



Full wwPDB EM Validation Report ⓘ

Nov 3, 2024 – 03:37 PM EST

PDB ID : 7N16
EMDB ID : EMD-24114
Title : Structure of TAX-4_R421W apo closed state
Authors : Zheng, X.; Li, H.; Hu, Z.; Su, D.; Yang, J.
Deposited on : 2021-05-27
Resolution : 3.20 Å (reported)
Based on initial model : 6WEJ

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

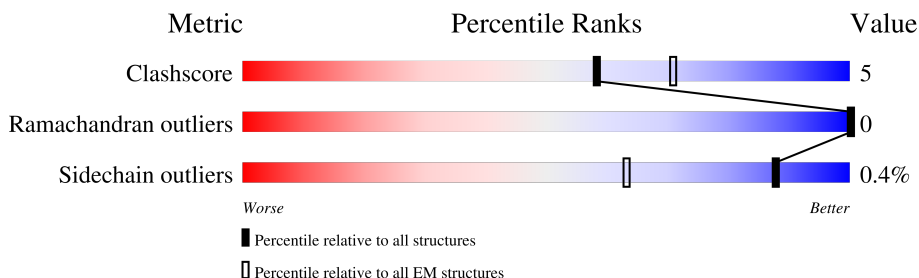
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	738	<div> <div>11%</div> <div>61%</div> <div>8%</div> <div>30%</div> </div>
1	B	738	<div> <div>11%</div> <div>61%</div> <div>8%</div> <div>30%</div> </div>
1	C	738	<div> <div>11%</div> <div>61%</div> <div>8%</div> <div>30%</div> </div>
1	D	738	<div> <div>11%</div> <div>62%</div> <div>8%</div> <div>30%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 17357 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	D	514	Total	C	N	O	S	0	0
			4252	2766	714	748	24		
1	A	514	Total	C	N	O	S	0	0
			4252	2766	714	748	24		
1	B	514	Total	C	N	O	S	0	0
			4252	2766	714	748	24		
1	C	514	Total	C	N	O	S	0	0
			4252	2766	714	748	24		

There are 24 discrepancies between the modelled and reference sequences:

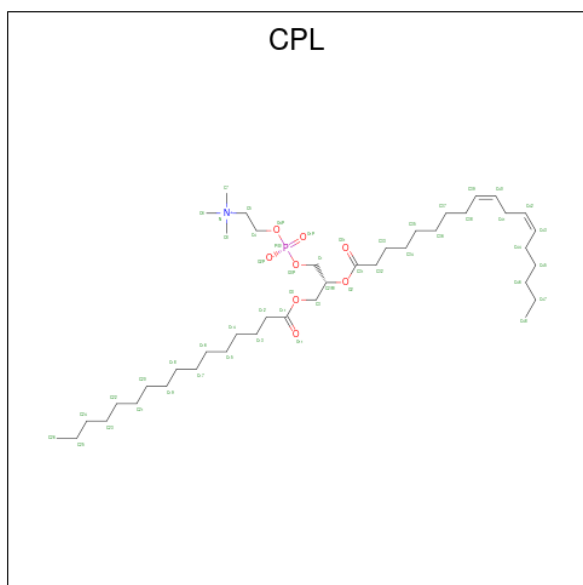
Chain	Residue	Modelled	Actual	Comment	Reference
D	-4	GLY	-	expression tag	UNP Q03611
D	-3	GLY	-	expression tag	UNP Q03611
D	-2	GLY	-	expression tag	UNP Q03611
D	-1	GLY	-	expression tag	UNP Q03611
D	0	SER	-	expression tag	UNP Q03611
D	421	TRP	ARG	engineered mutation	UNP Q03611
A	-4	GLY	-	expression tag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

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

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



Mol	Chain	Residues	Atoms					AltConf
2	D	1	Total	C	N	O	P	0
			28	18	1	8	1	
2	D	1	Total	C				0
			10	10				
2	D	1	Total	C	O	P		0
			27	18	8	1		
2	D	1	Total	C	O	P		0
			22	13	8	1		
2	A	1	Total	C	O	P		0
			22	13	8	1		
2	A	1	Total	C	N	O	P	0
			28	18	1	8	1	
2	A	1	Total	C				0
			10	10				
2	A	1	Total	C	O	P		0
			27	18	8	1		
2	B	1	Total	C	O	P		0
			22	13	8	1		

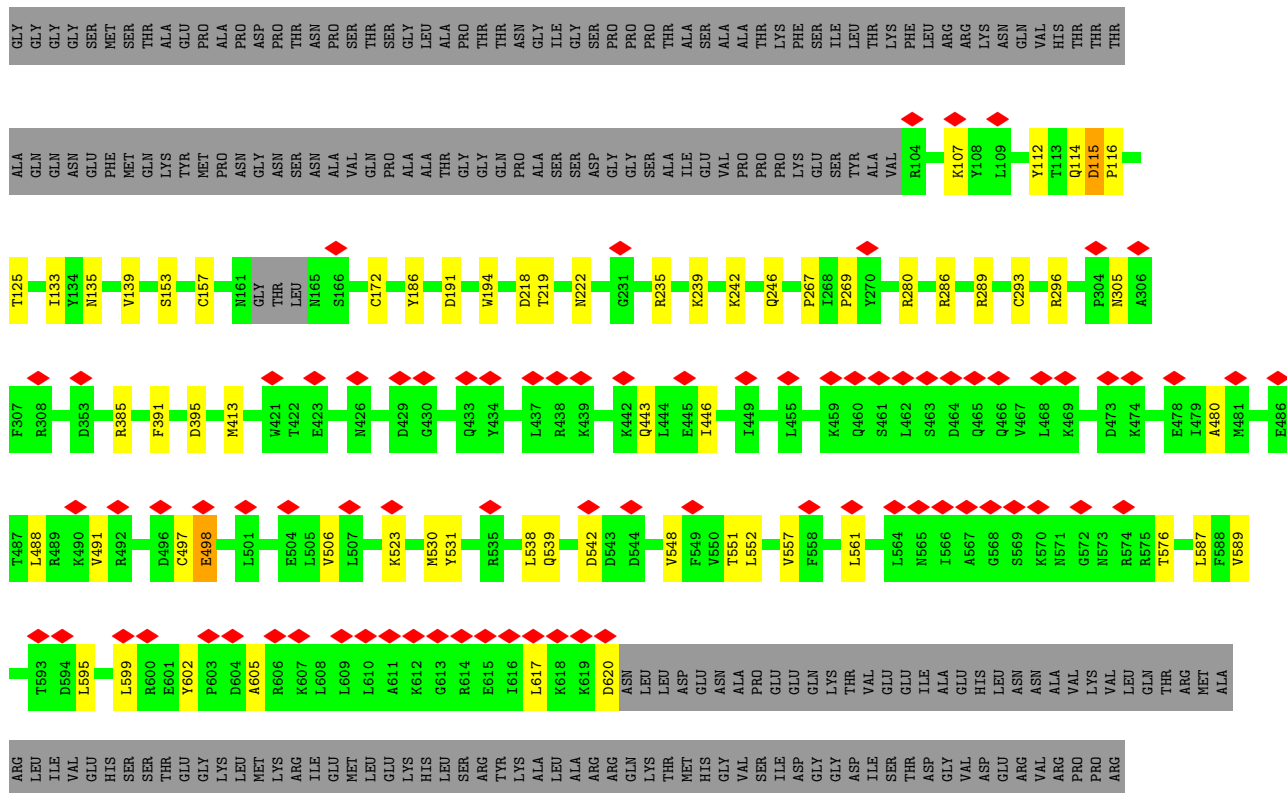
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Mol	Chain	Residues	Atoms					AltConf
2	B	1	Total	C	N	O	P	0
			28	18	1	8	1	
2	B	1	Total	C				0
			10	10				
2	B	1	Total	C	O	P		0
			27	18	8	1		
2	C	1	Total	C	O	P		0
			22	13	8	1		
2	C	1	Total	C	N	O	P	0
			28	18	1	8	1	
2	C	1	Total	C				0
			10	10				
2	C	1	Total	C	O	P		0
			27	18	8	1		

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

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



LEU
ARG
GLN
THR
GLY
LYS
THR
THR
ILE
ASP
LEU
PRO
THR
THR
GLY
THR
GLU
SER
SER
SER
LEU
LEU
LYS

● Molecule 1: Cyclic nucleotide-gated cation channel



GLY
GLY
GLY
GLY
ASN
SER
GLU
MET
SER
SER
THR
ALA
GLU
GLU
MET
PRO
ALA
PRO
ASP
PRO
THR
THR
THR
ASN
GLY
ALA
LEU
GLY
ALA
PRO
THR
THR
THR
GLY
ILE
SER
GLY
SER
PRO
PRO
GLY
GLY
THR
ALA
SER
SER
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GLU
SER
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LEU
ALA
THR
LYS
PHE
LEU
ARG
LYS
ASN
GLN
VAL
HIS
THR
THR
THR

ALA
GLN
GLN
ASN
GLU
PHE
MET
GLN
LYS
TYR
MET
PRO
ALA
ASN
GLY
ASN
THR
SER
ASN
ASN
ALA
VAL
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PRO
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ILE
ASP
GLY
GLY
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GLY
ILE
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VAL
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PRO
LYS
PHE
GLU
SER
TYR
VAL
R104
K107
Y108
I109
Y112
T113
Q114
D115
P116

T125
I133
Y134
N135
V139
S153
C157
H161
GLY
THR
LEU
N165
S166
C172
Y186
D191
W194
D218
T219
N222
C231
R236
K242
Q246
P267
I268
P269
R280
R286
R289
C293
R296
P304
N305
A306
F307
R308

R385
F391
D395
M413
W421
T422
E423
W426
D429
G430
Q433
Y434
L437
R438
K439
K442
Q443
L444
E445
I446
I449
L455
K459
Q460
S461
L462
S463
D464
Q465
Q466
V467
L468
K469
D473
K474
A480
M481
E486
T487
L488
R489
K490
V491
R492

D496
C497
E498
L501
E504
L505
V506
L507
K523
M530
Y531
R535
L538
Q539
D542
D543
D544
V548
F549
V550
T551
L552
V557
F558
L561
L564
N565
I566
A567
G568
S569
K570
G571
G572
M573
R574
T576
L587
F588
V589
T593
D594
L595
L599
R600

R601
Y602
P603
D604
A605
R606
R607
L608
L609
L610
A611
R612
G613
HIS
R614
E615
I616
L617
K618
K619
D620
ASN
LEU
LEU
ASP
GLU
GLU
ASN
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LYS
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THR
ILE

ASP
LEU
PRO
THR
THR
THR
GLU
SER
GLU
SER
SER
LEU
LEU
LYS

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	66523	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	2.561	Depositor
Minimum map value	-1.504	Depositor
Average map value	0.006	Depositor
Map value standard deviation	0.092	Depositor
Recommended contour level	0.39	Depositor
Map size (\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 (\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: NA, 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	0.40	0/4356	0.59	1/5909 (0.0%)
1	B	0.40	0/4356	0.59	1/5909 (0.0%)
1	C	0.41	0/4356	0.59	1/5909 (0.0%)
1	D	0.40	0/4356	0.59	1/5909 (0.0%)
All	All	0.40	0/17424	0.59	4/23636 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	620	ASP	CB-CG-OD1	6.40	124.06	118.30
1	A	620	ASP	CB-CG-OD1	6.39	124.05	118.30
1	D	620	ASP	CB-CG-OD1	6.38	124.05	118.30
1	B	620	ASP	CB-CG-OD1	6.33	124.00	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4252	0	4284	41	0
1	B	4252	0	4284	40	0
1	C	4252	0	4284	39	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	4252	0	4284	37	0
2	A	87	0	88	2	0
2	B	87	0	88	2	0
2	C	87	0	88	2	0
2	D	87	0	88	2	0
3	A	1	0	0	0	0
All	All	17357	0	17488	157	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 5.

All (157) 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:A:531:TYR:CD1	1:A:589:VAL:HG12	2.30	0.67
1:D:531:TYR:CD1	1:D:589:VAL:HG12	2.30	0.67
1:B:531:TYR:CD1	1:B:589:VAL:HG12	2.30	0.67
1:C:531:TYR:CD1	1:C:589:VAL:HG12	2.30	0.66
1:B:191:ASP:HA	1:B:269:PRO:HB3	1.79	0.64
1:D:191:ASP:HA	1:D:269:PRO:HB3	1.79	0.64
1:C:191:ASP:HA	1:C:269:PRO:HB3	1.79	0.63
1:D:135:ASN:O	1:D:139:VAL:HB	1.99	0.63
1:A:135:ASN:O	1:A:139:VAL:HB	1.99	0.62
1:C:135:ASN:O	1:C:139:VAL:HB	1.99	0.62
1:B:135:ASN:O	1:B:139:VAL:HB	1.99	0.62
1:A:191:ASP:HA	1:A:269:PRO:HB3	1.79	0.62
1:D:222:ASN:OD1	1:D:289:ARG:NH2	2.38	0.57
1:A:443:GLN:HA	1:A:446:ILE:HD12	1.87	0.57
1:B:222:ASN:OD1	1:B:289:ARG:NH2	2.38	0.57
1:C:222:ASN:OD1	1:C:289:ARG:NH2	2.38	0.57
1:D:115:ASP:OD2	1:D:235:ARG:NH1	2.38	0.56
1:A:222:ASN:OD1	1:A:289:ARG:NH2	2.38	0.56
1:C:115:ASP:OD2	1:C:235:ARG:NH1	2.38	0.56
1:C:191:ASP:O	1:C:191:ASP:OD1	2.23	0.56
1:D:443:GLN:HA	1:D:446:ILE:HD12	1.87	0.56
1:B:191:ASP:O	1:B:191:ASP:OD1	2.24	0.56
1:D:191:ASP:OD1	1:D:191:ASP:O	2.24	0.56
1:A:523:LYS:HG3	1:A:576:THR:HA	1.88	0.56
1:B:443:GLN:HA	1:B:446:ILE:HD12	1.87	0.56
1:B:523:LYS:HG3	1:B:576:THR:HA	1.88	0.56
1:B:115:ASP:OD2	1:B:235:ARG:NH1	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:ASP:OD2	1:A:235:ARG:NH1	2.38	0.56
1:B:385:ARG:NH2	2:B:1801:CPL:O2P	2.39	0.56
1:A:191:ASP:O	1:A:191:ASP:OD1	2.23	0.56
1:D:523:LYS:HG3	1:D:576:THR:HA	1.88	0.56
1:C:443:GLN:HA	1:C:446:ILE:HD12	1.87	0.56
1:C:523:LYS:HG3	1:C:576:THR:HA	1.88	0.55
1:B:135:ASN:OD1	1:B:280:ARG:NH1	2.40	0.55
1:B:531:TYR:HD1	1:B:589:VAL:HG12	1.72	0.55
1:D:135:ASN:OD1	1:D:280:ARG:NH1	2.40	0.55
1:C:135:ASN:OD1	1:C:280:ARG:NH1	2.40	0.54
1:A:135:ASN:OD1	1:A:280:ARG:NH1	2.40	0.54
1:C:531:TYR:HD1	1:C:589:VAL:HG12	1.72	0.54
1:B:497:CYS:SG	1:B:498:GLU:N	2.82	0.53
1:C:539:GLN:HB3	1:C:551:THR:HG23	1.90	0.53
1:B:125:THR:HG22	1:B:289:ARG:HD2	1.90	0.53
1:C:497:CYS:SG	1:C:498:GLU:N	2.81	0.53
1:C:218:ASP:OD1	1:C:289:ARG:NH1	2.42	0.53
1:D:218:ASP:OD1	1:D:289:ARG:NH1	2.42	0.53
1:B:491:VAL:HG13	1:B:557:VAL:HG11	1.90	0.53
1:A:218:ASP:OD1	1:A:289:ARG:NH1	2.42	0.53
1:A:539:GLN:HB3	1:A:551:THR:HG23	1.90	0.53
1:D:497:CYS:SG	1:D:498:GLU:N	2.81	0.53
1:B:218:ASP:OD1	1:B:289:ARG:NH1	2.42	0.53
1:A:497:CYS:SG	1:A:498:GLU:N	2.81	0.53
1:D:531:TYR:HD1	1:D:589:VAL:HG12	1.72	0.53
1:C:125:THR:HG22	1:C:289:ARG:HD2	1.90	0.53
1:D:491:VAL:HG13	1:D:557:VAL:HG11	1.90	0.52
1:D:125:THR:HG22	1:D:289:ARG:HD2	1.90	0.52
1:B:539:GLN:HB3	1:B:551:THR:HG23	1.90	0.52
1:A:531:TYR:HD1	1:A:589:VAL:HG12	1.72	0.52
1:D:539:GLN:HB3	1:D:551:THR:HG23	1.90	0.52
1:C:491:VAL:HG13	1:C:557:VAL:HG11	1.90	0.52
1:A:125:THR:HG22	1:A:289:ARG:HD2	1.90	0.51
1:A:491:VAL:HG13	1:A:557:VAL:HG11	1.90	0.51
1:B:305:ASN:HB3	1:B:413:MET:HG2	1.93	0.51
1:D:305:ASN:HB3	1:D:413:MET:HG2	1.93	0.51
1:B:538:LEU:HB2	1:B:552:LEU:HB2	1.92	0.51
1:D:538:LEU:HB2	1:D:552:LEU:HB2	1.92	0.51
1:C:538:LEU:HB2	1:C:552:LEU:HB2	1.92	0.51
1:A:305:ASN:HB3	1:A:413:MET:HG2	1.93	0.50
1:A:112:TYR:OH	1:A:114:GLN:NE2	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:538:LEU:HB2	1:A:552:LEU:HB2	1.92	0.50
1:C:112:TYR:OH	1:C:114:GLN:NE2	2.45	0.50
1:A:385:ARG:NH2	2:A:1801:CPL:O2P	2.45	0.49
1:B:112:TYR:OH	1:B:114:GLN:NE2	2.45	0.49
1:D:112:TYR:OH	1:D:114:GLN:NE2	2.45	0.49
1:C:305:ASN:HB3	1:C:413:MET:HG2	1.93	0.49
1:D:385:ARG:NH2	2:D:804:CPL:O2P	2.46	0.48
1:B:133:ILE:HD11	2:B:1803:CPL:H132	1.95	0.48
1:A:133:ILE:HD11	2:A:1803:CPL:H132	1.95	0.48
1:C:116:PRO:O	1:C:296:ARG:NH2	2.46	0.48
1:C:385:ARG:NH2	2:C:1801:CPL:O2P	2.47	0.47
1:D:133:ILE:HD11	2:D:802:CPL:H132	1.95	0.47
1:B:219:THR:OG1	1:B:286:ARG:NH2	2.48	0.47
1:D:219:THR:OG1	1:D:286:ARG:NH2	2.48	0.47
1:C:133:ILE:HD11	2:C:1803:CPL:H132	1.95	0.47
1:A:219:THR:OG1	1:A:286:ARG:NH2	2.48	0.47
1:D:194:TRP:NE1	1:D:267:PRO:O	2.39	0.47
1:A:116:PRO:O	1:A:296:ARG:NH2	2.46	0.47
1:B:194:TRP:NE1	1:B:267:PRO:O	2.39	0.47
1:B:595:LEU:O	1:B:599:LEU:HB2	2.15	0.47
1:C:595:LEU:O	1:C:599:LEU:HB2	2.15	0.47
1:C:219:THR:OG1	1:C:286:ARG:NH2	2.48	0.46
1:D:116:PRO:O	1:D:296:ARG:NH2	2.46	0.46
1:B:116:PRO:O	1:B:296:ARG:NH2	2.46	0.46
1:D:595:LEU:O	1:D:599:LEU:HB2	2.15	0.46
1:A:595:LEU:O	1:A:599:LEU:HB2	2.15	0.46
1:D:538:LEU:HD21	1:D:587:LEU:HD21	1.99	0.45
1:A:194:TRP:NE1	1:A:267:PRO:O	2.39	0.45
1:A:538:LEU:HD21	1:A:587:LEU:HD21	1.99	0.45
1:C:391:PHE:O	1:C:395:ASP:HB2	2.17	0.45
1:D:391:PHE:O	1:D:395:ASP:HB2	2.17	0.44
1:B:391:PHE:O	1:B:395:ASP:HB2	2.17	0.44
1:C:107:LYS:HD2	1:C:107:LYS:HA	1.78	0.44
1:C:538:LEU:HD21	1:C:587:LEU:HD21	1.99	0.44
1:A:391:PHE:O	1:A:395:ASP:HB2	2.17	0.44
1:B:480:ALA:HB1	1:B:506:VAL:HG12	1.99	0.44
1:D:480:ALA:HB1	1:D:506:VAL:HG12	1.99	0.44
1:B:538:LEU:HD21	1:B:587:LEU:HD21	1.99	0.44
1:C:194:TRP:NE1	1:C:267:PRO:O	2.38	0.44
1:C:480:ALA:HB1	1:C:506:VAL:HG12	1.99	0.43
1:B:107:LYS:HA	1:B:107:LYS:HD2	1.78	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:242:LYS:O	1:C:246:GLN:HB2	2.18	0.43
1:C:561:LEU:HD11	1:C:617:LEU:HD13	2.01	0.43
1:A:242:LYS:O	1:A:246:GLN:HB2	2.18	0.43
1:A:480:ALA:HB1	1:A:506:VAL:HG12	1.99	0.43
1:D:157:CYS:N	1:D:172:CYS:SG	2.92	0.43
1:A:561:LEU:HD11	1:A:617:LEU:HD13	2.01	0.43
1:B:157:CYS:N	1:B:172:CYS:SG	2.92	0.42
1:D:242:LYS:O	1:D:246:GLN:HB2	2.18	0.42
1:A:289:ARG:HA	1:A:289:ARG:HD3	1.84	0.42
1:D:561:LEU:HD11	1:D:617:LEU:HD13	2.01	0.42
1:A:157:CYS:N	1:A:172:CYS:SG	2.92	0.42
1:D:602:TYR:HB3	1:D:605:ALA:HB3	2.02	0.42
1:B:289:ARG:HD3	1:B:289:ARG:HA	1.84	0.42
1:A:125:THR:HB	1:A:293:CYS:HB2	2.02	0.42
1:C:157:CYS:N	1:C:172:CYS:SG	2.92	0.42
1:C:542:ASP:HB2	1:C:548:VAL:HG22	2.02	0.42
1:A:373:ILE:HD13	1:A:373:ILE:HA	1.94	0.42
1:A:602:TYR:HB3	1:A:605:ALA:HB3	2.02	0.42
1:A:348:LYS:HA	1:A:348:LYS:HD3	1.86	0.41
1:A:542:ASP:HB2	1:A:548:VAL:HG22	2.02	0.41
1:B:125:THR:HB	1:B:293:CYS:HB2	2.02	0.41
1:B:242:LYS:O	1:B:246:GLN:HB2	2.18	0.41
1:D:538:LEU:O	1:D:552:LEU:N	2.54	0.41
1:D:542:ASP:HB2	1:D:548:VAL:HG22	2.02	0.41
1:C:602:TYR:HB3	1:C:605:ALA:HB3	2.02	0.41
1:D:488:LEU:HD13	1:D:506:VAL:HG22	2.02	0.41
1:A:153:SER:HB2	1:A:186:TYR:HB3	2.03	0.41
1:B:542:ASP:HB2	1:B:548:VAL:HG22	2.02	0.41
1:B:561:LEU:HD11	1:B:617:LEU:HD13	2.01	0.41
1:D:153:SER:HB2	1:D:186:TYR:HB3	2.03	0.41
1:D:494:PHE:HB3	1:D:502:LEU:HD21	2.03	0.41
1:B:153:SER:HB2	1:B:186:TYR:HB3	2.03	0.41
1:B:538:LEU:O	1:B:552:LEU:N	2.54	0.41
1:B:602:TYR:HB3	1:B:605:ALA:HB3	2.02	0.41
1:B:488:LEU:HD13	1:B:506:VAL:HG22	2.02	0.41
1:C:505:LEU:HD12	1:C:505:LEU:HA	1.91	0.41
1:C:153:SER:HB2	1:C:186:TYR:HB3	2.03	0.41
1:C:488:LEU:HD13	1:C:506:VAL:HG22	2.02	0.41
1:C:530:MET:O	1:C:589:VAL:HA	2.21	0.41
1:A:538:LEU:O	1:A:552:LEU:N	2.54	0.41
1:B:239:LYS:HE2	1:B:239:LYS:HB2	1.96	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:530:MET:O	1:B:589:VAL:HA	2.21	0.41
1:C:125:THR:HB	1:C:293:CYS:HB2	2.02	0.41
1:D:289:ARG:HD3	1:D:289:ARG:HA	1.84	0.40
1:A:494:PHE:HB3	1:A:502:LEU:HD21	2.03	0.40
1:A:438:ARG:HD3	1:A:438:ARG:HA	1.87	0.40
1:C:538:LEU:O	1:C:552:LEU:N	2.54	0.40
1:A:530:MET:O	1:A:589:VAL:HA	2.21	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	510/738 (69%)	481 (94%)	29 (6%)	0	100	100
1	B	510/738 (69%)	481 (94%)	29 (6%)	0	100	100
1	C	510/738 (69%)	481 (94%)	29 (6%)	0	100	100
1	D	510/738 (69%)	481 (94%)	29 (6%)	0	100	100
All	All	2040/2952 (69%)	1924 (94%)	116 (6%)	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	466/652 (72%)	464 (100%)	2 (0%)	89	94
1	B	466/652 (72%)	464 (100%)	2 (0%)	89	94
1	C	466/652 (72%)	464 (100%)	2 (0%)	89	94
1	D	466/652 (72%)	464 (100%)	2 (0%)	89	94
All	All	1864/2608 (72%)	1856 (100%)	8 (0%)	88	94

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

Mol	Chain	Res	Type
1	D	115	ASP
1	D	498	GLU
1	A	115	ASP
1	A	498	GLU
1	B	115	ASP
1	B	498	GLU
1	C	115	ASP
1	C	498	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	114	GLN
1	D	154	GLN
1	D	179	ASN
1	D	349	GLN
1	D	416	ASN
1	D	539	GLN
1	A	114	GLN
1	A	154	GLN
1	A	179	ASN
1	A	349	GLN
1	A	416	ASN
1	B	114	GLN
1	B	154	GLN
1	B	179	ASN
1	B	349	GLN
1	B	416	ASN
1	C	114	GLN
1	C	154	GLN
1	C	179	ASN

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Mol	Chain	Res	Type
1	C	349	GLN
1	C	416	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 1 is monoatomic - leaving 16 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	1801	-	21,21,51	1.31	4 (19%)	24,26,59	1.33	2 (8%)
2	CPL	C	1804	-	26,26,51	1.27	5 (19%)	29,31,59	1.31	2 (6%)
2	CPL	A	1802	-	27,27,51	1.32	4 (14%)	33,35,59	1.03	2 (6%)
2	CPL	B	1801	-	21,21,51	1.31	4 (19%)	24,26,59	1.34	2 (8%)
2	CPL	A	1801	-	21,21,51	1.31	4 (19%)	24,26,59	1.33	2 (8%)
2	CPL	A	1804	-	26,26,51	1.27	5 (19%)	29,31,59	1.32	2 (6%)
2	CPL	B	1804	-	26,26,51	1.27	5 (19%)	29,31,59	1.31	2 (6%)
2	CPL	B	1802	-	27,27,51	1.32	4 (14%)	33,35,59	1.03	2 (6%)
2	CPL	D	801	-	27,27,51	1.32	4 (14%)	33,35,59	1.03	2 (6%)
2	CPL	B	1803	-	9,9,51	0.28	0	8,8,59	0.75	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	CPL	D	804	-	21,21,51	1.32	4 (19%)	24,26,59	1.33	2 (8%)
2	CPL	C	1803	-	9,9,51	0.28	0	8,8,59	0.75	0
2	CPL	C	1802	-	27,27,51	1.31	4 (14%)	33,35,59	1.04	2 (6%)
2	CPL	D	802	-	9,9,51	0.28	0	8,8,59	0.75	0
2	CPL	A	1803	-	9,9,51	0.28	0	8,8,59	0.75	0
2	CPL	D	803	-	26,26,51	1.27	5 (19%)	29,31,59	1.31	2 (6%)

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	1801	-	-	11/25/25/55	-
2	CPL	C	1804	-	-	9/28/28/55	-
2	CPL	A	1802	-	-	14/31/31/55	-
2	CPL	B	1801	-	-	11/25/25/55	-
2	CPL	A	1801	-	-	11/25/25/55	-
2	CPL	A	1804	-	-	9/28/28/55	-
2	CPL	B	1804	-	-	9/28/28/55	-
2	CPL	B	1802	-	-	14/31/31/55	-
2	CPL	D	801	-	-	14/31/31/55	-
2	CPL	B	1803	-	-	5/7/7/55	-
2	CPL	D	804	-	-	11/25/25/55	-
2	CPL	C	1803	-	-	5/7/7/55	-
2	CPL	C	1802	-	-	14/31/31/55	-
2	CPL	D	802	-	-	5/7/7/55	-
2	CPL	A	1803	-	-	5/7/7/55	-
2	CPL	D	803	-	-	9/28/28/55	-

All (52) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	801	CPL	O2-C2	-2.83	1.39	1.46
2	B	1802	CPL	O2-C2	-2.83	1.40	1.46
2	A	1802	CPL	O2-C2	-2.82	1.40	1.46
2	C	1802	CPL	O2-C2	-2.81	1.40	1.46
2	C	1804	CPL	P-O4P	2.78	1.65	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	803	CPL	P-O4P	2.77	1.65	1.54
2	A	1804	CPL	P-O4P	2.77	1.65	1.54
2	B	1804	CPL	P-O4P	2.76	1.65	1.54
2	C	1804	CPL	O2-C2	-2.68	1.40	1.46
2	D	803	CPL	O2-C2	-2.65	1.40	1.46
2	A	1804	CPL	O2-C2	-2.65	1.40	1.46
2	B	1804	CPL	O2-C2	-2.63	1.40	1.46
2	D	804	CPL	O2-C2	-2.60	1.40	1.46
2	B	1801	CPL	O2-C2	-2.59	1.40	1.46
2	C	1801	CPL	O2-C2	-2.58	1.40	1.46
2	A	1801	CPL	O2-C2	-2.57	1.40	1.46
2	B	1804	CPL	O3-C11	2.47	1.40	1.33
2	D	803	CPL	O3-C11	2.46	1.40	1.33
2	C	1804	CPL	O3-C11	2.45	1.40	1.33
2	A	1804	CPL	O3-C11	2.44	1.40	1.33
2	C	1801	CPL	O3-C11	2.38	1.40	1.33
2	A	1801	CPL	O3-C11	2.37	1.40	1.33
2	B	1801	CPL	O3-C11	2.35	1.40	1.33
2	D	804	CPL	O3-C11	2.34	1.40	1.33
2	B	1804	CPL	O2-C31	2.29	1.40	1.34
2	C	1804	CPL	O2-C31	2.29	1.40	1.34
2	C	1801	CPL	O2-C31	2.28	1.40	1.34
2	D	803	CPL	O2-C31	2.28	1.40	1.34
2	D	804	CPL	O2-C31	2.28	1.40	1.34
2	A	1801	CPL	O2-C31	2.28	1.40	1.34
2	B	1802	CPL	O3-C11	2.27	1.40	1.33
2	A	1804	CPL	O2-C31	2.26	1.40	1.34
2	B	1801	CPL	O2-C31	2.26	1.40	1.34
2	D	801	CPL	O3-C11	2.25	1.39	1.33
2	C	1802	CPL	O3-C11	2.25	1.39	1.33
2	A	1802	CPL	O3-C11	2.24	1.39	1.33
2	A	1802	CPL	O3-C3	-2.24	1.40	1.45
2	D	801	CPL	O3-C3	-2.24	1.40	1.45
2	B	1802	CPL	O3-C3	-2.23	1.40	1.45
2	B	1802	CPL	O2-C31	2.23	1.40	1.34
2	D	801	CPL	O2-C31	2.21	1.40	1.34
2	A	1802	CPL	O2-C31	2.21	1.40	1.34
2	C	1802	CPL	O2-C31	2.20	1.40	1.34
2	C	1802	CPL	O3-C3	-2.20	1.40	1.45
2	D	804	CPL	O3-C3	-2.15	1.40	1.45
2	C	1801	CPL	O3-C3	-2.15	1.40	1.45
2	A	1801	CPL	O3-C3	-2.14	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	803	CPL	O3-C3	-2.14	1.40	1.45
2	B	1804	CPL	O3-C3	-2.14	1.40	1.45
2	B	1801	CPL	O3-C3	-2.13	1.40	1.45
2	A	1804	CPL	O3-C3	-2.10	1.40	1.45
2	C	1804	CPL	O3-C3	-2.10	1.40	1.45

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1801	CPL	O2-C31-C32	4.43	121.07	111.48
2	A	1801	CPL	O2-C31-C32	4.41	121.01	111.48
2	D	804	CPL	O2-C31-C32	4.41	121.01	111.48
2	C	1801	CPL	O2-C31-C32	4.40	121.01	111.48
2	D	803	CPL	O2-C31-C32	4.06	120.26	111.48
2	A	1804	CPL	O2-C31-C32	4.06	120.26	111.48
2	B	1804	CPL	O2-C31-C32	4.05	120.25	111.48
2	C	1804	CPL	O2-C31-C32	4.04	120.22	111.48
2	C	1802	CPL	O2-C31-C32	3.47	118.99	111.48
2	D	801	CPL	O2-C31-C32	3.46	118.96	111.48
2	A	1802	CPL	O2-C31-C32	3.46	118.96	111.48
2	B	1802	CPL	O2-C31-C32	3.45	118.94	111.48
2	B	1804	CPL	O3-C11-C12	2.85	120.52	111.83
2	D	803	CPL	O3-C11-C12	2.83	120.47	111.83
2	C	1804	CPL	O3-C11-C12	2.83	120.46	111.83
2	A	1804	CPL	O3-C11-C12	2.83	120.45	111.83
2	B	1801	CPL	O3-C11-C12	2.76	120.25	111.83
2	A	1801	CPL	O3-C11-C12	2.75	120.23	111.83
2	D	804	CPL	O3-C11-C12	2.75	120.21	111.83
2	C	1801	CPL	O3-C11-C12	2.75	120.21	111.83
2	A	1802	CPL	O3-C11-C12	2.64	119.87	111.83
2	D	801	CPL	O3-C11-C12	2.63	119.84	111.83
2	C	1802	CPL	O3-C11-C12	2.62	119.84	111.83
2	B	1802	CPL	O3-C11-C12	2.62	119.81	111.83

There are no chirality outliers.

All (156) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	801	CPL	C1-O3P-P-O2P
2	D	801	CPL	C1-O3P-P-O4P
2	D	803	CPL	C32-C31-O2-C2
2	D	803	CPL	C1-O3P-P-O4P

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Mol	Chain	Res	Type	Atoms
2	D	804	CPL	O31-C31-O2-C2
2	D	804	CPL	C1-O3P-P-O2P
2	D	804	CPL	C1-O3P-P-O4P
2	D	804	CPL	C4-O4P-P-O1P
2	D	804	CPL	C4-O4P-P-O2P
2	D	804	CPL	C4-O4P-P-O3P
2	A	1801	CPL	O31-C31-O2-C2
2	A	1801	CPL	C1-O3P-P-O2P
2	A	1801	CPL	C1-O3P-P-O4P
2	A	1801	CPL	C4-O4P-P-O1P
2	A	1801	CPL	C4-O4P-P-O2P
2	A	1801	CPL	C4-O4P-P-O3P
2	A	1802	CPL	C1-O3P-P-O2P
2	A	1802	CPL	C1-O3P-P-O4P
2	A	1804	CPL	C32-C31-O2-C2
2	A	1804	CPL	C1-O3P-P-O4P
2	B	1801	CPL	O31-C31-O2-C2
2	B	1801	CPL	C1-O3P-P-O2P
2	B	1801	CPL	C1-O3P-P-O4P
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	C1-O3P-P-O2P
2	B	1802	CPL	C1-O3P-P-O4P
2	B	1804	CPL	C32-C31-O2-C2
2	B	1804	CPL	C1-O3P-P-O4P
2	C	1801	CPL	O31-C31-O2-C2
2	C	1801	CPL	C1-O3P-P-O2P
2	C	1801	CPL	C1-O3P-P-O4P
2	C	1801	CPL	C4-O4P-P-O1P
2	C	1801	CPL	C4-O4P-P-O2P
2	C	1801	CPL	C4-O4P-P-O3P
2	C	1802	CPL	C1-O3P-P-O2P
2	C	1802	CPL	C1-O3P-P-O4P
2	C	1804	CPL	C32-C31-O2-C2
2	C	1804	CPL	C1-O3P-P-O4P
2	D	803	CPL	O31-C31-O2-C2
2	A	1804	CPL	O31-C31-O2-C2
2	B	1804	CPL	O31-C31-O2-C2
2	C	1804	CPL	O31-C31-O2-C2
2	D	804	CPL	C32-C31-O2-C2
2	A	1801	CPL	C32-C31-O2-C2

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Mol	Chain	Res	Type	Atoms
2	B	1801	CPL	C32-C31-O2-C2
2	C	1801	CPL	C32-C31-O2-C2
2	D	803	CPL	C31-C32-C33-C34
2	A	1804	CPL	C31-C32-C33-C34
2	B	1804	CPL	C31-C32-C33-C34
2	C	1804	CPL	C31-C32-C33-C34
2	B	1804	CPL	C11-C12-C13-C14
2	D	803	CPL	C11-C12-C13-C14
2	A	1804	CPL	C11-C12-C13-C14
2	C	1804	CPL	C11-C12-C13-C14
2	D	804	CPL	C12-C11-O3-C3
2	A	1801	CPL	C12-C11-O3-C3
2	B	1801	CPL	C12-C11-O3-C3
2	C	1801	CPL	C12-C11-O3-C3
2	D	801	CPL	C32-C31-O2-C2
2	A	1802	CPL	C32-C31-O2-C2
2	B	1802	CPL	C32-C31-O2-C2
2	C	1802	CPL	C32-C31-O2-C2
2	D	801	CPL	O31-C31-O2-C2
2	A	1802	CPL	O31-C31-O2-C2
2	B	1802	CPL	O31-C31-O2-C2
2	C	1802	CPL	O31-C31-O2-C2
2	D	804	CPL	O11-C11-O3-C3
2	A	1801	CPL	O11-C11-O3-C3
2	B	1801	CPL	O11-C11-O3-C3
2	C	1801	CPL	O11-C11-O3-C3
2	D	804	CPL	C1-C2-C3-O3
2	A	1801	CPL	C1-C2-C3-O3
2	B	1801	CPL	C1-C2-C3-O3
2	C	1801	CPL	C1-C2-C3-O3
2	D	801	CPL	C12-C11-O3-C3
2	A	1802	CPL	C12-C11-O3-C3
2	B	1802	CPL	C12-C11-O3-C3
2	C	1802	CPL	C12-C11-O3-C3
2	D	801	CPL	O3P-C1-C2-O2
2	A	1802	CPL	O3P-C1-C2-O2
2	B	1802	CPL	O3P-C1-C2-O2
2	C	1802	CPL	O3P-C1-C2-O2
2	D	802	CPL	C18-C19-C20-C21
2	A	1803	CPL	C18-C19-C20-C21
2	B	1803	CPL	C18-C19-C20-C21
2	C	1803	CPL	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
2	D	801	CPL	O11-C11-O3-C3
2	A	1802	CPL	O11-C11-O3-C3
2	B	1802	CPL	O11-C11-O3-C3
2	C	1802	CPL	O11-C11-O3-C3
2	D	802	CPL	C16-C17-C18-C19
2	A	1803	CPL	C16-C17-C18-C19
2	B	1803	CPL	C16-C17-C18-C19
2	C	1803	CPL	C16-C17-C18-C19
2	B	1802	CPL	C31-C32-C33-C34
2	D	801	CPL	C31-C32-C33-C34
2	A	1802	CPL	C31-C32-C33-C34
2	C	1802	CPL	C31-C32-C33-C34
2	D	801	CPL	O2-C31-C32-C33
2	A	1802	CPL	O2-C31-C32-C33
2	B	1802	CPL	O2-C31-C32-C33
2	C	1802	CPL	O2-C31-C32-C33
2	D	801	CPL	O3P-C1-C2-C3
2	A	1802	CPL	O3P-C1-C2-C3
2	B	1802	CPL	O3P-C1-C2-C3
2	C	1802	CPL	O3P-C1-C2-C3
2	D	802	CPL	C14-C15-C16-C17
2	A	1803	CPL	C14-C15-C16-C17
2	C	1803	CPL	C14-C15-C16-C17
2	B	1803	CPL	C14-C15-C16-C17
2	D	801	CPL	O4P-C4-C5-N
2	A	1802	CPL	O4P-C4-C5-N
2	B	1802	CPL	O4P-C4-C5-N
2	C	1802	CPL	O4P-C4-C5-N
2	D	803	CPL	C12-C11-O3-C3
2	A	1804	CPL	C12-C11-O3-C3
2	B	1804	CPL	C12-C11-O3-C3
2	C	1804	CPL	C12-C11-O3-C3
2	D	803	CPL	O11-C11-O3-C3
2	A	1804	CPL	O11-C11-O3-C3
2	B	1804	CPL	O11-C11-O3-C3
2	C	1804	CPL	O11-C11-O3-C3
2	D	804	CPL	O2-C2-C3-O3
2	A	1801	CPL	O2-C2-C3-O3
2	B	1801	CPL	O2-C2-C3-O3
2	C	1801	CPL	O2-C2-C3-O3
2	D	801	CPL	C3-C2-O2-C31
2	A	1802	CPL	C3-C2-O2-C31

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Mol	Chain	Res	Type	Atoms
2	B	1802	CPL	C3-C2-O2-C31
2	C	1802	CPL	C3-C2-O2-C31
2	B	1804	CPL	C33-C34-C35-C36
2	C	1804	CPL	C33-C34-C35-C36
2	D	803	CPL	C33-C34-C35-C36
2	A	1804	CPL	C33-C34-C35-C36
2	A	1803	CPL	C12-C13-C14-C15
2	B	1803	CPL	C12-C13-C14-C15
2	C	1803	CPL	C12-C13-C14-C15
2	D	802	CPL	C12-C13-C14-C15
2	D	803	CPL	C1-C2-C3-O3
2	A	1804	CPL	C1-C2-C3-O3
2	B	1804	CPL	C1-C2-C3-O3
2	C	1804	CPL	C1-C2-C3-O3
2	D	801	CPL	O31-C31-C32-C33
2	A	1802	CPL	O31-C31-C32-C33
2	B	1802	CPL	O31-C31-C32-C33
2	C	1802	CPL	O31-C31-C32-C33
2	D	801	CPL	C1-C2-O2-C31
2	A	1802	CPL	C1-C2-O2-C31
2	B	1802	CPL	C1-C2-O2-C31
2	C	1802	CPL	C1-C2-O2-C31
2	D	802	CPL	C15-C16-C17-C18
2	B	1803	CPL	C15-C16-C17-C18
2	C	1803	CPL	C15-C16-C17-C18
2	A	1803	CPL	C15-C16-C17-C18

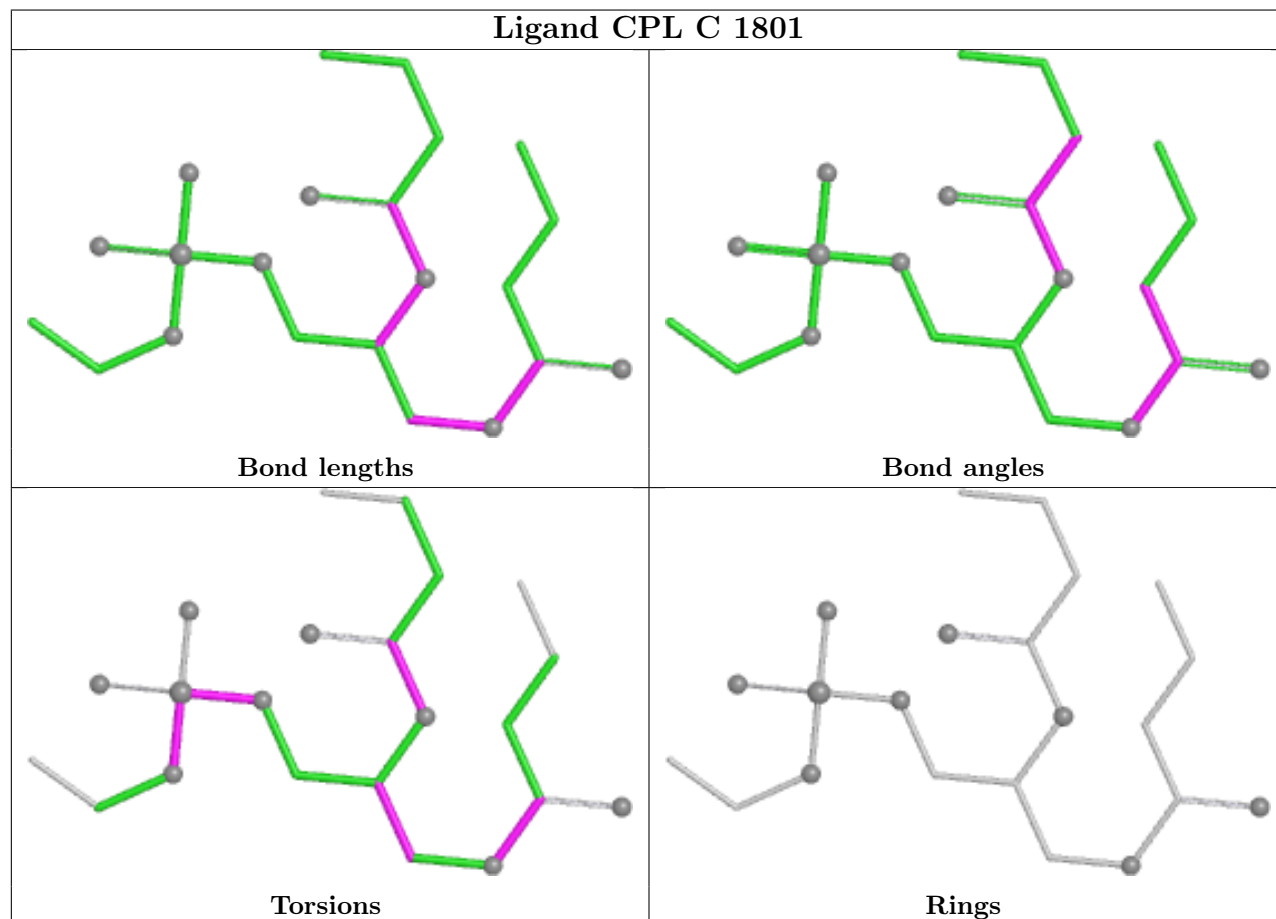
There are no ring outliers.

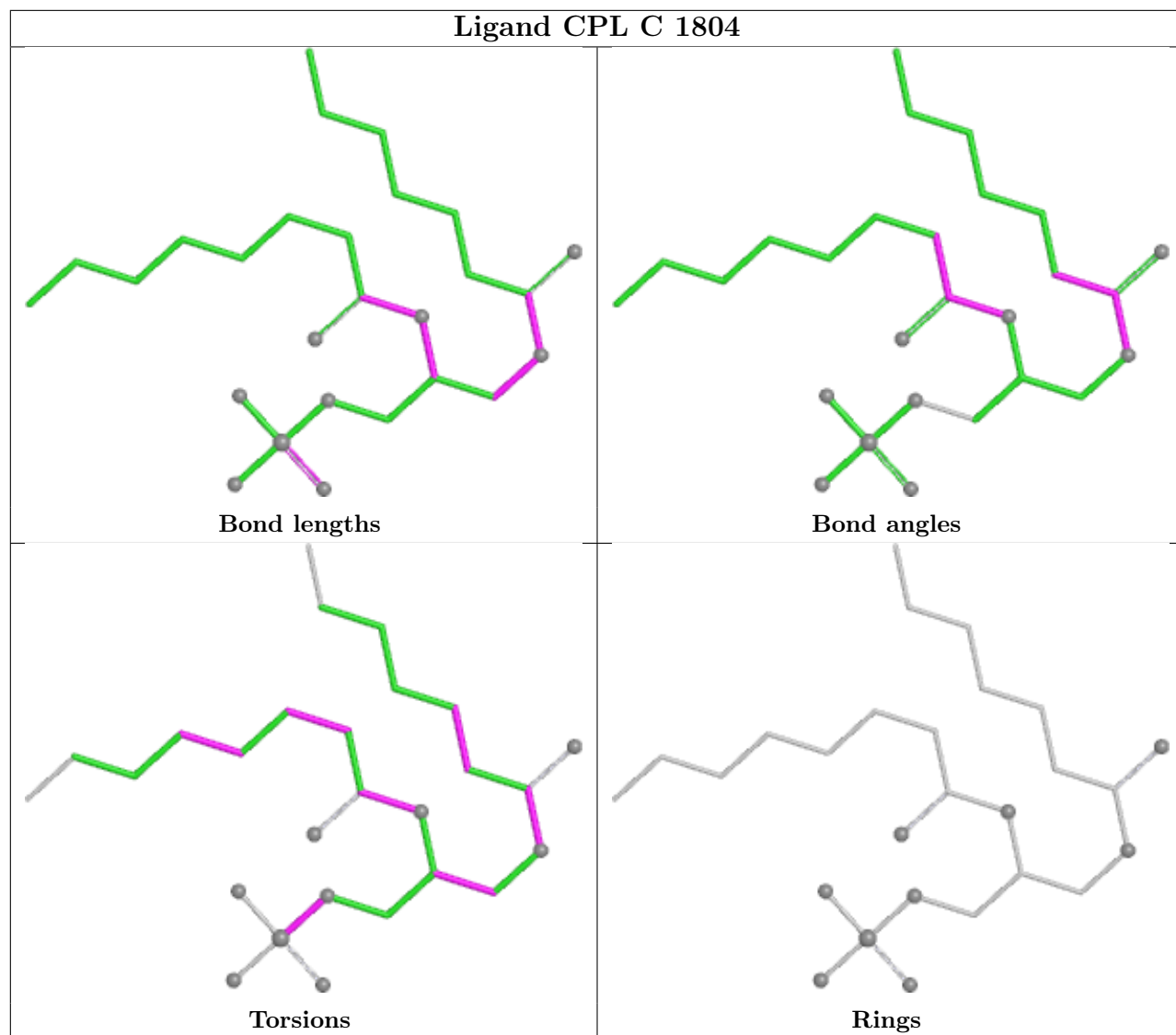
8 monomers are involved in 8 short contacts:

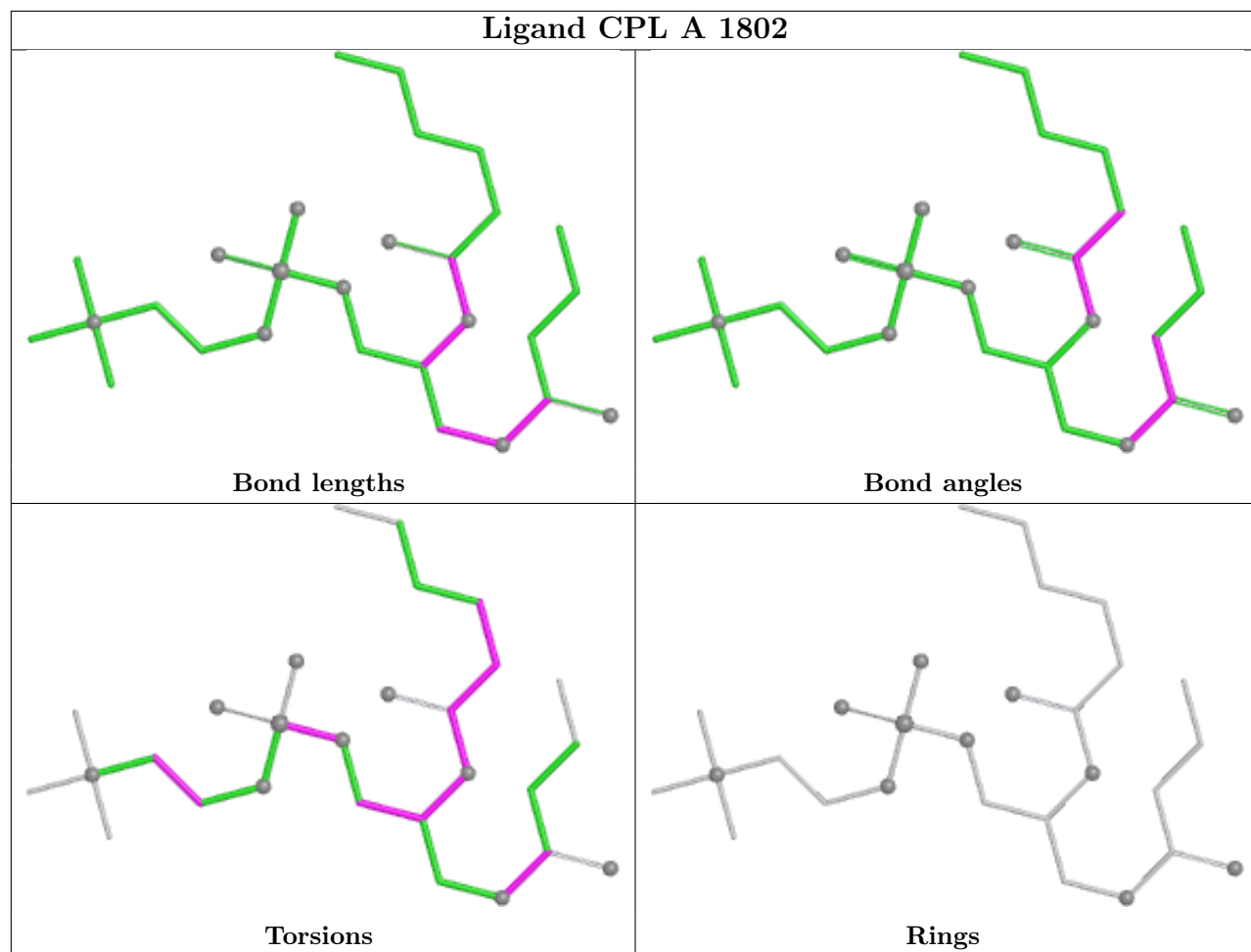
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1801	CPL	1	0
2	B	1801	CPL	1	0
2	A	1801	CPL	1	0
2	B	1803	CPL	1	0
2	D	804	CPL	1	0
2	C	1803	CPL	1	0
2	D	802	CPL	1	0
2	A	1803	CPL	1	0

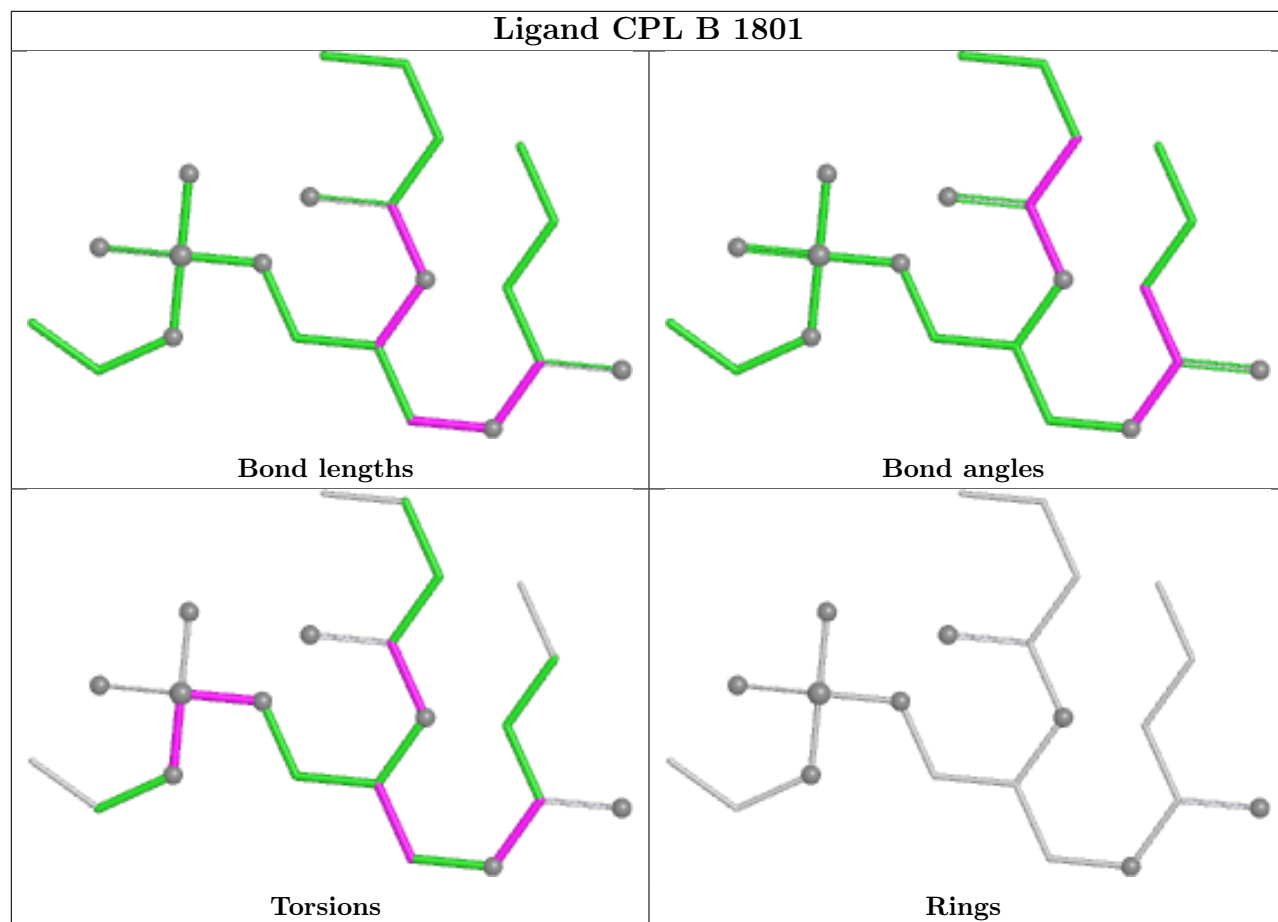
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

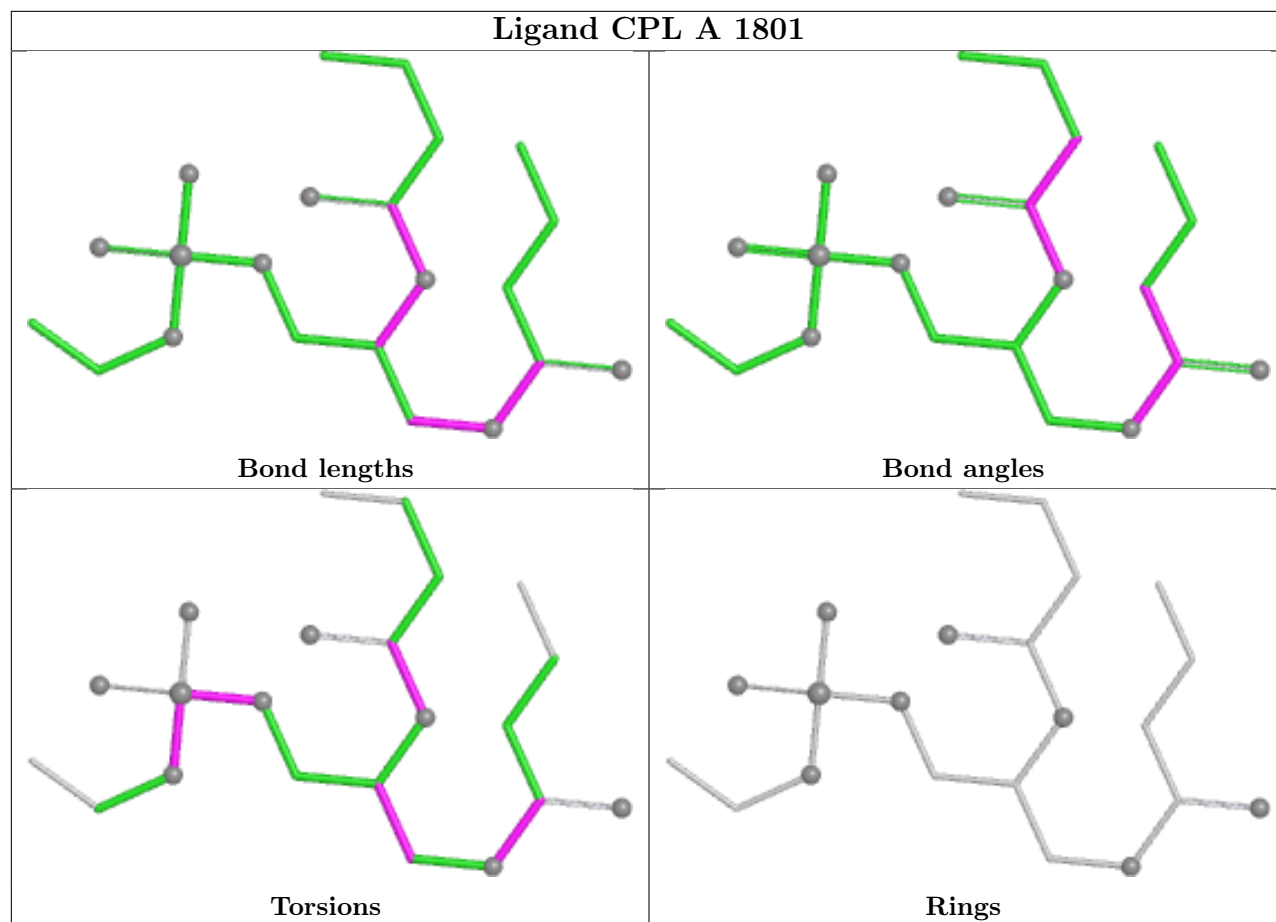
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. 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.

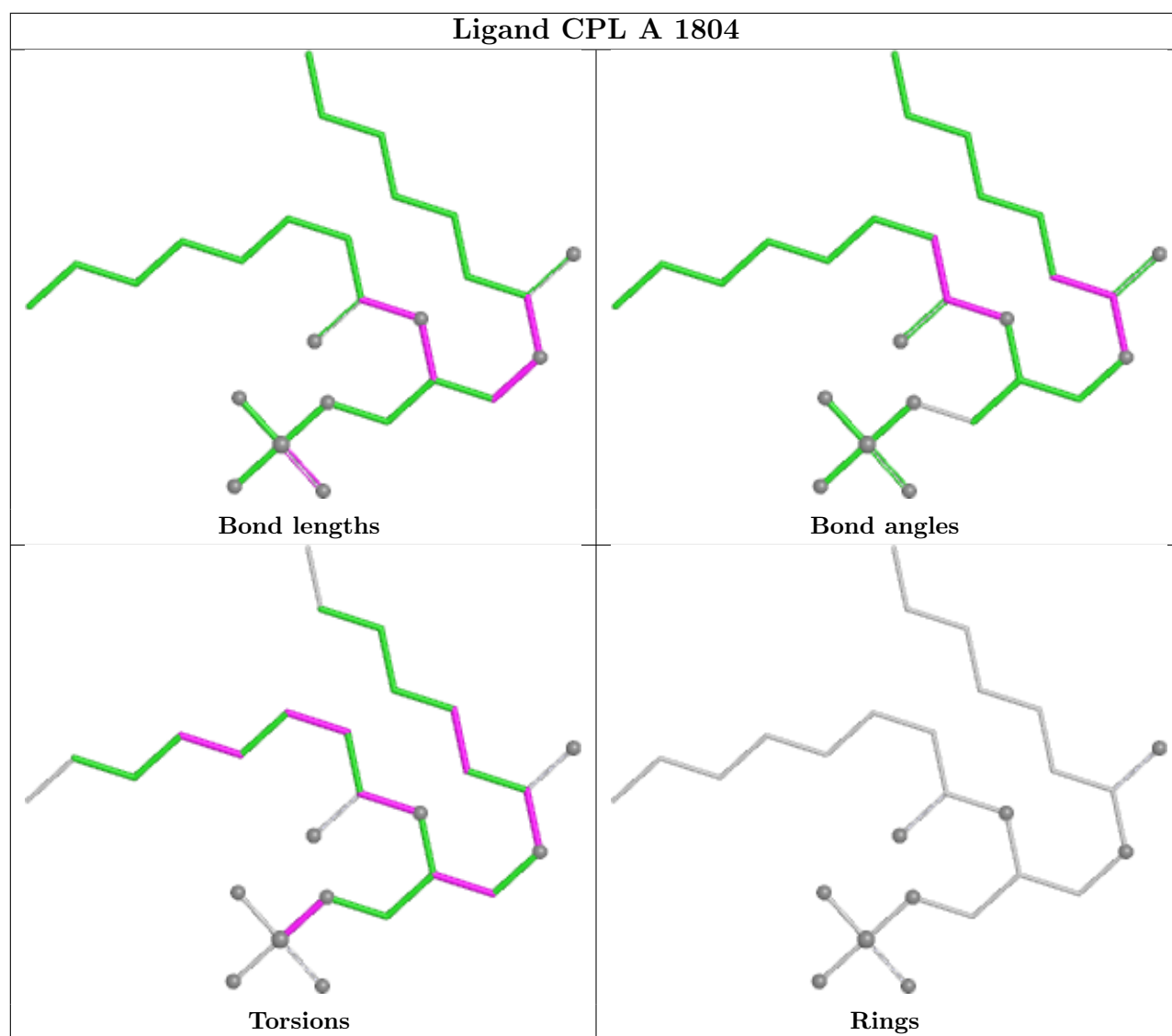


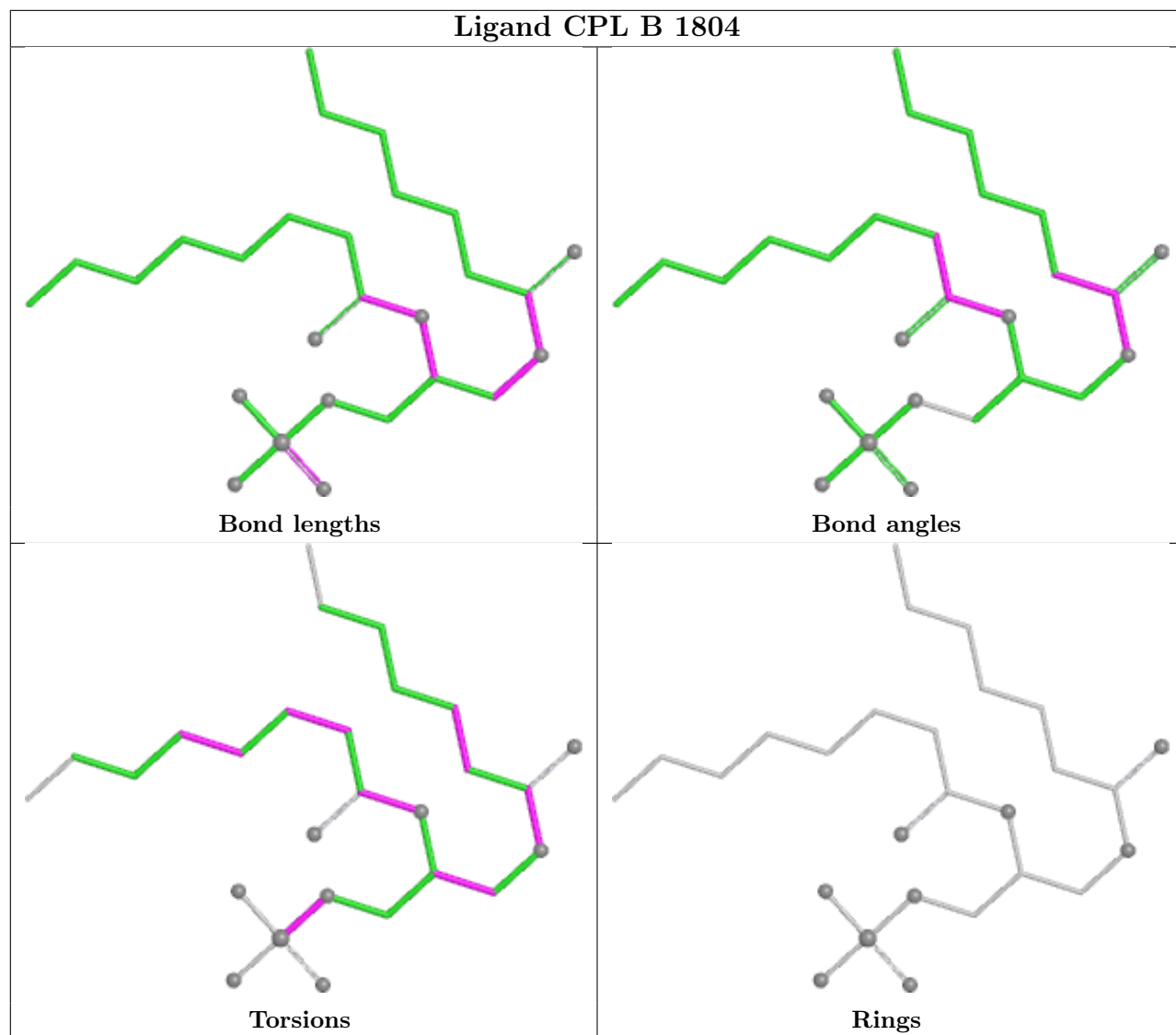


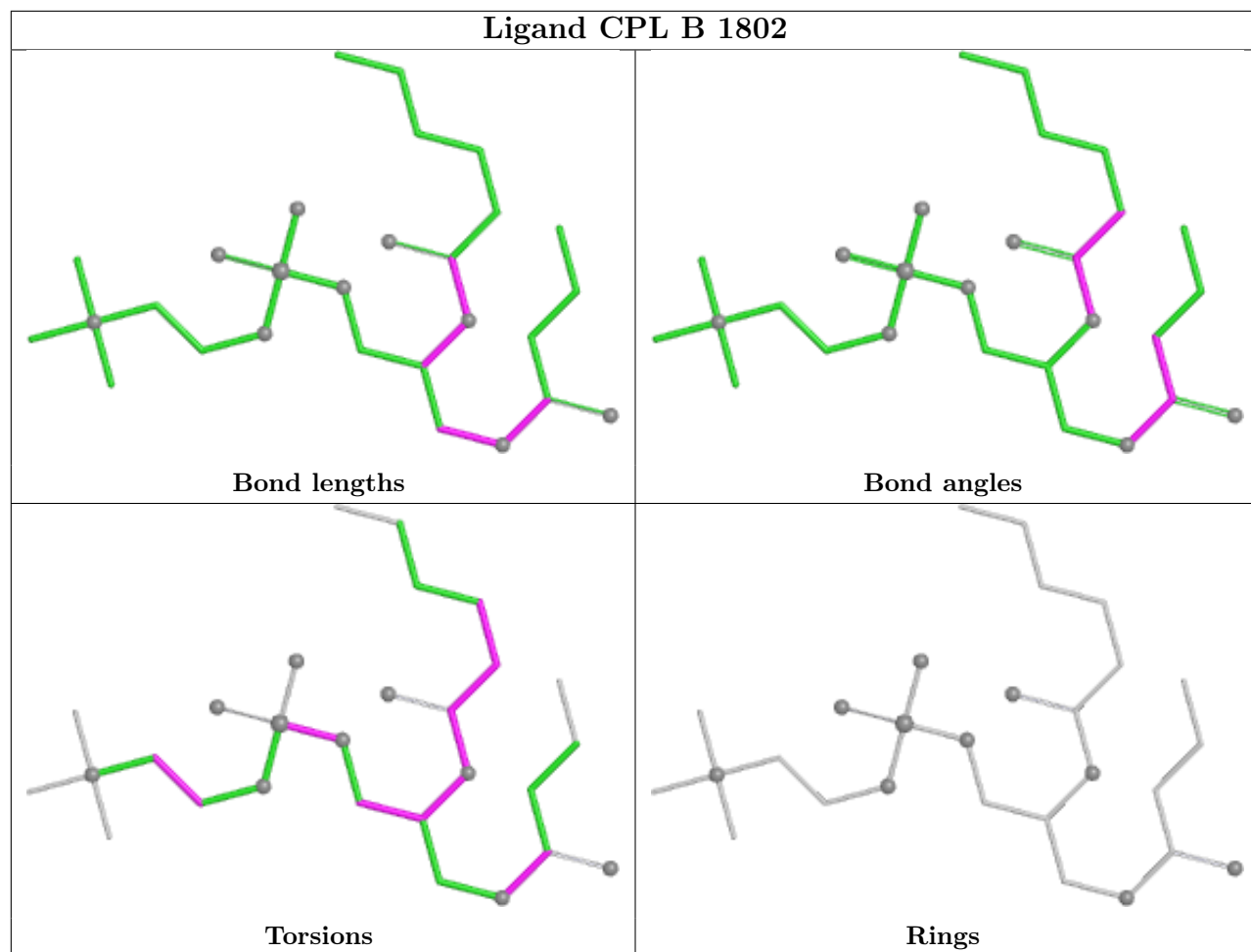


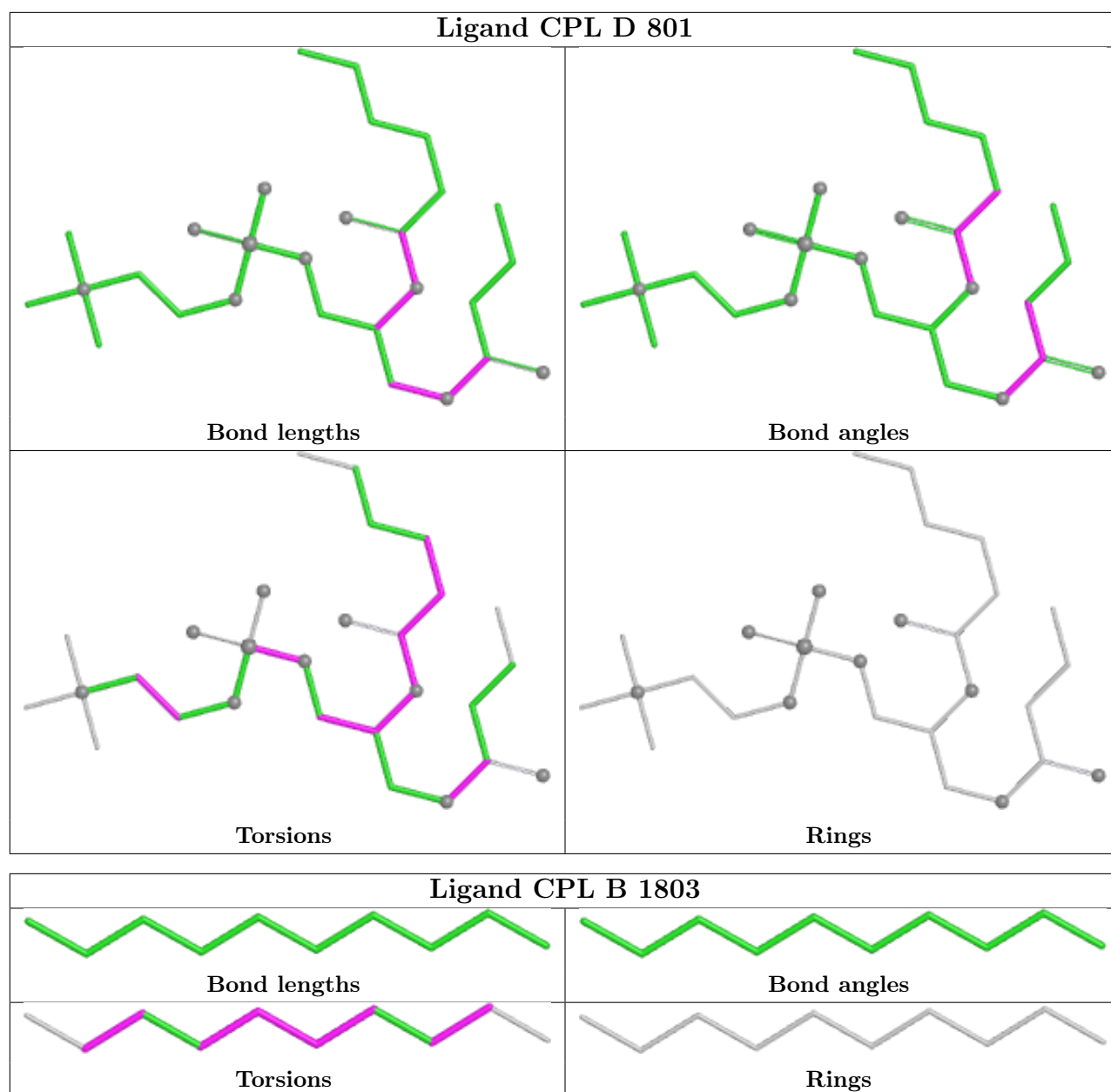


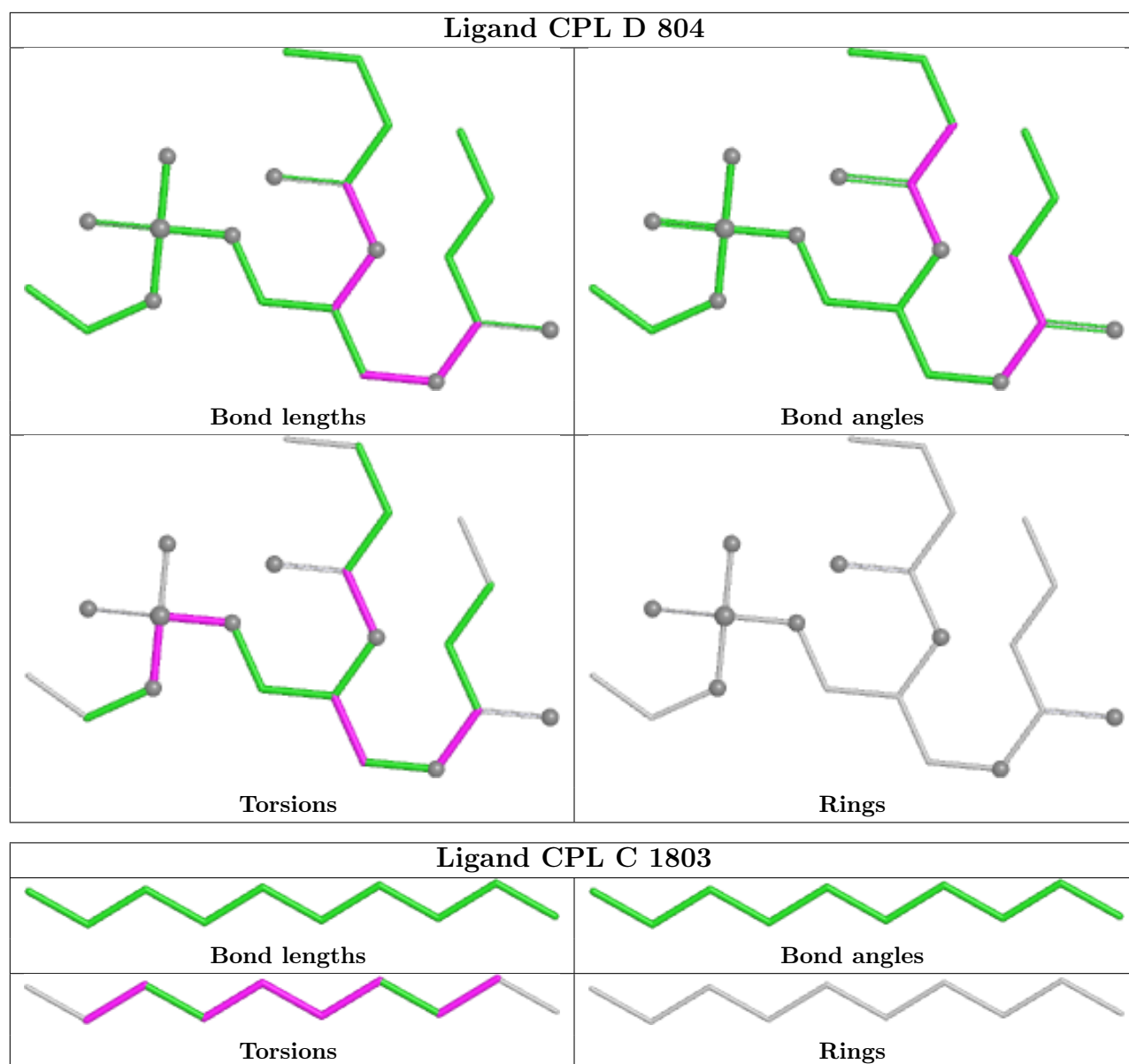


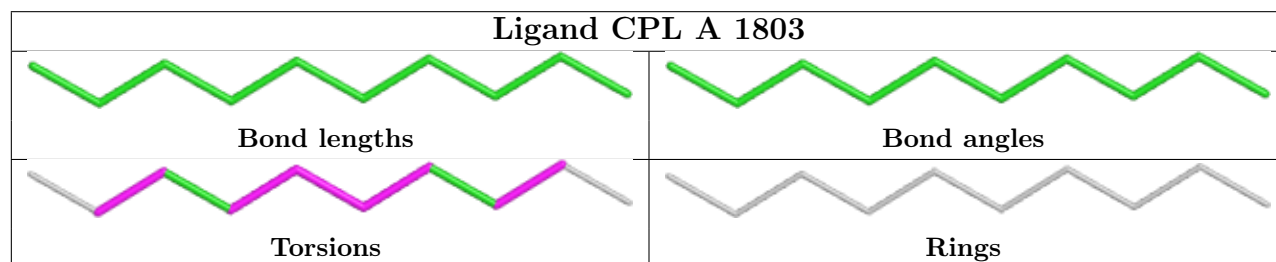
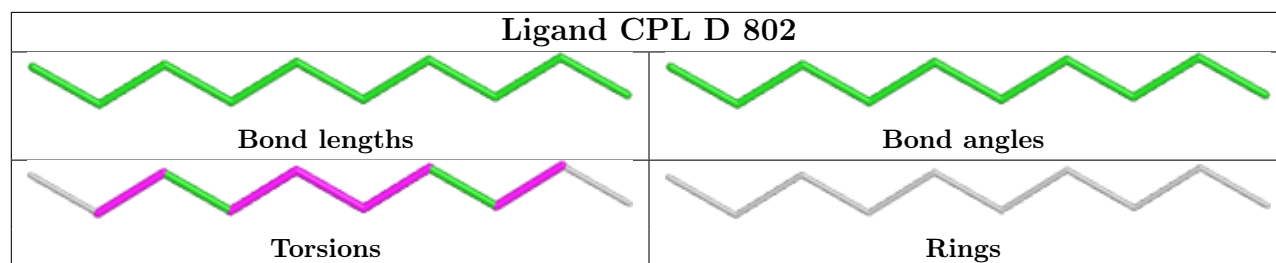
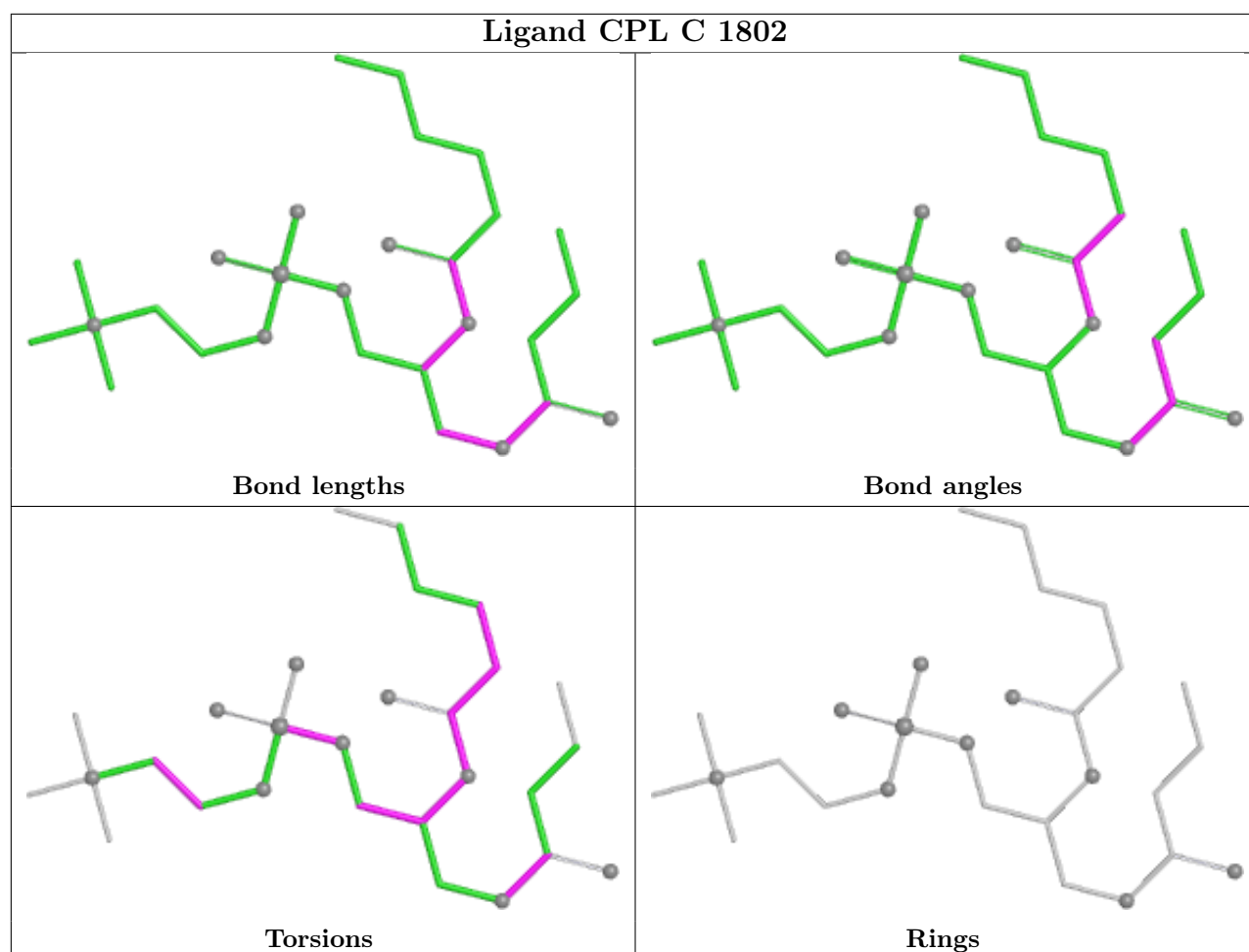


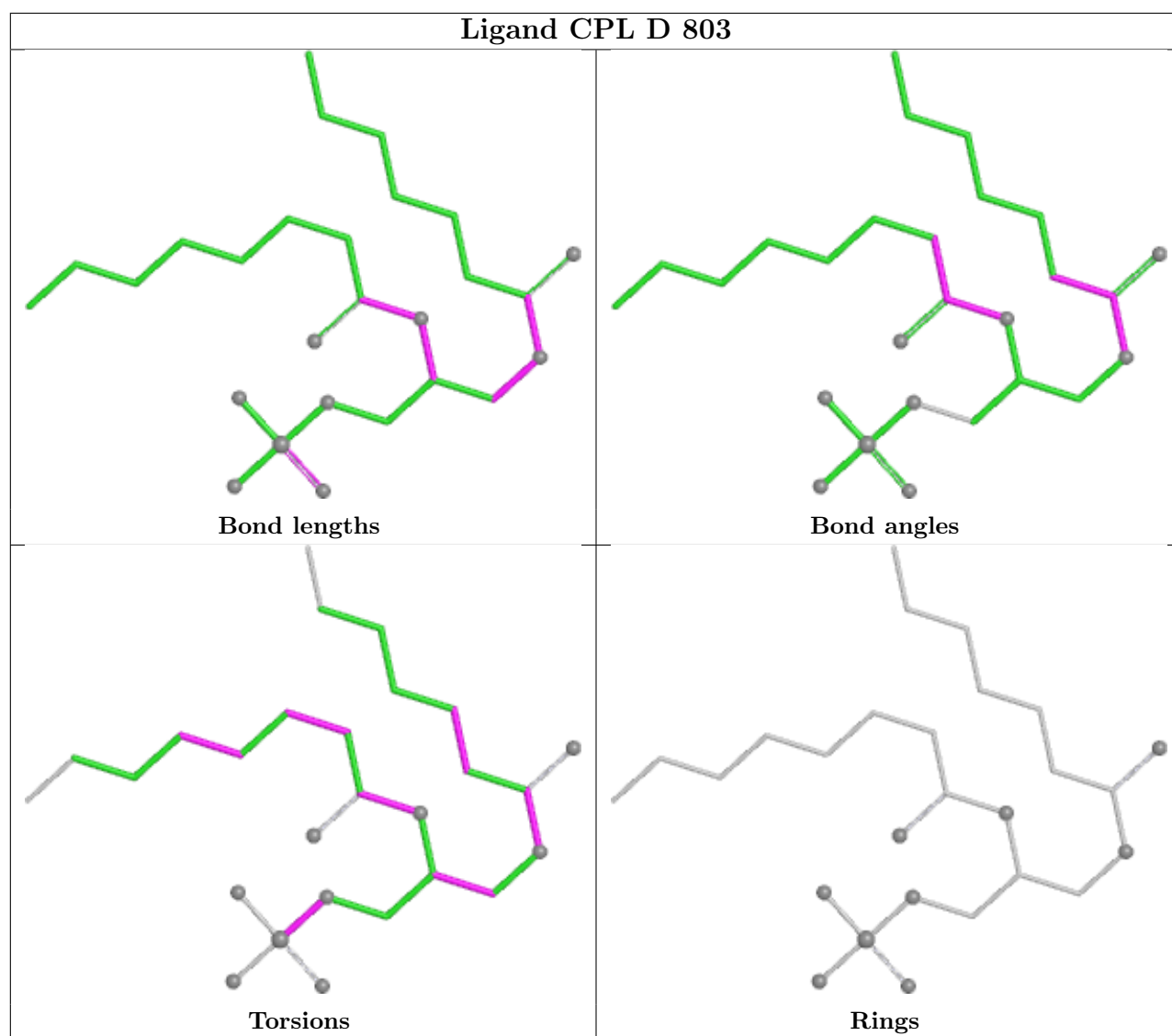












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

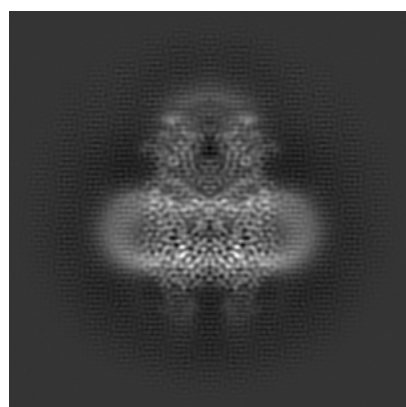
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-24114. These allow visual inspection of the internal detail of the map and identification of artifacts.

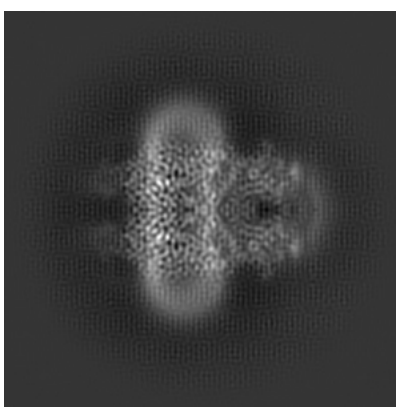
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

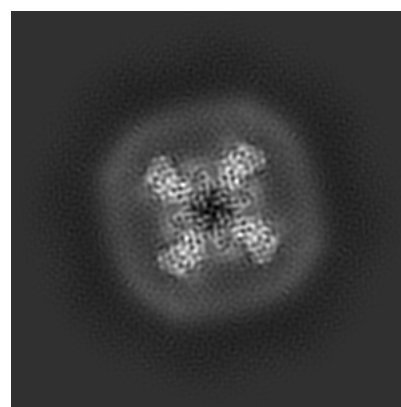
6.1.1 Primary map



X



Y

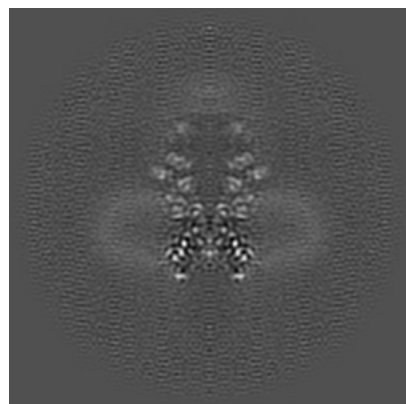


Z

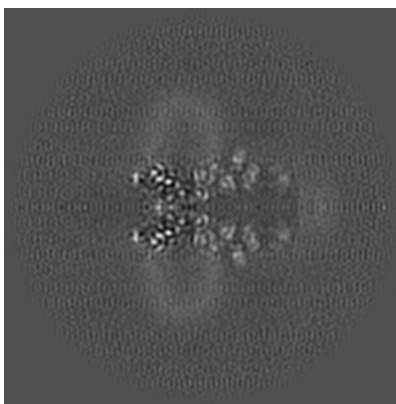
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

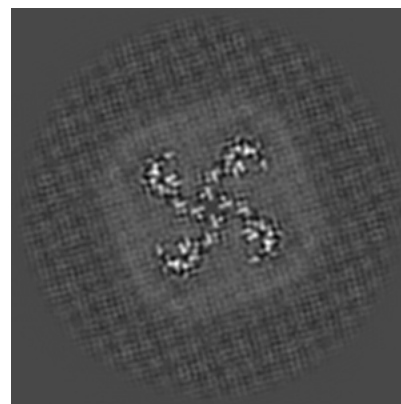
6.2.1 Primary map



X Index: 148



Y Index: 148

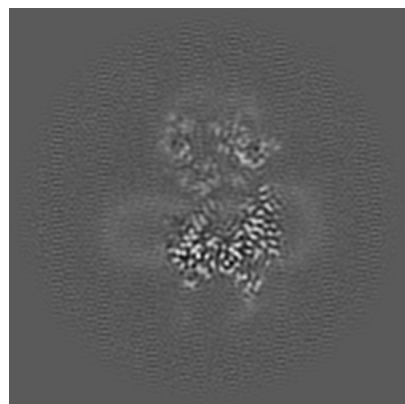


Z Index: 148

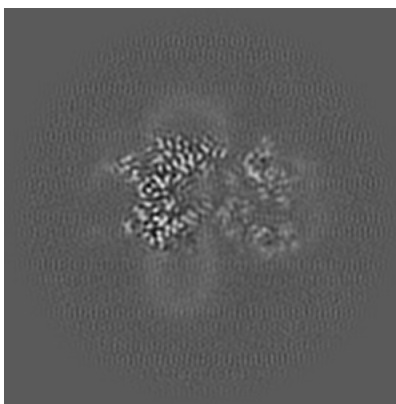
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

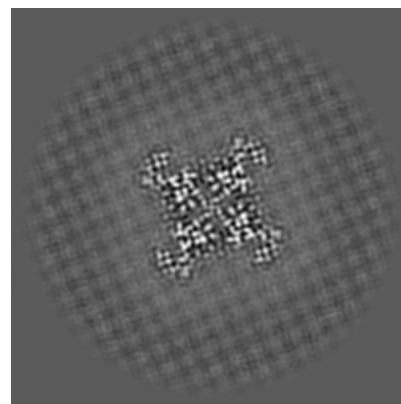
6.3.1 Primary map



X Index: 167



Y Index: 129

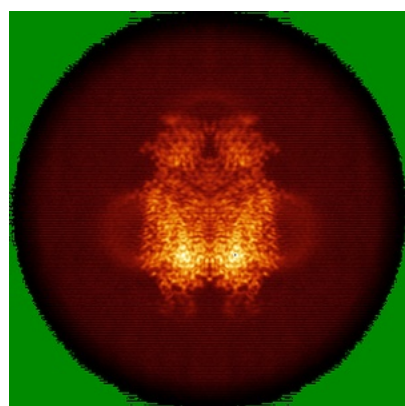


Z Index: 115

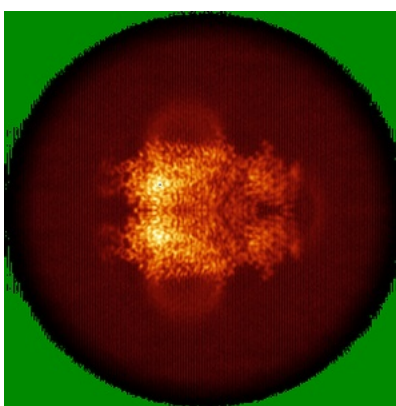
The images above show the largest variance slices of the map in three orthogonal directions.

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

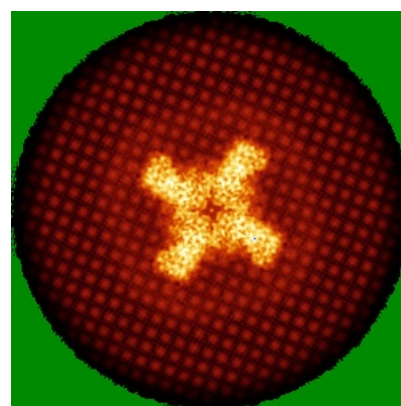
6.4.1 Primary map



X



Y

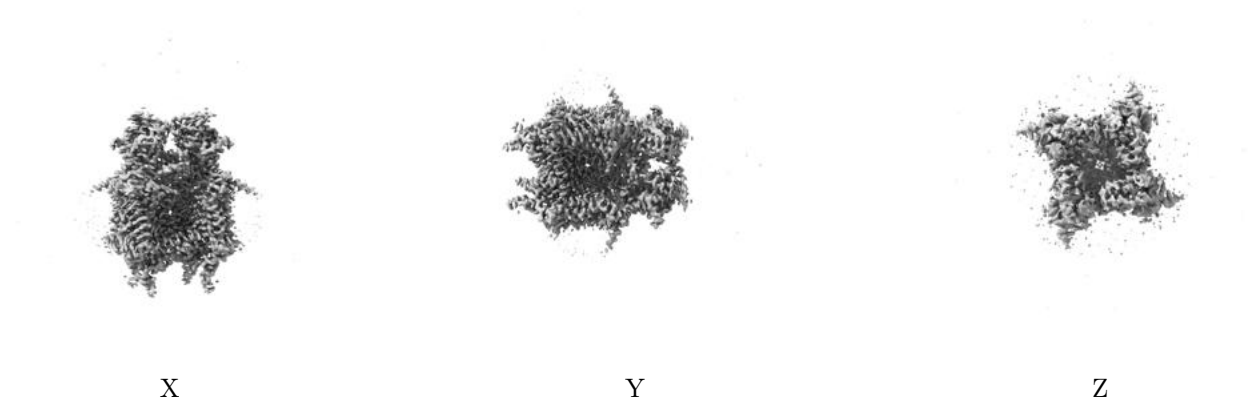


Z

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



The images above show the 3D surface view of the map at the recommended contour level 0.39. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

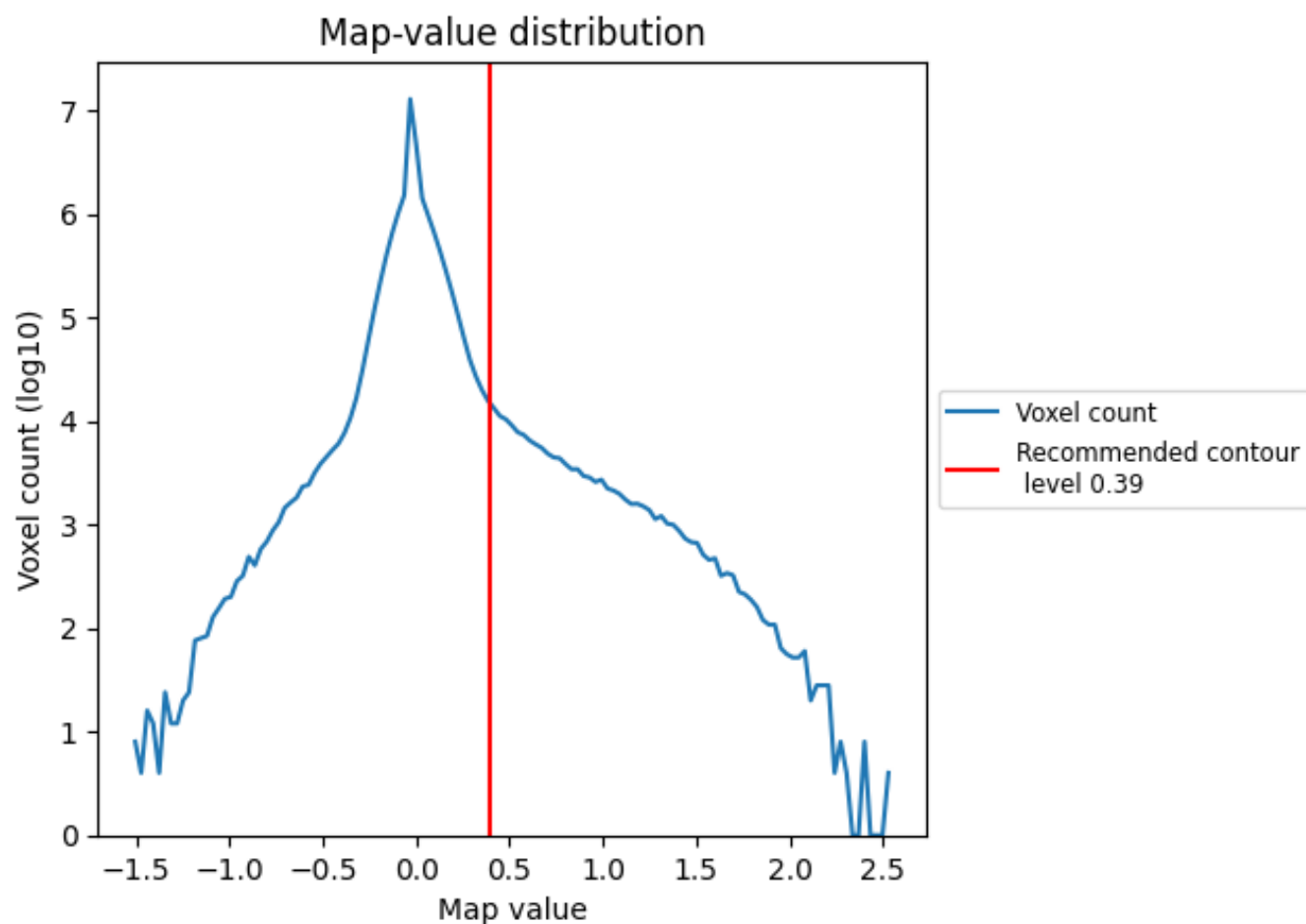
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

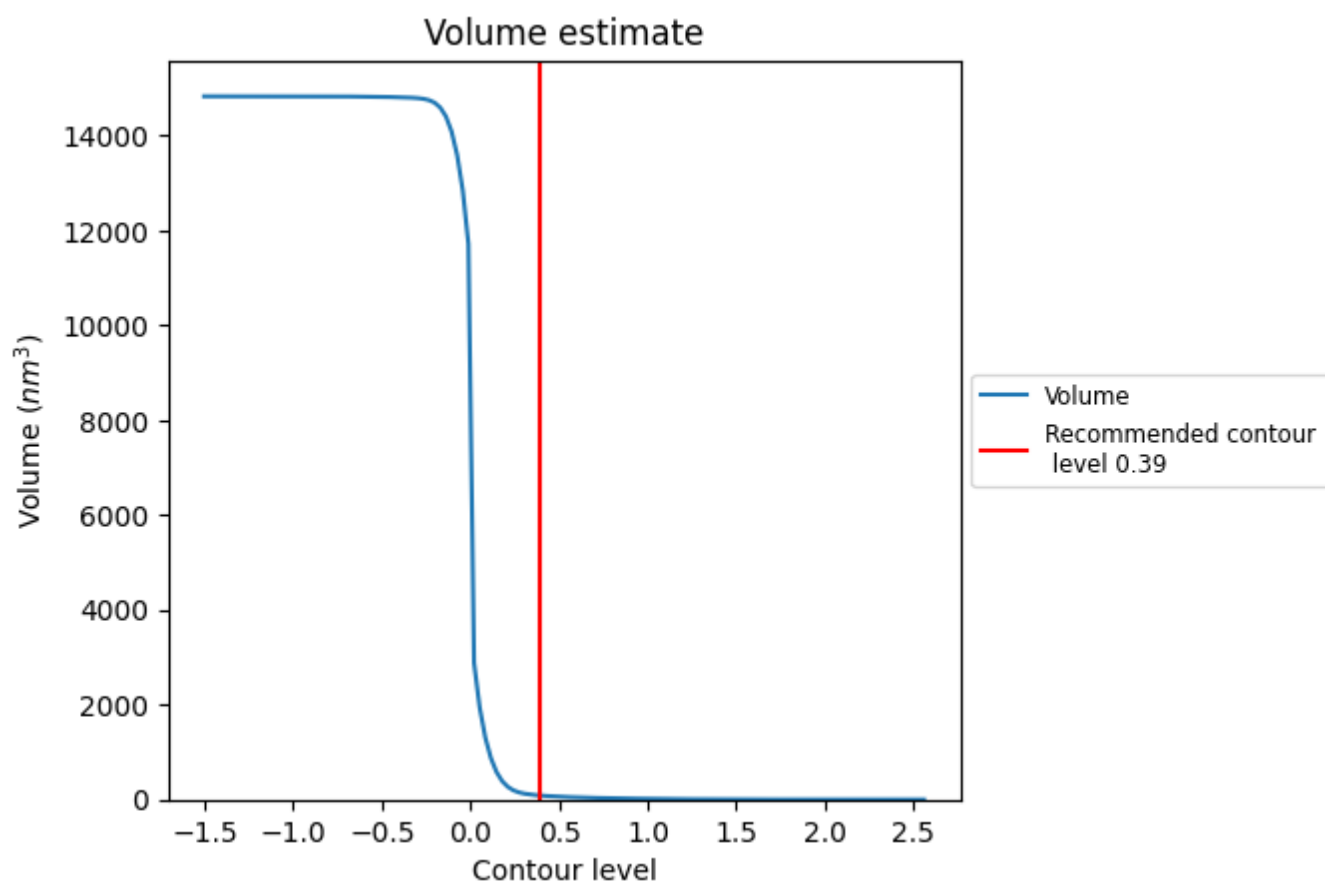
This section contains the results of statistical analysis of the map.

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.

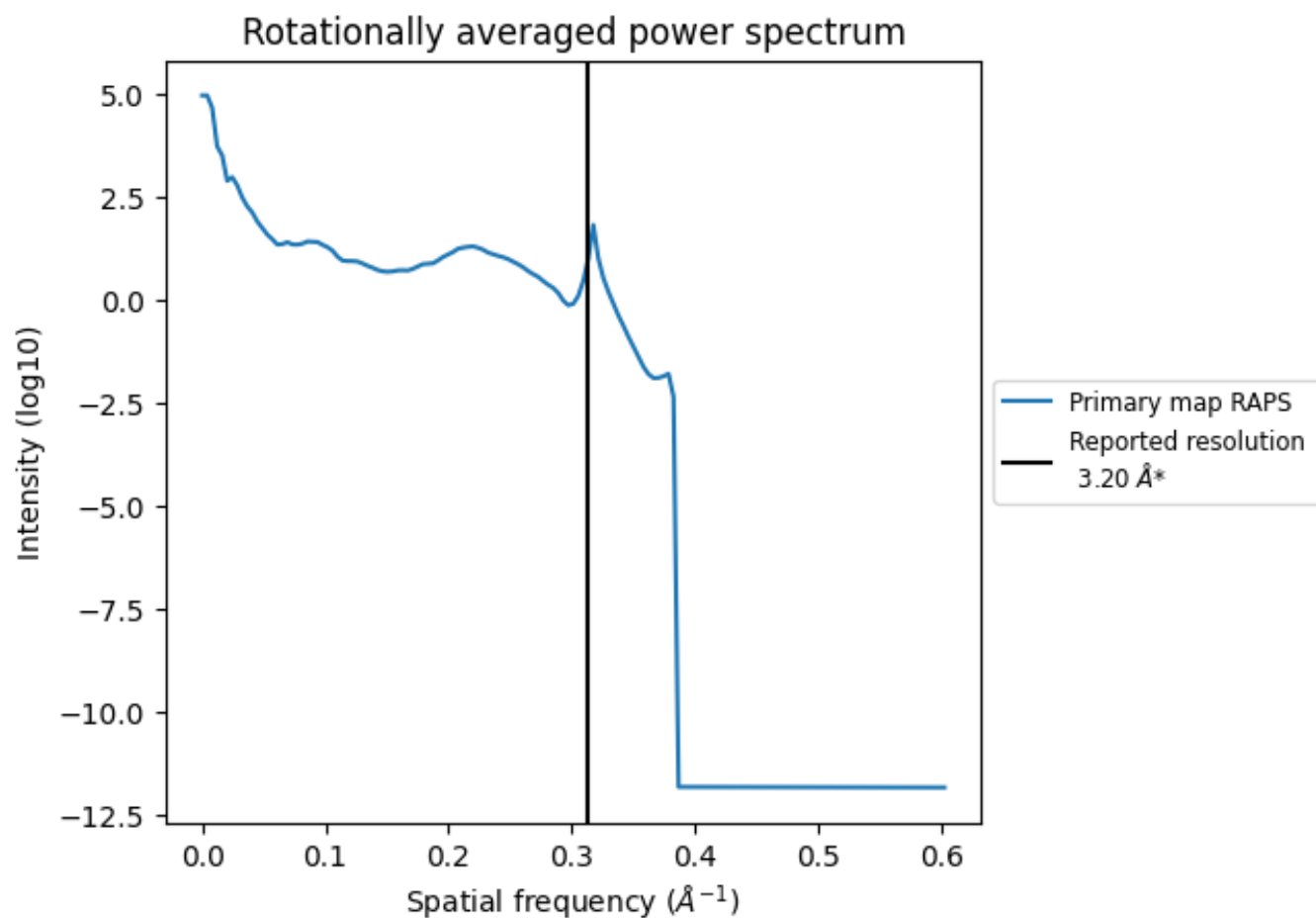
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 86 nm^3 ; this corresponds to an approximate mass of 78 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 0.312 Å⁻¹

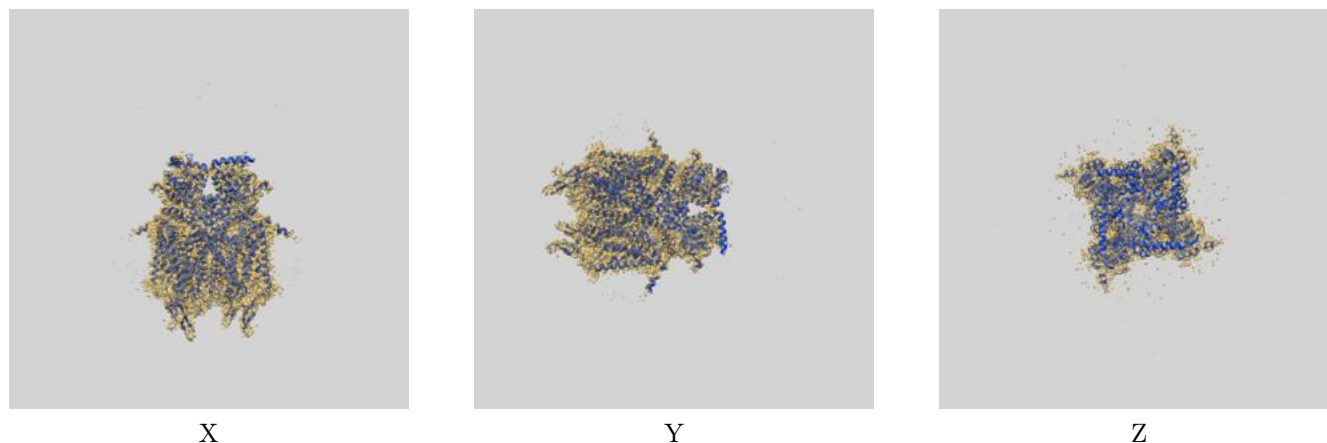
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

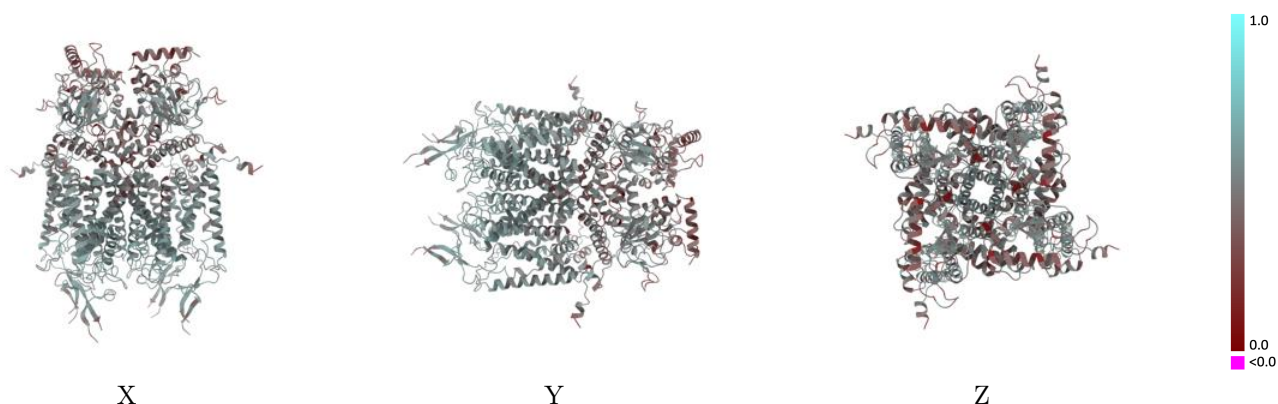
This section contains information regarding the fit between EMDB map EMD-24114 and PDB model 7N16. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

9.1 Map-model overlay [i](#)



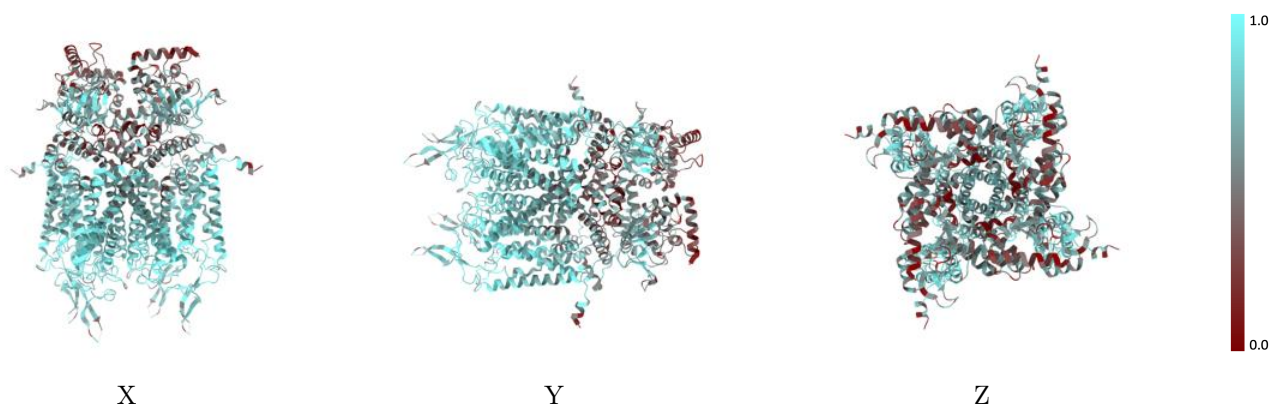
The images above show the 3D surface view of the map at the recommended contour level 0.39 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



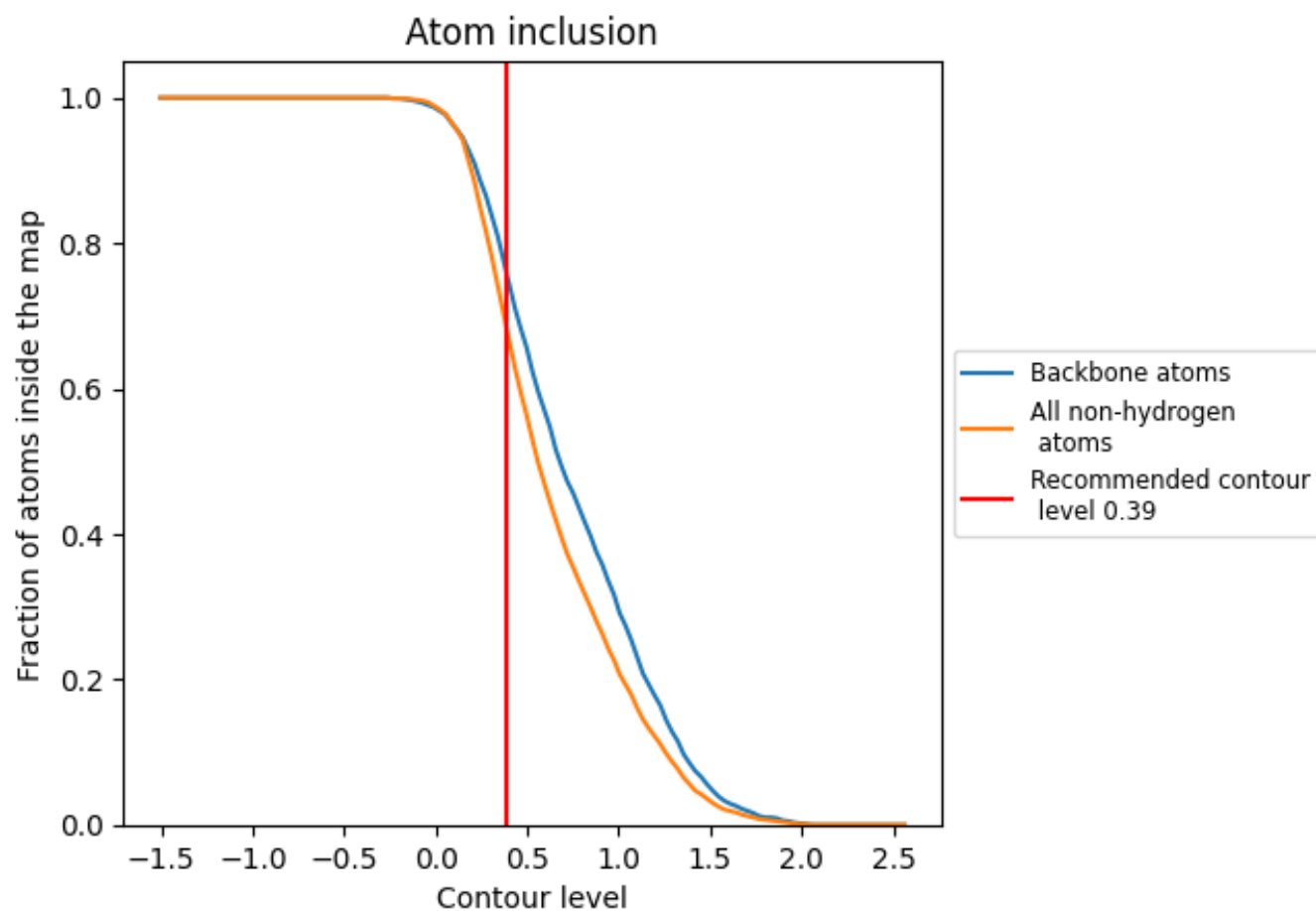
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.39).

9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 68% 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 (0.39) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6790	<div></div> 0.4900
A	<div></div> 0.6800	<div></div> 0.4890
B	<div></div> 0.6780	<div></div> 0.4900
C	<div></div> 0.6790	<div></div> 0.4900
D	<div></div> 0.6790	<div></div> 0.4890

