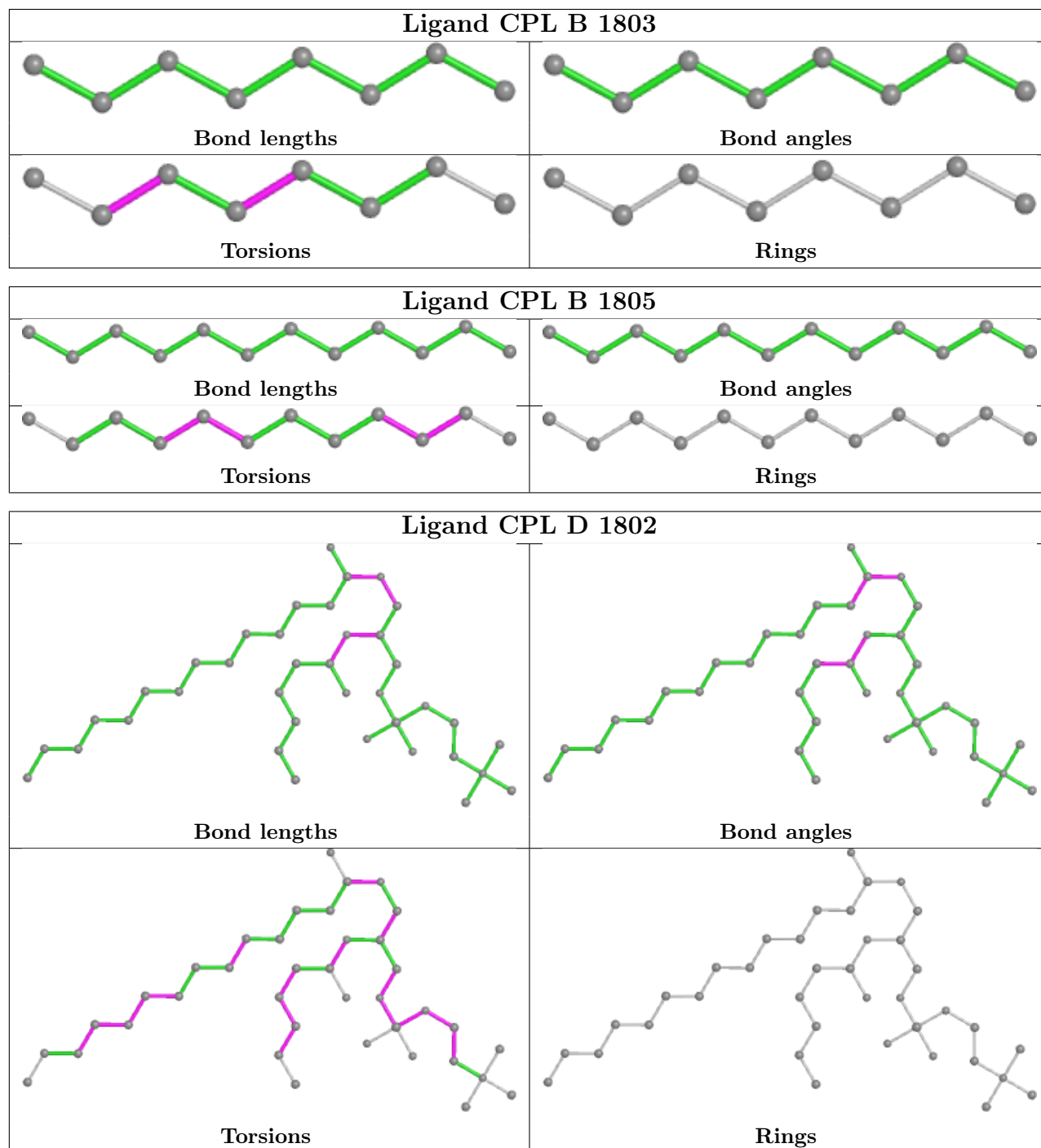
There are no ring outliers.

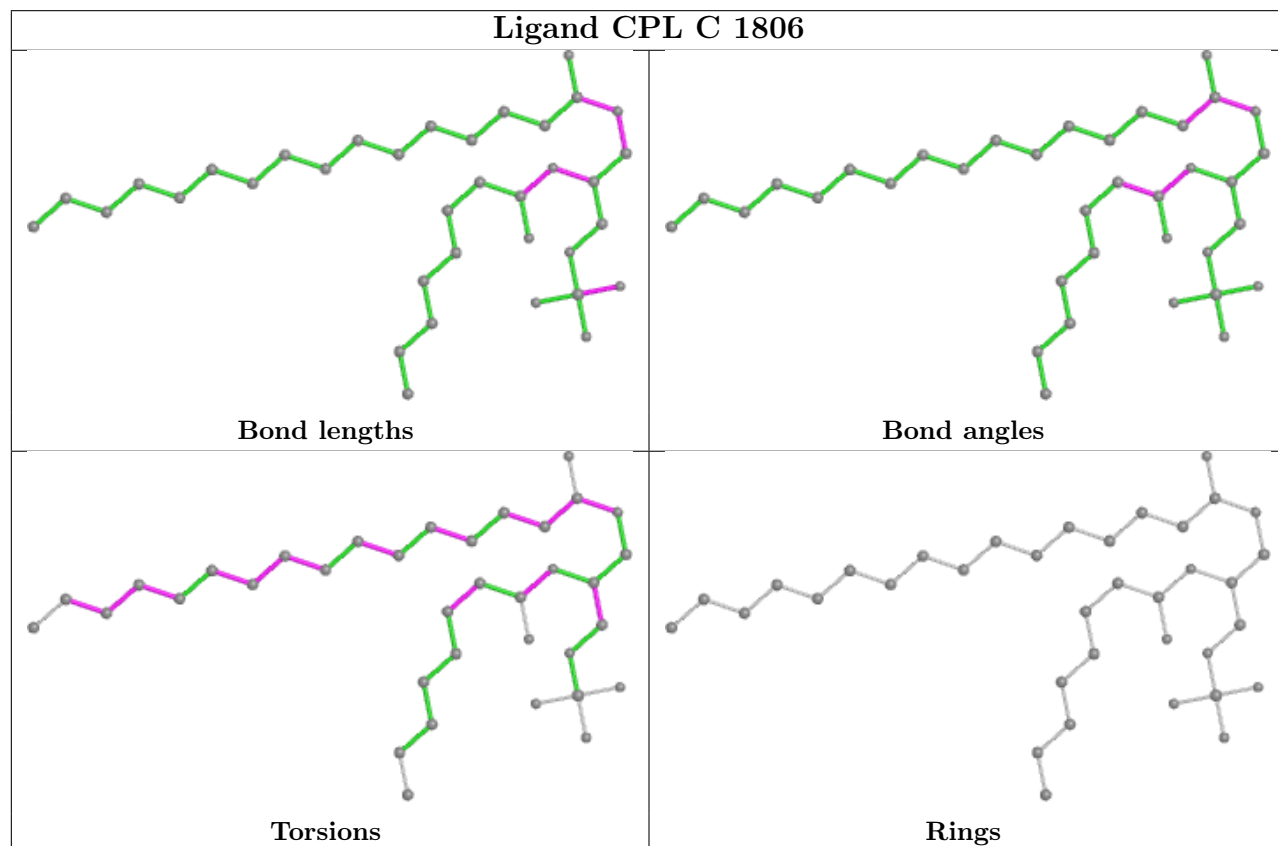
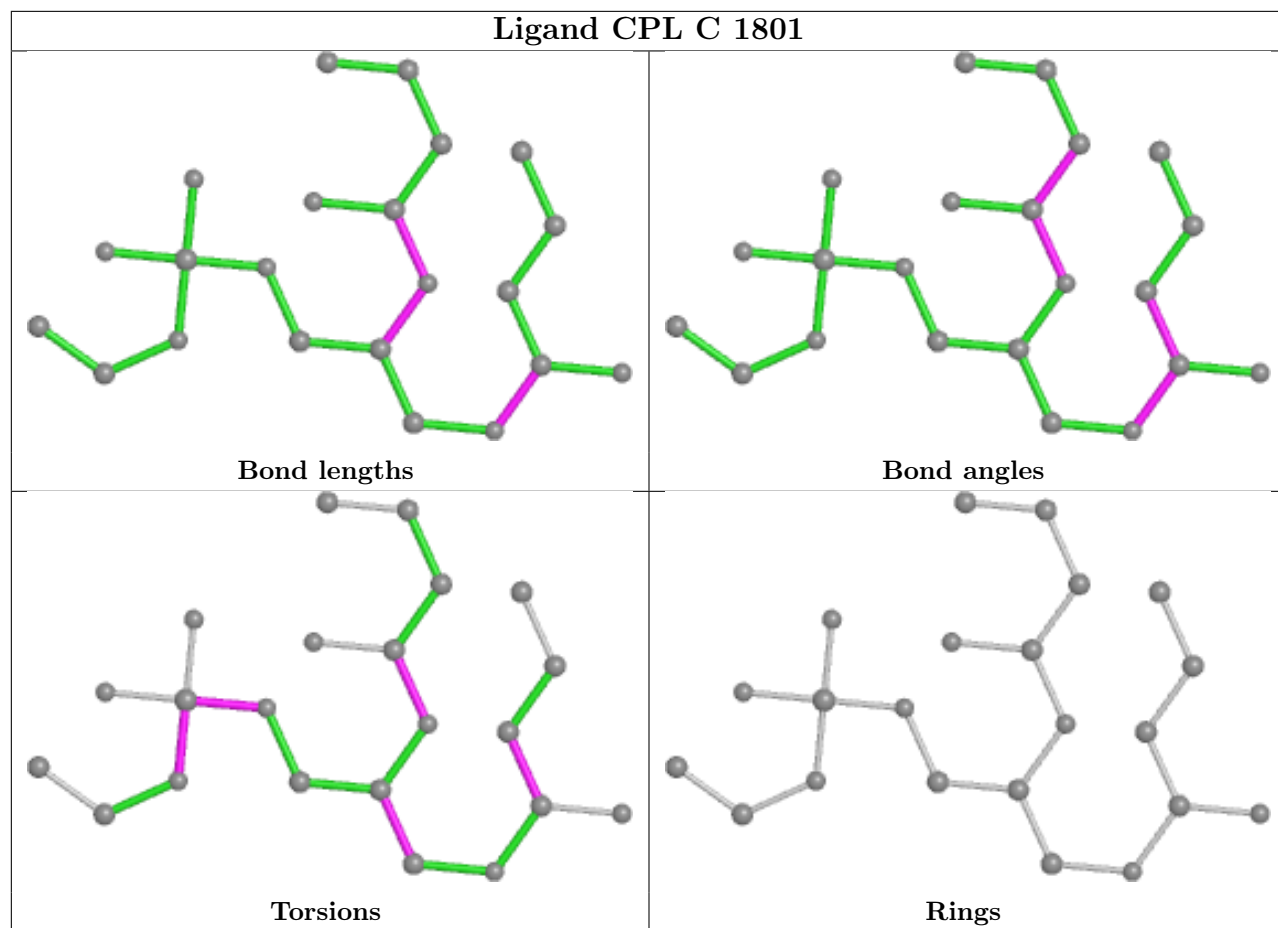
8 monomers are involved in 8 short contacts:

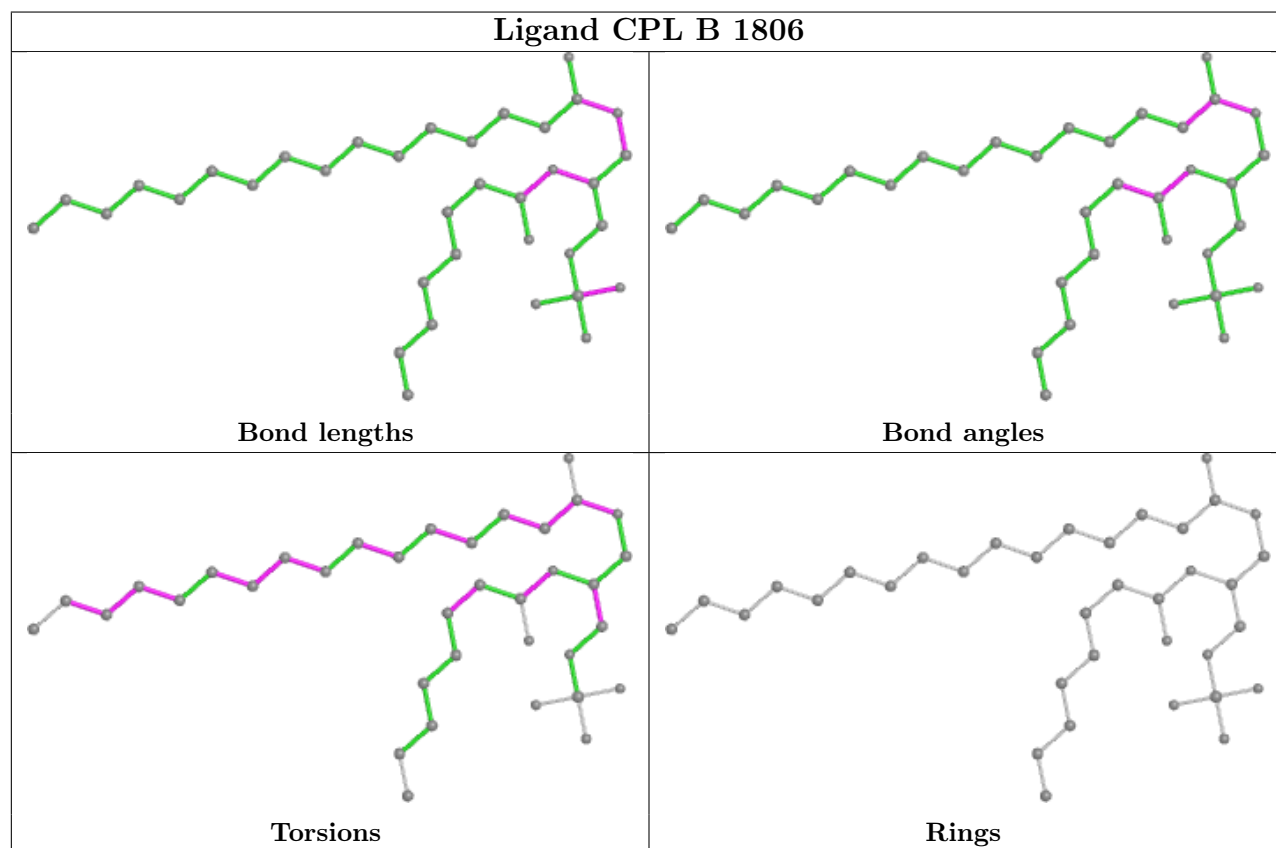
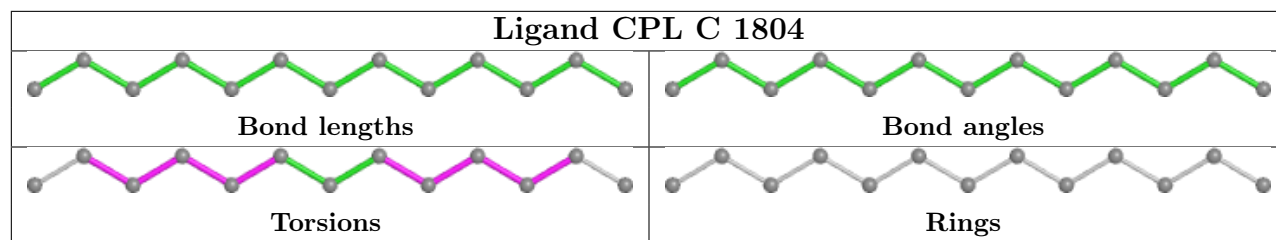
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1801	CPL	1	0
2	C	1804	CPL	1	0
2	D	1801	CPL	1	0
2	A	803	CPL	1	0
2	B	1804	CPL	1	0
2	D	1804	CPL	1	0
2	B	1801	CPL	1	0
2	A	806	CPL	1	0

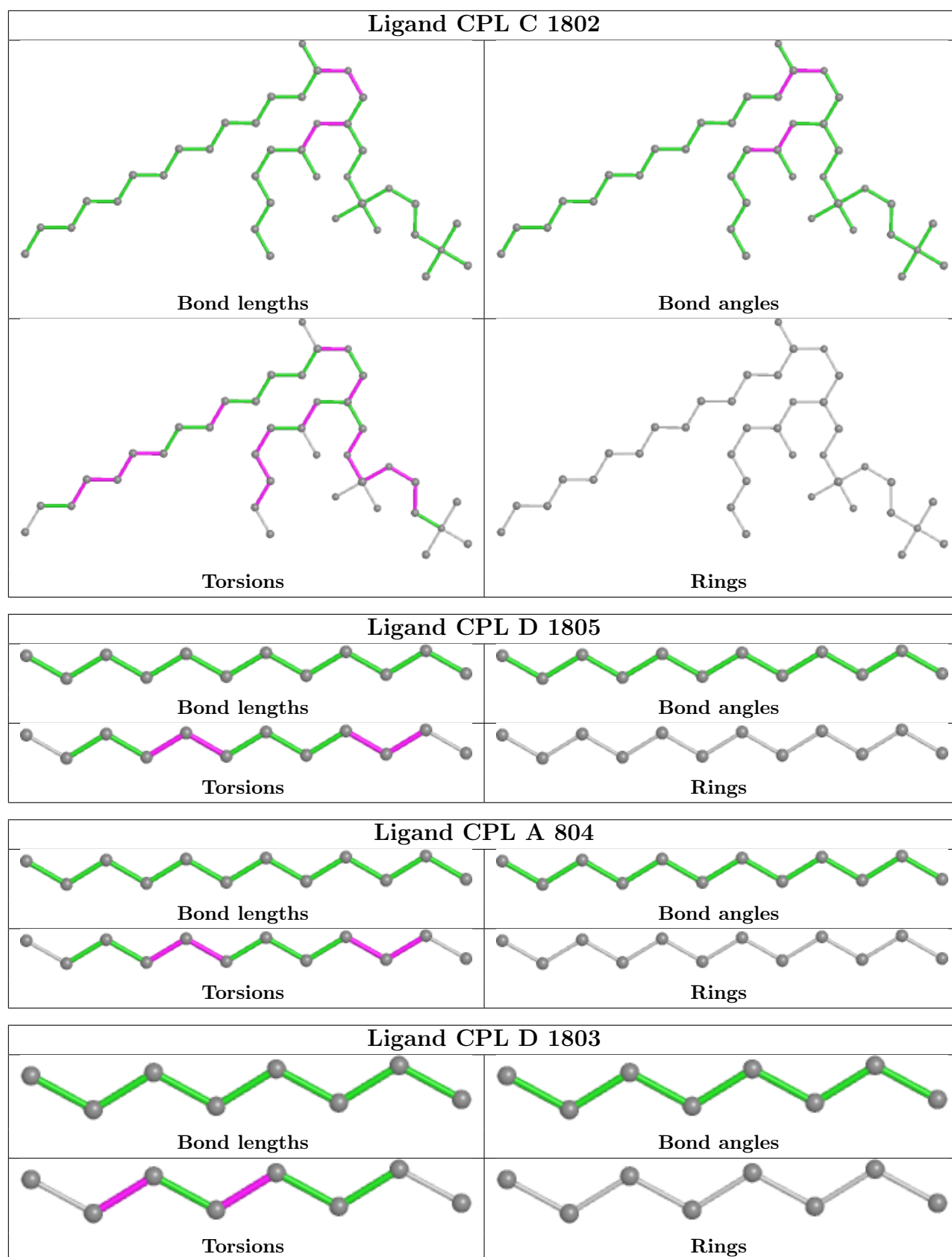
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

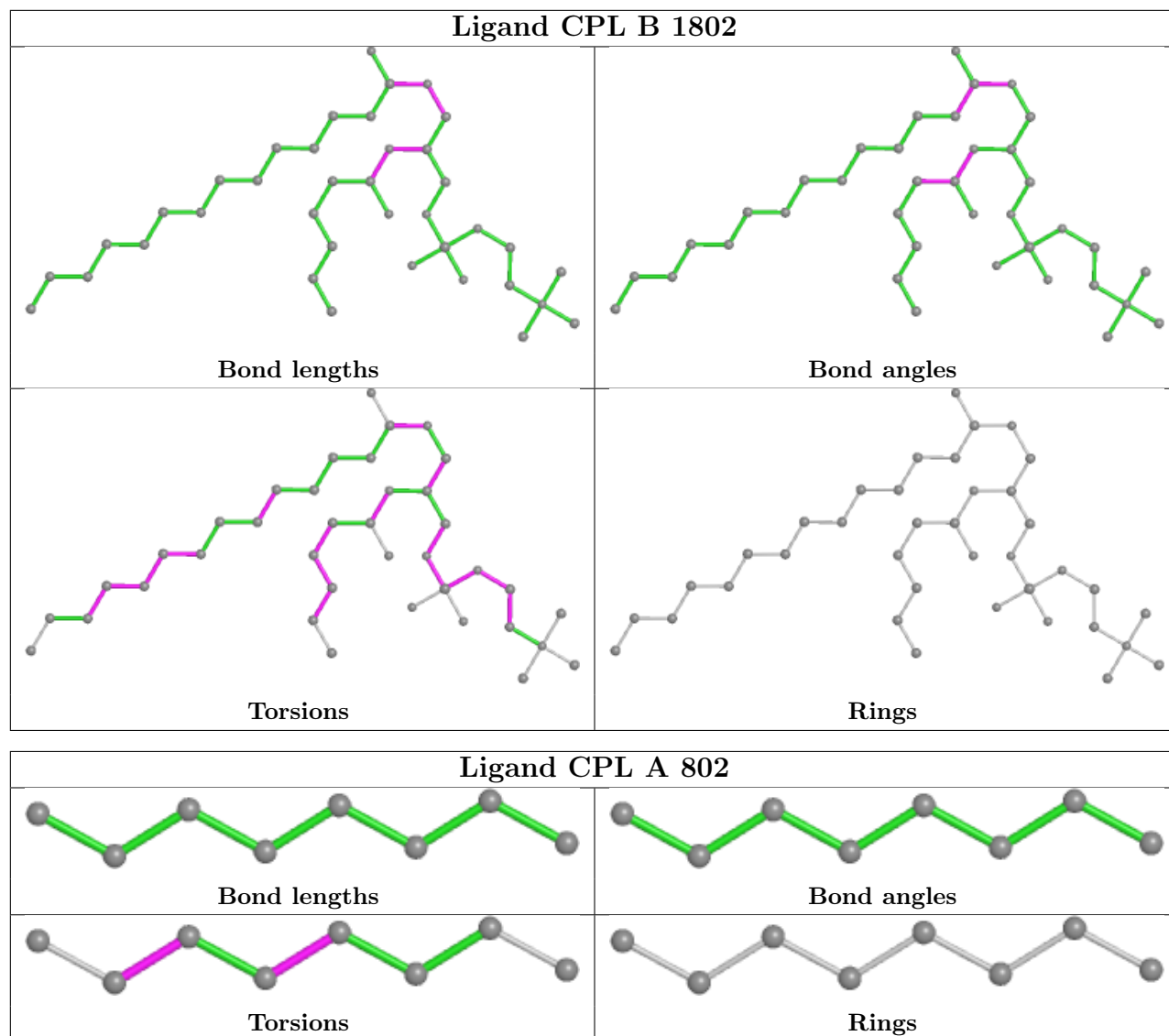
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

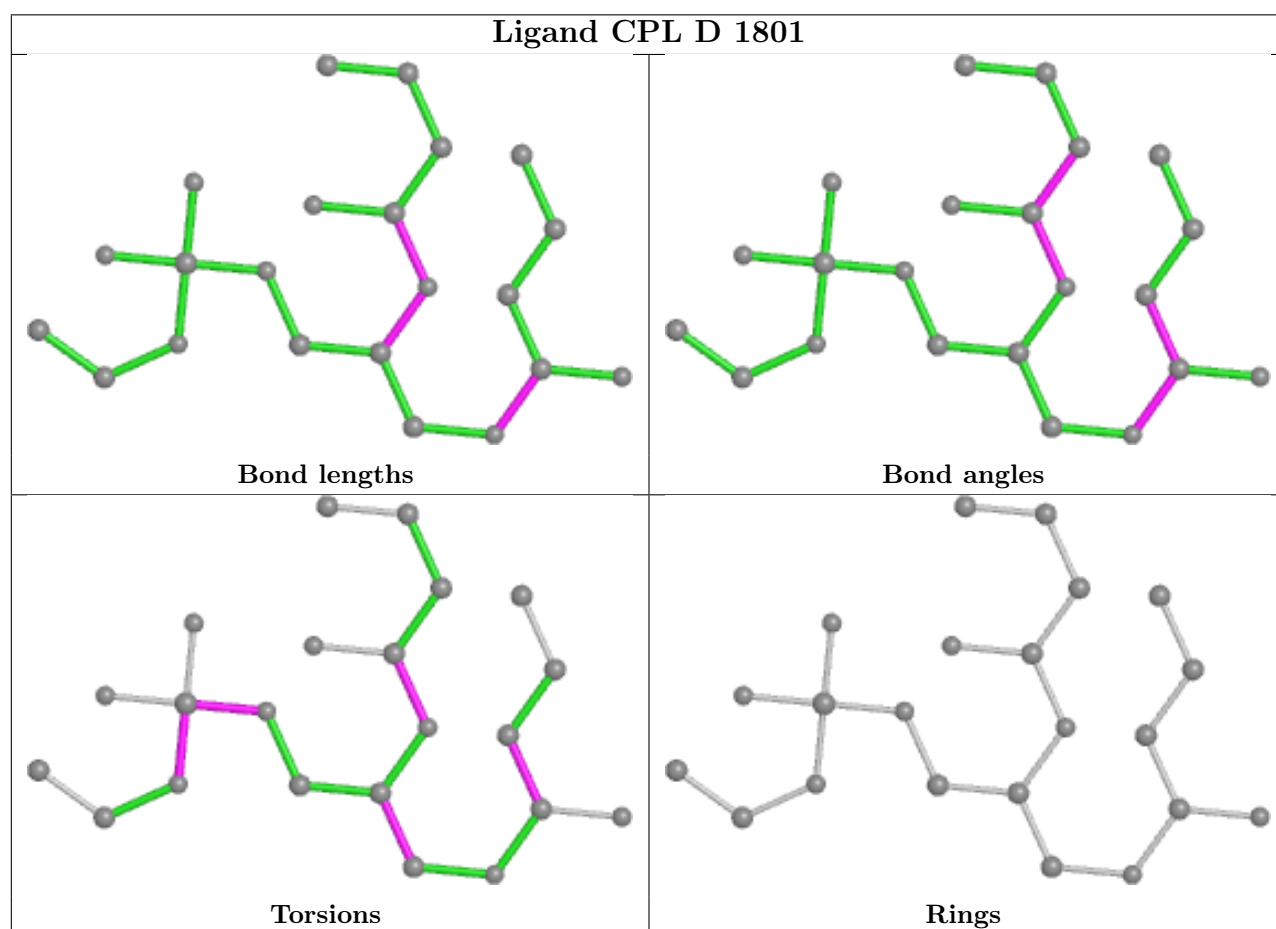
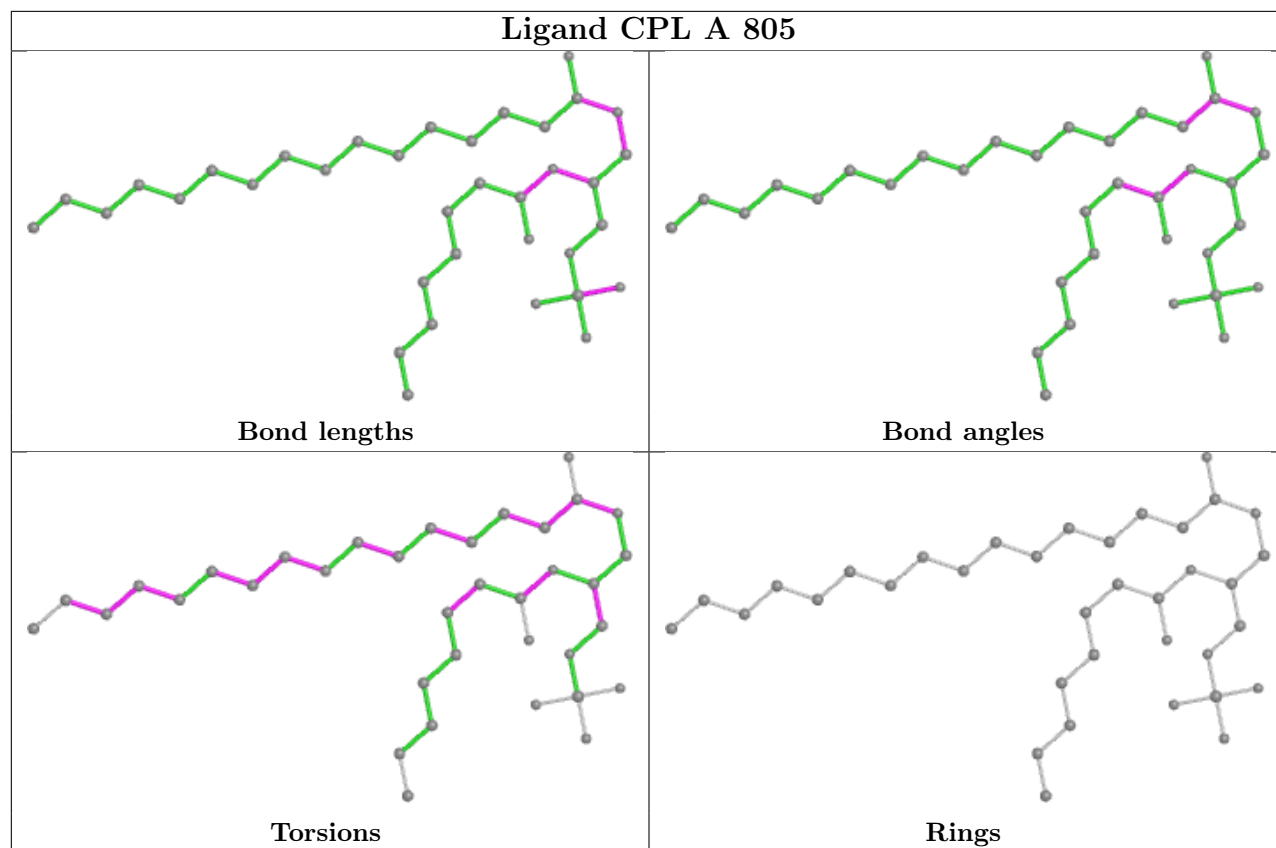




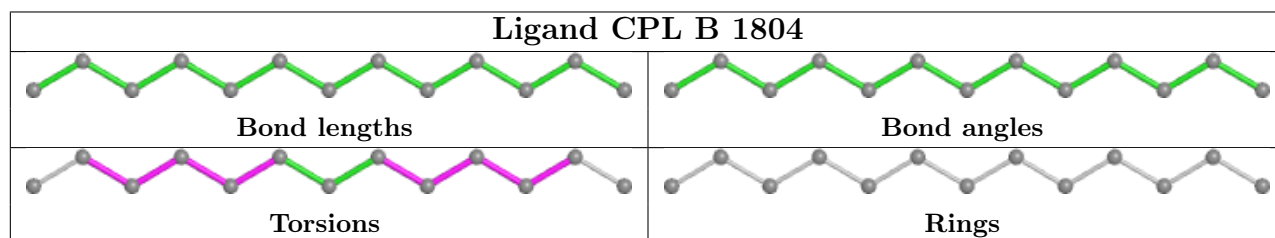
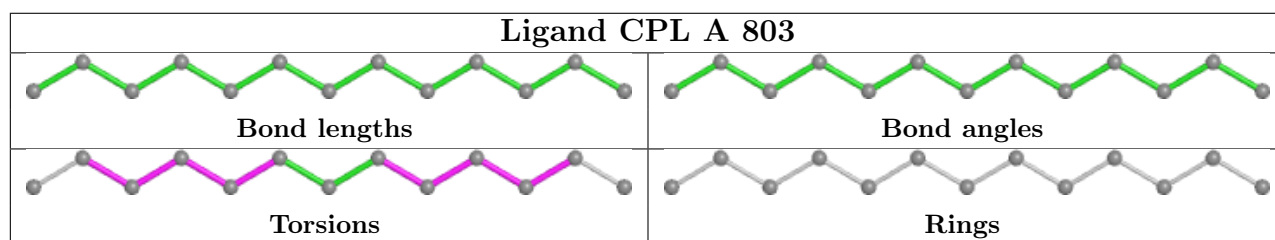
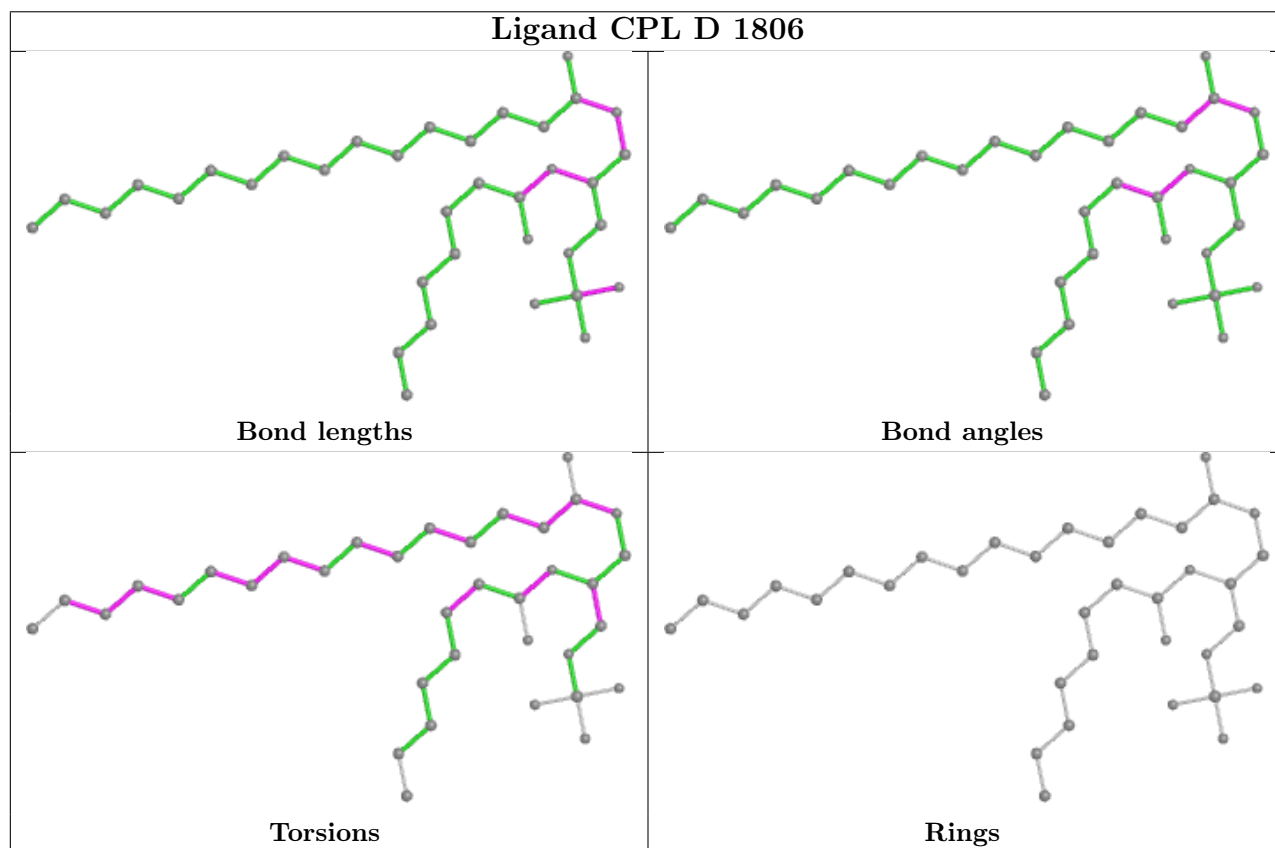
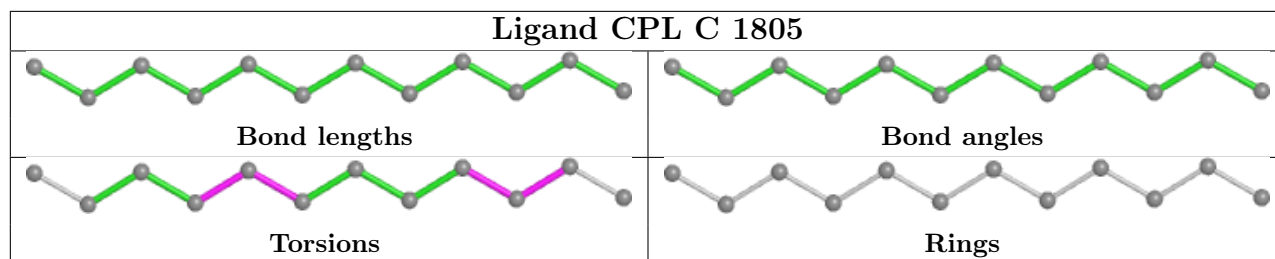


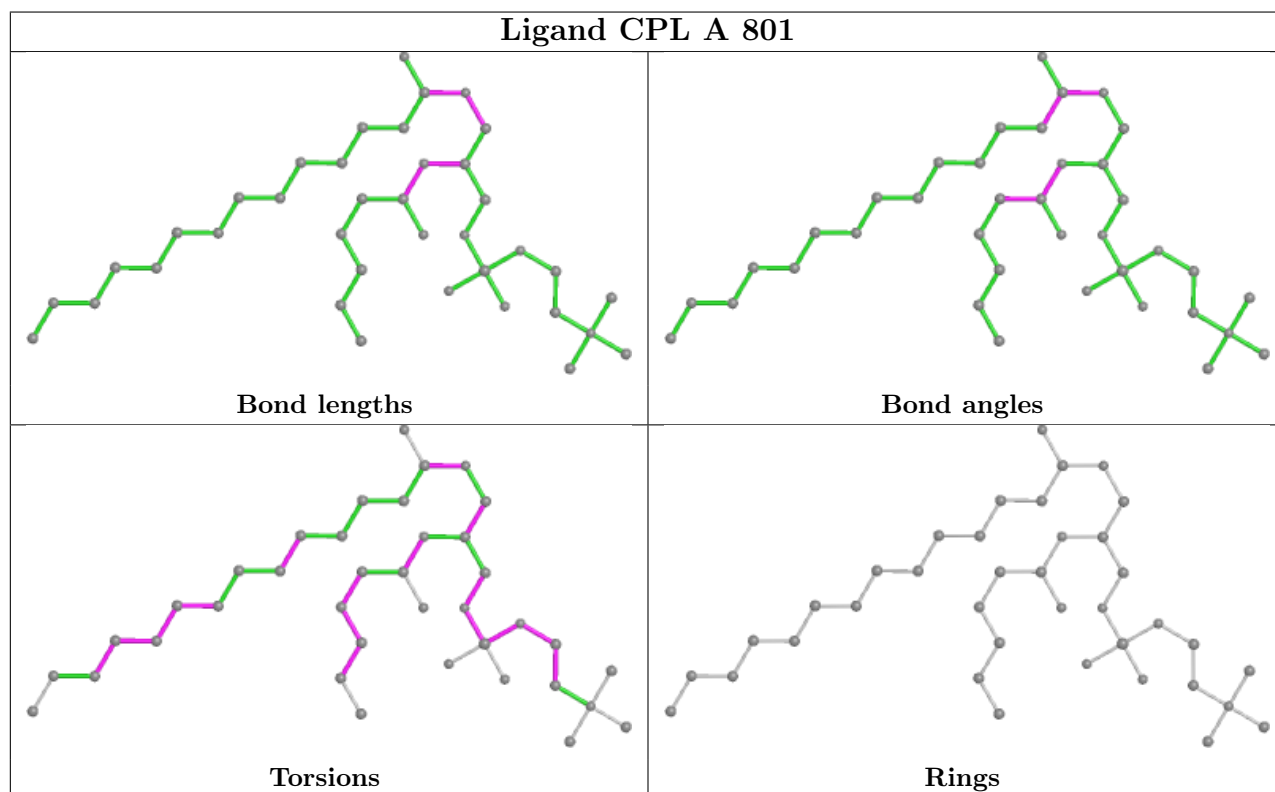
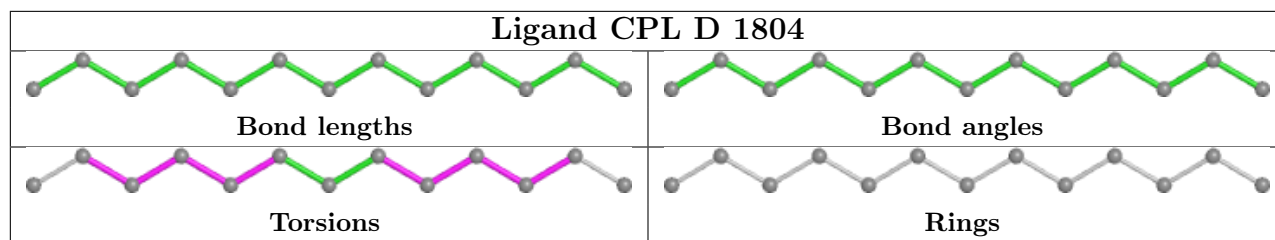


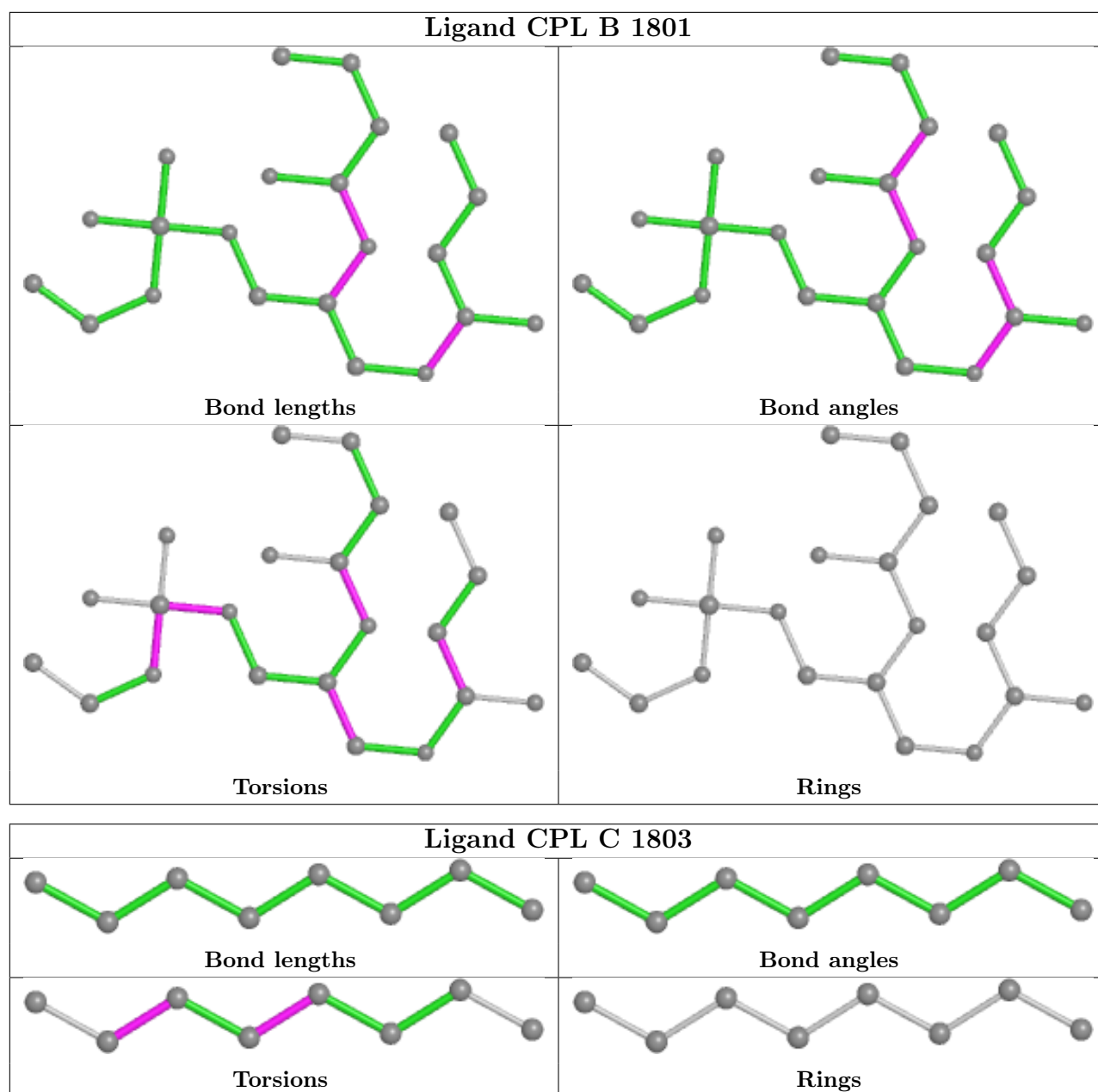


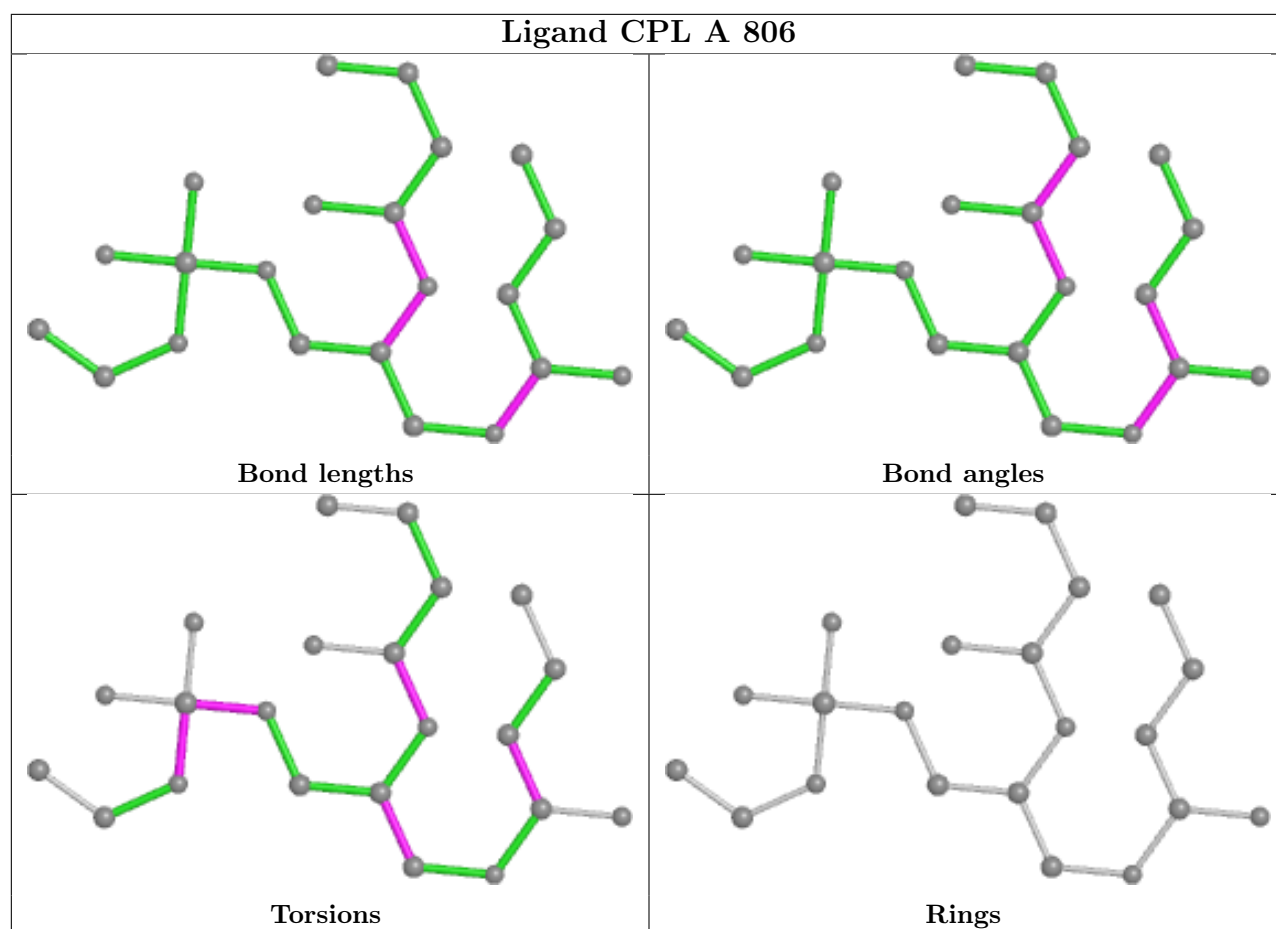












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

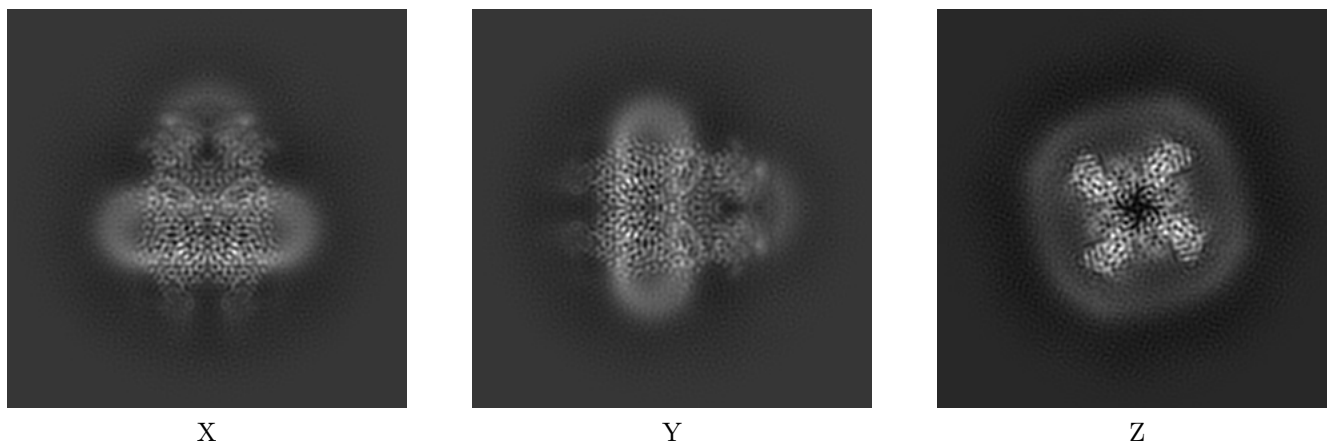
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-24115. 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](#)

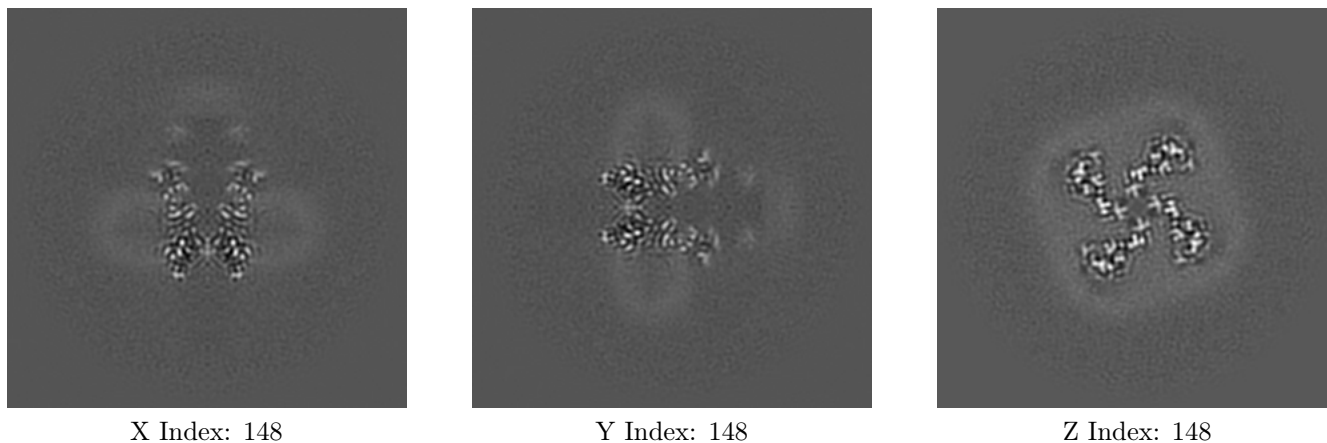
#### 6.1.1 Primary map



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

### 6.2 Central slices [i](#)

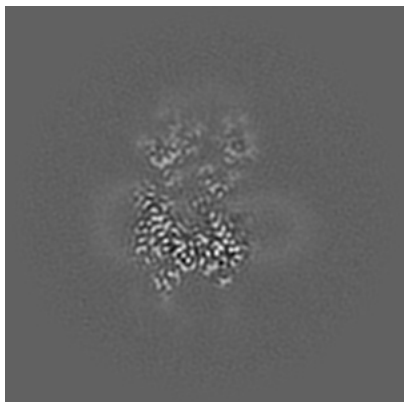
#### 6.2.1 Primary map



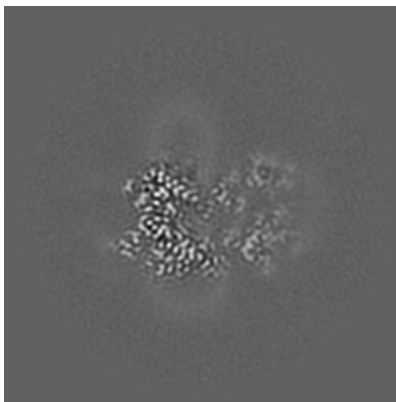
The images above show central slices of the map in three orthogonal directions.

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

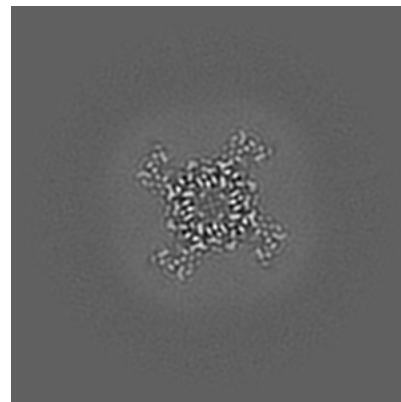
### 6.3.1 Primary map



X Index: 129



Y Index: 167

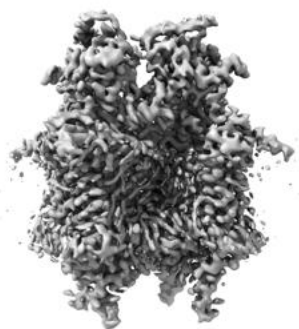


Z Index: 112

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

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

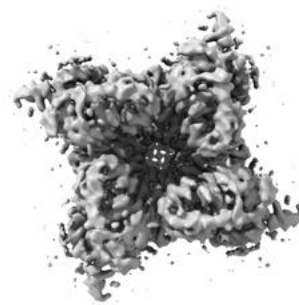
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.33. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

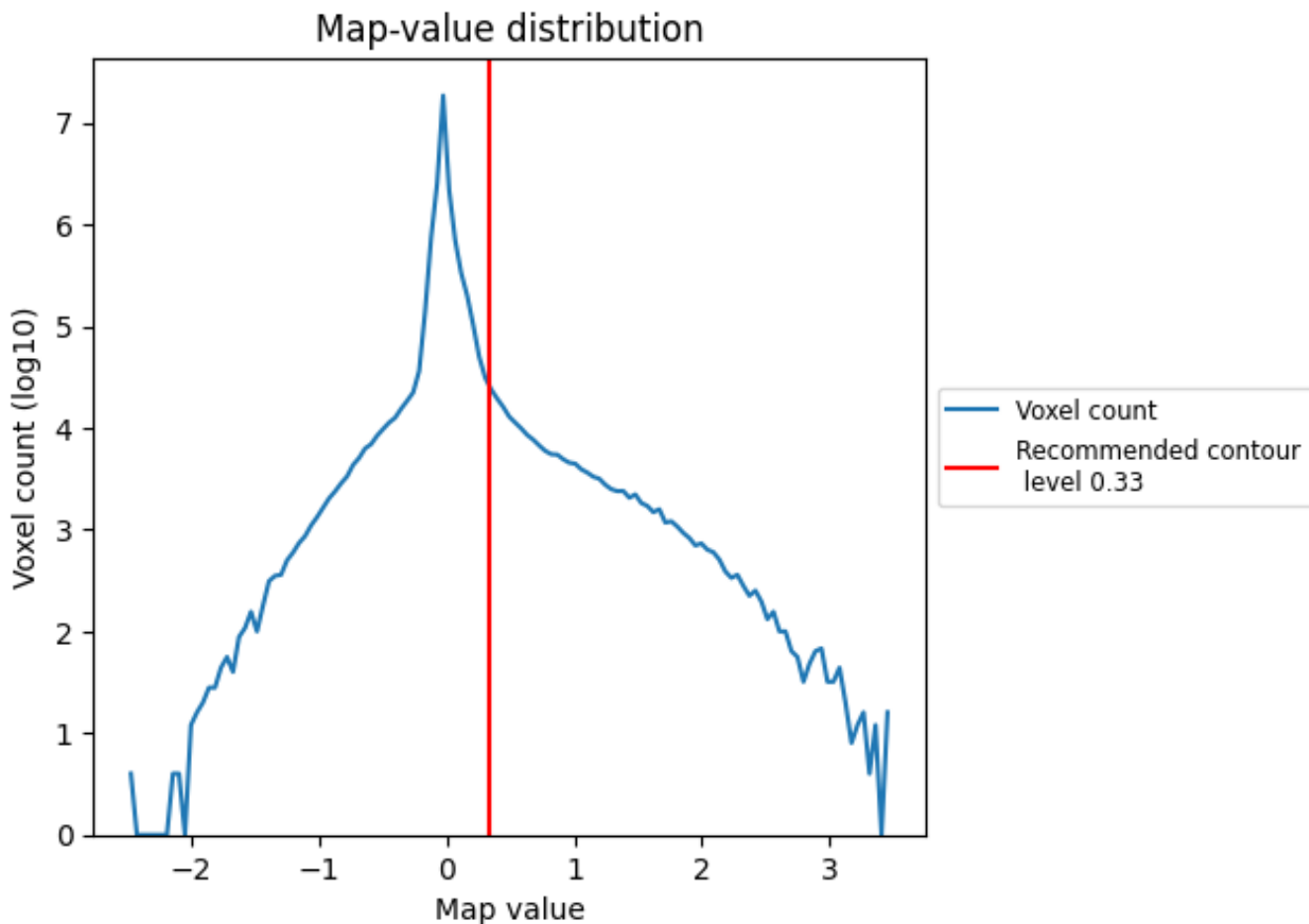
## 6.5 Mask visualisation

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.

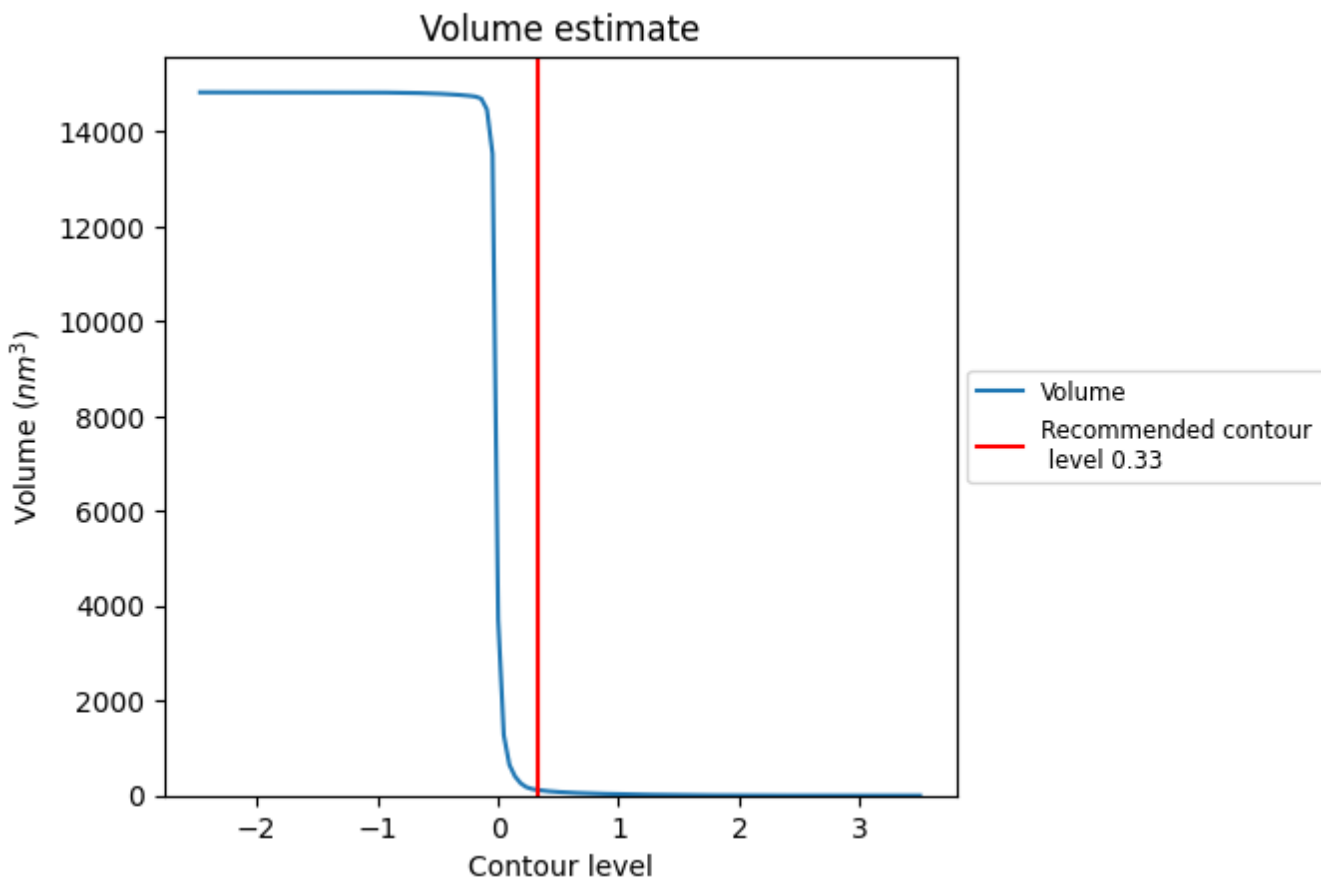
### 7.1 Map-value distribution [i](#)



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.



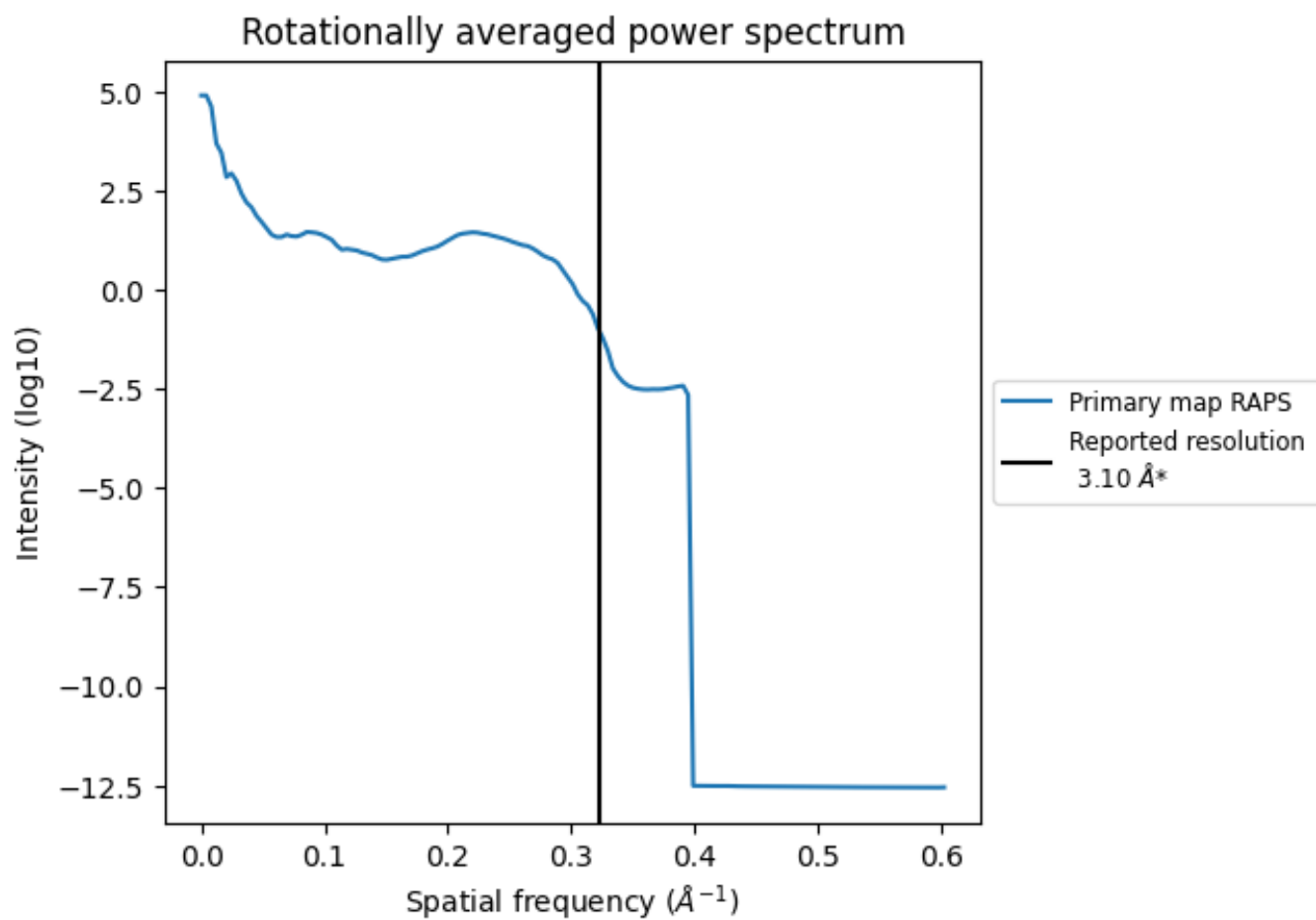
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 118 nm<sup>3</sup>; this corresponds to an approximate mass of 106 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum [i](#)



\*Reported resolution corresponds to spatial frequency of 0.323 Å<sup>-1</sup>

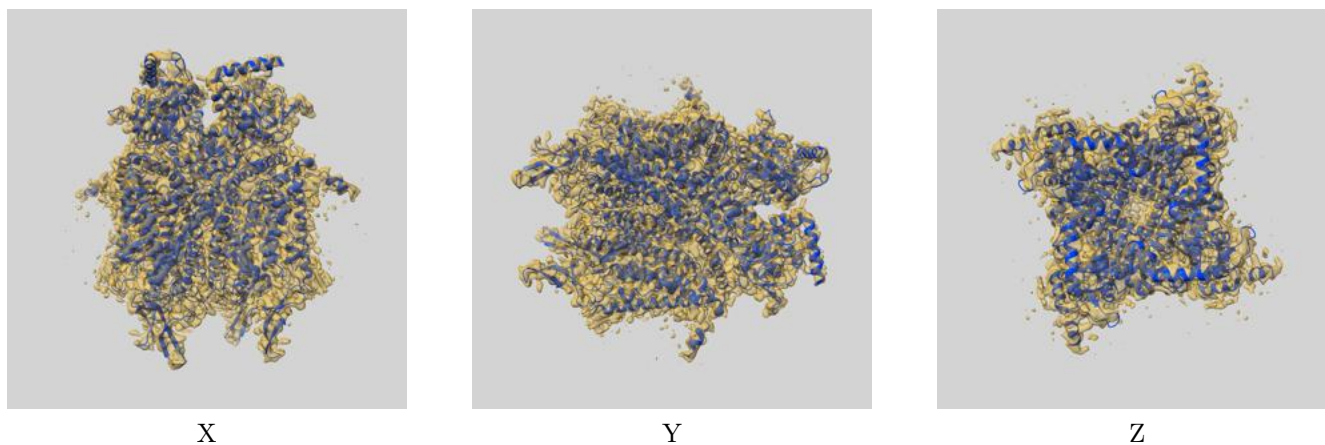
## 8 Fourier-Shell correlation

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

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

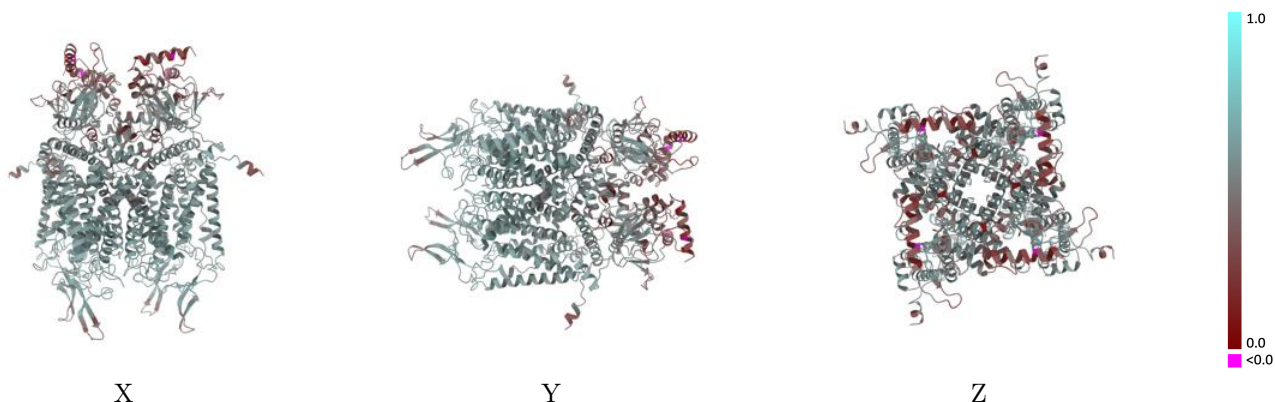
This section contains information regarding the fit between EMDB map EMD-24115 and PDB model 7N17. Per-residue inclusion information can be found in section 3 on page 6.

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



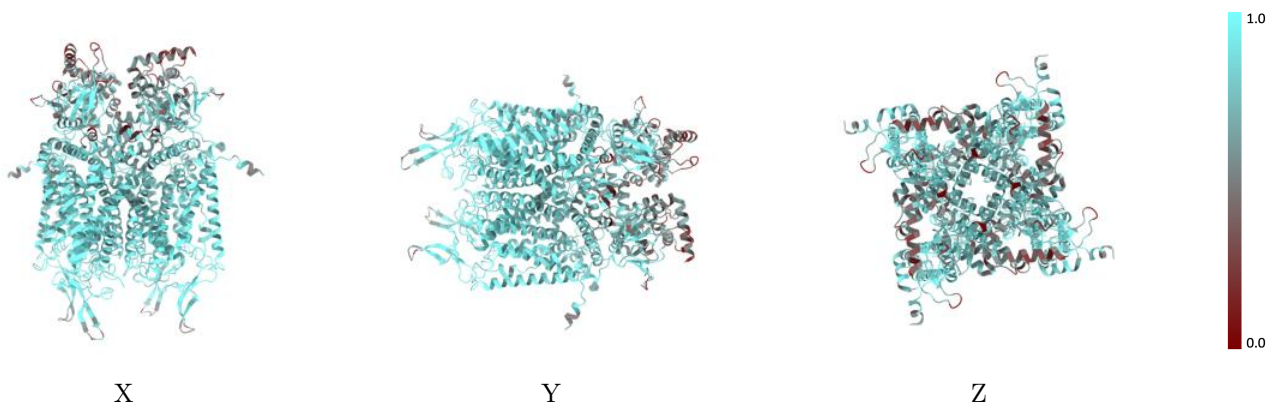
The images above show the 3D surface view of the map at the recommended contour level 0.33 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



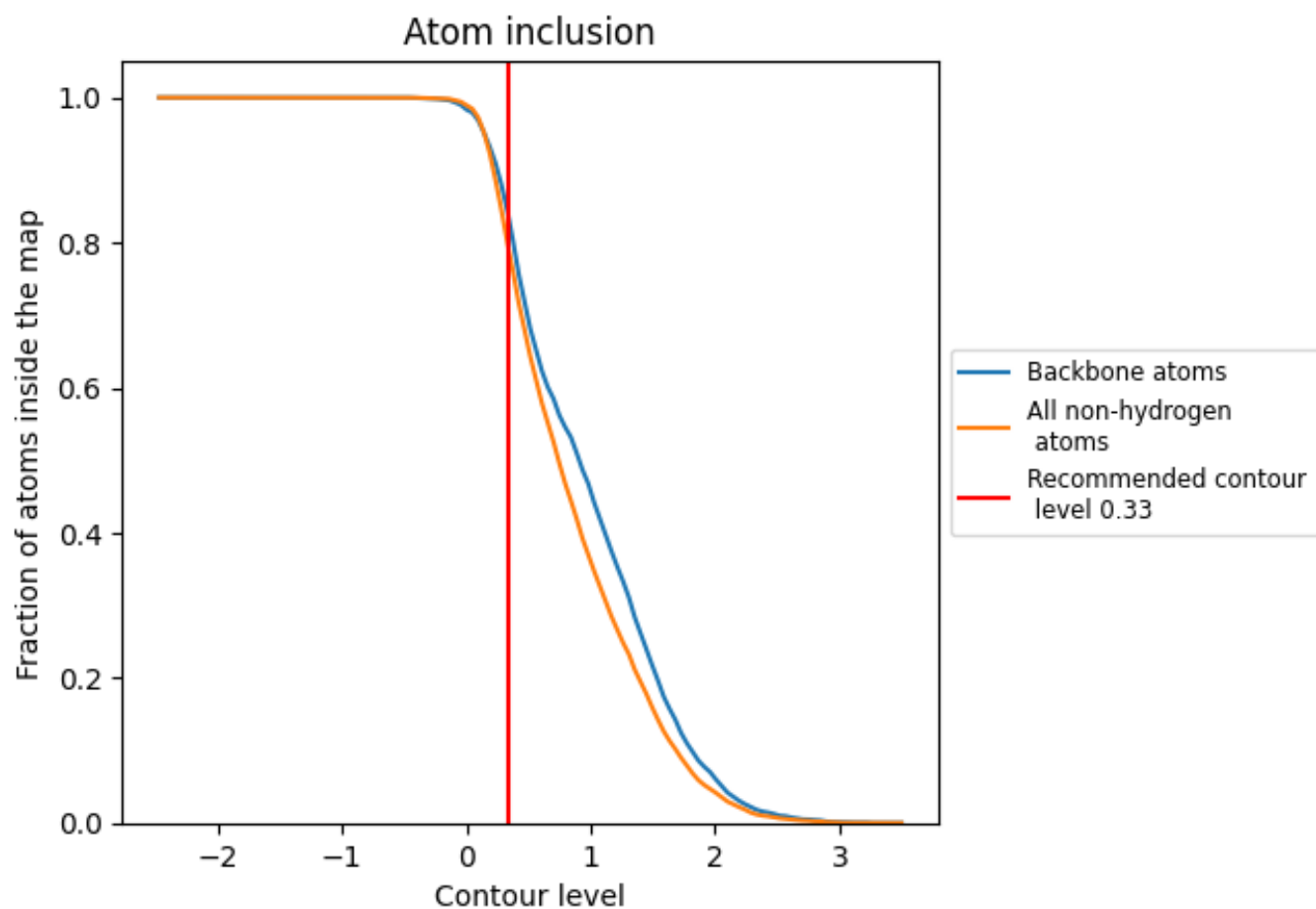
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.33).





## 9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 80% 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 (0.33) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7995	 0.5140
A	 0.8002	 0.5140
B	 0.7981	 0.5140
C	 0.7986	 0.5140
D	 0.8012	 0.5140

