



## Full wwPDB EM Validation Report ⓘ

Jul 9, 2025 – 02:07 am BST

PDB ID : 8R0P / pdb\_00008r0p  
EMDB ID : EMD-18800  
Title : Cryo-EM structure of the microbial rhodopsin CryoR2 at pH 8.0 in detergent  
Authors : Kovalev, K.; Marin, E.; Stetsenko, A.; Guskov, A.; Lamm, G.H.U.  
Deposited on : 2023-10-31  
Resolution : 2.44 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev118  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0rc1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.44

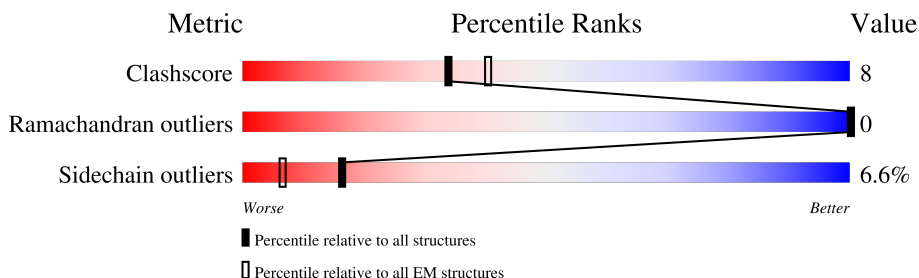
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.44 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	327	
1	B	327	
1	C	327	
1	D	327	
1	E	327	

## 2 Entry composition [i](#)

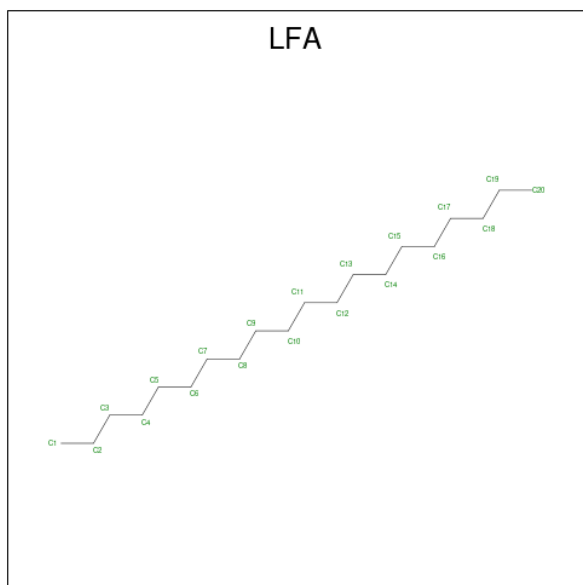
There are 4 unique types of molecules in this entry. The entry contains 11154 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 microbial rhodopsin CryoR2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	282	Total	C	N	O	S	0	0
			2109	1385	347	371	6		
1	B	282	Total	C	N	O	S	0	0
			2109	1385	347	371	6		
1	C	282	Total	C	N	O	S	0	0
			2109	1385	347	371	6		
1	D	282	Total	C	N	O	S	0	0
			2109	1385	347	371	6		
1	E	282	Total	C	N	O	S	0	0
			2109	1385	347	371	6		

- Molecule 2 is EICOSANE (CCD ID: LFA) (formula:  $C_{20}H_{42}$ ).



Mol	Chain	Residues	Atoms		AltConf
2	A	1	Total	C	0
			11	11	
2	A	1	Total	C	0
			13	13	

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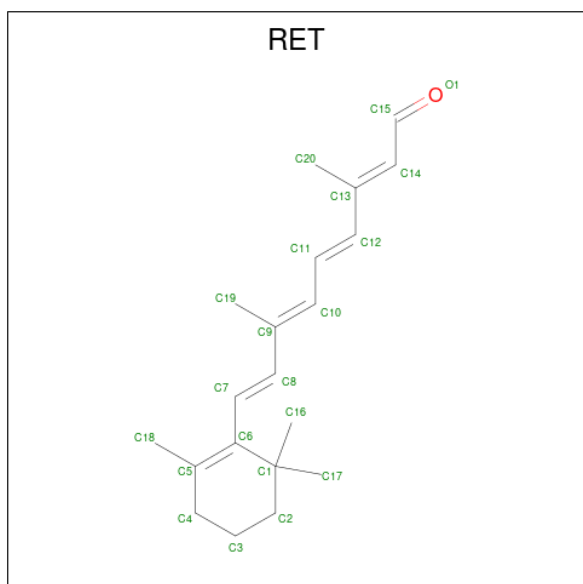
Mol	Chain	Residues	Atoms	AltConf
2	A	1	Total C 9 9	0
2	A	1	Total C 10 10	0
2	A	1	Total C 6 6	0
2	A	1	Total C 11 11	0
2	A	1	Total C 10 10	0
2	B	1	Total C 11 11	0
2	B	1	Total C 11 11	0
2	B	1	Total C 11 11	0
2	B	1	Total C 9 9	0
2	B	1	Total C 11 11	0
2	B	1	Total C 7 7	0
2	B	1	Total C 9 9	0
2	C	1	Total C 11 11	0
2	C	1	Total C 12 12	0
2	C	1	Total C 10 10	0
2	C	1	Total C 10 10	0
2	C	1	Total C 7 7	0
2	C	1	Total C 12 12	0
2	C	1	Total C 11 11	0
2	D	1	Total C 11 11	0
2	D	1	Total C 12 12	0

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Mol	Chain	Residues	Atoms	AltConf
2	D	1	Total C 13 13	0
2	D	1	Total C 10 10	0
2	D	1	Total C 10 10	0
2	D	1	Total C 6 6	0
2	D	1	Total C 9 9	0
2	E	1	Total C 11 11	0
2	E	1	Total C 11 11	0
2	E	1	Total C 12 12	0
2	E	1	Total C 10 10	0
2	E	1	Total C 11 11	0
2	E	1	Total C 6 6	0
2	E	1	Total C 10 10	0

- Molecule 3 is RETINAL (CCD ID: RET) (formula:  $C_{20}H_{28}O$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
3	A	1	Total C 20 20	0
3	B	1	Total C 20 20	0
3	C	1	Total C 20 20	0
3	D	1	Total C 20 20	0
3	E	1	Total C 20 20	0

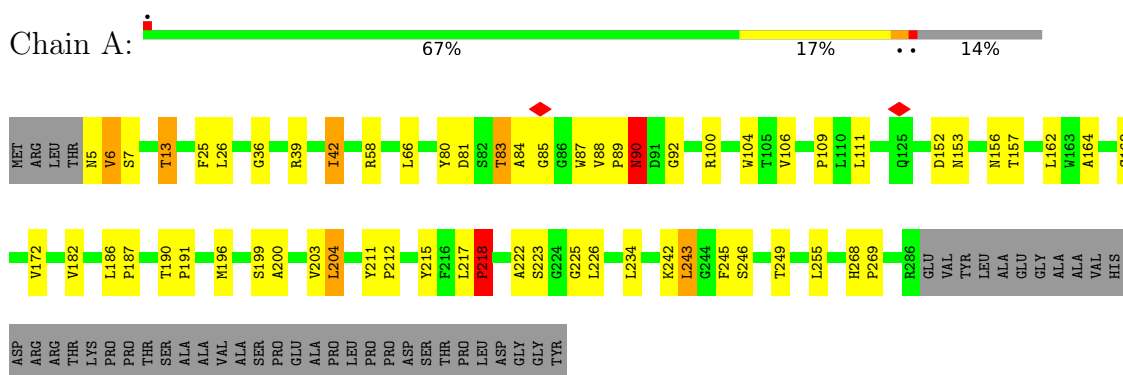
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	AltConf
4	A	31	Total O 31 31	0
4	B	31	Total O 31 31	0
4	C	32	Total O 32 32	0
4	D	30	Total O 30 30	0
4	E	31	Total O 31 31	0

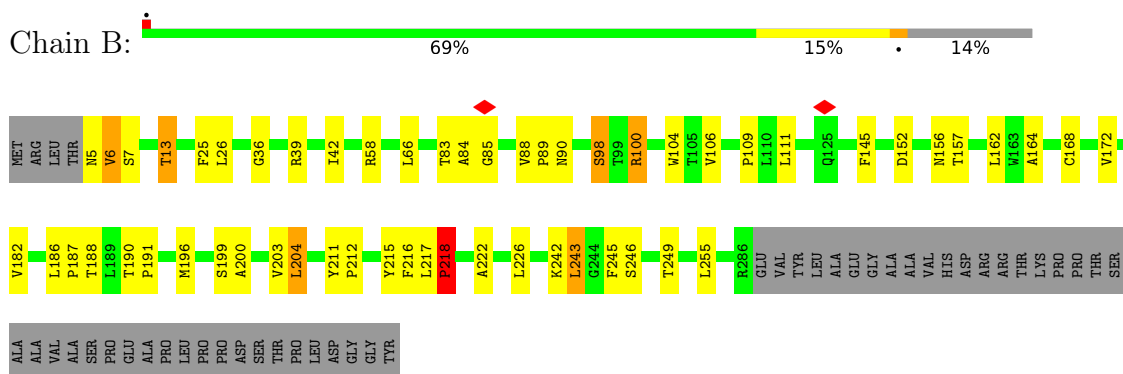
### 3 Residue-property plots [i](#)

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.

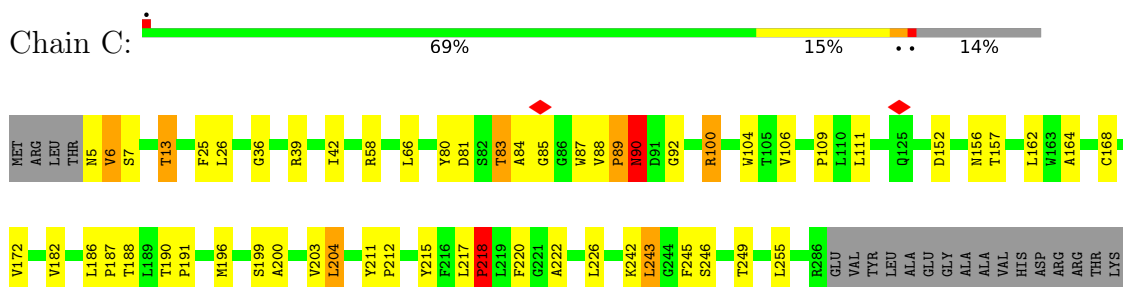
- Molecule 1: microbial rhodopsin CryoR2



- Molecule 1: microbial rhodopsin CryoR2



- Molecule 1: microbial rhodopsin CryoR2



PRO  
PRO  
THR  
SER  
ALA  
ALA  
VAL  
ALA  
SER  
PRO  
GLU  
ALA  
PRO  
LEU  
PRO  
PRO  
ASP  
SER  
THR  
PRO  
LEU  
ASP  
GLY  
GLY  
TYR

● Molecule 1: microbial rhodopsin CryoR2



MET ARG LEU THR N5 V6 S7 T13 Q20 L21 F25 L26 G36 R39 I42 I45 R58 L66 Y80 T83 A94 G85 G86 W87 V88 P89 N90 S98 T99 R100 W104 T105 V106 P109 L110 L111 Q125 F145 D152 N153 N156 T157 L162

V163 A164 C168 V172 V182 L186 P187 T188 L189 T190 P191 M196 S199 A200 A201 I202 V203 L204 G207 Y211 P212 Y215 F216 L217 P218 A222 L226 K242 L243 G244 F245 S246 T249 L255 P269 E270 R286 GLU VAL TYR LEU ALA GLY

ALA  
ALA  
VAL  
HIS  
ASP  
ARG  
ARG  
THR  
LYS  
PRO  
PRO  
THR  
SER  
ALA  
ALA  
VAL  
SER  
PRO  
GLU  
ALA  
PRO  
LEU  
LEU  
ASP  
PRO  
SER  
THR  
PRO  
LEU  
LEU  
ASP  
GLY  
GLY  
TYR

● Molecule 1: microbial rhodopsin CryoR2



MET ARG LEU THR N5 V6 S7 T13 F25 L26 G36 R39 I42 R58 L66 D81 S82 T83 A84 G85 V88 P89 N90 A93 R100 W104 T105 V106 P109 L110 L111 Q125 I149 D152 N156 T157 L162 V163 A164 C168

V172 V182 R183 L186 P187 T188 L189 P191 M196 S199 A200 A201 I202 V203 L204 Y211 P212 Y215 F216 L217 P218 A222 L226 K242 L243 G244 F245 S246 T249 L255 R286 GLU VAL TYR LEU ALA GLY ALA VAL HIS ASP ARG ARG THR LYS

PRO  
PRO  
THR  
SER  
ALA  
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VAL  
ALA  
SER  
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GLU  
ALA  
PRO  
LEU  
PRO  
PRO  
ASP  
SER  
THR  
PRO  
LEU  
ASP  
GLY  
GLY  
TYR



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C5	Depositor
Number of particles used	486732	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.860	Depositor
Minimum map value	-1.873	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.048	Depositor
Recommended contour level	0.316	Depositor
Map size (Å)	321.02402, 321.02402, 321.02402	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.836, 0.836, 0.836	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: RET, LFA

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	0.84	1/2156 (0.0%)	1.25	7/2959 (0.2%)
1	B	0.81	1/2156 (0.0%)	1.22	5/2959 (0.2%)
1	C	0.80	1/2156 (0.0%)	1.22	6/2959 (0.2%)
1	D	0.80	1/2156 (0.0%)	1.22	7/2959 (0.2%)
1	E	0.80	1/2156 (0.0%)	1.22	6/2959 (0.2%)
All	All	0.81	5/10780 (0.0%)	1.23	31/14795 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
1	C	0	2
1	D	0	2
1	E	0	2
All	All	0	9

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	218	PRO	C-O	-5.43	1.17	1.24
1	A	218	PRO	C-O	-5.40	1.17	1.24
1	D	218	PRO	C-O	-5.29	1.16	1.24
1	E	218	PRO	C-O	-5.29	1.16	1.24
1	C	218	PRO	C-O	-5.14	1.17	1.24

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	218	PRO	CB-CA-C	8.96	124.71	111.62
1	C	218	PRO	CB-CA-C	8.88	124.58	111.62
1	E	218	PRO	CB-CA-C	8.35	123.82	111.62
1	B	218	PRO	CB-CA-C	8.17	123.45	111.85
1	B	90	ASN	CA-CB-CG	7.82	120.42	112.60
1	A	90	ASN	CA-CB-CG	7.59	120.19	112.60
1	C	90	ASN	CA-CB-CG	7.48	120.08	112.60
1	E	90	ASN	CA-CB-CG	7.39	120.00	112.60
1	D	90	ASN	CA-CB-CG	7.25	119.86	112.60
1	A	218	PRO	N-CA-CB	-7.04	96.44	103.48
1	C	218	PRO	N-CA-CB	-6.97	96.90	103.52
1	A	218	PRO	CB-CA-C	6.96	121.73	111.85
1	B	218	PRO	N-CA-CB	-6.89	96.59	103.48
1	D	218	PRO	N-CA-CB	-6.82	97.04	103.52
1	C	220	PHE	CB-CA-C	6.73	121.54	109.29
1	C	89	PRO	N-CA-CB	-6.71	97.23	103.27
1	E	218	PRO	N-CA-CB	-6.69	97.17	103.52
1	D	89	PRO	N-CA-CB	-6.17	97.72	103.27
1	A	89	PRO	N-CA-CB	-5.91	97.95	103.27
1	E	89	PRO	N-CA-CB	-5.83	98.02	103.27
1	B	216	PHE	CA-CB-CG	5.80	119.60	113.80
1	A	223	SER	CA-C-O	-5.71	115.12	121.23
1	B	89	PRO	N-CA-CB	-5.54	98.28	103.27
1	E	83	THR	CA-C-O	-5.50	115.47	121.20
1	A	225	GLY	CA-C-O	-5.48	115.11	120.75
1	D	270	GLU	CB-CG-CD	5.47	121.90	112.60
1	E	93	ALA	N-CA-C	-5.36	106.25	112.89
1	A	83	THR	CA-C-O	-5.33	115.65	121.20
1	C	83	THR	CA-C-O	-5.24	115.75	121.20
1	D	216	PHE	CA-CB-CG	5.07	118.87	113.80
1	D	269	PRO	CB-CA-C	-5.01	104.73	111.85

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	39	ARG	Sidechain
1	B	100	ARG	Sidechain
1	B	39	ARG	Sidechain
1	C	100	ARG	Sidechain
1	C	39	ARG	Sidechain
1	D	100	ARG	Sidechain
1	D	39	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	E	100	ARG	Sidechain
1	E	39	ARG	Sidechain

## 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	2109	0	2166	36	0
1	B	2109	0	2166	30	0
1	C	2109	0	2166	33	0
1	D	2109	0	2166	36	0
1	E	2109	0	2166	37	0
2	A	70	0	133	0	0
2	B	69	0	131	1	0
2	C	73	0	129	0	0
2	D	71	0	129	3	0
2	E	71	0	132	3	0
3	A	20	0	27	2	0
3	B	20	0	27	1	0
3	C	20	0	27	2	0
3	D	20	0	27	2	0
3	E	20	0	27	2	0
4	A	31	0	0	0	0
4	B	31	0	0	0	0
4	C	32	0	0	0	0
4	D	30	0	0	0	0
4	E	31	0	0	1	0
All	All	11154	0	11619	180	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 8.

All (180) 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)
3:C:408:RET:H161	3:C:408:RET:H8	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:408:RET:H161	3:A:408:RET:H8	1.80	0.63
3:B:408:RET:H161	3:B:408:RET:H8	1.80	0.63
1:C:83:THR:O	1:C:85:GLY:N	2.31	0.63
1:D:83:THR:O	1:D:85:GLY:N	2.31	0.63
1:A:90:ASN:HD22	1:A:92:GLY:H	1.44	0.63
3:E:408:RET:H8	3:E:408:RET:H161	1.80	0.63
3:D:408:RET:H161	3:D:408:RET:H8	1.80	0.62
1:B:83:THR:O	1:B:85:GLY:N	2.33	0.60
1:E:83:THR:O	1:E:85:GLY:N	2.32	0.60
1:A:106:VAL:O	1:A:109:PRO:HD2	2.03	0.59
1:C:106:VAL:O	1:C:109:PRO:HD2	2.03	0.59
1:E:106:VAL:O	1:E:109:PRO:HD2	2.03	0.58
1:B:106:VAL:O	1:B:109:PRO:HD2	2.03	0.58
1:D:106:VAL:O	1:D:109:PRO:HD2	2.03	0.57
1:A:83:THR:O	1:A:85:GLY:N	2.32	0.57
1:B:243:LEU:HD11	2:B:401:LFA:H121	1.87	0.56
1:C:182:VAL:O	1:C:186:LEU:HG	2.07	0.54
1:E:182:VAL:O	1:E:186:LEU:HG	2.08	0.54
1:B:182:VAL:O	1:B:186:LEU:HG	2.07	0.54
1:A:182:VAL:O	1:A:186:LEU:HG	2.07	0.54
1:E:243:LEU:HD11	2:E:401:LFA:H41	1.89	0.54
1:D:182:VAL:O	1:D:186:LEU:HG	2.07	0.54
1:C:111:LEU:C	1:C:111:LEU:HD23	2.34	0.52
1:C:168:CYS:O	1:C:172:VAL:HG23	2.10	0.52
1:E:168:CYS:O	1:E:172:VAL:HG23	2.10	0.52
1:A:168:CYS:O	1:A:172:VAL:HG23	2.10	0.52
1:D:186:LEU:N	1:D:187:PRO:CD	2.74	0.51
1:A:211:TYR:HB2	1:A:212:PRO:HD3	1.93	0.51
1:B:211:TYR:HB2	1:B:212:PRO:HD3	1.93	0.51
1:D:168:CYS:O	1:D:172:VAL:HG23	2.10	0.51
1:C:211:TYR:HB2	1:C:212:PRO:HD3	1.93	0.51
1:B:168:CYS:O	1:B:172:VAL:HG23	2.10	0.51
1:E:186:LEU:N	1:E:187:PRO:CD	2.74	0.51
1:E:211:TYR:HB2	1:E:212:PRO:HD3	1.93	0.51
1:C:186:LEU:N	1:C:187:PRO:CD	2.74	0.51
1:C:58:ARG:NH1	1:C:242:LYS:O	2.44	0.51
1:A:7:SER:HB3	1:A:222:ALA:HB2	1.94	0.50
1:B:58:ARG:NH1	1:B:242:LYS:O	2.44	0.50
1:C:100:ARG:HG2	1:C:104:TRP:CZ2	2.47	0.50
1:E:58:ARG:NH1	1:E:242:LYS:O	2.44	0.50
1:B:186:LEU:N	1:B:187:PRO:CD	2.74	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:LEU:N	1:A:187:PRO:CD	2.73	0.50
1:D:100:ARG:HG2	1:D:104:TRP:CZ2	2.47	0.50
1:B:100:ARG:HG2	1:B:104:TRP:CZ2	2.47	0.50
1:A:199:SER:O	1:A:203:VAL:HG23	2.12	0.50
1:C:199:SER:O	1:C:203:VAL:HG23	2.12	0.50
1:D:58:ARG:NH1	1:D:242:LYS:O	2.44	0.50
1:D:211:TYR:HB2	1:D:212:PRO:HD3	1.93	0.50
1:E:100:ARG:HG2	1:E:104:TRP:CZ2	2.47	0.50
1:E:217:LEU:N	1:E:218:PRO:CD	2.74	0.50
1:A:58:ARG:NH1	1:A:242:LYS:O	2.44	0.49
1:A:100:ARG:HG2	1:A:104:TRP:CZ2	2.47	0.49
1:B:111:LEU:C	1:B:111:LEU:HD23	2.38	0.49
1:E:255:LEU:HD12	1:E:255:LEU:O	2.13	0.49
1:A:255:LEU:HD12	1:A:255:LEU:O	2.12	0.49
1:C:255:LEU:HD12	1:C:255:LEU:O	2.13	0.49
1:D:111:LEU:HD23	1:D:111:LEU:O	2.13	0.49
1:A:111:LEU:O	1:A:111:LEU:HD23	2.13	0.48
1:A:217:LEU:N	1:A:218:PRO:CD	2.75	0.48
1:E:111:LEU:C	1:E:111:LEU:HD23	2.38	0.48
1:E:111:LEU:HD23	1:E:111:LEU:O	2.13	0.48
1:B:255:LEU:HD12	1:B:255:LEU:O	2.13	0.48
1:D:36:GLY:HA3	1:D:243:LEU:HD21	1.96	0.48
1:D:255:LEU:O	1:D:255:LEU:HD12	2.13	0.48
1:B:58:ARG:CZ	1:B:246:SER:HA	2.44	0.47
1:C:217:LEU:N	1:C:218:PRO:CD	2.77	0.47
1:A:83:THR:O	1:A:84:ALA:HB3	2.13	0.47
1:C:90:ASN:HD22	1:C:92:GLY:H	1.60	0.47
1:C:36:GLY:HA3	1:C:243:LEU:HD21	1.97	0.47
1:A:58:ARG:CZ	1:A:246:SER:HA	2.44	0.47
1:A:83:THR:C	1:A:85:GLY:N	2.73	0.47
1:C:58:ARG:CZ	1:C:246:SER:HA	2.44	0.47
1:B:36:GLY:HA3	1:B:243:LEU:HD21	1.96	0.47
1:D:111:LEU:HD23	1:D:111:LEU:C	2.40	0.47
1:E:36:GLY:HA3	1:E:243:LEU:HD21	1.96	0.47
1:D:58:ARG:CZ	1:D:246:SER:HA	2.44	0.47
1:E:83:THR:O	1:E:84:ALA:HB3	2.15	0.47
1:E:83:THR:C	1:E:85:GLY:N	2.73	0.47
1:B:13:THR:OG1	1:B:88:VAL:HG22	2.15	0.47
1:B:111:LEU:HD23	1:B:111:LEU:O	2.14	0.47
1:C:111:LEU:HD23	1:C:111:LEU:O	2.14	0.46
1:E:58:ARG:CZ	1:E:246:SER:HA	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:LEU:HD23	1:A:111:LEU:C	2.40	0.46
1:A:36:GLY:HA3	1:A:243:LEU:HD21	1.97	0.46
1:E:199:SER:O	1:E:203:VAL:HG23	2.14	0.46
1:C:200:ALA:O	1:C:204:LEU:HB2	2.16	0.46
1:E:200:ALA:O	1:E:204:LEU:HB2	2.16	0.46
1:B:98:SER:OG	1:B:145:PHE:HE1	1.99	0.45
1:B:200:ALA:O	1:B:204:LEU:HB2	2.16	0.45
3:D:408:RET:H191	3:D:408:RET:H11	1.65	0.45
1:D:200:ALA:O	1:D:204:LEU:HB2	2.16	0.45
1:E:7:SER:HB3	1:E:222:ALA:HB2	1.99	0.45
3:A:408:RET:H11	3:A:408:RET:H191	1.65	0.45
1:A:200:ALA:O	1:A:204:LEU:HB2	2.16	0.45
1:C:83:THR:C	1:C:85:GLY:N	2.75	0.44
1:E:25:PHE:CZ	2:E:402:LFA:H22	2.51	0.44
1:C:83:THR:O	1:C:84:ALA:HB3	2.15	0.44
1:D:7:SER:HB3	1:D:222:ALA:HB2	1.99	0.44
1:A:100:ARG:NH1	1:A:234:LEU:HB2	2.33	0.44
1:B:152:ASP:OD2	1:B:156:ASN:HB2	2.18	0.44
1:C:13:THR:OG1	1:C:88:VAL:HG22	2.17	0.44
1:B:83:THR:O	1:B:84:ALA:HB3	2.17	0.44
1:D:98:SER:OG	1:D:145:PHE:HE1	1.99	0.44
1:E:202:ILE:HG12	2:E:405:LFA:H61	2.00	0.44
1:B:7:SER:HB3	1:B:222:ALA:HB2	1.99	0.43
1:C:80:TYR:HB3	1:C:87:TRP:HB3	2.00	0.43
1:D:152:ASP:OD2	1:D:156:ASN:HB2	2.18	0.43
1:C:243:LEU:HD23	1:C:243:LEU:HA	1.89	0.43
1:C:152:ASP:OD2	1:C:156:ASN:HB2	2.18	0.43
1:D:199:SER:O	1:D:203:VAL:HG23	2.18	0.43
1:B:199:SER:O	1:B:203:VAL:HG23	2.19	0.43
1:C:7:SER:HB3	1:C:222:ALA:HB2	1.99	0.43
1:D:21:LEU:HD11	2:D:402:LFA:H101	2.00	0.43
1:D:217:LEU:N	1:D:218:PRO:CD	2.81	0.43
1:A:203:VAL:HG12	1:A:245:PHE:CD2	2.54	0.43
1:D:203:VAL:HG12	1:D:245:PHE:CD2	2.54	0.43
1:A:152:ASP:OD2	1:A:156:ASN:HB2	2.18	0.43
1:B:83:THR:C	1:B:85:GLY:N	2.75	0.43
1:C:203:VAL:HG12	1:C:245:PHE:CD2	2.54	0.43
1:D:13:THR:OG1	1:D:88:VAL:HG22	2.19	0.43
1:E:25:PHE:O	1:E:26:LEU:C	2.60	0.43
3:E:408:RET:H11	3:E:408:RET:H191	1.65	0.43
1:E:152:ASP:OD2	1:E:156:ASN:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:106:VAL:C	1:D:109:PRO:HD2	2.44	0.42
1:E:164:ALA:HB2	1:E:215:TYR:CE1	2.55	0.42
1:B:203:VAL:HG12	1:B:245:PHE:CD2	2.54	0.42
1:D:164:ALA:HB2	1:D:215:TYR:CE1	2.55	0.42
1:E:190:THR:O	1:E:191:PRO:C	2.63	0.42
1:E:203:VAL:HG12	1:E:245:PHE:CD2	2.54	0.42
1:A:164:ALA:HB2	1:A:215:TYR:CE1	2.55	0.42
1:A:13:THR:OG1	1:A:88:VAL:HG22	2.20	0.42
1:A:25:PHE:O	1:A:26:LEU:C	2.60	0.42
1:A:190:THR:O	1:A:191:PRO:C	2.63	0.42
1:C:164:ALA:HB2	1:C:215:TYR:CE1	2.54	0.42
1:C:106:VAL:C	1:C:109:PRO:HD2	2.44	0.42
1:A:106:VAL:C	1:A:109:PRO:HD2	2.44	0.42
1:D:190:THR:O	1:D:191:PRO:C	2.63	0.42
1:E:13:THR:OG1	1:E:88:VAL:HG22	2.20	0.42
1:D:83:THR:C	1:D:85:GLY:N	2.78	0.41
1:E:106:VAL:C	1:E:109:PRO:HD2	2.45	0.41
1:B:83:THR:C	1:B:85:GLY:H	2.26	0.41
1:B:164:ALA:HB2	1:B:215:TYR:CE1	2.55	0.41
1:B:25:PHE:O	1:B:26:LEU:C	2.60	0.41
3:C:408:RET:H11	3:C:408:RET:H191	1.65	0.41
1:E:217:LEU:N	1:E:218:PRO:HD3	2.36	0.41
1:B:106:VAL:C	1:B:109:PRO:HD2	2.45	0.41
1:D:243:LEU:HD23	1:D:243:LEU:HA	1.89	0.41
1:A:42:ILE:HA	1:A:42:ILE:HD12	1.81	0.41
1:A:80:TYR:HB3	1:A:87:TRP:HB3	2.02	0.41
1:B:217:LEU:N	1:B:218:PRO:CD	2.83	0.41
1:C:6:VAL:CG2	1:C:157:THR:HA	2.51	0.41
1:C:242:LYS:O	1:C:246:SER:HB3	2.21	0.41
1:E:42:ILE:HA	1:E:42:ILE:HD12	1.81	0.41
1:E:243:LEU:HD23	1:E:243:LEU:HA	1.89	0.41
1:B:190:THR:O	1:B:191:PRO:C	2.63	0.41
1:D:6:VAL:CG2	1:D:157:THR:HA	2.51	0.41
1:D:25:PHE:O	1:D:26:LEU:C	2.60	0.41
1:D:80:TYR:HB3	1:D:87:TRP:HB3	2.02	0.41
1:D:152:ASP:C	1:D:153:ASN:HD22	2.29	0.41
1:E:6:VAL:CG2	1:E:157:THR:HA	2.51	0.41
1:A:242:LYS:O	1:A:246:SER:HB3	2.21	0.41
1:D:20:GLN:HG2	1:E:149:ILE:HG22	2.03	0.41
1:E:6:VAL:HG23	1:E:157:THR:OG1	2.21	0.41
1:A:6:VAL:HG23	1:A:157:THR:OG1	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:6:VAL:HG23	1:C:157:THR:OG1	2.21	0.40
1:D:83:THR:O	1:D:84:ALA:HB3	2.21	0.40
1:E:111:LEU:HD12	4:E:527:HOH:O	2.21	0.40
1:A:6:VAL:CG2	1:A:157:THR:HA	2.51	0.40
1:D:207:GLY:HA3	2:D:404:LFA:H42	2.03	0.40
1:A:243:LEU:HD23	1:A:243:LEU:HA	1.89	0.40
1:A:268:HIS:HA	1:A:269:PRO:HD3	1.81	0.40
1:B:6:VAL:CG2	1:B:157:THR:HA	2.51	0.40
1:C:25:PHE:O	1:C:26:LEU:C	2.60	0.40
1:C:190:THR:O	1:C:191:PRO:C	2.63	0.40
1:D:202:ILE:HG13	2:D:405:LFA:H52	2.04	0.40
1:D:242:LYS:O	1:D:246:SER:HB3	2.21	0.40
1:E:88:VAL:HA	1:E:89:PRO:HD2	1.83	0.40
1:A:152:ASP:C	1:A:153:ASN:HD22	2.29	0.40
1:C:88:VAL:HA	1:C:89:PRO:HD2	1.81	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	280/327 (86%)	269 (96%)	11 (4%)	0	100	100
1	B	280/327 (86%)	270 (96%)	10 (4%)	0	100	100
1	C	280/327 (86%)	270 (96%)	10 (4%)	0	100	100
1	D	280/327 (86%)	269 (96%)	11 (4%)	0	100	100
1	E	280/327 (86%)	268 (96%)	12 (4%)	0	100	100
All	All	1400/1635 (86%)	1346 (96%)	54 (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	220/261 (84%)	206 (94%)	14 (6%)	14	18
1	B	220/261 (84%)	206 (94%)	14 (6%)	14	18
1	C	220/261 (84%)	205 (93%)	15 (7%)	13	15
1	D	220/261 (84%)	205 (93%)	15 (7%)	13	15
1	E	220/261 (84%)	205 (93%)	15 (7%)	13	15
All	All	1100/1305 (84%)	1027 (93%)	73 (7%)	16	17

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	A	6	VAL
1	A	13	THR
1	A	42	ILE
1	A	66	LEU
1	A	81	ASP
1	A	90	ASN
1	A	162	LEU
1	A	196	MET
1	A	204	LEU
1	A	218	PRO
1	A	226	LEU
1	A	243	LEU
1	A	249	THR
1	B	5	ASN
1	B	6	VAL
1	B	13	THR
1	B	42	ILE
1	B	66	LEU
1	B	98	SER
1	B	162	LEU
1	B	188	THR
1	B	196	MET

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Mol	Chain	Res	Type
1	B	204	LEU
1	B	218	PRO
1	B	226	LEU
1	B	243	LEU
1	B	249	THR
1	C	5	ASN
1	C	6	VAL
1	C	13	THR
1	C	42	ILE
1	C	66	LEU
1	C	81	ASP
1	C	90	ASN
1	C	162	LEU
1	C	188	THR
1	C	196	MET
1	C	204	LEU
1	C	218	PRO
1	C	226	LEU
1	C	243	LEU
1	C	249	THR
1	D	5	ASN
1	D	6	VAL
1	D	13	THR
1	D	42	ILE
1	D	66	LEU
1	D	98	SER
1	D	162	LEU
1	D	188	THR
1	D	196	MET
1	D	204	LEU
1	D	218	PRO
1	D	226	LEU
1	D	243	LEU
1	D	249	THR
1	D	270	GLU
1	E	5	ASN
1	E	6	VAL
1	E	13	THR
1	E	42	ILE
1	E	66	LEU
1	E	81	ASP
1	E	162	LEU

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Mol	Chain	Res	Type
1	E	183	ARG
1	E	188	THR
1	E	196	MET
1	E	204	LEU
1	E	218	PRO
1	E	226	LEU
1	E	243	LEU
1	E	249	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	A	90	ASN
1	A	153	ASN
1	B	153	ASN
1	B	248	GLN
1	C	5	ASN
1	C	90	ASN
1	C	248	GLN
1	D	5	ASN
1	D	153	ASN
1	D	248	GLN
1	E	5	ASN
1	E	248	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

40 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	LFA	C	407	-	10,10,19	0.19	0	9,9,18	0.20	0
2	LFA	E	401	-	10,10,19	0.13	0	9,9,18	0.17	0
2	LFA	E	404	-	9,9,19	0.14	0	8,8,18	0.20	0
2	LFA	B	404	-	8,8,19	0.18	0	7,7,18	0.21	0
2	LFA	C	404	-	9,9,19	0.19	0	8,8,18	0.26	0
2	LFA	A	405	-	5,5,19	0.24	0	4,4,18	0.42	0
3	RET	B	408	1	20,20,21	1.35	3 (15%)	27,27,28	1.80	7 (25%)
2	LFA	D	402	-	11,11,19	0.23	0	10,10,18	0.29	0
2	LFA	E	406	-	5,5,19	0.28	0	4,4,18	0.39	0
2	LFA	E	407	-	9,9,19	0.23	0	8,8,18	0.12	0
2	LFA	C	403	-	9,9,19	0.16	0	8,8,18	0.17	0
2	LFA	A	404	-	9,9,19	0.18	0	8,8,18	0.22	0
2	LFA	E	403	-	11,11,19	0.20	0	10,10,18	0.20	0
2	LFA	A	407	-	9,9,19	0.20	0	8,8,18	0.16	0
3	RET	C	408	1	20,20,21	1.34	3 (15%)	27,27,28	1.79	7 (25%)
2	LFA	B	405	-	10,10,19	0.14	0	9,9,18	0.10	0
2	LFA	A	402	-	12,12,19	0.23	0	11,11,18	0.19	0
2	LFA	E	402	-	10,10,19	0.22	0	9,9,18	0.19	0
2	LFA	A	401	-	10,10,19	0.22	0	9,9,18	0.17	0
2	LFA	D	405	-	9,9,19	0.19	0	8,8,18	0.10	0
2	LFA	D	407	-	8,8,19	0.28	0	7,7,18	0.10	0
2	LFA	A	403	-	8,8,19	0.19	0	7,7,18	0.25	0
3	RET	E	408	1	20,20,21	1.34	3 (15%)	27,27,28	1.79	7 (25%)
2	LFA	A	406	-	10,10,19	0.25	0	9,9,18	0.20	0
2	LFA	C	405	-	6,6,19	0.28	0	5,5,18	0.18	0
2	LFA	B	403	-	10,10,19	0.23	0	9,9,18	0.18	0
3	RET	A	408	1	20,20,21	1.35	3 (15%)	27,27,28	1.80	6 (22%)
2	LFA	B	406	-	6,6,19	0.28	0	5,5,18	0.18	0
2	LFA	D	406	-	5,5,19	0.28	0	4,4,18	0.39	0
2	LFA	E	405	-	10,10,19	0.14	0	9,9,18	0.14	0
2	LFA	B	402	-	10,10,19	0.22	0	9,9,18	0.17	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	LFA	B	401	-	10,10,19	0.17	0	9,9,18	0.43	0
2	LFA	C	406	-	10,10,19	0.30	0	8,8,18	0.20	0
2	LFA	D	403	-	12,12,19	0.17	0	11,11,18	0.18	0
2	LFA	D	404	-	9,9,19	0.14	0	8,8,18	0.12	0
2	LFA	C	401	-	10,10,19	0.25	0	9,9,18	0.27	0
2	LFA	B	407	-	8,8,19	0.26	0	7,7,18	0.17	0
3	RET	D	408	1	20,20,21	1.34	3 (15%)	27,27,28	1.79	7 (25%)
2	LFA	D	401	-	10,10,19	0.13	0	9,9,18	0.12	0
2	LFA	C	402	-	11,11,19	0.21	0	10,10,18	0.29	0

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	LFA	C	407	-	-	5/8/8/17	-
2	LFA	E	401	-	-	1/8/8/17	-
2	LFA	E	404	-	-	1/7/7/17	-
2	LFA	B	404	-	-	1/6/6/17	-
2	LFA	C	404	-	-	2/7/7/17	-
2	LFA	A	405	-	-	1/3/3/17	-
3	RET	B	408	1	-	0/13/30/31	0/1/1/1
2	LFA	D	402	-	-	2/9/9/17	-
2	LFA	E	406	-	-	1/3/3/17	-
2	LFA	E	407	-	-	5/7/7/17	-
2	LFA	C	403	-	-	1/7/7/17	-
2	LFA	A	404	-	-	2/7/7/17	-
2	LFA	E	403	-	-	0/9/9/17	-
2	LFA	A	407	-	-	4/7/7/17	-
3	RET	C	408	1	-	0/13/30/31	0/1/1/1
2	LFA	B	405	-	-	6/8/8/17	-
2	LFA	A	402	-	-	3/10/10/17	-
2	LFA	E	402	-	-	0/8/8/17	-
2	LFA	A	401	-	-	0/8/8/17	-
2	LFA	D	405	-	-	1/7/7/17	-
2	LFA	D	407	-	-	4/6/6/17	-
2	LFA	A	403	-	-	0/6/6/17	-
3	RET	E	408	1	-	0/13/30/31	0/1/1/1
2	LFA	A	406	-	-	2/8/8/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LFA	C	405	-	-	2/4/4/17	-
2	LFA	B	403	-	-	1/8/8/17	-
3	RET	A	408	1	-	0/13/30/31	0/1/1/1
2	LFA	B	406	-	-	1/4/4/17	-
2	LFA	D	406	-	-	1/3/3/17	-
2	LFA	E	405	-	-	1/8/8/17	-
2	LFA	B	402	-	-	0/8/8/17	-
2	LFA	B	401	-	-	1/8/8/17	-
2	LFA	C	406	-	-	4/7/7/17	-
2	LFA	D	403	-	-	3/10/10/17	-
2	LFA	D	404	-	-	2/7/7/17	-
2	LFA	C	401	-	-	0/8/8/17	-
2	LFA	B	407	-	-	1/6/6/17	-
3	RET	D	408	1	-	0/13/30/31	0/1/1/1
2	LFA	D	401	-	-	2/8/8/17	-
2	LFA	C	402	-	-	0/9/9/17	-

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	408	RET	C10-C9	3.48	1.40	1.35
3	B	408	RET	C10-C9	3.48	1.40	1.35
3	A	408	RET	C10-C9	3.46	1.40	1.35
3	E	408	RET	C10-C9	3.45	1.40	1.35
3	C	408	RET	C10-C9	3.43	1.40	1.35
3	B	408	RET	C11-C10	-2.88	1.34	1.43
3	A	408	RET	C11-C10	-2.88	1.34	1.43
3	D	408	RET	C11-C10	-2.85	1.34	1.43
3	E	408	RET	C11-C10	-2.84	1.34	1.43
3	C	408	RET	C11-C10	-2.82	1.34	1.43
3	B	408	RET	C11-C12	2.46	1.40	1.34
3	C	408	RET	C11-C12	2.43	1.40	1.34
3	E	408	RET	C11-C12	2.43	1.40	1.34
3	A	408	RET	C11-C12	2.43	1.40	1.34
3	D	408	RET	C11-C12	2.42	1.40	1.34

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	408	RET	C19-C9-C10	-5.77	114.84	122.92
3	B	408	RET	C19-C9-C10	-5.76	114.86	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	408	RET	C19-C9-C10	-5.74	114.89	122.92
3	C	408	RET	C19-C9-C10	-5.73	114.89	122.92
3	E	408	RET	C19-C9-C10	-5.71	114.92	122.92
3	B	408	RET	C19-C9-C8	3.50	123.59	118.08
3	D	408	RET	C19-C9-C8	3.47	123.55	118.08
3	E	408	RET	C19-C9-C8	3.45	123.52	118.08
3	C	408	RET	C19-C9-C8	3.44	123.49	118.08
3	A	408	RET	C19-C9-C8	3.43	123.48	118.08
3	A	408	RET	C10-C11-C12	2.82	132.03	123.22
3	D	408	RET	C10-C11-C12	2.81	132.00	123.22
3	C	408	RET	C10-C11-C12	2.81	131.98	123.22
3	B	408	RET	C10-C11-C12	2.81	131.98	123.22
3	E	408	RET	C10-C11-C12	2.80	131.97	123.22
3	A	408	RET	C1-C6-C5	-2.26	119.42	122.61
3	B	408	RET	C1-C6-C5	-2.26	119.44	122.61
3	E	408	RET	C1-C6-C5	-2.25	119.45	122.61
3	D	408	RET	C1-C6-C5	-2.24	119.45	122.61
3	C	408	RET	C1-C6-C5	-2.21	119.50	122.61
3	E	408	RET	C1-C6-C7	2.19	121.96	115.78
3	B	408	RET	C1-C6-C7	2.18	121.94	115.78
3	D	408	RET	C1-C6-C7	2.17	121.93	115.78
3	A	408	RET	C1-C6-C7	2.17	121.92	115.78
3	C	408	RET	C1-C6-C7	2.17	121.91	115.78
3	C	408	RET	C20-C13-C14	-2.10	117.49	123.71
3	B	408	RET	C20-C13-C14	-2.10	117.52	123.71
3	D	408	RET	C20-C13-C14	-2.08	117.55	123.71
3	E	408	RET	C20-C13-C14	-2.07	117.59	123.71
3	C	408	RET	C12-C13-C14	2.07	125.35	118.80
3	A	408	RET	C20-C13-C14	-2.07	117.60	123.71
3	B	408	RET	C12-C13-C14	2.04	125.28	118.80
3	E	408	RET	C12-C13-C14	2.03	125.23	118.80
3	D	408	RET	C12-C13-C14	2.02	125.21	118.80

There are no chirality outliers.

All (61) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	406	LFA	C11-C12-C13-C14
2	D	403	LFA	C11-C10-C9-C8
2	D	404	LFA	C6-C7-C8-C9
2	A	402	LFA	C9-C10-C11-C12
2	B	405	LFA	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
2	A	402	LFA	C2-C3-C4-C5
2	A	407	LFA	C3-C4-C5-C6
2	E	407	LFA	C2-C3-C4-C5
2	D	403	LFA	C7-C8-C9-C10
2	A	402	LFA	C6-C7-C8-C9
2	C	406	LFA	C5-C6-C7-C8
2	D	404	LFA	C7-C8-C9-C10
2	B	401	LFA	C13-C14-C15-C16
2	C	407	LFA	C11-C12-C13-C14
2	E	407	LFA	C4-C5-C6-C7
2	D	407	LFA	C4-C5-C6-C7
2	B	403	LFA	C10-C11-C12-C13
2	C	404	LFA	C6-C7-C8-C9
2	D	406	LFA	C15-C16-C17-C18
2	E	406	LFA	C15-C16-C17-C18
2	A	405	LFA	C3-C4-C5-C6
2	C	407	LFA	C14-C15-C16-C17
2	C	407	LFA	C13-C14-C15-C16
2	D	407	LFA	C3-C4-C5-C6
2	C	406	LFA	C2-C3-C4-C5
2	B	405	LFA	C14-C15-C16-C17
2	C	406	LFA	C7-C8-C9-C10
2	D	401	LFA	C3-C4-C5-C6
2	C	407	LFA	C12-C13-C14-C15
2	B	405	LFA	C11-C12-C13-C14
2	A	407	LFA	C6-C7-C8-C9
2	A	407	LFA	C4-C5-C6-C7
2	A	404	LFA	C13-C14-C15-C16
2	B	406	LFA	C14-C15-C16-C17
2	C	405	LFA	C4-C5-C6-C7
2	D	402	LFA	C11-C10-C9-C8
2	E	407	LFA	C5-C6-C7-C8
2	E	401	LFA	C5-C6-C7-C8
2	A	407	LFA	C5-C6-C7-C8
2	B	405	LFA	C13-C14-C15-C16
2	E	407	LFA	C3-C4-C5-C6
2	B	405	LFA	C16-C17-C18-C19
2	C	404	LFA	C5-C6-C7-C8
2	C	407	LFA	C9-C10-C11-C12
2	D	403	LFA	C9-C10-C11-C12
2	D	407	LFA	C2-C3-C4-C5
2	E	405	LFA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
2	D	407	LFA	C5-C6-C7-C8
2	D	402	LFA	C10-C11-C12-C13
2	A	404	LFA	C17-C18-C19-C20
2	B	405	LFA	C17-C18-C19-C20
2	B	407	LFA	C13-C14-C15-C16
2	B	404	LFA	C12-C13-C14-C15
2	C	403	LFA	C7-C8-C9-C10
2	E	407	LFA	C6-C7-C8-C9
2	A	406	LFA	C16-C17-C18-C19
2	D	405	LFA	C4-C5-C6-C7
2	E	404	LFA	C11-C12-C13-C14
2	C	405	LFA	C3-C4-C5-C6
2	D	401	LFA	C7-C8-C9-C10
2	C	406	LFA	C4-C5-C6-C7

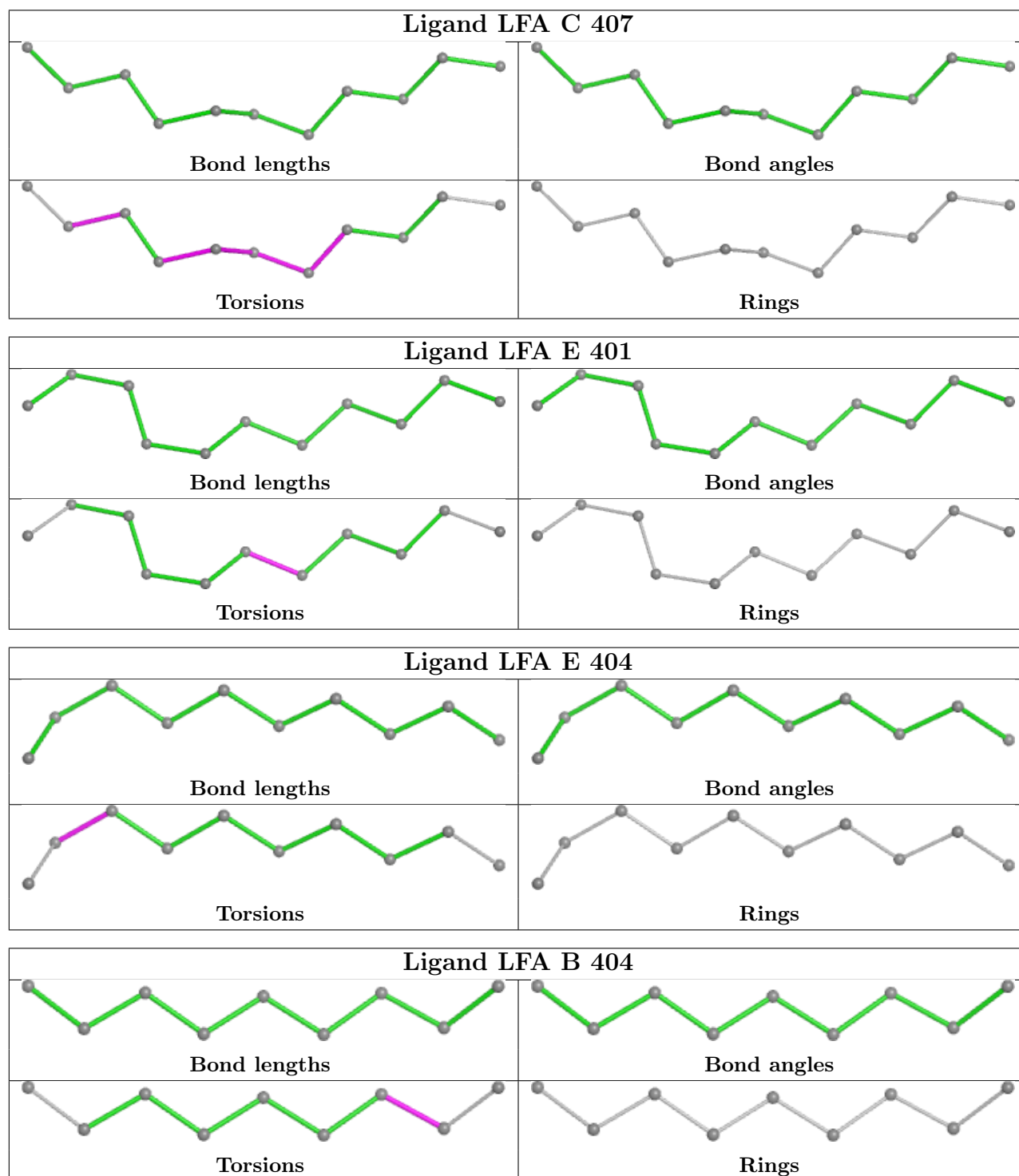
There are no ring outliers.

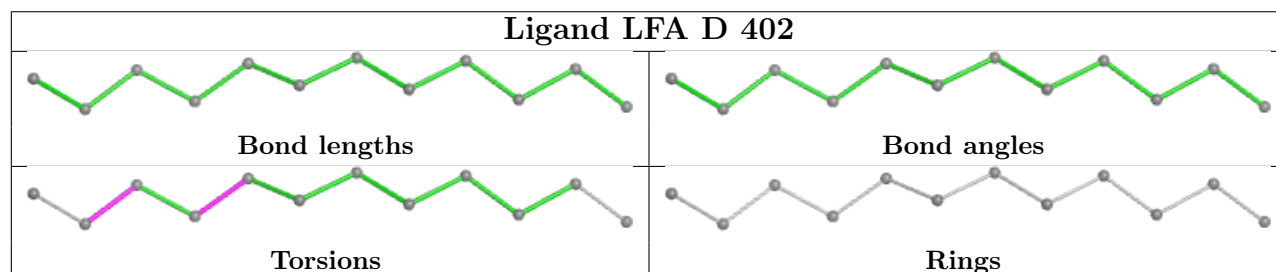
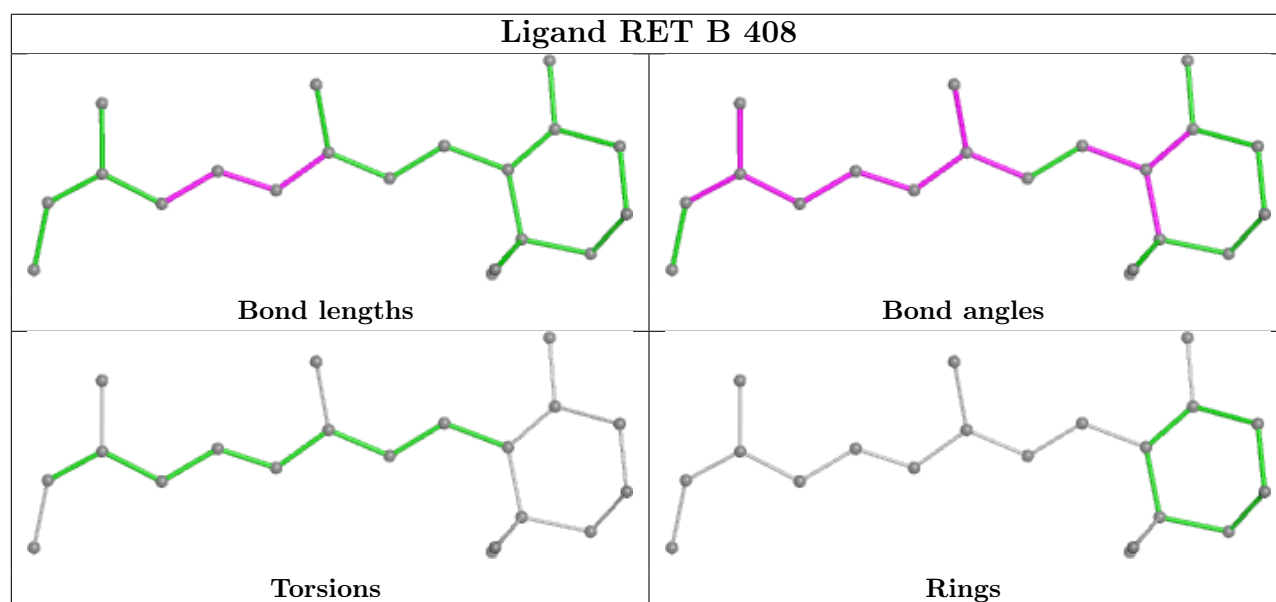
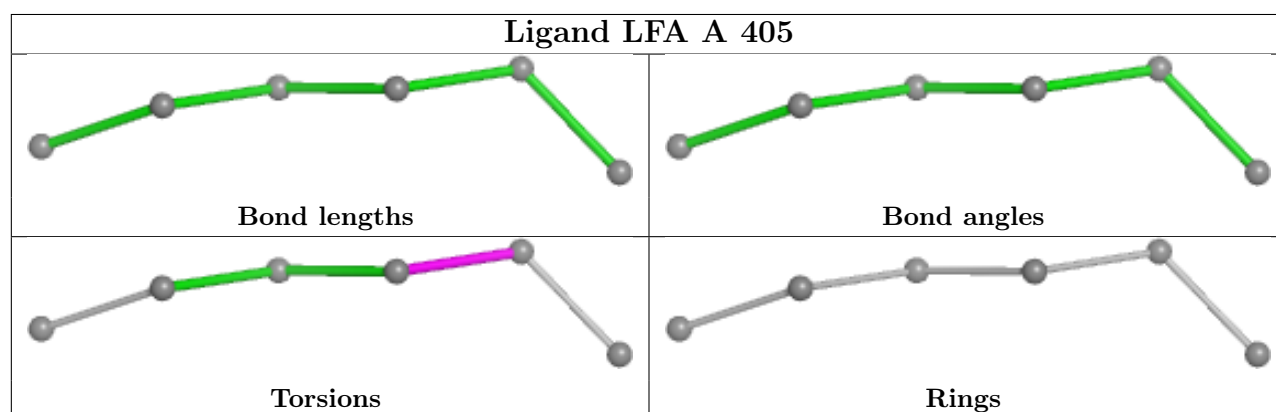
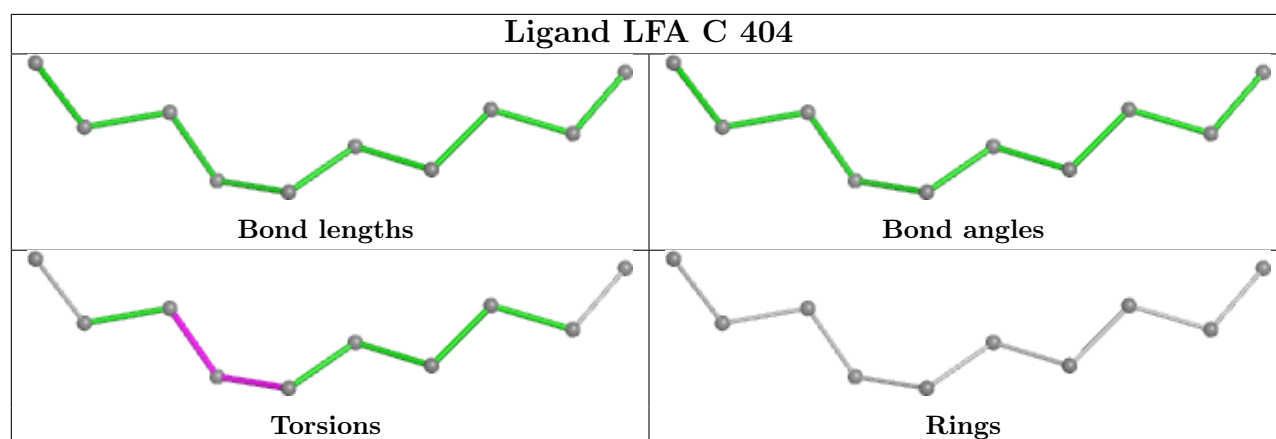
12 monomers are involved in 16 short contacts:

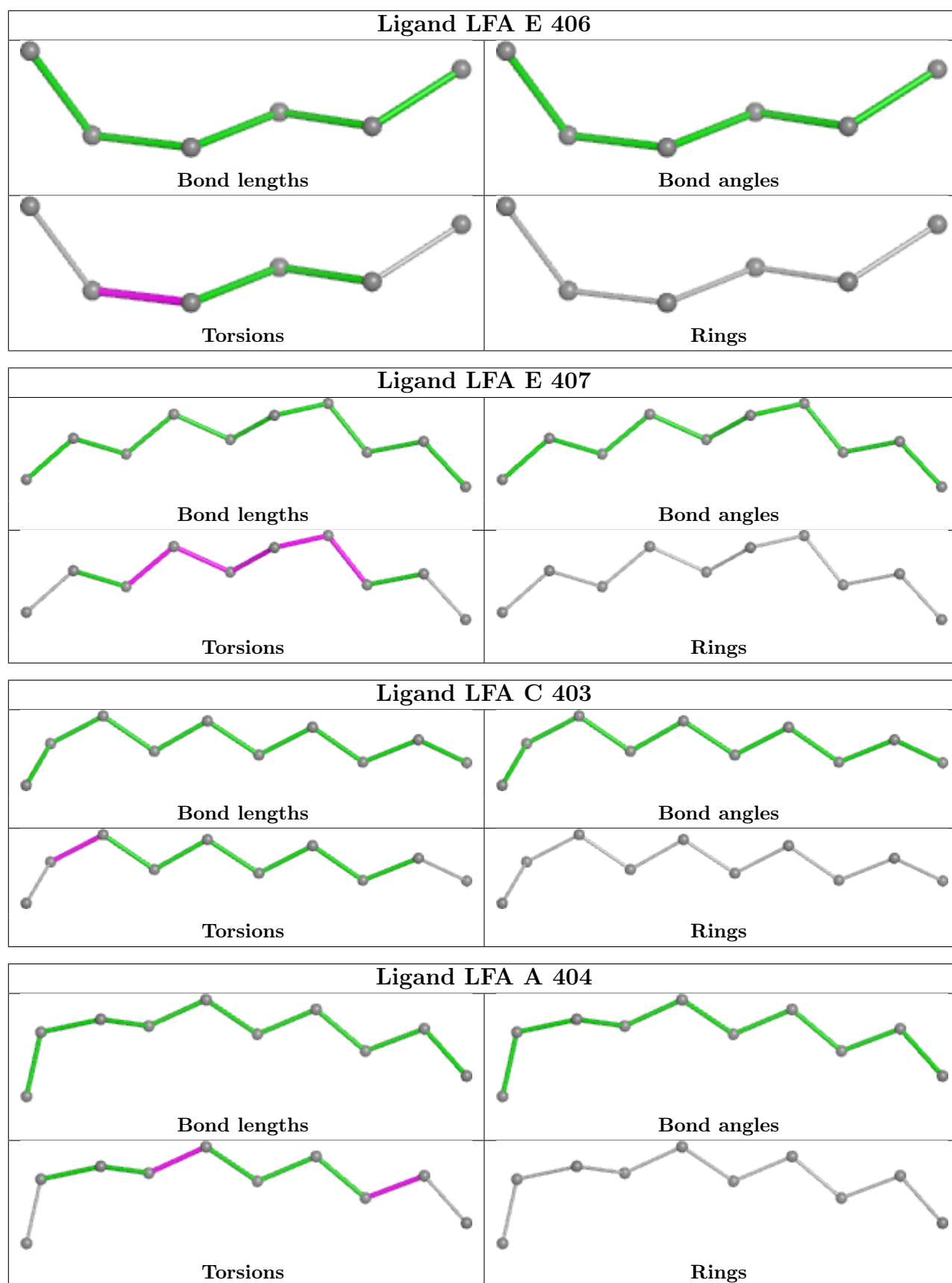
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	401	LFA	1	0
3	B	408	RET	1	0
2	D	402	LFA	1	0
3	C	408	RET	2	0
2	E	402	LFA	1	0
2	D	405	LFA	1	0
3	E	408	RET	2	0
3	A	408	RET	2	0
2	E	405	LFA	1	0
2	B	401	LFA	1	0
2	D	404	LFA	1	0
3	D	408	RET	2	0

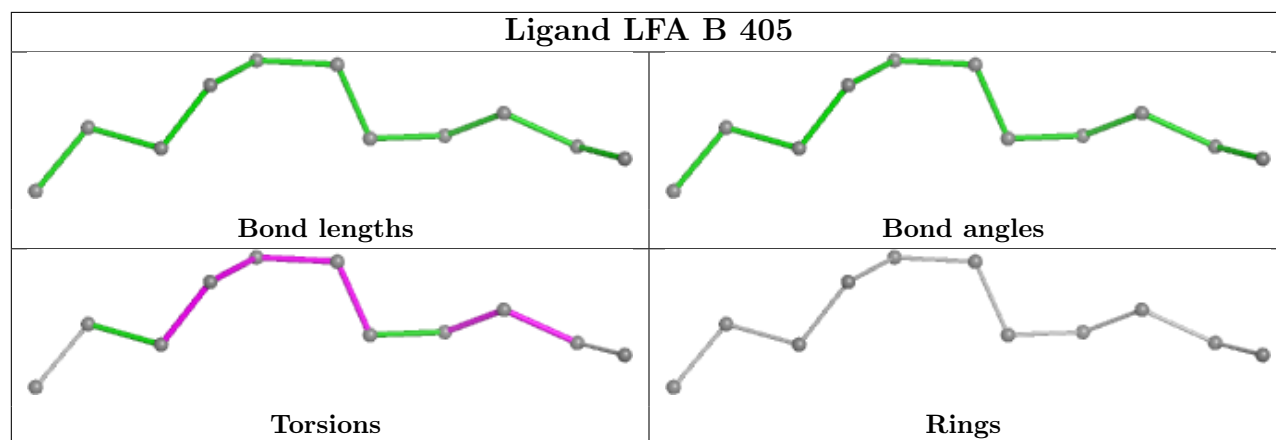
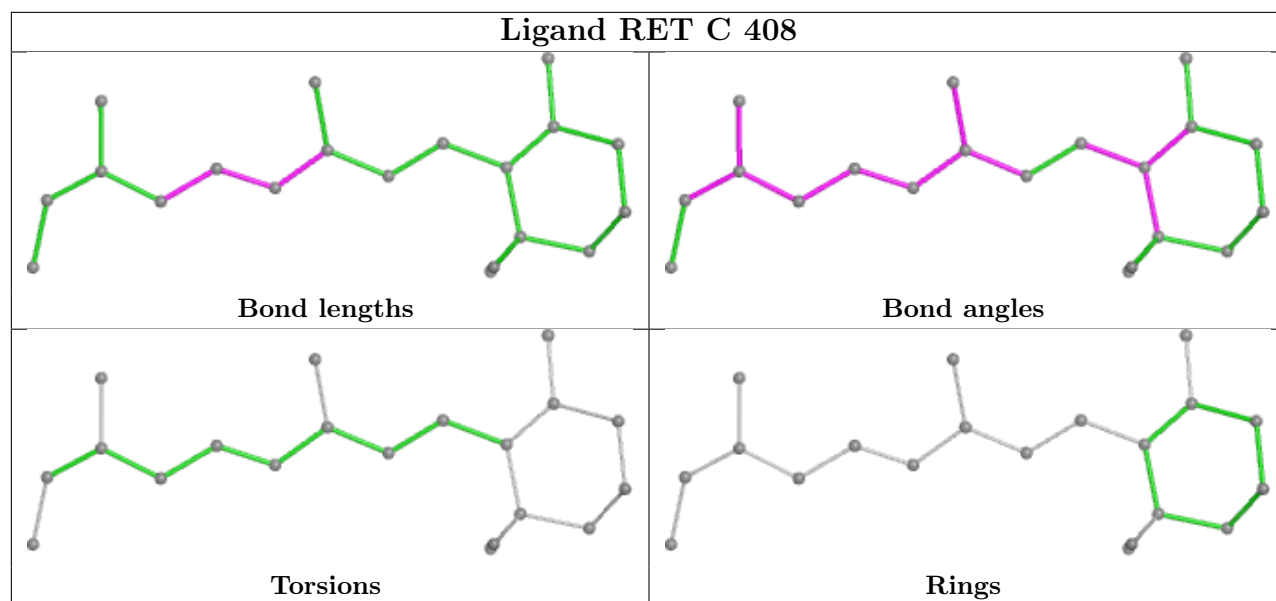
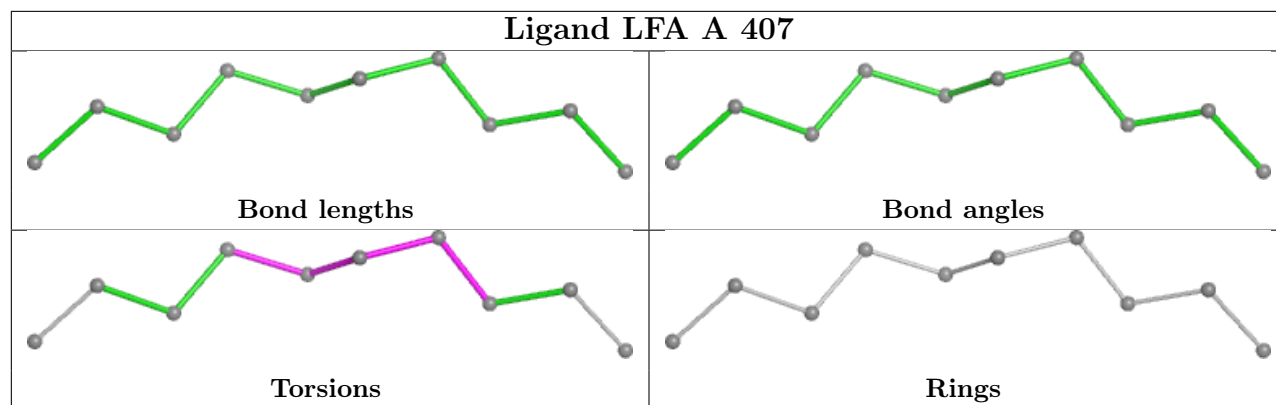
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

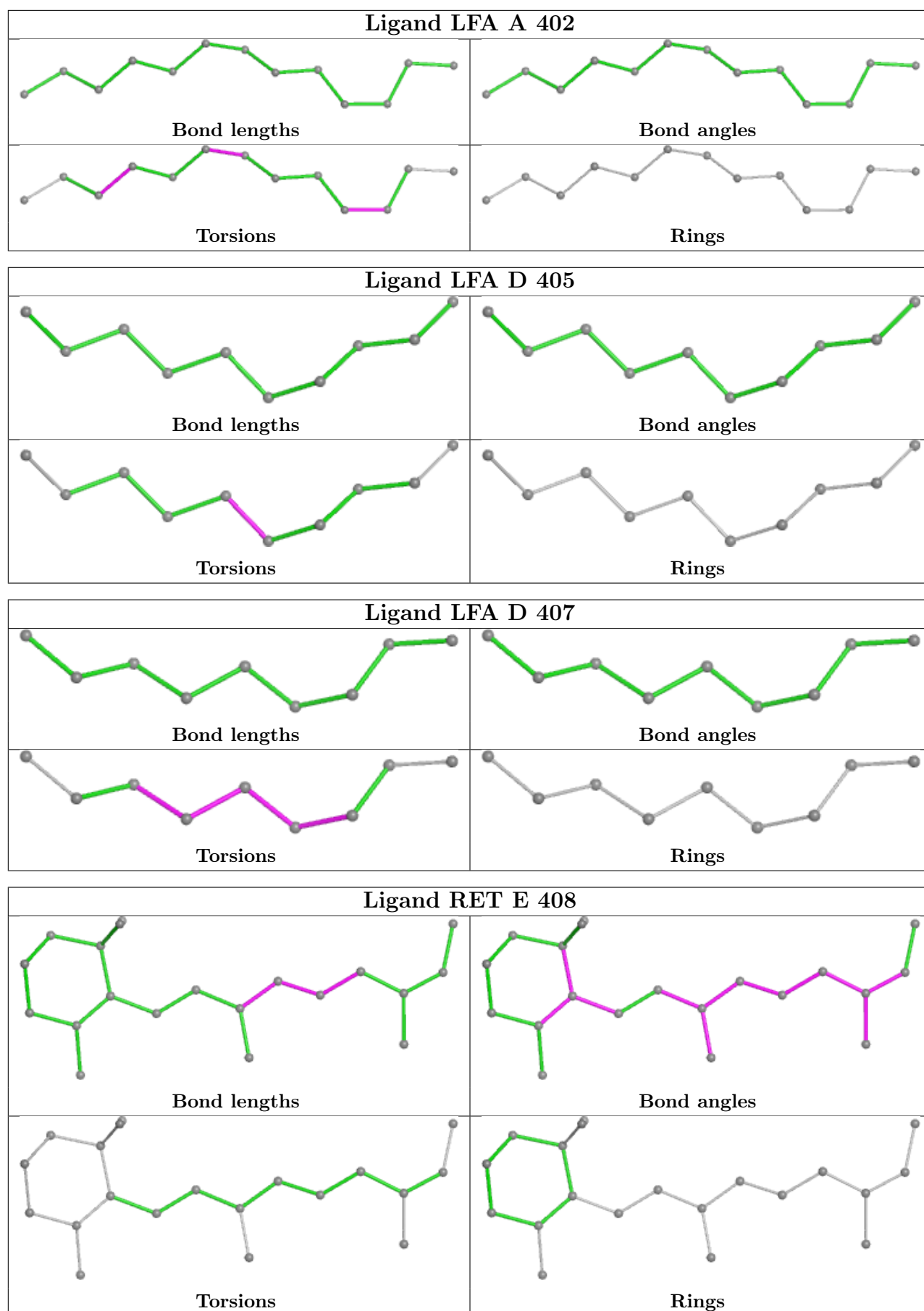
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

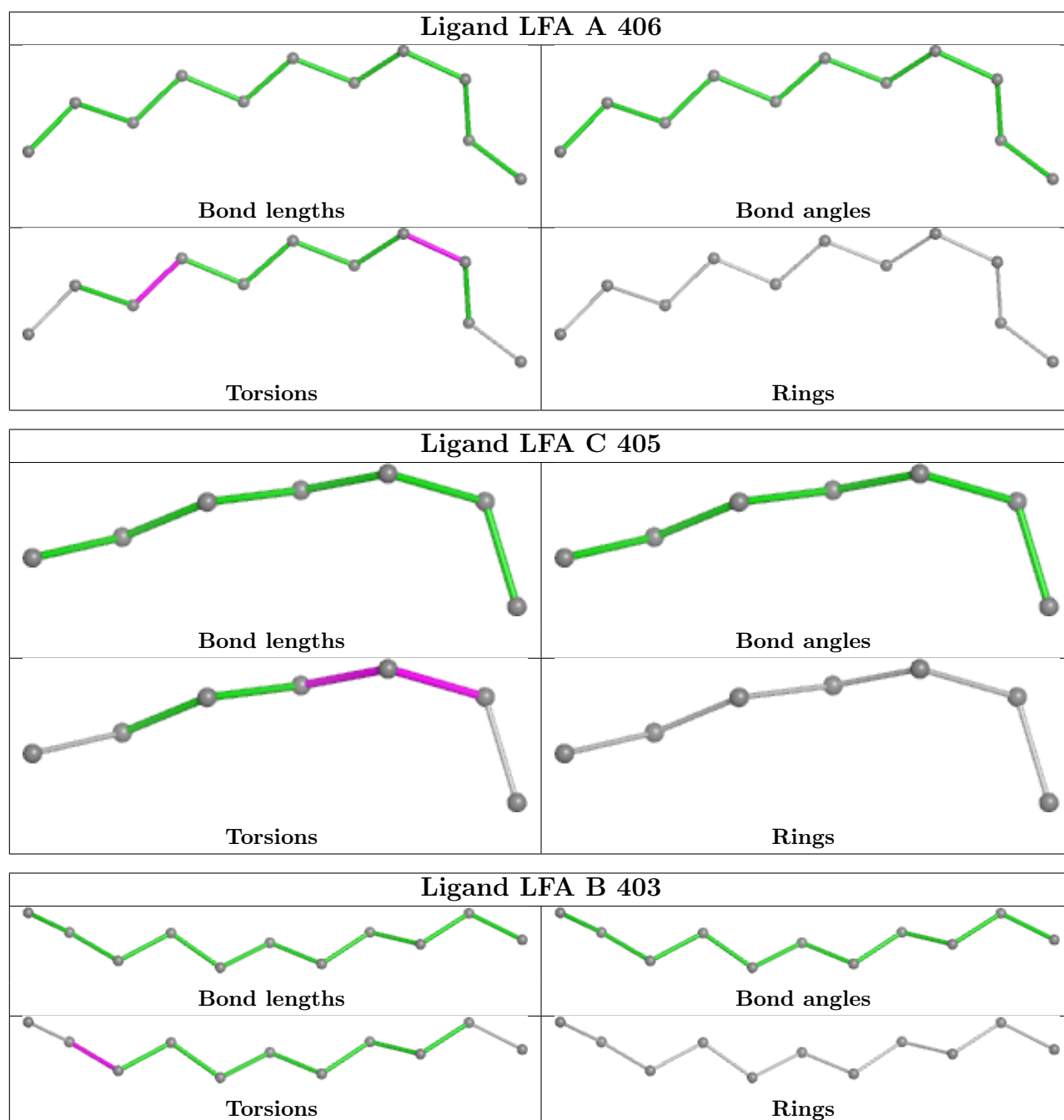




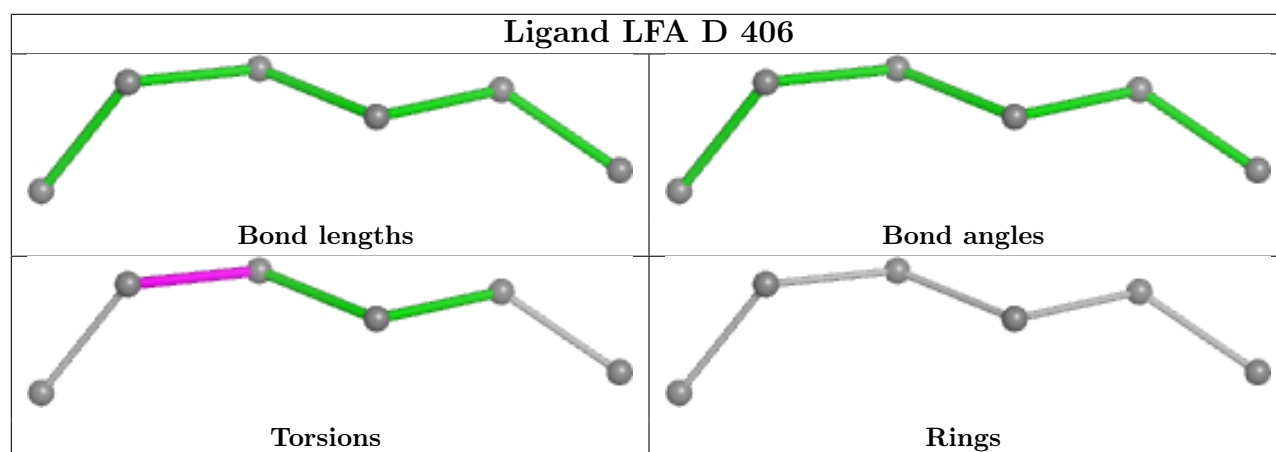
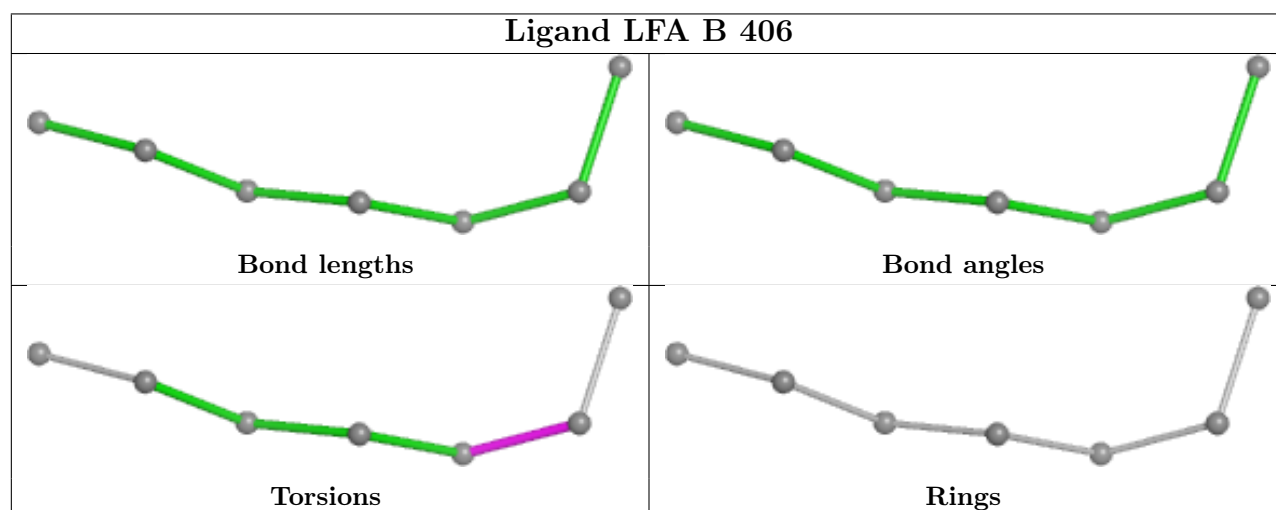
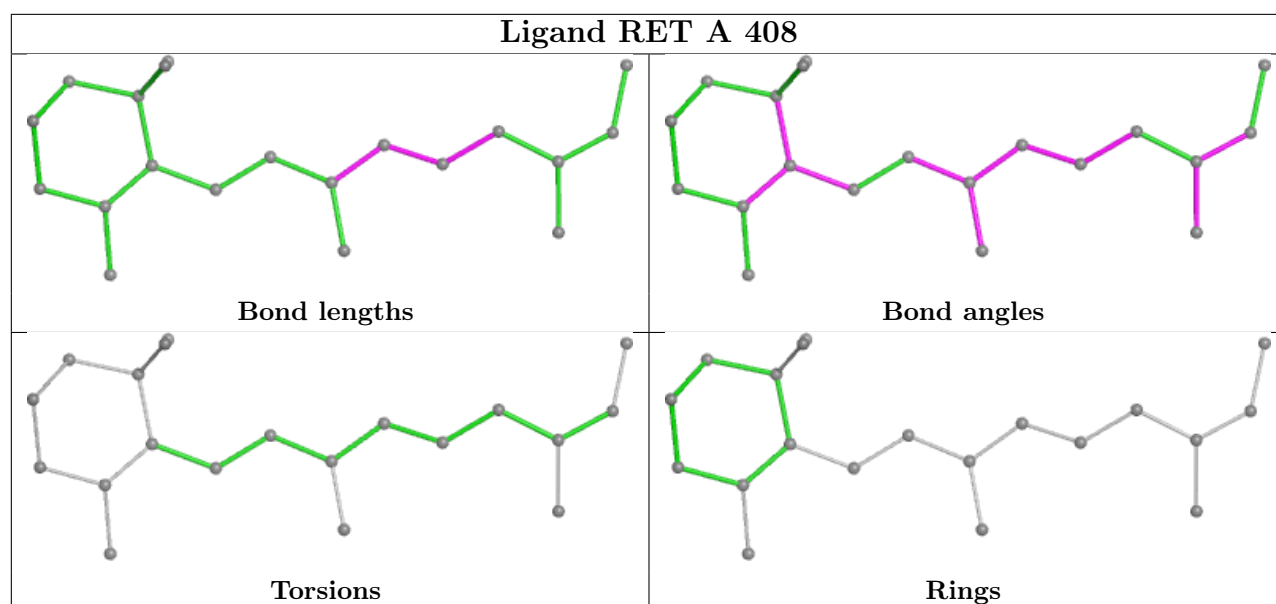


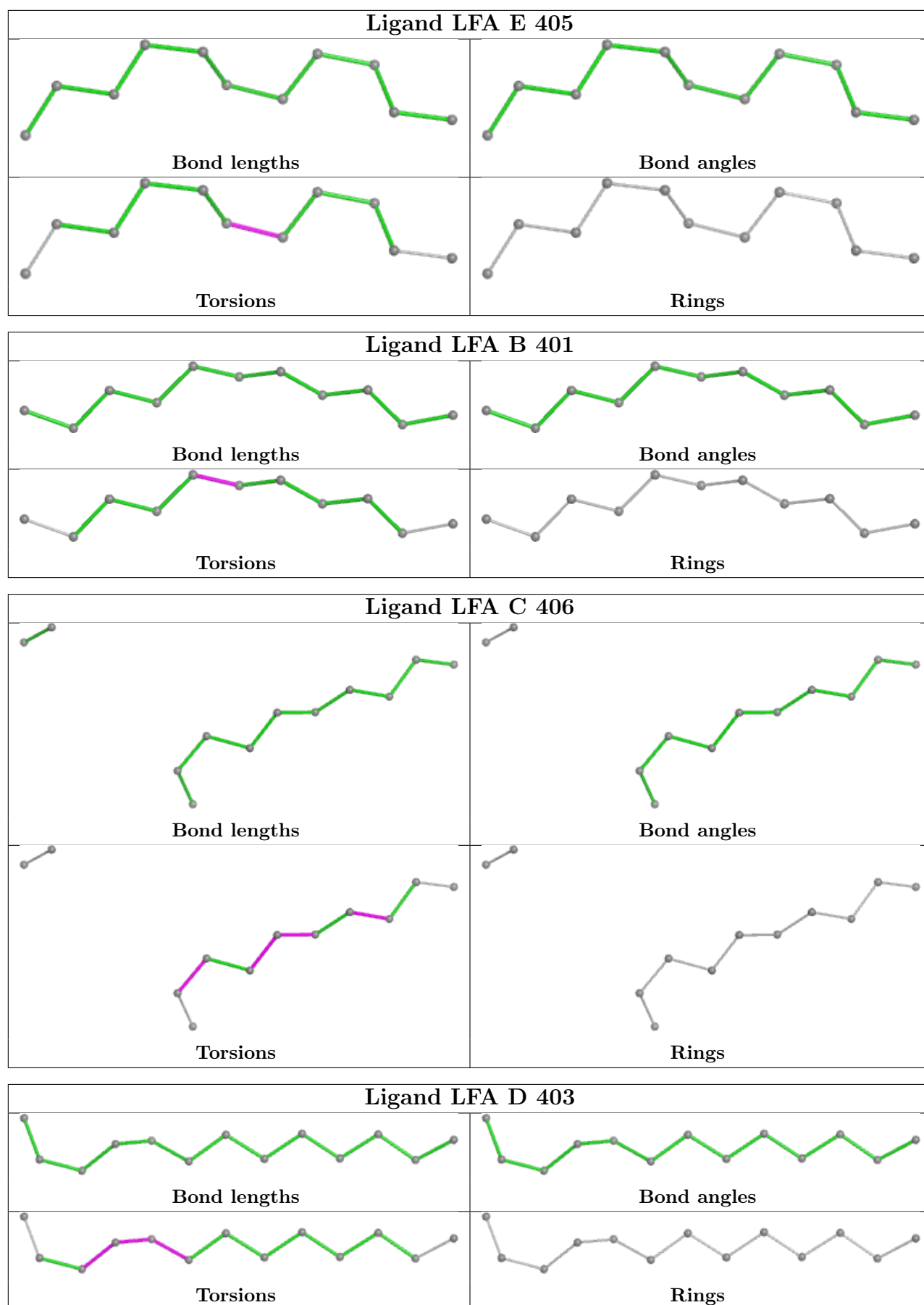


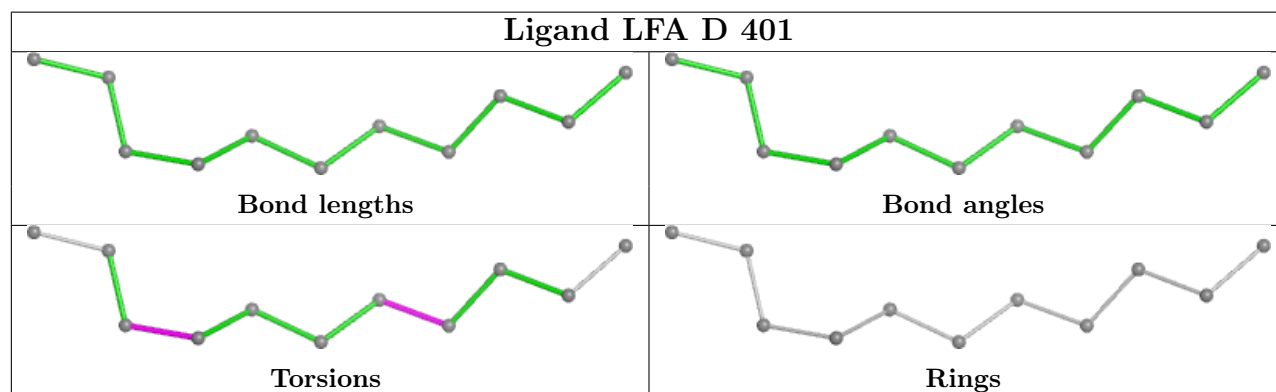
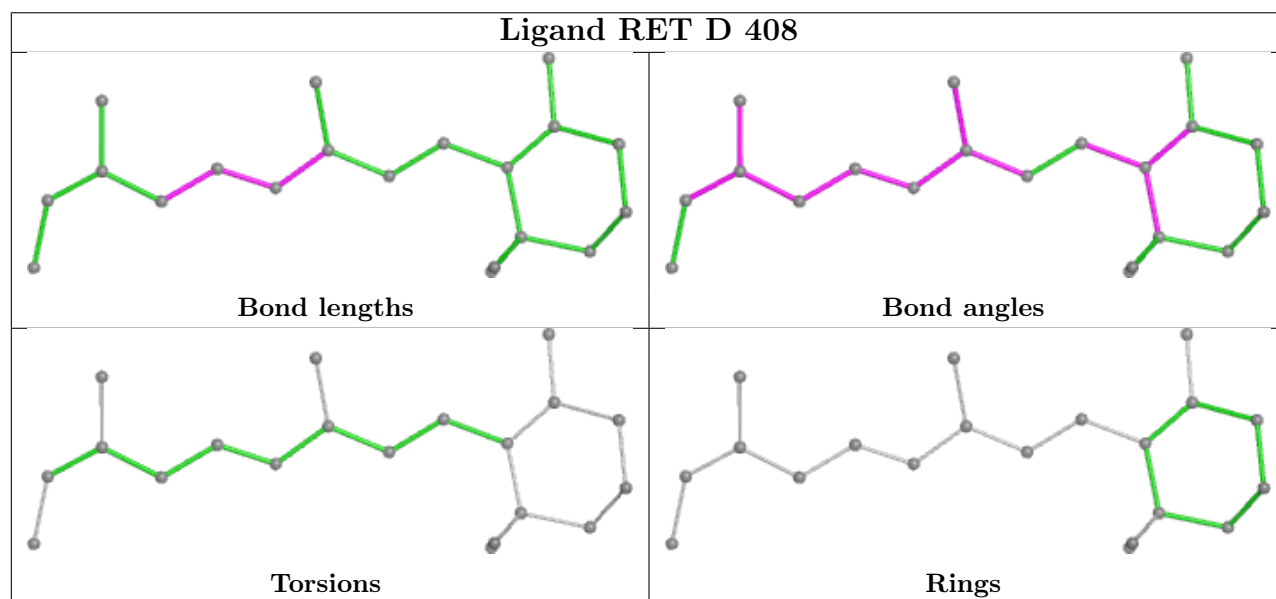
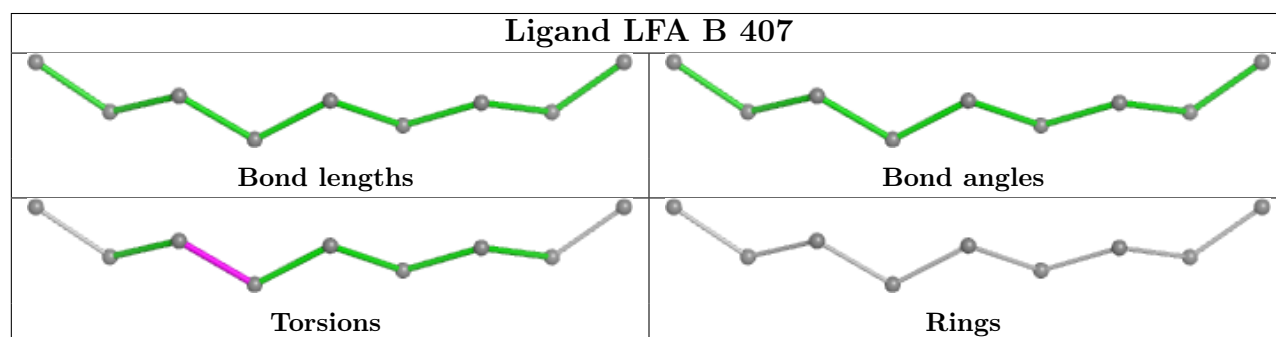
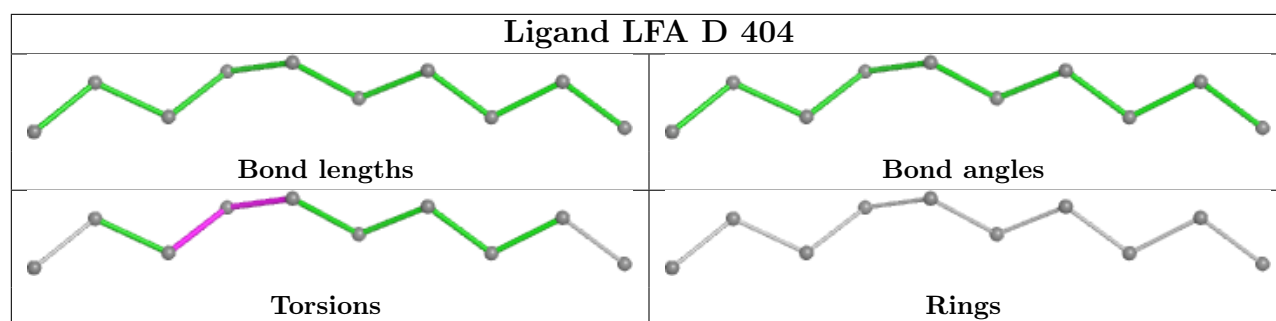












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

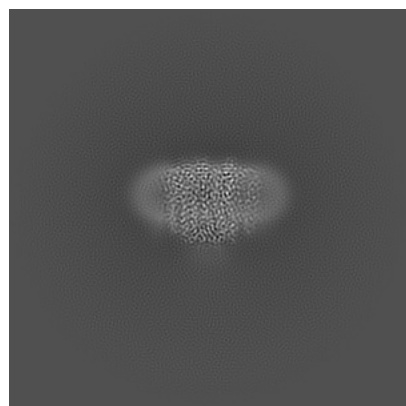
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18800. These allow visual inspection of the internal detail of the map and identification of artifacts.

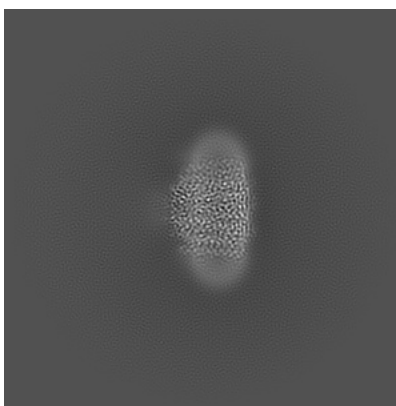
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

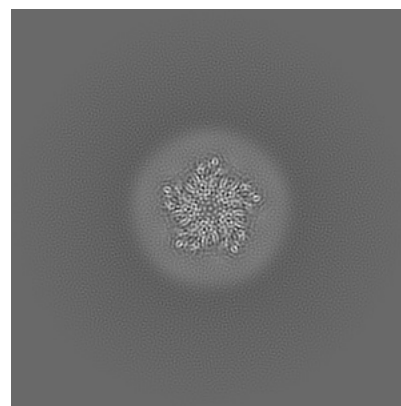
#### 6.1.1 Primary map



X

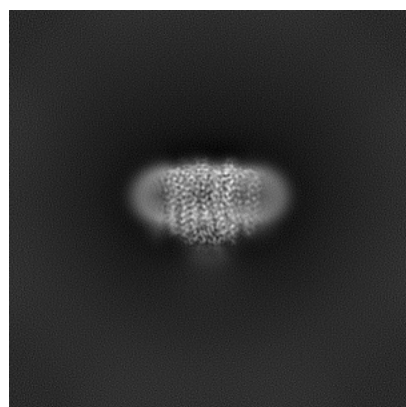


Y

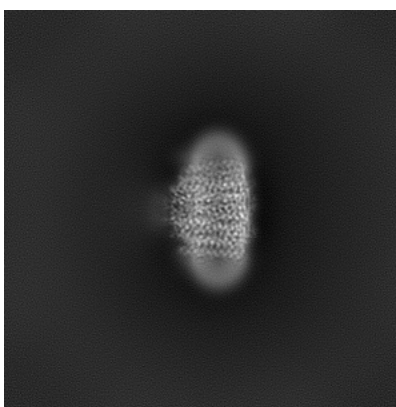


Z

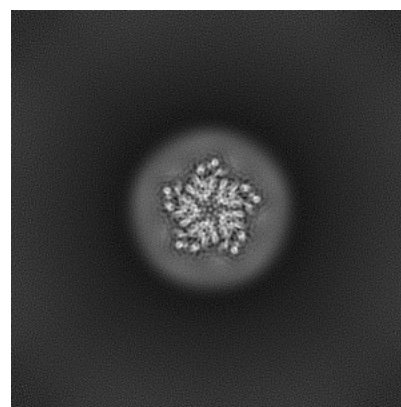
#### 6.1.2 Raw map



X



Y

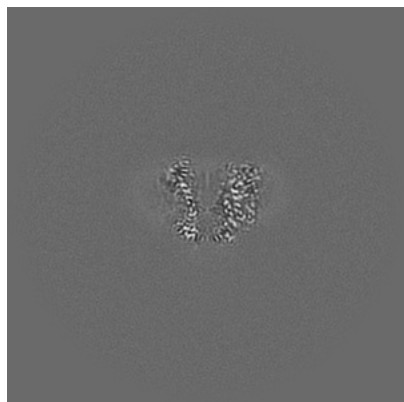


Z

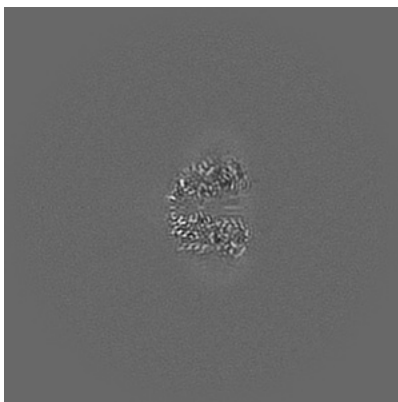
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

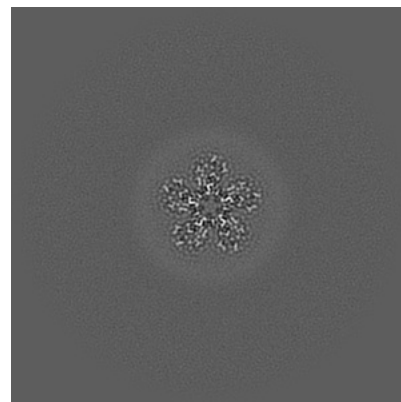
### 6.2.1 Primary map



X Index: 192

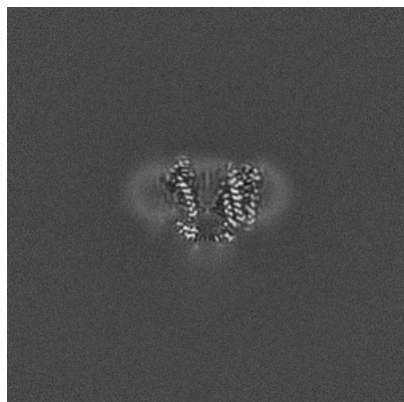


Y Index: 192

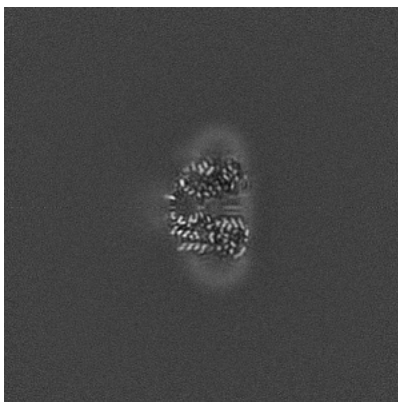


Z Index: 192

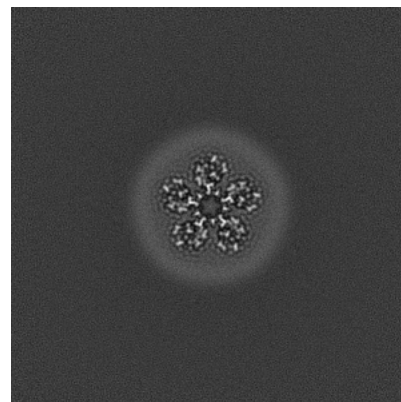
### 6.2.2 Raw map



X Index: 192



Y Index: 192

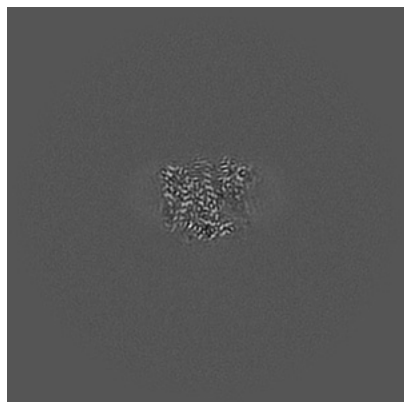


Z Index: 192

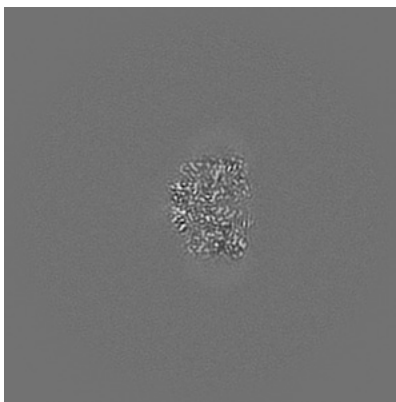
The images above show central slices of the map in three orthogonal directions.

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

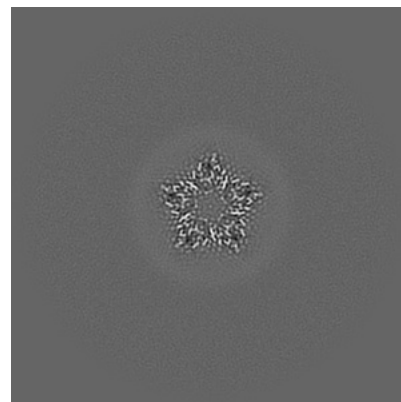
### 6.3.1 Primary map



X Index: 174

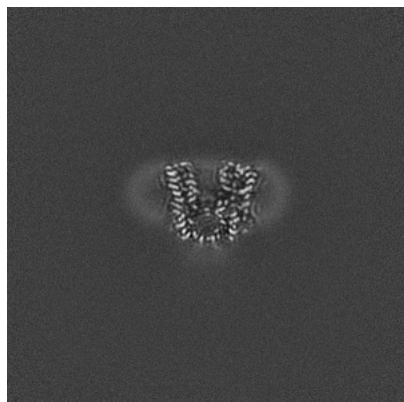


Y Index: 206

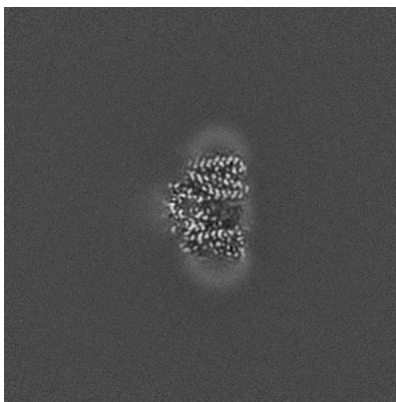


Z Index: 213

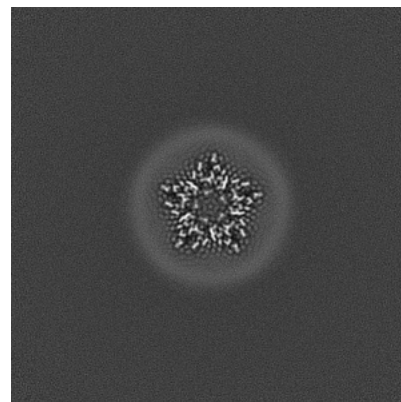
### 6.3.2 Raw map



X Index: 184



Y Index: 201



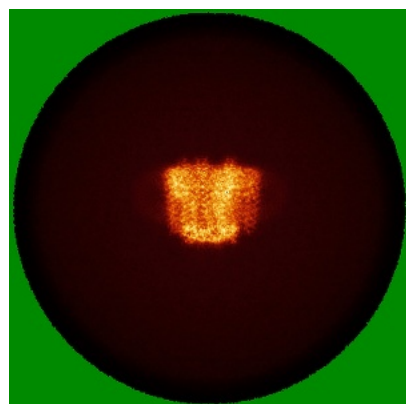
Z Index: 213

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

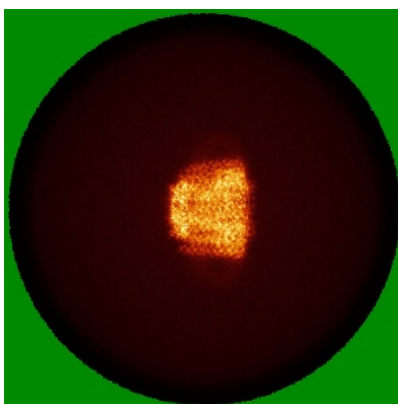


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

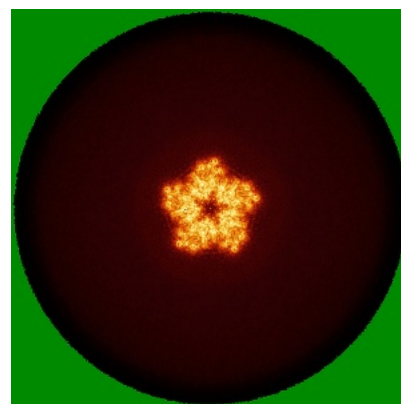
### 6.4.1 Primary map



X

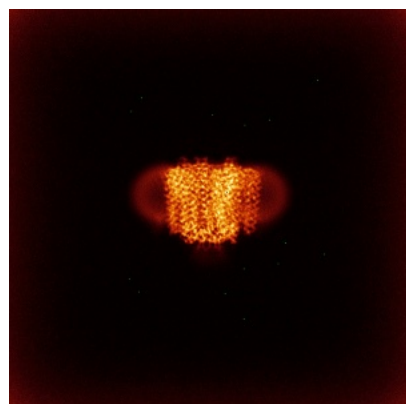


Y

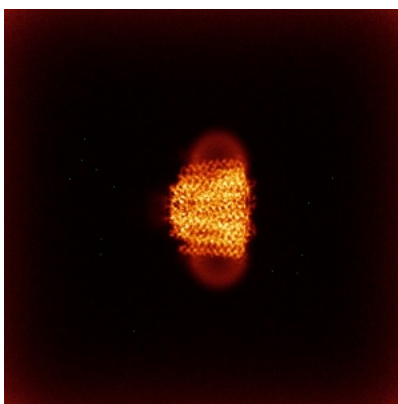


Z

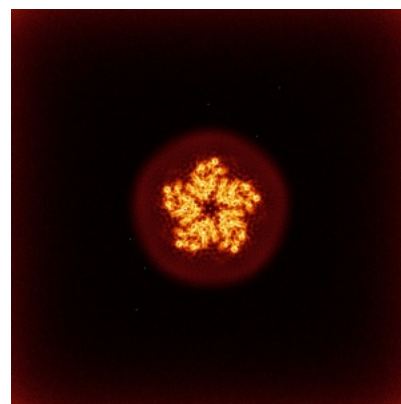
### 6.4.2 Raw map



X



Y



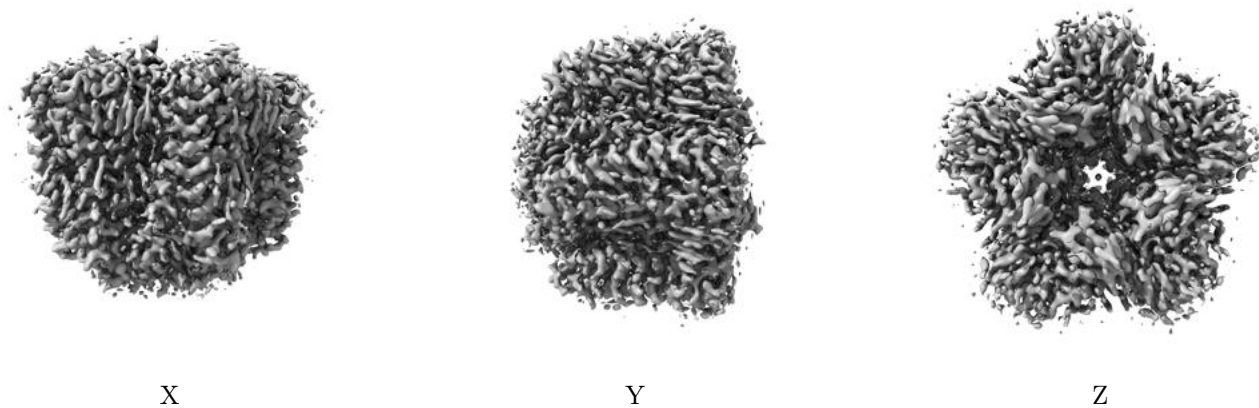
Z

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



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

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.316. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

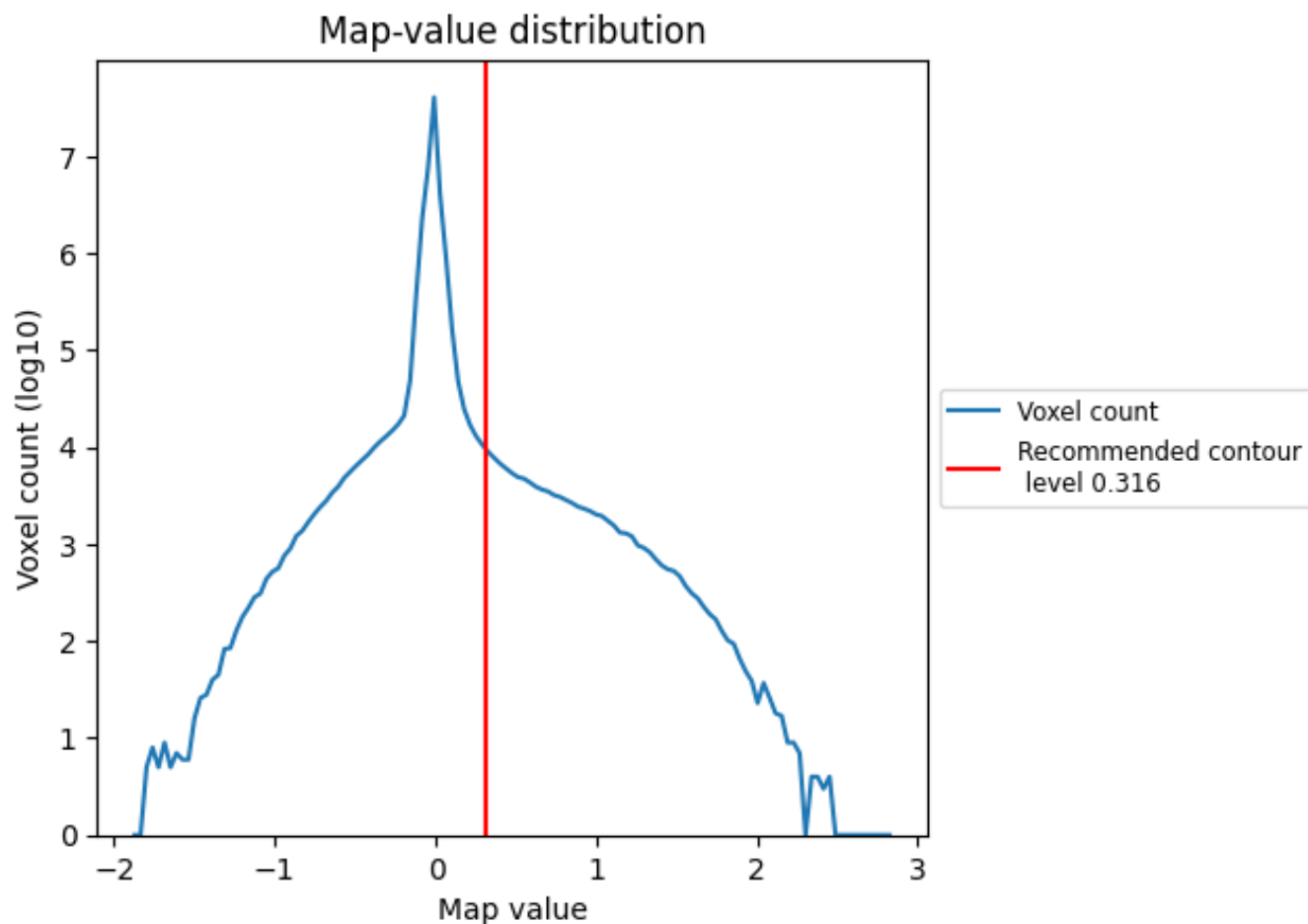
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

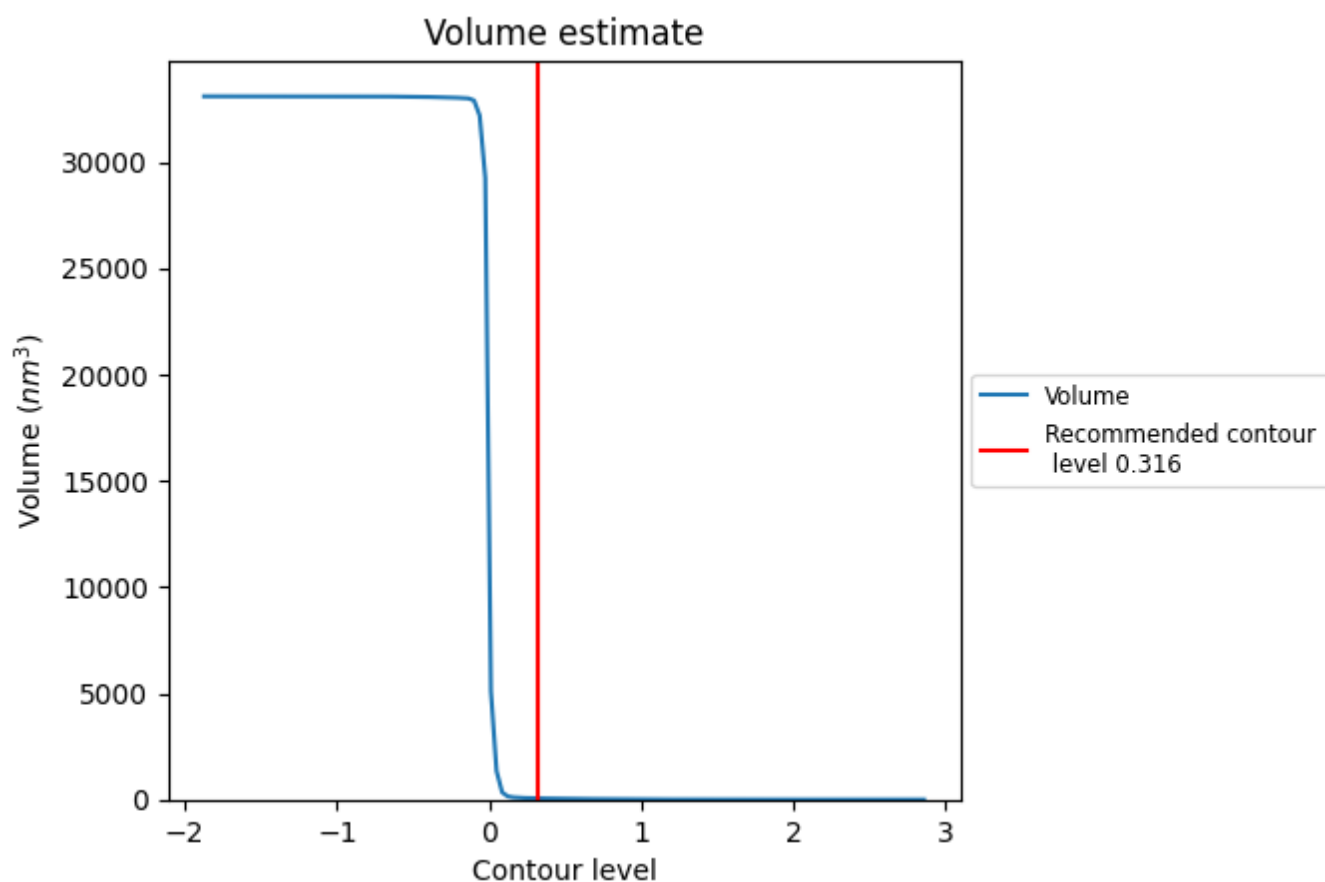
This section contains the results of statistical analysis of the map.

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



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

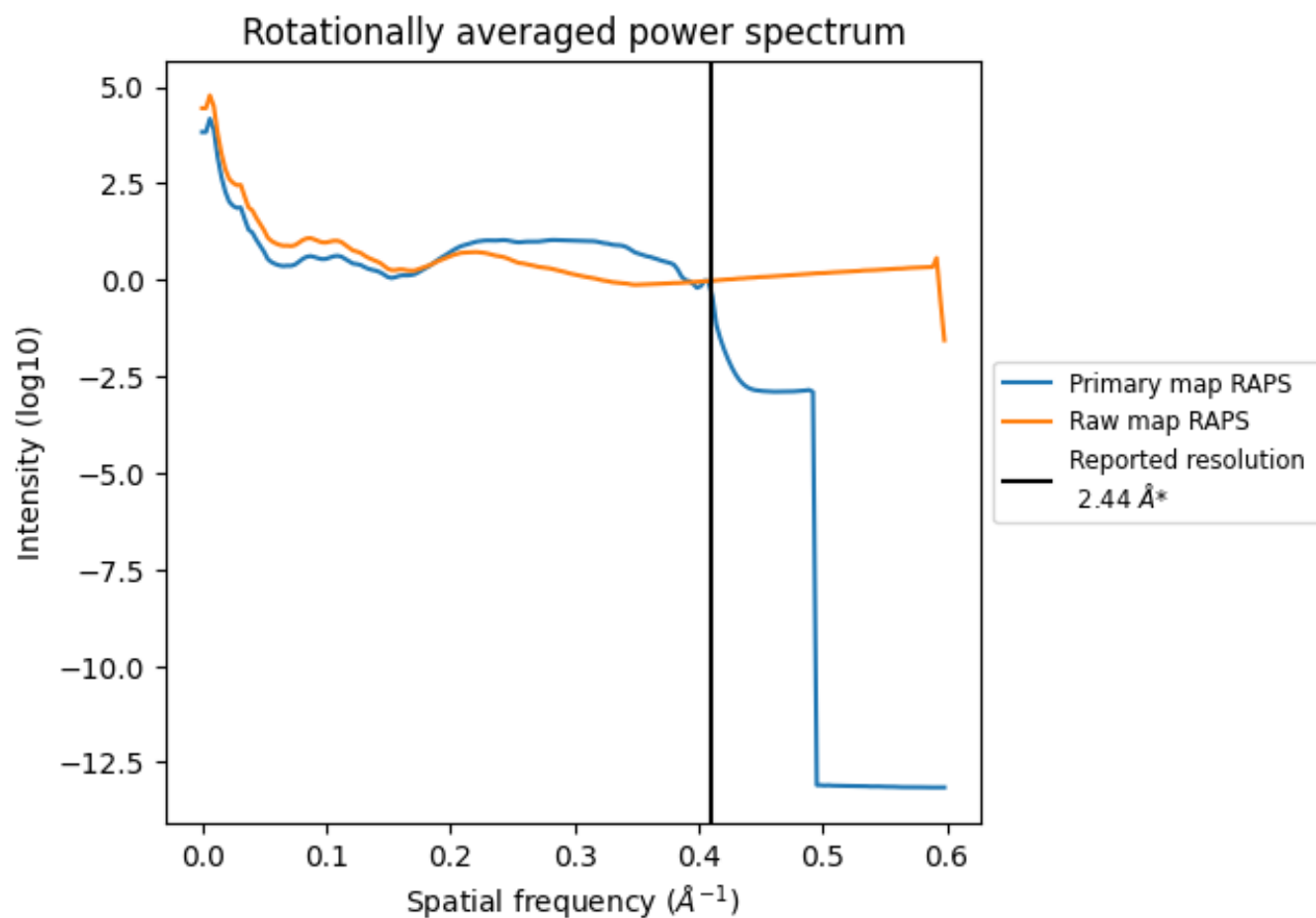
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 59  $\text{nm}^3$ ; this corresponds to an approximate mass of 53 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 ⓘ

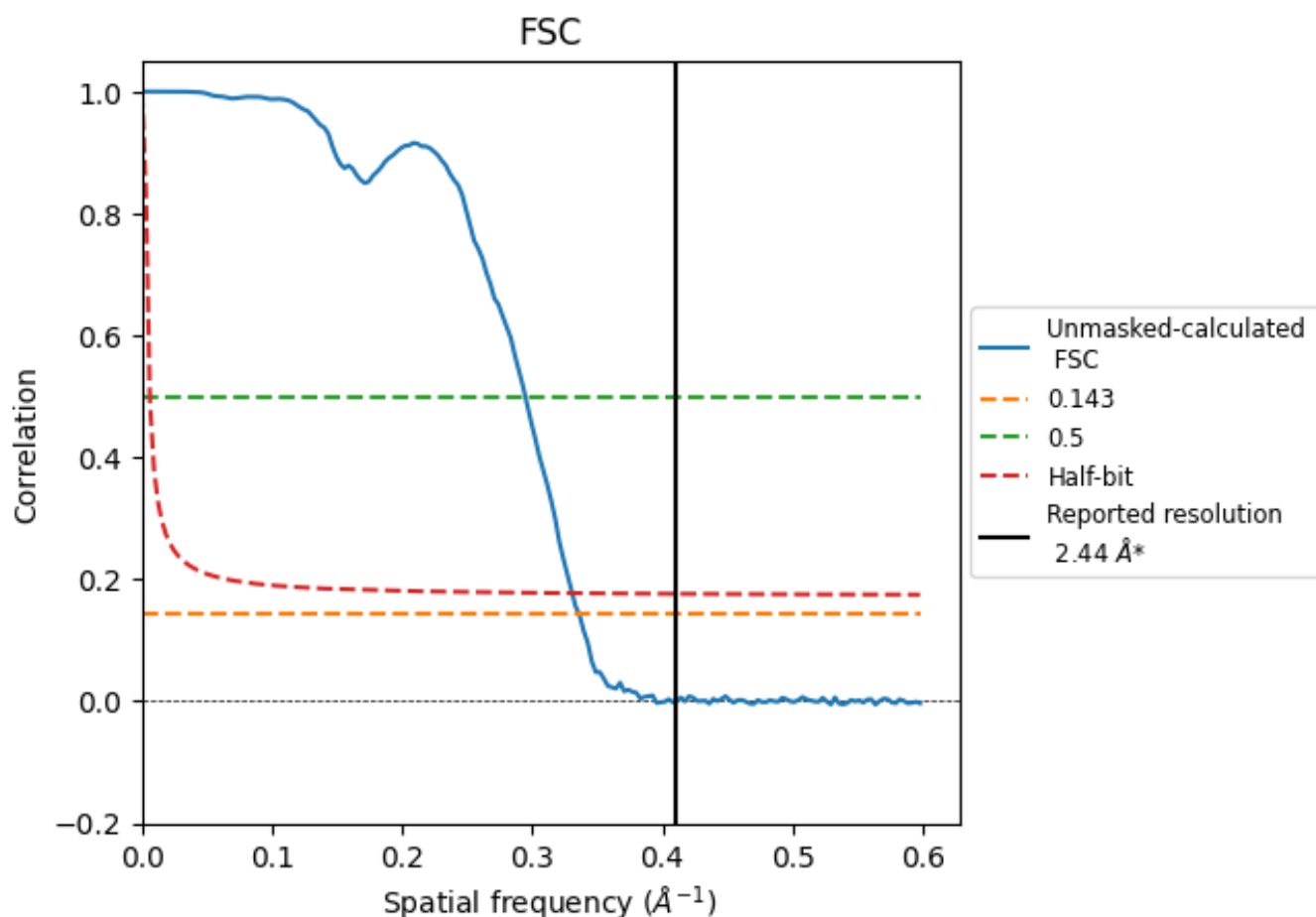


\*Reported resolution corresponds to spatial frequency of 0.410  $\text{\AA}^{-1}$

## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of  $0.410 \text{ \AA}^{-1}$

## 8.2 Resolution estimates [i](#)

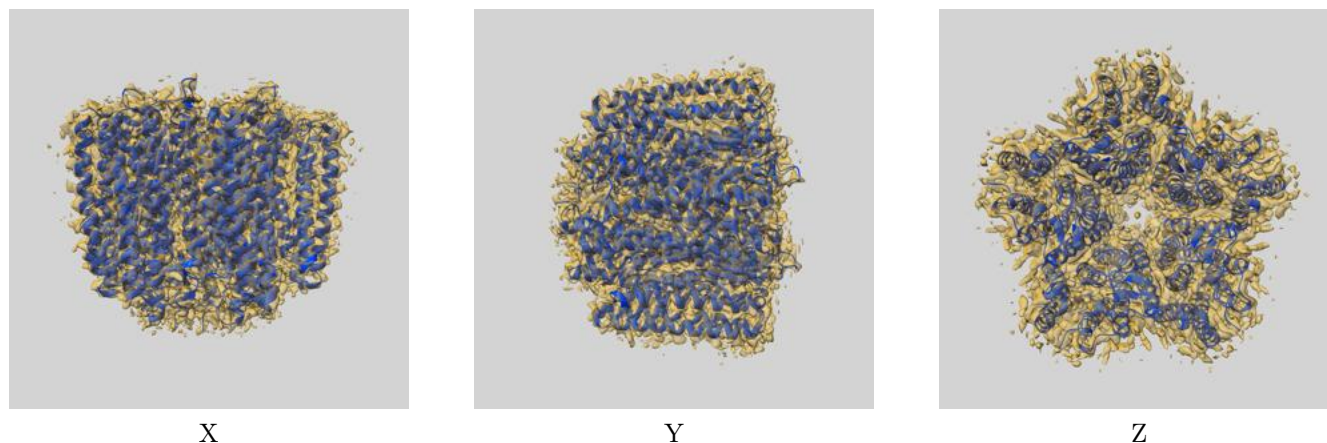
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.44	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.98	3.39	3.02

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.98 differs from the reported value 2.44 by more than 10 %

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

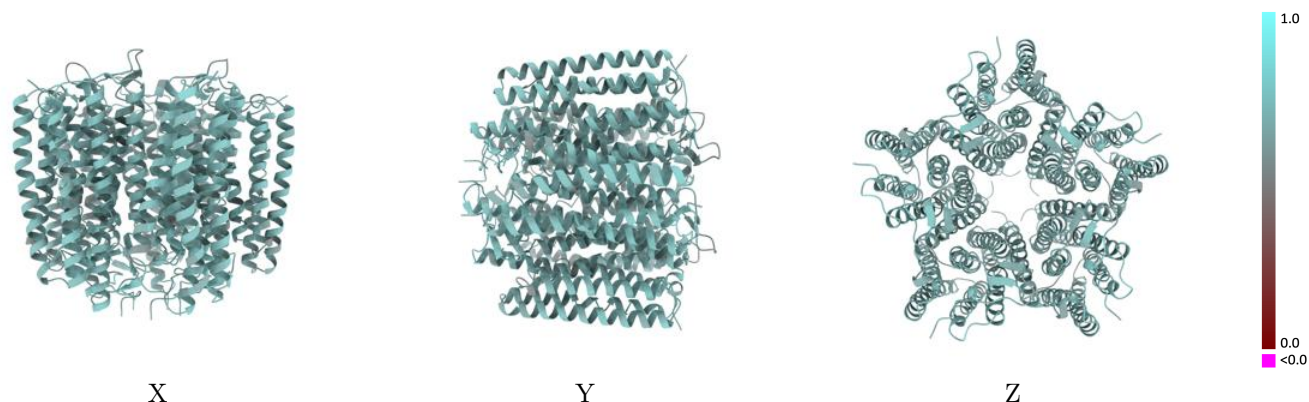
This section contains information regarding the fit between EMDB map EMD-18800 and PDB model 8R0P. Per-residue inclusion information can be found in section [3](#) on page [7](#).

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



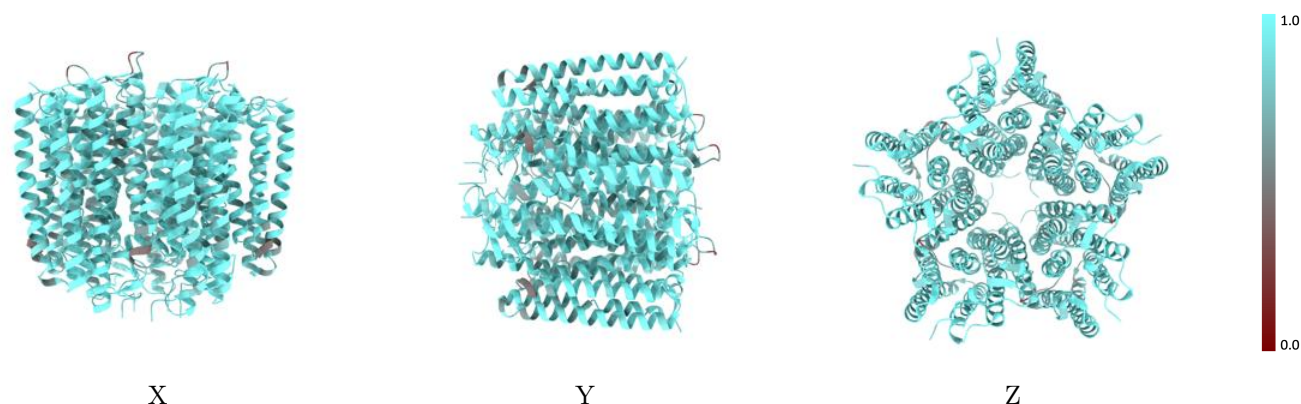
The images above show the 3D surface view of the map at the recommended contour level 0.316 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



The images above show the model with each residue coloured according 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.

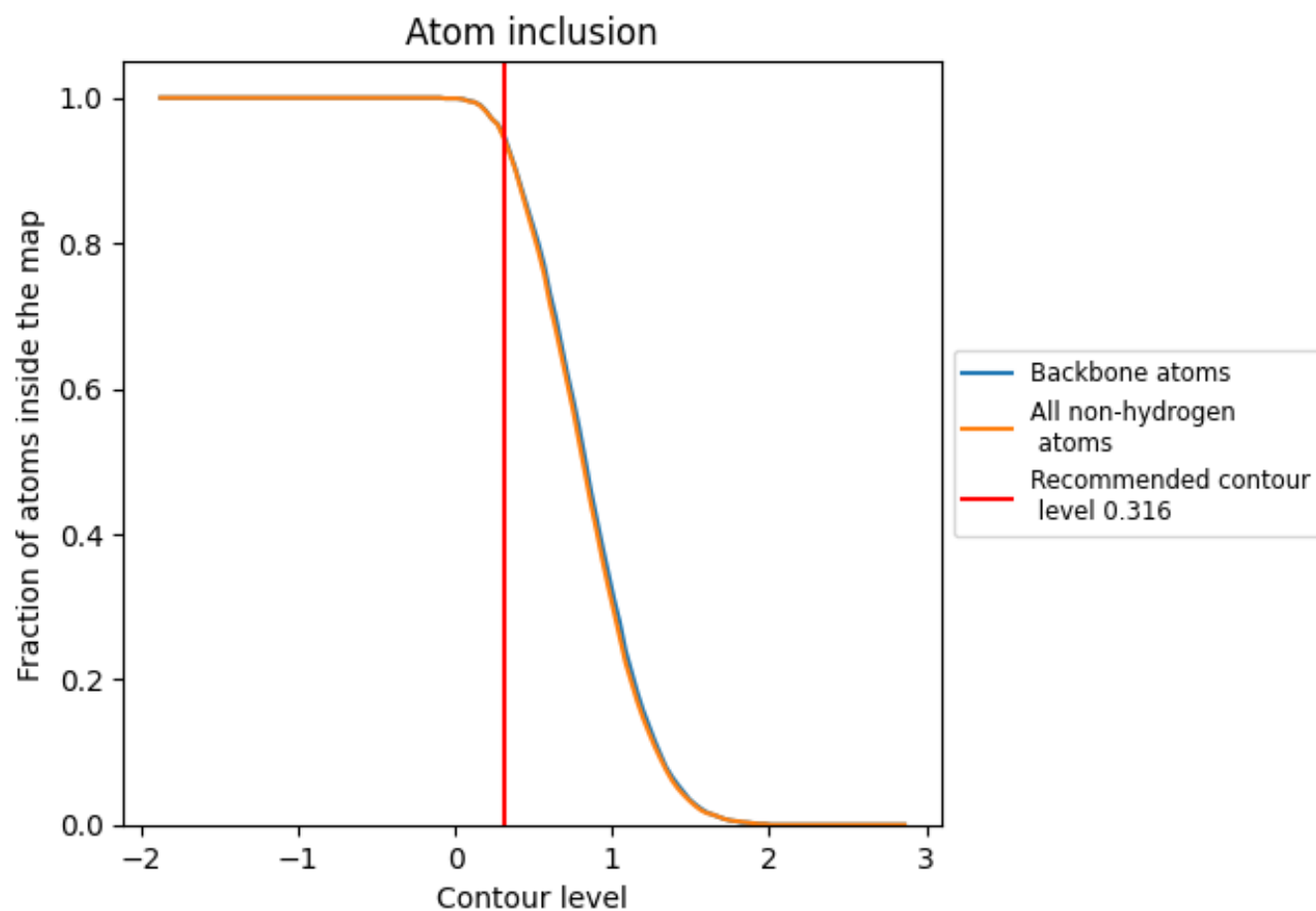
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.316).



## 9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 94% 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 (0.316) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.9420	<div></div> 0.6660
A	<div></div> 0.9450	<div></div> 0.6660
B	<div></div> 0.9430	<div></div> 0.6650
C	<div></div> 0.9450	<div></div> 0.6660
D	<div></div> 0.9460	<div></div> 0.6650
E	<div></div> 0.9420	<div></div> 0.6650

