



Full wwPDB EM Validation Report ⓘ

Oct 4, 2025 – 02:01 PM EDT

PDB ID : 9O62 / pdb_00009o62
EMDB ID : EMD-70157
Title : 1C5H TCR bound to R-phycoerythrin
Authors : Rashleigh, L.; Venugopal, H.; Rossjohn, J.; Gully, B.S.
Deposited on : 2025-04-10
Resolution : 2.03 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

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:

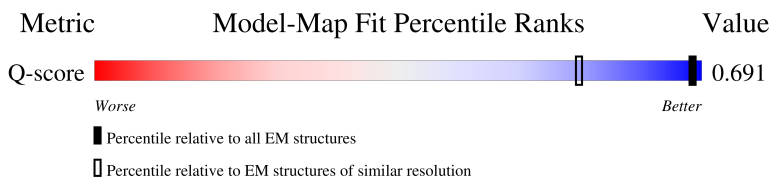
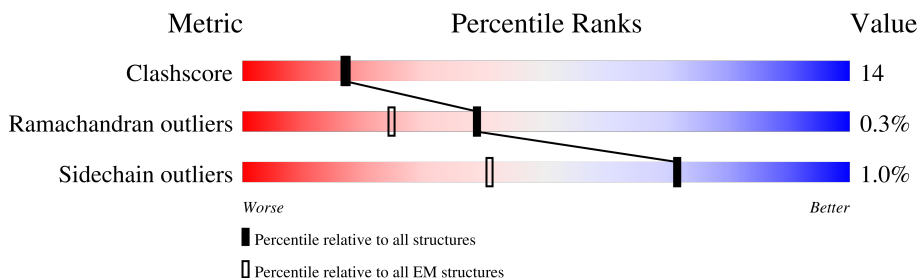
EMDB validation analysis : 0.0.1.dev129
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.46

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 2.03 Å.

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











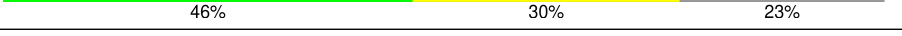

Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	1771 (1.55 - 2.53)

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	164	
1	C	164	
1	E	164	
1	G	164	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	I	164	 73% 27% .
1	K	164	 71% 29%
2	B	176	 78% 21% .
2	D	176	 72% 28%
2	F	176	 76% 23% .
2	H	176	 74% 26%
2	J	176	 79% 20% .
2	L	176	 76% 24% .
3	a	239	 46% 30% 23%
4	b	237	 51% 33% . 15%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 19376 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 R-phycoerythrin class I alpha subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	164	Total	C	N	O	S	0	0
			1242	775	217	243	7		
1	C	164	Total	C	N	O	S	0	0
			1242	775	217	243	7		
1	E	164	Total	C	N	O	S	0	0
			1242	775	217	243	7		
1	G	164	Total	C	N	O	S	0	0
			1242	775	217	243	7		
1	I	164	Total	C	N	O	S	0	0
			1242	775	217	243	7		
1	K	164	Total	C	N	O	S	0	0
			1242	775	217	243	7		

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	64	PRO	SER	conflict	UNP A0A1C9C9A7
A	109	GLY	CYS	conflict	UNP A0A1C9C9A7
A	119	ALA	THR	conflict	UNP A0A1C9C9A7
A	124	GLY	SER	conflict	UNP A0A1C9C9A7
A	128	ILE	VAL	conflict	UNP A0A1C9C9A7
A	149	ALA	GLY	conflict	UNP A0A1C9C9A7
A	152	PHE	TYR	conflict	UNP A0A1C9C9A7
A	153	SER	GLY	conflict	UNP A0A1C9C9A7
A	154	GLY	ALA	conflict	UNP A0A1C9C9A7
C	64	PRO	SER	conflict	UNP A0A1C9C9A7
C	109	GLY	CYS	conflict	UNP A0A1C9C9A7
C	119	ALA	THR	conflict	UNP A0A1C9C9A7
C	124	GLY	SER	conflict	UNP A0A1C9C9A7
C	128	ILE	VAL	conflict	UNP A0A1C9C9A7
C	149	ALA	GLY	conflict	UNP A0A1C9C9A7
C	152	PHE	TYR	conflict	UNP A0A1C9C9A7
C	153	SER	GLY	conflict	UNP A0A1C9C9A7
C	154	GLY	ALA	conflict	UNP A0A1C9C9A7

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	64	PRO	SER	conflict	UNP A0A1C9C9A7
E	109	GLY	CYS	conflict	UNP A0A1C9C9A7
E	119	ALA	THR	conflict	UNP A0A1C9C9A7
E	124	GLY	SER	conflict	UNP A0A1C9C9A7
E	128	ILE	VAL	conflict	UNP A0A1C9C9A7
E	149	ALA	GLY	conflict	UNP A0A1C9C9A7
E	152	PHE	TYR	conflict	UNP A0A1C9C9A7
E	153	SER	GLY	conflict	UNP A0A1C9C9A7
E	154	GLY	ALA	conflict	UNP A0A1C9C9A7
G	64	PRO	SER	conflict	UNP A0A1C9C9A7
G	109	GLY	CYS	conflict	UNP A0A1C9C9A7
G	119	ALA	THR	conflict	UNP A0A1C9C9A7
G	124	GLY	SER	conflict	UNP A0A1C9C9A7
G	128	ILE	VAL	conflict	UNP A0A1C9C9A7
G	149	ALA	GLY	conflict	UNP A0A1C9C9A7
G	152	PHE	TYR	conflict	UNP A0A1C9C9A7
G	153	SER	GLY	conflict	UNP A0A1C9C9A7
G	154	GLY	ALA	conflict	UNP A0A1C9C9A7
I	64	PRO	SER	conflict	UNP A0A1C9C9A7
I	109	GLY	CYS	conflict	UNP A0A1C9C9A7
I	119	ALA	THR	conflict	UNP A0A1C9C9A7
I	124	GLY	SER	conflict	UNP A0A1C9C9A7
I	128	ILE	VAL	conflict	UNP A0A1C9C9A7
I	149	ALA	GLY	conflict	UNP A0A1C9C9A7
I	152	PHE	TYR	conflict	UNP A0A1C9C9A7
I	153	SER	GLY	conflict	UNP A0A1C9C9A7
I	154	GLY	ALA	conflict	UNP A0A1C9C9A7
K	64	PRO	SER	conflict	UNP A0A1C9C9A7
K	109	GLY	CYS	conflict	UNP A0A1C9C9A7
K	119	ALA	THR	conflict	UNP A0A1C9C9A7
K	124	GLY	SER	conflict	UNP A0A1C9C9A7
K	128	ILE	VAL	conflict	UNP A0A1C9C9A7
K	149	ALA	GLY	conflict	UNP A0A1C9C9A7
K	152	PHE	TYR	conflict	UNP A0A1C9C9A7
K	153	SER	GLY	conflict	UNP A0A1C9C9A7
K	154	GLY	ALA	conflict	UNP A0A1C9C9A7

- Molecule 2 is a protein called R-phycoerythrin class I beta subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	176	Total	C	N	O	S	0	0
			1275	783	222	258	12		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	176	Total	C	N	O	S	0	0
			1275	783	222	258	12		
2	F	176	Total	C	N	O	S	0	0
			1275	783	222	258	12		
2	H	176	Total	C	N	O	S	0	0
			1275	783	222	258	12		
2	J	176	Total	C	N	O	S	0	0
			1275	783	222	258	12		
2	L	176	Total	C	N	O	S	0	0
			1275	783	222	258	12		

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	20	SER	GLY	conflict	UNP A0A1C9C989
B	127	THR	SER	conflict	UNP A0A1C9C989
B	128	ALA	VAL	conflict	UNP A0A1C9C989
B	137	SER	ALA	conflict	UNP A0A1C9C989
B	147	PRO	SER	conflict	UNP A0A1C9C989
B	154	ALA	THR	conflict	UNP A0A1C9C989
B	155	ALA	ASP	conflict	UNP A0A1C9C989
B	173	SER	ALA	conflict	UNP A0A1C9C989
D	20	SER	GLY	conflict	UNP A0A1C9C989
D	127	THR	SER	conflict	UNP A0A1C9C989
D	128	ALA	VAL	conflict	UNP A0A1C9C989
D	137	SER	ALA	conflict	UNP A0A1C9C989
D	147	PRO	SER	conflict	UNP A0A1C9C989
D	154	ALA	THR	conflict	UNP A0A1C9C989
D	155	ALA	ASP	conflict	UNP A0A1C9C989
D	173	SER	ALA	conflict	UNP A0A1C9C989
F	20	SER	GLY	conflict	UNP A0A1C9C989
F	127	THR	SER	conflict	UNP A0A1C9C989
F	128	ALA	VAL	conflict	UNP A0A1C9C989
F	137	SER	ALA	conflict	UNP A0A1C9C989
F	147	PRO	SER	conflict	UNP A0A1C9C989
F	154	ALA	THR	conflict	UNP A0A1C9C989
F	155	ALA	ASP	conflict	UNP A0A1C9C989
F	173	SER	ALA	conflict	UNP A0A1C9C989
H	20	SER	GLY	conflict	UNP A0A1C9C989
H	127	THR	SER	conflict	UNP A0A1C9C989
H	128	ALA	VAL	conflict	UNP A0A1C9C989
H	137	SER	ALA	conflict	UNP A0A1C9C989
H	147	PRO	SER	conflict	UNP A0A1C9C989

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
H	154	ALA	THR	conflict	UNP A0A1C9C989
H	155	ALA	ASP	conflict	UNP A0A1C9C989
H	173	SER	ALA	conflict	UNP A0A1C9C989
J	20	SER	GLY	conflict	UNP A0A1C9C989
J	127	THR	SER	conflict	UNP A0A1C9C989
J	128	ALA	VAL	conflict	UNP A0A1C9C989
J	137	SER	ALA	conflict	UNP A0A1C9C989
J	147	PRO	SER	conflict	UNP A0A1C9C989
J	154	ALA	THR	conflict	UNP A0A1C9C989
J	155	ALA	ASP	conflict	UNP A0A1C9C989
J	173	SER	ALA	conflict	UNP A0A1C9C989
L	20	SER	GLY	conflict	UNP A0A1C9C989
L	127	THR	SER	conflict	UNP A0A1C9C989
L	128	ALA	VAL	conflict	UNP A0A1C9C989
L	137	SER	ALA	conflict	UNP A0A1C9C989
L	147	PRO	SER	conflict	UNP A0A1C9C989
L	154	ALA	THR	conflict	UNP A0A1C9C989
L	155	ALA	ASP	conflict	UNP A0A1C9C989
L	173	SER	ALA	conflict	UNP A0A1C9C989

- Molecule 3 is a protein called 1C5H TCR delta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	a	184	Total	C	N	O	S	0	0
			1403	911	234	252	6		

- Molecule 4 is a protein called TCR gamma chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	b	201	Total	C	N	O	S	0	0
			1581	1016	261	298	6		

- Molecule 5 is PHYCOERYTHROBILIN (CCD ID: PEB) (formula: C₃₃H₄₀N₄O₆) (labeled as "Ligand of Interest" by depositor).

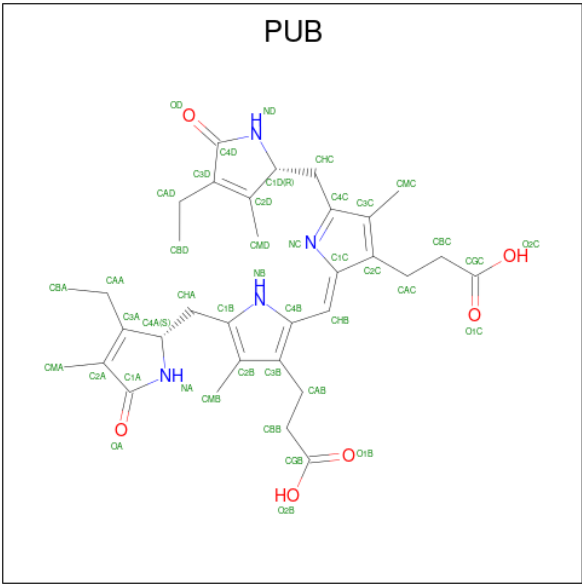


Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
5	G	1	Total 43	33	4	6	0
5	H	1	Total 43	33	4	6	0
5	H	1	Total 43	33	4	6	0
5	I	1	Total 43	33	4	6	0
5	I	1	Total 43	33	4	6	0
5	J	1	Total 43	33	4	6	0
5	K	1	Total 43	33	4	6	0
5	K	1	Total 43	33	4	6	0
5	L	1	Total 43	33	4	6	0
5	L	1	Total 43	33	4	6	0

- Molecule 6 is PHYCOUROBILIN (CCD ID: PUB) (formula: C₃₃H₄₂N₄O₆) (labeled as "Lig- and of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
6	B	1	Total 43	C 33	N 4	O 6	0

Continued on next page...

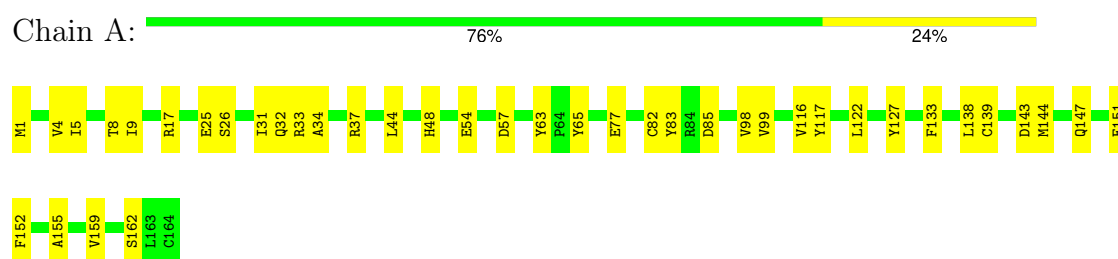
Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
6	D	1	Total	C	N	O	0
			43	33	4	6	
6	F	1	Total	C	N	O	0
			43	33	4	6	
6	H	1	Total	C	N	O	0
			43	33	4	6	
6	J	1	Total	C	N	O	0
			43	33	4	6	
6	L	1	Total	C	N	O	0
			43	33	4	6	

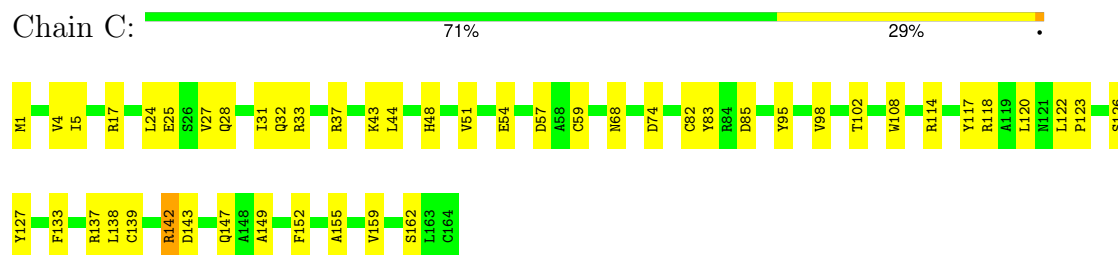
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

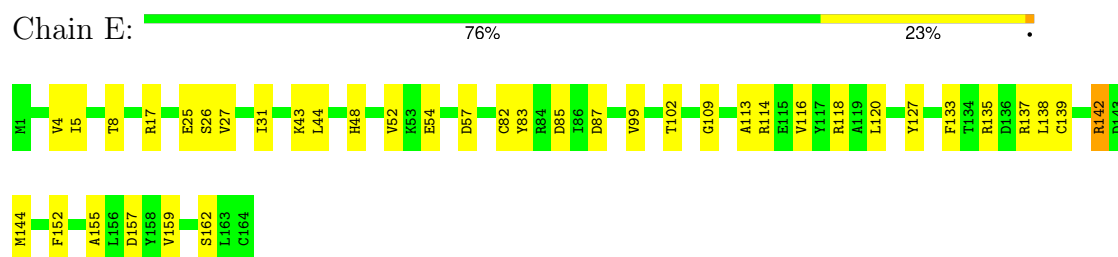
• Molecule 1: R-phycoerythrin class I alpha subunit



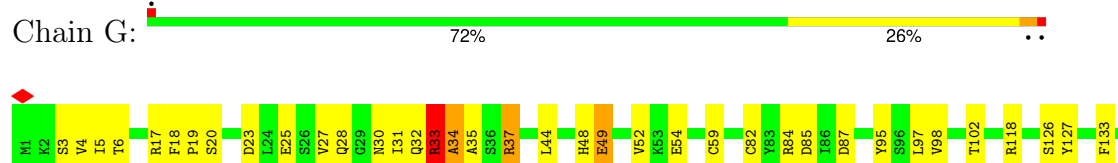
• Molecule 1: R-phycoerythrin class I alpha subunit

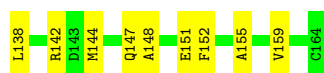


• Molecule 1: R-phycoerythrin class I alpha subunit



• Molecule 1: R-phycoerythrin class I alpha subunit





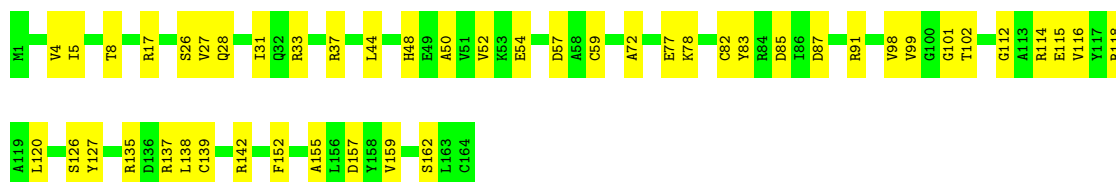
- Molecule 1: R-phycoerythrin class I alpha subunit

Chain I: 73% 27%



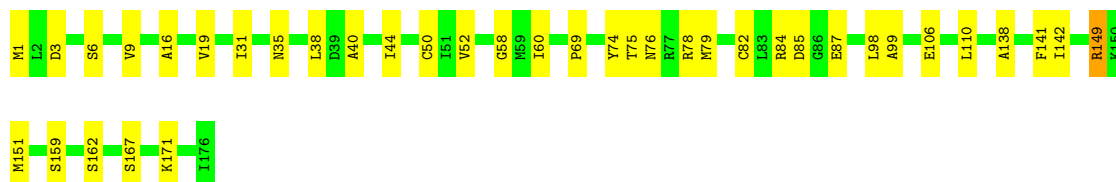
- Molecule 1: R-phycoerythrin class I alpha subunit

Chain K: 71% 29%



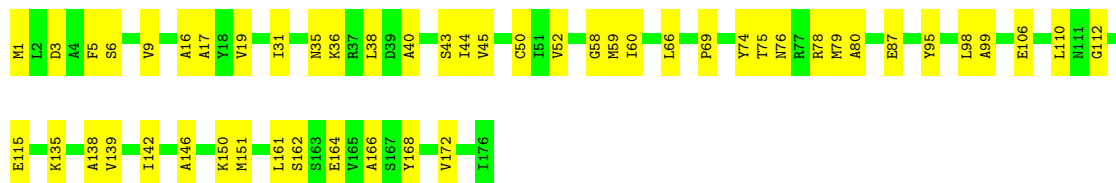
- Molecule 2: R-phycoerythrin class I beta subunit

Chain B: 78% 21%



- Molecule 2: R-phycoerythrin class I beta subunit

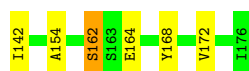
Chain D: 72% 28%



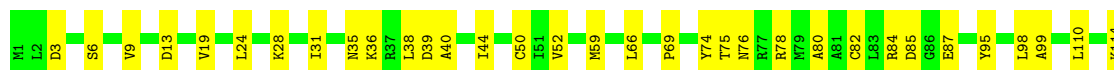
- Molecule 2: R-phycoerythrin class I beta subunit

Chain F: 76% 23%

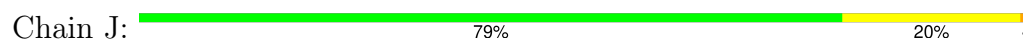




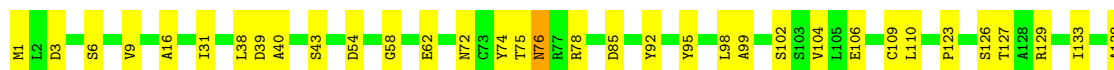
• Molecule 2: R-phycoerythrin class I beta subunit



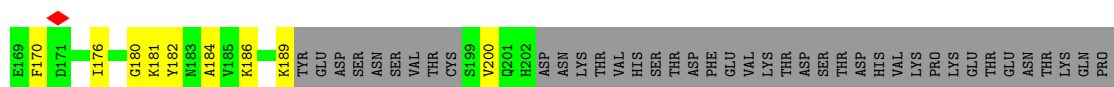
• Molecule 2: R-phycoerythrin class I beta subunit



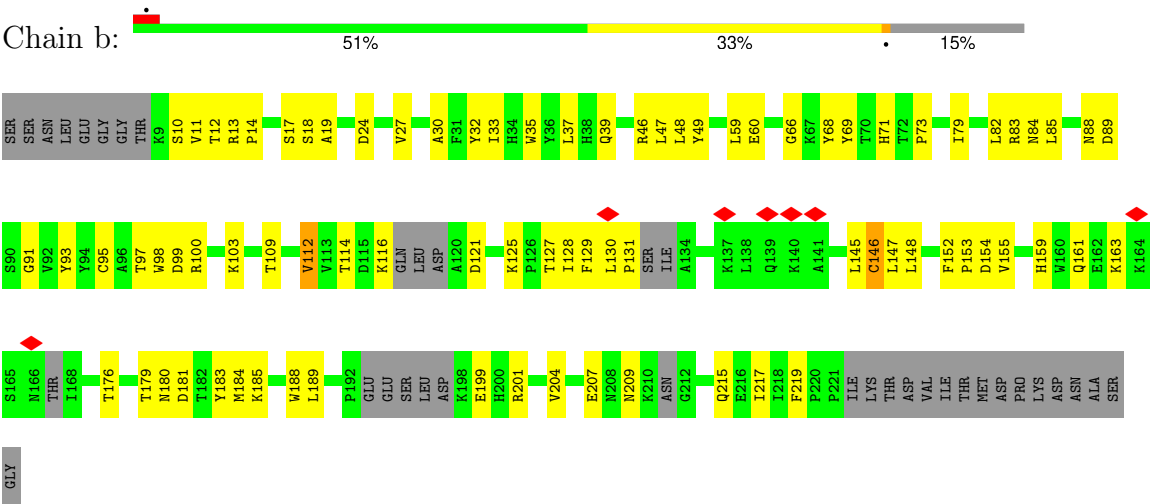
• Molecule 2: R-phycoerythrin class I beta subunit



• Molecule 3: 1C5H TCR delta chain



● Molecule 4: TCR gamma chain



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	45513	Depositor
Resolution determination method	OTHER	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60.0	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	45.702	Depositor
Minimum map value	-32.661	Depositor
Average map value	0.003	Depositor
Map value standard deviation	1.036	Depositor
Recommended contour level	3.7	Depositor
Map size (Å)	295.2, 295.2, 295.2	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.82000005, 0.82000005, 0.82000005	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PUB, PEB

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	0.13	0/1264	0.31	0/1709
1	C	0.24	0/1264	0.41	0/1709
1	E	0.22	0/1264	0.37	0/1709
1	G	0.30	0/1264	0.43	0/1709
1	I	0.14	0/1264	0.33	0/1709
1	K	0.15	0/1264	0.32	0/1709
2	B	0.26	0/1287	0.41	0/1741
2	D	0.14	0/1287	0.34	0/1741
2	F	0.13	0/1287	0.29	0/1741
2	H	0.20	0/1287	0.36	0/1741
2	J	0.14	0/1287	0.31	0/1741
2	L	0.14	0/1287	0.33	0/1741
3	a	0.29	0/1439	0.50	0/1955
4	b	0.23	0/1622	0.44	0/2211
All	All	0.20	0/18367	0.37	0/24866

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	C	0	1
1	E	0	1
1	G	0	1
2	B	0	1
3	a	0	1
All	All	0	5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	149	ARG	Sidechain
1	C	142	ARG	Sidechain
1	E	142	ARG	Sidechain
1	G	33	ARG	Sidechain
3	a	16	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	1242	0	1211	33	0
1	C	1242	0	1214	53	0
1	E	1242	0	1215	37	0
1	G	1242	0	1214	44	0
1	I	1242	0	1214	39	0
1	K	1242	0	1213	44	0
2	B	1275	0	1283	32	0
2	D	1275	0	1283	41	0
2	F	1275	0	1283	37	0
2	H	1275	0	1280	39	0
2	J	1275	0	1282	32	0
2	L	1275	0	1283	34	0
3	a	1403	0	1339	63	0
4	b	1581	0	1483	70	0
5	A	172	0	146	11	0
5	B	43	0	37	3	0
5	C	86	0	74	19	0
5	D	86	0	75	3	0
5	E	86	0	75	13	0
5	F	86	0	74	10	0
5	G	86	0	75	9	0
5	H	86	0	72	13	0
5	I	86	0	74	11	0
5	J	43	0	38	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	K	86	0	73	14	0
5	L	86	0	75	5	0
6	B	43	0	40	2	0
6	D	43	0	40	1	0
6	F	43	0	40	3	0
6	H	43	0	40	1	0
6	J	43	0	38	1	0
6	L	43	0	39	3	0
All	All	19376	0	18922	525	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 14.

All (525) 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:C:142:ARG:NH2	1:C:143:ASP:OD1	1.77	1.17
3:a:159:ILE:HD12	3:a:186:LYS:HD3	1.11	1.10
2:B:149:ARG:NH2	2:B:151:MET:SD	2.30	1.04
3:a:159:ILE:CD1	3:a:186:LYS:HD3	1.90	1.01
4:b:68:TYR:CE1	4:b:82:LEU:HD21	1.99	0.98
3:a:68:LYS:HD2	3:a:73:SER:HB3	1.45	0.95
4:b:68:TYR:CE1	4:b:82:LEU:CD2	2.49	0.95
3:a:12:SER:HB3	3:a:125:GLU:OE2	1.68	0.94
4:b:68:TYR:HE1	4:b:82:LEU:HD21	1.31	0.93
1:E:142:ARG:HG2	5:E:202:PEB:HHA1	1.57	0.86
1:C:32:GLN:HG3	1:G:32:GLN:HG3	1.58	0.85
1:A:32:GLN:HG3	1:I:32:GLN:HG3	1.59	0.85
1:C:114:ARG:HD3	1:K:114:ARG:HD2	1.63	0.78
1:G:28:GLN:HA	1:G:31:ILE:HD12	1.69	0.74
1:A:31:ILE:HA	2:J:31:ILE:HD12	1.71	0.73
4:b:130:LEU:HD12	4:b:131:PRO:HD2	1.70	0.73
2:J:40:ALA:HB1	2:J:142:ILE:HD12	1.72	0.71
3:a:159:ILE:HD12	3:a:186:LYS:CD	2.06	0.71
1:C:143:ASP:CG	5:C:202:PEB:H1D1	2.15	0.71
2:D:31:ILE:HD12	1:G:31:ILE:HA	1.73	0.71
1:I:78:LYS:HB3	5:I:201:PEB:HMB1	1.71	0.70
4:b:11:VAL:HG13	4:b:13:ARG:HH21	1.57	0.70
1:C:25:GLU:OE1	1:G:30:ASN:ND2	2.25	0.69
2:F:85:ASP:OD2	5:F:202:PEB:H1D1	1.92	0.69
2:L:40:ALA:HB1	2:L:142:ILE:HD12	1.74	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:b:114:THR:CG2	4:b:152:PHE:CE2	2.76	0.69
1:K:157:ASP:OD2	2:L:149:ARG:NH2	2.26	0.68
4:b:114:THR:HG21	4:b:152:PHE:CE2	2.28	0.68
1:C:31:ILE:HA	2:H:31:ILE:HD12	1.75	0.68
4:b:159:HIS:NE2	4:b:161:GLN:OE1	2.25	0.68
2:B:31:ILE:HD12	1:I:31:ILE:HA	1.75	0.68
2:F:40:ALA:HB1	2:F:142:ILE:HD12	1.74	0.68
4:b:99:ASP:OD1	4:b:100:ARG:N	2.26	0.68
2:L:127:THR:HG22	2:L:176:ILE:HD12	1.76	0.67
1:I:77:GLU:OE1	4:b:100:ARG:NH2	2.27	0.67
4:b:112:VAL:HG11	4:b:153:PRO:HB3	1.77	0.66
2:F:60:ILE:HD13	5:I:201:PEB:HBC2	1.78	0.66
2:B:16:ALA:HB2	2:F:69:PRO:HG3	1.78	0.65
3:a:35:PHE:HB2	3:a:92:ALA:HB3	1.78	0.65
4:b:114:THR:CG2	4:b:152:PHE:HE2	2.11	0.64
2:B:141:PHE:HE1	2:B:149:ARG:HB3	1.62	0.63
1:C:44:LEU:O	1:C:48:HIS:HB3	1.98	0.63
2:B:167:SER:O	2:B:171:LYS:HG3	1.98	0.63
3:a:33:TYR:HA	3:a:52:GLY:HA2	1.80	0.62
2:J:138:ALA:O	2:J:142:ILE:HG12	2.00	0.62
1:I:76:GLN:NE2	3:a:31:SER:OG	2.29	0.62
1:I:78:LYS:HA	1:I:81:LYS:HB2	1.82	0.62
1:A:33:ARG:NH1	1:A:151:GLU:OE1	2.32	0.62
3:a:144:ASN:OD1	3:a:189:LYS:NZ	2.32	0.62
4:b:24:ASP:N	4:b:24:ASP:OD1	2.33	0.62
4:b:146:CYS:HB2	4:b:219:PHE:HZ	1.65	0.62
2:H:85:ASP:OD1	5:H:202:PEB:H1D1	1.99	0.62
1:E:43:LYS:NZ	5:E:202:PEB:OD	2.33	0.61
1:C:118:ARG:NH2	1:K:162:SER:O	2.33	0.61
4:b:14:PRO:HB3	4:b:116:LYS:HA	1.81	0.61
2:D:3:ASP:N	2:D:6:SER:OG	2.32	0.61
5:G:201:PEB:HMB1	5:G:201:PEB:HNA	1.64	0.61
3:a:68:LYS:HB2	3:a:73:SER:H	1.64	0.61
3:a:97:HIS:NE2	4:b:100:ARG:O	2.26	0.60
3:a:159:ILE:HD13	3:a:186:LYS:HB2	1.82	0.60
3:a:8:GLN:HE22	3:a:11:VAL:HB	1.67	0.60
2:F:110:LEU:HD21	2:F:172:VAL:HG22	1.82	0.60
1:I:54:GLU:HB3	1:I:133:PHE:HE2	1.66	0.60
4:b:181:ASP:OD1	4:b:181:ASP:O	2.19	0.60
1:C:143:ASP:OD1	5:C:202:PEB:H1D1	2.00	0.60
1:A:127:TYR:CZ	5:A:202:PEB:HAA1	2.37	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:78:ARG:HA	5:H:202:PEB:HAB1	1.83	0.60
2:H:154:ALA:HB3	5:H:203:PEB:HBB1	1.83	0.60
4:b:176:THR:HB	4:b:185:LYS:HE3	1.82	0.60
2:D:36:LYS:HB3	2:D:161:LEU:HD11	1.83	0.59
2:D:40:ALA:HB1	2:D:142:ILE:HD12	1.83	0.59
1:G:82:CYS:HA	5:G:201:PEB:HHA1	1.84	0.59
4:b:204:VAL:HB	4:b:215:GLN:HB3	1.85	0.59
2:D:1:MET:HE2	1:G:6:THR:HA	1.85	0.59
1:G:33:ARG:O	1:G:34:ALA:C	2.46	0.59
2:H:3:ASP:N	2:H:6:SER:OG	2.35	0.59
1:A:54:GLU:HB3	1:A:133:PHE:HE2	1.67	0.58
1:A:162:SER:O	1:G:118:ARG:NH2	2.36	0.58
2:F:3:ASP:H	2:F:6:SER:HB2	1.68	0.58
3:a:102:ILE:HG22	3:a:103:SER:H	1.67	0.58
3:a:155:LYS:O	3:a:155:LYS:HG3	2.02	0.58
3:a:134:PRO:HB3	3:a:152:PHE:HB3	1.85	0.58
1:C:33:ARG:O	1:C:37:ARG:HG2	2.03	0.58
2:B:75:THR:O	2:B:78:ARG:N	2.35	0.58
1:I:53:LYS:HZ2	3:a:30:TRP:CD1	2.21	0.58
1:C:33:ARG:NH1	1:C:147:GLN:OE1	2.37	0.58
1:E:135:ARG:NH1	1:E:157:ASP:OD1	2.33	0.58
2:D:79:MET:HE2	1:K:120:LEU:HD11	1.86	0.58
1:E:114:ARG:HD2	1:I:114:ARG:HD2	1.86	0.58
5:C:201:PEB:NA	5:C:201:PEB:HMB1	2.19	0.58
1:E:57:ASP:OD1	1:E:83:TYR:OH	2.21	0.57
1:G:54:GLU:HB3	1:G:133:PHE:HE2	1.69	0.57
2:D:138:ALA:O	2:D:142:ILE:HG12	2.03	0.57
2:J:69:PRO:HG3	2:L:16:ALA:HB2	1.86	0.57
1:E:31:ILE:HA	2:L:31:ILE:HD12	1.85	0.57
4:b:163:LYS:NZ	4:b:199:GLU:OE2	2.32	0.57
3:a:68:LYS:HD3	3:a:71:ALA:HB3	1.85	0.57
1:A:33:ARG:NH2	1:A:147:GLN:OE1	2.37	0.57
2:F:138:ALA:O	2:F:142:ILE:HG12	2.04	0.57
2:H:13:ASP:OD1	2:L:74:TYR:OH	2.18	0.57
2:H:24:LEU:O	2:H:28:LYS:HG3	2.05	0.57
2:H:69:PRO:HG2	2:J:16:ALA:HB2	1.87	0.57
1:A:37:ARG:NH1	1:A:98:VAL:O	2.36	0.57
3:a:38:LYS:HB3	3:a:48:LEU:HD11	1.86	0.57
2:F:75:THR:O	2:F:78:ARG:N	2.38	0.56
4:b:68:TYR:CD1	4:b:82:LEU:CD2	2.88	0.56
1:A:25:GLU:OE1	1:I:30:ASN:ND2	2.38	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:98:LEU:HD11	1:I:27:VAL:HG21	1.88	0.56
2:F:99:ALA:HA	1:K:5:ILE:HG21	1.88	0.56
2:F:139:VAL:HG13	2:F:162:SER:HB3	1.86	0.56
2:D:98:LEU:HD11	1:G:27:VAL:HG21	1.87	0.56
1:E:27:VAL:HG21	2:L:98:LEU:HD11	1.88	0.56
1:E:155:ALA:O	1:E:159:VAL:HG23	2.06	0.56
1:C:17:ARG:NH2	1:G:102:THR:OG1	2.34	0.56
1:G:155:ALA:O	1:G:159:VAL:HG23	2.05	0.56
4:b:209:ASN:ND2	4:b:215:GLN:OE1	2.39	0.56
5:I:201:PEB:HNA	5:I:201:PEB:HMB3	1.70	0.55
2:J:75:THR:O	2:J:78:ARG:N	2.39	0.55
1:A:155:ALA:O	1:A:159:VAL:HG23	2.06	0.55
1:C:82:CYS:HB2	5:C:201:PEB:NA	2.21	0.55
1:C:155:ALA:O	1:C:159:VAL:HG23	2.07	0.55
2:D:75:THR:O	2:D:78:ARG:N	2.38	0.55
1:K:44:LEU:O	1:K:48:HIS:HB3	2.06	0.55
3:a:47:PHE:HZ	3:a:50:ARG:HB2	1.70	0.55
1:E:102:THR:OG1	1:K:17:ARG:NH2	2.32	0.55
2:F:31:ILE:HD12	1:K:31:ILE:HA	1.88	0.55
2:L:85:ASP:OD1	5:L:202:PEB:H1D1	2.07	0.55
2:B:106:GLU:HA	2:B:110:LEU:HB2	1.89	0.55
1:C:82:CYS:SG	5:C:201:PEB:HAA2	2.47	0.55
1:C:85:ASP:CG	5:C:201:PEB:HNC	2.14	0.55
1:I:155:ALA:O	1:I:159:VAL:HG23	2.07	0.55
1:G:85:ASP:OD1	5:G:201:PEB:H1D1	2.07	0.55
3:a:167:ILE:HD12	3:a:189:LYS:HB3	1.88	0.55
1:K:82:CYS:HA	5:K:201:PEB:HHA1	1.89	0.54
1:E:120:LEU:HD13	5:E:201:PEB:HBB1	1.89	0.54
2:D:99:ALA:HA	1:G:5:ILE:HG21	1.89	0.54
1:G:142:ARG:HD3	5:G:202:PEB:HHA1	1.88	0.54
2:F:95:TYR:OH	1:K:17:ARG:O	2.24	0.54
4:b:68:TYR:CD1	4:b:82:LEU:HD23	2.42	0.54
4:b:154:ASP:OD1	4:b:154:ASP:N	2.37	0.54
2:L:138:ALA:O	2:L:142:ILE:HG12	2.07	0.54
4:b:35:TRP:CZ3	4:b:95:CYS:HB3	2.43	0.54
1:E:127:TYR:CZ	5:E:201:PEB:HAA1	2.43	0.53
1:E:114:ARG:HG3	1:I:118:ARG:NH1	2.23	0.53
1:E:118:ARG:NH2	1:I:162:SER:O	2.40	0.53
1:I:138:LEU:HD22	1:I:152:PHE:HD2	1.72	0.53
2:B:84:ARG:NH2	2:B:85:ASP:OD1	2.42	0.53
4:b:27:VAL:HG23	4:b:30:ALA:HB2	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3:ASP:N	2:B:6:SER:OG	2.34	0.53
3:a:159:ILE:CD1	3:a:186:LYS:CD	2.77	0.53
1:C:51:VAL:HG21	5:C:202:PEB:HBD1	1.90	0.53
1:E:17:ARG:O	2:L:95:TYR:OH	2.25	0.53
1:E:82:CYS:HB2	5:E:201:PEB:NA	2.23	0.53
2:F:52:VAL:HG21	2:F:87:GLU:HA	1.90	0.53
1:G:34:ALA:O	1:G:35:ALA:C	2.52	0.53
2:H:40:ALA:HB1	2:H:142:ILE:HD12	1.90	0.53
1:K:155:ALA:O	1:K:159:VAL:HG23	2.09	0.53
1:I:82:CYS:HA	5:I:201:PEB:HHA1	1.90	0.53
3:a:13:MET:HG2	3:a:19:VAL:HB	1.91	0.53
1:C:4:VAL:HG21	1:G:25:GLU:HB3	1.92	0.52
2:L:54:ASP:HB2	6:L:201:PUB:HHA1	1.91	0.52
1:A:138:LEU:HD11	1:A:144:MET:HE3	1.90	0.52
2:B:40:ALA:HB1	2:B:142:ILE:HD12	1.91	0.52
1:C:17:ARG:O	2:H:95:TYR:OH	2.27	0.52
1:K:82:CYS:HB2	5:K:201:PEB:NA	2.24	0.52
1:A:82:CYS:HA	5:A:202:PEB:HHA1	1.92	0.52
1:I:80:ASN:OD1	3:a:99:TYR:N	2.35	0.52
2:L:62:GLU:OE1	2:L:129:ARG:NE	2.40	0.52
4:b:47:LEU:HG	4:b:68:TYR:CZ	2.44	0.52
1:A:139:CYS:HB2	5:A:203:PEB:HHA1	1.91	0.52
4:b:121:ASP:O	4:b:125:LYS:NZ	2.35	0.52
2:J:110:LEU:HD21	2:J:172:VAL:HG22	1.91	0.52
1:K:72:ALA:HA	1:K:78:LYS:HE3	1.92	0.52
3:a:83:LEU:HD11	3:a:176:ILE:HG21	1.90	0.52
2:H:158:CYS:SG	5:H:203:PEB:HAA1	2.49	0.52
1:I:44:LEU:O	1:I:48:HIS:HB3	2.10	0.52
1:A:138:LEU:HD22	1:A:152:PHE:HD2	1.75	0.52
1:C:122:LEU:HD21	5:C:201:PEB:HBB2	1.91	0.52
1:E:44:LEU:O	1:E:48:HIS:HB3	2.10	0.52
2:F:39:ASP:CB	5:F:203:PEB:HHA1	2.40	0.51
1:E:85:ASP:OD1	5:E:201:PEB:H1D1	2.11	0.51
2:H:110:LEU:HD21	2:H:172:VAL:HG22	1.92	0.51
5:J:202:PEB:CMB	5:J:202:PEB:HNA	2.22	0.51
1:I:82:CYS:SG	5:I:201:PEB:HAA2	2.51	0.51
4:b:163:LYS:HA	4:b:201:ARG:HE	1.76	0.51
2:H:138:ALA:O	2:H:142:ILE:HG12	2.09	0.51
2:H:59:MET:HE3	2:H:66:LEU:HD13	1.93	0.51
2:D:69:PRO:HG2	2:F:16:ALA:HB2	1.92	0.51
2:F:58:GLY:O	2:F:62:GLU:HG3	2.11	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:74:TYR:O	2:J:75:THR:OG1	2.22	0.51
3:a:6:GLN:HE22	3:a:120:ILE:HG22	1.75	0.51
3:a:136:VAL:HG21	3:a:200:VAL:HG12	1.93	0.51
4:b:27:VAL:HG21	4:b:97:THR:HG21	1.92	0.51
1:A:8:THR:HG21	1:A:26:SER:OG	2.11	0.51
4:b:10:SER:HB3	4:b:155:VAL:HB	1.92	0.51
2:F:84:ARG:NH2	5:F:202:PEB:O1C	2.44	0.51
2:H:74:TYR:CD2	2:H:75:THR:HG23	2.45	0.51
1:I:57:ASP:OD1	1:I:83:TYR:OH	2.30	0.51
2:B:1:MET:HE2	1:I:6:THR:HG22	1.93	0.50
1:A:9:ILE:HG22	2:J:1:MET:HE1	1.92	0.50
1:A:57:ASP:OD1	1:A:83:TYR:OH	2.27	0.50
2:B:138:ALA:O	2:B:142:ILE:HG12	2.11	0.50
1:C:120:LEU:HD13	5:C:201:PEB:HBB1	1.92	0.50
1:I:82:CYS:HB2	5:I:201:PEB:NA	2.26	0.50
1:A:34:ALA:HA	1:A:37:ARG:HG2	1.93	0.50
1:A:116:VAL:HG23	2:H:80:ALA:HB2	1.93	0.50
1:C:24:LEU:C	5:H:203:PEB:HBD2	2.36	0.50
2:D:6:SER:HA	2:D:9:VAL:HG22	1.93	0.50
1:C:138:LEU:HD22	1:C:152:PHE:HD2	1.76	0.50
2:J:58:GLY:HA3	6:J:201:PUB:HHC2	1.93	0.50
1:A:5:ILE:HG21	2:J:99:ALA:HA	1.93	0.50
1:C:5:ILE:HG21	2:H:99:ALA:HA	1.94	0.50
2:D:17:ALA:O	1:G:95:TYR:OH	2.30	0.50
1:E:137:ARG:HH22	5:E:202:PEB:CGB	2.25	0.50
2:B:149:ARG:CZ	2:B:151:MET:SD	2.99	0.50
2:D:74:TYR:CD2	2:D:75:THR:HG23	2.47	0.50
6:B:201:PUB:HBB1	6:B:201:PUB:HBB1	1.93	0.50
4:b:17:SER:OG	4:b:18:SER:N	2.45	0.50
5:E:201:PEB:HAC1	2:J:79:MET:HE2	1.94	0.49
2:B:74:TYR:O	2:B:78:ARG:HB2	2.12	0.49
1:C:43:LYS:HB3	5:C:202:PEB:HAD1	1.93	0.49
2:L:74:TYR:CD2	2:L:75:THR:HG23	2.46	0.49
2:H:52:VAL:HG21	2:H:87:GLU:HA	1.95	0.49
1:K:50:ALA:O	1:K:54:GLU:HB2	2.12	0.49
3:a:159:ILE:O	3:a:159:ILE:HG13	2.12	0.49
1:A:82:CYS:HB2	5:A:202:PEB:NA	2.28	0.49
2:D:58:GLY:HA3	6:D:201:PUB:HHC2	1.94	0.49
2:D:74:TYR:O	2:D:75:THR:OG1	2.23	0.49
5:G:201:PEB:HMB1	5:G:201:PEB:NA	2.26	0.49
3:a:19:VAL:HG12	3:a:81:LEU:HD11	1.93	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:a:111:THR:HB	4:b:49:TYR:CZ	2.47	0.49
2:D:164:GLU:HG2	2:D:168:TYR:CE2	2.47	0.49
3:a:149:VAL:HG22	3:a:184:ALA:HB3	1.94	0.49
2:F:74:TYR:O	2:F:78:ARG:HB2	2.13	0.49
1:G:33:ARG:HH12	1:G:147:GLN:HB3	1.78	0.49
2:D:110:LEU:HD21	2:D:172:VAL:HG22	1.93	0.49
3:a:159:ILE:CD1	3:a:186:LYS:HB2	2.41	0.49
2:D:60:ILE:HD13	5:K:201:PEB:HBC2	1.93	0.49
2:D:95:TYR:CE1	1:G:19:PRO:HD3	2.48	0.49
1:K:4:VAL:O	1:K:8:THR:HG23	2.12	0.49
4:b:19:ALA:HB2	4:b:85:LEU:HD11	1.94	0.49
2:D:45:VAL:HG22	1:G:18:PHE:HB3	1.95	0.49
1:E:5:ILE:HG21	2:L:99:ALA:HA	1.95	0.49
2:J:74:TYR:CD2	2:J:75:THR:HG23	2.48	0.49
1:K:57:ASP:OD1	1:K:83:TYR:OH	2.22	0.49
4:b:39:GLN:NE2	4:b:88:ASN:O	2.46	0.49
2:F:58:GLY:HA3	6:F:201:PUB:HHC2	1.95	0.48
4:b:127:THR:HB	4:b:147:LEU:HB3	1.95	0.48
2:D:52:VAL:HG21	2:D:87:GLU:HA	1.95	0.48
1:E:54:GLU:HB3	1:E:133:PHE:HE2	1.79	0.48
1:E:162:SER:O	1:I:118:ARG:NH2	2.39	0.48
2:F:98:LEU:HD11	1:K:27:VAL:HG21	1.95	0.48
2:H:75:THR:O	2:H:78:ARG:N	2.46	0.48
2:B:159:SER:HA	2:B:162:SER:OG	2.12	0.48
2:L:1:MET:HE3	2:L:104:VAL:HB	1.95	0.48
2:B:74:TYR:CD2	2:B:75:THR:HG23	2.49	0.48
1:C:59:CYS:HG	1:C:126:SER:HB2	1.78	0.48
1:K:28:GLN:HA	1:K:31:ILE:HD12	1.96	0.48
1:E:116:VAL:HG23	2:J:80:ALA:HB2	1.96	0.48
5:K:201:PEB:NA	5:K:201:PEB:HMB1	2.29	0.48
2:L:123:PRO:HG2	2:L:126:SER:HB2	1.96	0.48
2:D:44:ILE:HG13	2:D:142:ILE:HD11	1.96	0.48
1:E:27:VAL:HB	2:L:38:LEU:HD21	1.96	0.48
2:H:59:MET:HB3	2:H:59:MET:HE2	1.76	0.48
2:H:84:ARG:NH2	5:H:202:PEB:O1C	2.47	0.48
3:a:6:GLN:NE2	3:a:120:ILE:HG22	2.28	0.48
3:a:20:THR:OG1	3:a:77:THR:OG1	2.32	0.48
4:b:46:ARG:HB3	4:b:60:GLU:OE2	2.13	0.48
1:C:31:ILE:HG23	2:H:31:ILE:HG23	1.96	0.48
1:C:57:ASP:OD1	1:C:83:TYR:OH	2.24	0.48
2:H:82:CYS:HA	5:H:202:PEB:CHA	2.44	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:75:THR:O	2:L:78:ARG:N	2.47	0.48
1:K:127:TYR:CZ	5:K:201:PEB:HAA1	2.49	0.48
2:B:52:VAL:HG21	2:B:87:GLU:HA	1.96	0.47
2:L:39:ASP:CB	5:L:203:PEB:HHA1	2.44	0.47
1:A:4:VAL:HG21	1:I:25:GLU:HB3	1.95	0.47
2:B:99:ALA:HA	1:I:5:ILE:HG21	1.96	0.47
1:E:139:CYS:HB2	5:E:202:PEB:H3A1	1.34	0.47
1:K:99:VAL:HG23	1:K:101:GLY:H	1.79	0.47
2:L:39:ASP:HB3	5:L:203:PEB:HHA1	1.96	0.47
4:b:145:LEU:HB2	4:b:188:TRP:HB3	1.97	0.47
1:I:127:TYR:CZ	5:I:201:PEB:HAA1	2.49	0.47
2:B:82:CYS:HA	5:B:202:PEB:HHA1	1.97	0.47
2:L:3:ASP:H	2:L:6:SER:HB2	1.80	0.47
1:A:85:ASP:CG	5:A:202:PEB:H1D1	2.40	0.47
2:B:44:ILE:HG13	2:B:142:ILE:HD11	1.97	0.47
1:C:54:GLU:HB3	1:C:133:PHE:HE2	1.80	0.47
2:F:19:VAL:HG21	1:K:98:VAL:HG21	1.97	0.47
4:b:154:ASP:HB3	4:b:183:TYR:CD2	2.50	0.47
1:A:1:MET:HA	1:A:1:MET:HE2	1.96	0.47
1:G:33:ARG:NE	1:G:151:GLU:OE2	2.48	0.47
2:H:39:ASP:HB3	5:H:203:PEB:HBA3	1.96	0.47
3:a:141:ASN:ND2	4:b:128:ILE:O	2.33	0.47
5:F:203:PEB:OD	1:K:28:GLN:NE2	2.45	0.47
2:H:74:TYR:C	2:H:75:THR:HG1	2.18	0.47
2:D:106:GLU:HA	2:D:110:LEU:HB2	1.97	0.47
2:F:44:ILE:HG13	2:F:142:ILE:HD11	1.97	0.47
2:B:58:GLY:HA3	6:B:201:PUB:HHC2	1.96	0.46
1:C:98:VAL:HG21	2:H:19:VAL:HG21	1.95	0.46
3:a:149:VAL:HG21	3:a:157:ILE:HG12	1.97	0.46
1:C:33:ARG:HB2	1:G:25:GLU:HG3	1.97	0.46
1:C:127:TYR:CZ	5:C:201:PEB:HAA1	2.50	0.46
2:D:74:TYR:OH	1:K:91:ARG:NH2	2.38	0.46
1:G:138:LEU:HD22	1:G:152:PHE:HD2	1.80	0.46
3:a:48:LEU:HD22	3:a:63:TYR:CZ	2.50	0.46
4:b:73:PRO:HG3	4:b:79:ILE:HD12	1.97	0.46
2:B:38:LEU:HD21	1:I:27:VAL:HB	1.98	0.46
1:C:95:TYR:CG	2:H:9:VAL:HG13	2.50	0.46
2:J:74:TYR:O	2:J:78:ARG:HB2	2.16	0.46
5:C:201:PEB:HMB1	5:C:201:PEB:HNA	1.77	0.46
2:D:139:VAL:HG13	2:D:162:SER:HB3	1.97	0.46
1:K:138:LEU:HD22	1:K:152:PHE:HD2	1.79	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:a:129:GLN:NE2	3:a:180:GLY:O	2.39	0.46
4:b:179:THR:OG1	4:b:180:ASN:N	2.48	0.46
2:B:74:TYR:C	2:B:75:THR:HG1	2.21	0.46
2:L:133:ILE:HG12	6:L:201:PUB:HBC1	1.98	0.46
5:A:202:PEB:HNA	5:A:202:PEB:HMB3	1.81	0.46
2:F:164:GLU:HG2	2:F:168:TYR:CE2	2.50	0.46
1:C:114:ARG:HD3	1:K:114:ARG:CD	2.42	0.46
2:D:19:VAL:HG21	1:G:98:VAL:HG21	1.96	0.46
5:E:201:PEB:NA	5:E:201:PEB:HMB1	2.31	0.46
1:G:84:ARG:NH1	5:G:201:PEB:O2C	2.40	0.46
1:A:44:LEU:O	1:A:48:HIS:HB3	2.16	0.45
3:a:132:THR:HG21	3:a:181:LYS:HE2	1.97	0.45
1:C:27:VAL:HG21	2:H:98:LEU:HD11	1.98	0.45
4:b:147:LEU:HD21	4:b:184:MET:HG3	1.99	0.45
2:F:36:LYS:HG2	5:F:203:PEB:C2B	2.47	0.45
1:G:3:SER:N	1:G:6:THR:OG1	2.47	0.45
1:G:49:GLU:CD	1:G:49:GLU:H	2.23	0.45
2:L:92:TYR:CD2	2:L:109:CYS:HB2	2.51	0.45
3:a:12:SER:HB3	3:a:125:GLU:CD	2.37	0.45
3:a:170:PHE:CE1	4:b:184:MET:HE1	2.51	0.45
1:I:33:ARG:NH1	1:I:147:GLN:OE1	2.44	0.45
1:C:1:MET:HE1	1:C:108:TRP:CZ2	2.51	0.45
2:D:35:ASN:HB2	5:D:203:PEB:HAB2	1.97	0.45
4:b:128:ILE:HD11	4:b:217:ILE:HG21	1.98	0.45
2:B:9:VAL:HG21	1:I:99:VAL:HG23	1.99	0.45
5:D:202:PEB:HNA	5:D:202:PEB:CMB	2.30	0.45
2:F:2:LEU:HD22	2:F:6:SER:HB3	1.98	0.45
2:J:52:VAL:HG21	2:J:87:GLU:HA	1.98	0.45
1:K:137:ARG:HH22	5:K:202:PEB:CGB	2.30	0.45
1:E:82:CYS:HA	5:E:201:PEB:HHA1	1.97	0.45
3:a:113:GLN:HB2	4:b:46:ARG:CZ	2.47	0.45
4:b:146:CYS:HB2	4:b:219:PHE:CZ	2.50	0.45
1:A:99:VAL:HG23	2:J:9:VAL:HG21	1.98	0.45
3:a:57:ASN:HB3	3:a:65:VAL:O	2.17	0.45
4:b:48:LEU:HB3	4:b:59:LEU:HD23	1.99	0.45
5:A:201:PEB:C1B	2:J:154:ALA:HB3	2.47	0.45
2:F:74:TYR:CD2	2:F:75:THR:HG23	2.52	0.45
5:F:202:PEB:CMB	5:F:202:PEB:HNA	2.30	0.45
1:K:37:ARG:NH1	1:K:98:VAL:O	2.42	0.45
2:J:82:CYS:HA	5:J:202:PEB:CHA	2.48	0.44
1:A:17:ARG:NH2	1:I:102:THR:OG1	2.44	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:202:PEB:HNA	5:B:202:PEB:CMB	2.31	0.44
1:C:28:GLN:HA	1:C:31:ILE:HD12	1.98	0.44
1:G:33:ARG:HD2	1:G:33:ARG:HA	1.45	0.44
1:I:133:PHE:CZ	1:I:137:ARG:HD3	2.52	0.44
2:J:3:ASP:H	2:J:6:SER:HG	1.60	0.44
1:K:135:ARG:NH1	1:K:157:ASP:OD1	2.43	0.44
1:K:139:CYS:HB2	5:K:202:PEB:H3A1	1.52	0.44
2:L:154:ALA:HB3	5:L:203:PEB:HBB1	1.99	0.44
5:L:202:PEB:CMB	5:L:202:PEB:HNA	2.30	0.44
2:H:75:THR:OG1	2:H:78:ARG:NH1	2.50	0.44
1:C:82:CYS:HA	5:C:201:PEB:HHA1	1.99	0.44
1:C:126:SER:OG	5:C:201:PEB:HMA1	2.16	0.44
5:C:201:PEB:HHC2	2:L:76:ASN:ND2	2.32	0.44
2:D:74:TYR:O	2:D:78:ARG:HB2	2.17	0.44
3:a:96:PRO:HB3	4:b:98:TRP:CE3	2.52	0.44
4:b:66:GLY:O	4:b:83:ARG:NE	2.38	0.44
1:E:138:LEU:HD11	1:E:144:MET:HG2	1.99	0.44
5:H:203:PEB:HBB1	5:H:203:PEB:O1B	2.17	0.44
2:B:79:MET:HE2	5:G:201:PEB:HAC1	2.00	0.44
1:C:102:THR:OG1	1:G:17:ARG:NH2	2.33	0.44
2:F:92:TYR:CD2	2:F:109:CYS:HB2	2.52	0.44
2:L:1:MET:HE3	2:L:1:MET:HB2	1.83	0.44
1:C:137:ARG:HH22	5:C:202:PEB:CGB	2.29	0.44
1:G:59:CYS:SG	1:G:126:SER:HB3	2.58	0.44
2:J:37:ARG:NH1	2:J:97:LEU:O	2.36	0.44
1:C:117:TYR:CD1	1:C:122:LEU:HD12	2.53	0.44
2:J:3:ASP:N	2:J:6:SER:OG	2.32	0.44
3:a:140:LYS:HA	3:a:144:ASN:O	2.17	0.44
3:a:109:TRP:HA	3:a:112:ARG:HG3	2.00	0.44
1:K:142:ARG:HG2	5:K:202:PEB:HAA2	1.99	0.43
1:A:139:CYS:N	1:A:143:ASP:OD2	2.42	0.43
2:B:19:VAL:HG21	1:I:98:VAL:HG21	2.00	0.43
2:D:69:PRO:CG	2:F:16:ALA:HB2	2.48	0.43
4:b:147:LEU:HD22	4:b:148:LEU:N	2.33	0.43
1:C:82:CYS:HA	5:C:201:PEB:CHA	2.48	0.43
2:H:82:CYS:HA	5:H:202:PEB:HHA1	2.00	0.43
3:a:63:TYR:HD2	3:a:76:LEU:HD11	1.82	0.43
1:E:82:CYS:SG	5:E:201:PEB:HAA2	2.58	0.43
1:G:147:GLN:OE1	5:H:203:PEB:HHC2	2.18	0.43
1:I:59:CYS:SG	1:I:126:SER:HB3	2.58	0.43
1:K:82:CYS:SG	5:K:201:PEB:HAA2	2.59	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:123:PRO:O	1:C:126:SER:OG	2.36	0.43
2:D:59:MET:HE3	2:D:66:LEU:HD13	2.01	0.43
5:A:201:PEB:ND	2:J:35:ASN:OD1	2.47	0.43
1:C:162:SER:O	1:K:118:ARG:NH2	2.51	0.43
1:I:109:GLY:O	1:I:113:ALA:HB2	2.18	0.43
4:b:37:LEU:HD11	4:b:91:GLY:HA3	2.01	0.43
1:A:116:VAL:HG11	5:A:202:PEB:HMC2	2.00	0.43
2:D:43:SER:HA	2:D:151:MET:SD	2.59	0.43
2:J:147:PRO:HB2	2:J:148:GLN:NE2	2.33	0.43
5:A:204:PEB:C1C	2:B:35:ASN:HB3	2.49	0.43
1:I:139:CYS:N	1:I:143:ASP:OD2	2.45	0.43
4:b:147:LEU:HD22	4:b:148:LEU:H	1.84	0.43
2:L:110:LEU:HD21	2:L:172:VAL:HG22	2.00	0.43
3:a:4:VAL:HG11	3:a:91:CYS:O	2.19	0.42
3:a:111:THR:HB	4:b:49:TYR:CE2	2.53	0.42
4:b:84:ASN:ND2	4:b:84:ASN:O	2.52	0.42
2:B:85:ASP:CG	5:B:202:PEB:H1D1	2.43	0.42
3:a:35:PHE:HZ	3:a:96:PRO:HG3	1.83	0.42
3:a:51:GLN:OE1	3:a:58:ALA:N	2.47	0.42
2:D:38:LEU:HD21	1:G:27:VAL:HB	2.00	0.42
1:E:52:VAL:HG21	1:E:87:ASP:HA	2.02	0.42
5:E:202:PEB:H2A1	5:E:202:PEB:HBA3	1.76	0.42
1:G:20:SER:N	1:G:23:ASP:OD2	2.51	0.42
1:K:8:THR:HG21	1:K:26:SER:HB2	2.00	0.42
2:L:58:GLY:HA3	6:L:201:PUB:HHC2	2.01	0.42
1:E:99:VAL:HG23	2:L:9:VAL:HG21	2.00	0.42
2:F:59:MET:HE2	2:F:59:MET:HB3	1.90	0.42
2:H:135:LYS:HG3	2:H:166:ALA:HA	2.01	0.42
1:I:78:LYS:HB3	5:I:201:PEB:CMB	2.46	0.42
3:a:36:TRP:HB2	3:a:49:ILE:HG22	2.01	0.42
3:a:113:GLN:HG2	3:a:114:MET:N	2.33	0.42
1:E:109:GLY:O	1:E:113:ALA:HB2	2.20	0.42
3:a:110:ASP:HB3	4:b:32:TYR:CD1	2.54	0.42
4:b:18:SER:HA	4:b:82:LEU:O	2.19	0.42
1:C:27:VAL:HB	2:H:38:LEU:HD21	2.01	0.42
2:D:146:ALA:O	2:D:150:LYS:NZ	2.37	0.42
2:F:154:ALA:HB3	5:F:203:PEB:HBB1	2.01	0.42
1:G:3:SER:H	1:G:6:THR:HG1	1.68	0.42
1:G:44:LEU:O	1:G:48:HIS:HB3	2.19	0.42
2:J:24:LEU:HD23	2:J:24:LEU:HA	1.79	0.42
2:J:59:MET:HE1	2:J:82:CYS:SG	2.60	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:85:ASP:OD1	5:K:201:PEB:H1D1	2.19	0.42
4:b:154:ASP:HB3	4:b:183:TYR:CG	2.54	0.42
1:A:98:VAL:HG21	2:J:19:VAL:HG21	2.01	0.42
2:F:140:ALA:HB3	6:F:201:PUB:HMB3	2.02	0.42
2:L:74:TYR:O	2:L:75:THR:OG1	2.22	0.42
2:L:106:GLU:OE1	2:L:110:LEU:HD12	2.20	0.42
4:b:69:TYR:HE1	4:b:71:HIS:HB2	1.84	0.42
1:G:44:LEU:HD22	1:G:152:PHE:HE1	1.85	0.42
1:G:52:VAL:HG21	1:G:87:ASP:HA	2.02	0.42
1:K:137:ARG:HG3	5:K:202:PEB:HHC1	2.01	0.42
2:D:80:ALA:HB2	1:K:116:VAL:HG23	2.00	0.42
1:E:25:GLU:OE1	1:K:33:ARG:HB3	2.20	0.42
2:F:35:ASN:HB3	5:F:203:PEB:C1C	2.49	0.42
2:F:39:ASP:HB3	5:F:203:PEB:HHA1	2.02	0.42
2:H:44:ILE:HG13	2:H:142:ILE:HD11	2.01	0.42
3:a:11:VAL:HB	3:a:120:ILE:HD11	2.01	0.42
4:b:12:THR:N	4:b:207:GLU:OE1	2.53	0.42
1:G:127:TYR:CZ	5:G:201:PEB:HAA1	2.54	0.42
1:C:139:CYS:HB2	5:C:202:PEB:H3A1	1.67	0.41
2:D:112:GLY:HA2	2:D:115:GLU:OE1	2.20	0.41
2:F:82:CYS:HA	5:F:202:PEB:HHA1	2.02	0.41
2:F:105:LEU:HD21	2:F:172:VAL:HG23	2.02	0.41
1:I:8:THR:HG21	1:I:26:SER:HB2	2.01	0.41
1:I:146:ALA:O	1:I:150:VAL:HG23	2.20	0.41
3:a:168:THR:O	3:a:189:LYS:N	2.44	0.41
1:C:68:ASN:O	1:C:74:ASP:HB3	2.20	0.41
2:F:38:LEU:HD21	1:K:27:VAL:HB	2.01	0.41
1:G:37:ARG:HB2	1:G:97:LEU:O	2.19	0.41
2:B:69:PRO:HG3	2:D:16:ALA:HB2	2.01	0.41
2:D:135:LYS:HG3	2:D:166:ALA:HA	2.03	0.41
2:H:164:GLU:HG2	2:H:168:TYR:CE2	2.55	0.41
3:a:21:LEU:HD12	3:a:76:LEU:HD23	2.02	0.41
1:E:85:ASP:OD2	1:E:127:TYR:OH	2.36	0.41
1:G:144:MET:HB2	1:G:148:ALA:HB3	2.03	0.41
2:L:43:SER:HA	2:L:151:MET:SD	2.60	0.41
2:F:36:LYS:HB2	2:F:36:LYS:HE3	1.87	0.41
2:H:36:LYS:HD2	2:H:158:CYS:SG	2.61	0.41
5:I:201:PEB:HMB3	5:I:201:PEB:NA	2.35	0.41
1:K:52:VAL:HG11	1:K:87:ASP:HB2	2.02	0.41
4:b:59:LEU:HD21	4:b:68:TYR:HB2	2.03	0.41
2:B:74:TYR:O	2:B:75:THR:OG1	2.22	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:60:ILE:HD13	5:G:201:PEB:HBC2	2.01	0.41
6:F:201:PUB:HBB1	6:F:201:PUB:HHB1	2.03	0.41
1:C:25:GLU:HB3	1:G:4:VAL:HG21	2.03	0.41
2:J:60:ILE:HD11	2:J:73:CYS:SG	2.61	0.41
1:K:112:GLY:HA2	1:K:115:GLU:OE1	2.20	0.41
2:L:164:GLU:OE2	2:L:168:TYR:OH	2.29	0.41
4:b:129:PHE:CD2	4:b:145:LEU:HD23	2.55	0.41
1:A:98:VAL:HG22	2:J:24:LEU:HD21	2.02	0.41
1:C:143:ASP:CG	5:C:202:PEB:C1D	2.91	0.41
1:E:4:VAL:HG11	1:E:26:SER:O	2.21	0.41
1:I:137:ARG:HH22	5:I:202:PEB:CGB	2.33	0.41
5:I:201:PEB:HBA2	5:I:201:PEB:H2A1	1.82	0.41
2:J:43:SER:HA	2:J:151:MET:SD	2.61	0.41
1:K:59:CYS:SG	1:K:126:SER:HB2	2.60	0.41
3:a:114:MET:HE1	4:b:103:LYS:HB3	2.03	0.41
4:b:179:THR:HG22	4:b:184:MET:HE2	2.02	0.41
5:A:201:PEB:C4D	2:J:38:LEU:HD12	2.51	0.41
1:C:138:LEU:HD21	1:C:149:ALA:HA	2.03	0.41
5:K:201:PEB:HMB1	5:K:201:PEB:HNA	1.85	0.41
4:b:100:ARG:HD2	4:b:100:ARG:HA	1.84	0.41
4:b:209:ASN:ND2	4:b:215:GLN:HB2	2.36	0.41
2:D:5:PHE:O	2:D:9:VAL:HG13	2.22	0.40
2:D:95:TYR:HE1	1:G:19:PRO:HD3	1.86	0.40
1:E:138:LEU:HD22	1:E:152:PHE:HD2	1.86	0.40
2:H:35:ASN:HB3	5:H:203:PEB:C1C	2.51	0.40
6:H:201:PUB:HHB1	6:H:201:PUB:HBB1	2.02	0.40
3:a:128:SER:HA	3:a:153:TYR:OH	2.21	0.40
3:a:152:PHE:O	3:a:182:TYR:HB2	2.21	0.40
4:b:128:ILE:HG23	4:b:219:PHE:CE2	2.56	0.40
1:E:4:VAL:O	1:E:8:THR:HG23	2.20	0.40
1:E:25:GLU:HB3	1:K:4:VAL:HG21	2.03	0.40
2:H:114:LYS:HB2	2:H:176:ILE:HA	2.03	0.40
2:H:156:GLY:HA3	5:H:203:PEB:HMB3	2.03	0.40
3:a:83:LEU:HD12	3:a:83:LEU:HA	1.82	0.40
4:b:33:ILE:HD13	4:b:97:THR:HB	2.02	0.40
1:A:63:TYR:HB3	1:A:65:TYR:CE1	2.57	0.40
1:C:59:CYS:SG	1:C:126:SER:HB2	2.62	0.40
2:D:95:TYR:OH	1:G:17:ARG:O	2.33	0.40
3:a:48:LEU:HD13	3:a:63:TYR:CE2	2.55	0.40
4:b:148:LEU:HD21	4:b:204:VAL:HG21	2.02	0.40
1:A:117:TYR:HB3	1:A:122:LEU:O	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:69:PRO:CG	2:J:16:ALA:HB2	2.50	0.40
2:L:173:SER:O	2:L:176:ILE:HG12	2.21	0.40
3:a:167:ILE:H	3:a:167:ILE:HG13	1.74	0.40
1:C:147:GLN:OE1	5:D:203:PEB:HHC2	2.21	0.40
1:E:17:ARG:NH2	1:K:102:THR:OG1	2.36	0.40
1:K:137:ARG:CG	5:K:202:PEB:HHC1	2.52	0.40
5:K:201:PEB:HBA2	5:K:201:PEB:H2A1	1.90	0.40
4:b:89:ASP:O	4:b:93:TYR:OH	2.37	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	162/164 (99%)	160 (99%)	2 (1%)	0	100	100
1	C	162/164 (99%)	160 (99%)	2 (1%)	0	100	100
1	E	162/164 (99%)	159 (98%)	3 (2%)	0	100	100
1	G	162/164 (99%)	158 (98%)	3 (2%)	1 (1%)	22	16
1	I	162/164 (99%)	161 (99%)	1 (1%)	0	100	100
1	K	162/164 (99%)	160 (99%)	2 (1%)	0	100	100
2	B	174/176 (99%)	170 (98%)	3 (2%)	1 (1%)	22	16
2	D	174/176 (99%)	171 (98%)	2 (1%)	1 (1%)	22	16
2	F	174/176 (99%)	171 (98%)	2 (1%)	1 (1%)	22	16
2	H	174/176 (99%)	170 (98%)	3 (2%)	1 (1%)	22	16
2	J	174/176 (99%)	171 (98%)	2 (1%)	1 (1%)	22	16
2	L	174/176 (99%)	172 (99%)	1 (1%)	1 (1%)	22	16
3	a	176/239 (74%)	164 (93%)	11 (6%)	1 (1%)	22	16

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	b	189/237 (80%)	168 (89%)	21 (11%)	0	100	100
All	All	2381/2516 (95%)	2315 (97%)	58 (2%)	8 (0%)	38	34

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	34	ALA
2	B	76	ASN
2	D	76	ASN
2	F	76	ASN
2	H	76	ASN
2	J	76	ASN
2	L	76	ASN
3	a	96	PRO

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	128/128 (100%)	127 (99%)	1 (1%)	79	83
1	C	128/128 (100%)	128 (100%)	0	100	100
1	E	128/128 (100%)	128 (100%)	0	100	100
1	G	128/128 (100%)	125 (98%)	3 (2%)	45	47
1	I	128/128 (100%)	126 (98%)	2 (2%)	58	62
1	K	128/128 (100%)	127 (99%)	1 (1%)	79	83
2	B	139/139 (100%)	138 (99%)	1 (1%)	81	85
2	D	139/139 (100%)	138 (99%)	1 (1%)	81	85
2	F	139/139 (100%)	138 (99%)	1 (1%)	81	85
2	H	139/139 (100%)	137 (99%)	2 (1%)	62	67
2	J	139/139 (100%)	138 (99%)	1 (1%)	81	85
2	L	139/139 (100%)	137 (99%)	2 (1%)	62	67

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	a	143/214 (67%)	143 (100%)	0	100	100
4	b	170/216 (79%)	166 (98%)	4 (2%)	44	46
All	All	1915/2032 (94%)	1896 (99%)	19 (1%)	71	77

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	GLU
2	B	50	CYS
2	D	50	CYS
2	F	162	SER
1	G	33	ARG
1	G	37	ARG
1	G	49	GLU
2	H	50	CYS
2	H	162	SER
1	I	99	VAL
1	I	125	SER
2	J	9	VAL
1	K	77	GLU
2	L	72	ASN
2	L	102	SER
4	b	109	THR
4	b	112	VAL
4	b	146	CYS
4	b	189	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
2	D	42	ASN
2	D	148	GLN
1	E	76	GLN
1	G	28	GLN
1	G	32	GLN
1	G	48	HIS
1	G	76	GLN
1	G	121	ASN
2	H	42	ASN
3	a	8	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	b	54	ASN
4	b	209	ASN

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 ⓘ

30 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	$\# Z > 2$
5	PEB	E	201	-	43,46,46	0.97	1 (2%)	49,67,67	1.05	3 (6%)
5	PEB	A	204	-	43,46,46	0.95	1 (2%)	49,67,67	0.95	1 (2%)
6	PUB	L	201	-	42,46,46	0.87	1 (2%)	38,67,67	1.29	4 (10%)
5	PEB	A	201	-	43,46,46	0.93	0	49,67,67	0.97	2 (4%)
6	PUB	F	201	-	42,46,46	1.01	1 (2%)	38,67,67	1.19	4 (10%)
6	PUB	D	201	-	42,46,46	0.99	2 (4%)	38,67,67	1.19	4 (10%)
5	PEB	B	202	-	43,46,46	0.95	1 (2%)	49,67,67	1.11	5 (10%)
5	PEB	G	201	-	43,46,46	0.94	1 (2%)	49,67,67	1.02	3 (6%)
5	PEB	K	201	-	43,46,46	0.95	1 (2%)	49,67,67	1.04	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	PEB	D	202	-	43,46,46	0.97	1 (2%)	49,67,67	1.02	3 (6%)
5	PEB	I	202	-	43,46,46	0.94	1 (2%)	49,67,67	0.87	2 (4%)
5	PEB	H	202	-	43,46,46	0.97	1 (2%)	49,67,67	1.27	3 (6%)
5	PEB	L	203	-	43,46,46	0.93	0	49,67,67	0.96	1 (2%)
5	PEB	A	202	-	43,46,46	0.94	1 (2%)	49,67,67	1.23	4 (8%)
6	PUB	H	201	-	42,46,46	0.98	2 (4%)	38,67,67	1.29	4 (10%)
5	PEB	C	201	-	43,46,46	0.97	0	49,67,67	1.21	5 (10%)
5	PEB	D	203	-	43,46,46	1.17	2 (4%)	49,67,67	1.16	4 (8%)
5	PEB	H	203	-	43,46,46	0.93	0	49,67,67	1.10	2 (4%)
5	PEB	I	201	-	43,46,46	0.97	1 (2%)	49,67,67	1.06	4 (8%)
5	PEB	A	203	-	43,46,46	0.94	1 (2%)	49,67,67	0.88	1 (2%)
5	PEB	C	202	-	43,46,46	0.91	2 (4%)	49,67,67	1.27	5 (10%)
5	PEB	E	202	-	43,46,46	0.96	2 (4%)	49,67,67	1.46	7 (14%)
6	PUB	B	201	-	42,46,46	1.00	1 (2%)	38,67,67	1.52	4 (10%)
6	PUB	J	201	-	42,46,46	0.99	2 (4%)	38,67,67	1.20	4 (10%)
5	PEB	F	202	-	43,46,46	0.95	0	49,67,67	1.03	3 (6%)
5	PEB	F	203	-	43,46,46	0.93	0	49,67,67	0.95	2 (4%)
5	PEB	G	202	-	43,46,46	0.96	1 (2%)	49,67,67	0.95	1 (2%)
5	PEB	L	202	-	43,46,46	0.98	1 (2%)	49,67,67	1.01	2 (4%)
5	PEB	K	202	-	43,46,46	0.89	0	49,67,67	1.15	2 (4%)
5	PEB	J	202	-	43,46,46	0.97	0	49,67,67	1.15	7 (14%)

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
5	PEB	E	201	-	-	8/24/74/74	0/4/4/4
5	PEB	A	204	-	-	12/24/74/74	0/4/4/4
6	PUB	L	201	-	-	8/24/74/74	0/4/4/4
5	PEB	A	201	-	-	8/24/74/74	0/4/4/4
6	PUB	F	201	-	-	8/24/74/74	0/4/4/4
6	PUB	D	201	-	-	8/24/74/74	0/4/4/4
5	PEB	B	202	-	-	9/24/74/74	0/4/4/4
5	PEB	G	201	-	-	10/24/74/74	0/4/4/4

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PEB	K	201	-	-	9/24/74/74	0/4/4/4
5	PEB	D	202	-	-	9/24/74/74	0/4/4/4
5	PEB	I	202	-	-	6/24/74/74	0/4/4/4
5	PEB	H	202	-	-	9/24/74/74	0/4/4/4
5	PEB	L	203	-	-	10/24/74/74	0/4/4/4
5	PEB	A	202	-	-	14/24/74/74	0/4/4/4
6	PUB	H	201	-	-	8/24/74/74	0/4/4/4
5	PEB	C	201	-	-	8/24/74/74	0/4/4/4
5	PEB	D	203	-	-	10/24/74/74	0/4/4/4
5	PEB	H	203	-	-	9/24/74/74	0/4/4/4
5	PEB	I	201	-	-	11/24/74/74	0/4/4/4
5	PEB	A	203	-	-	9/24/74/74	0/4/4/4
5	PEB	C	202	-	-	13/24/74/74	0/4/4/4
5	PEB	E	202	-	-	8/24/74/74	0/4/4/4
6	PUB	B	201	-	-	8/24/74/74	0/4/4/4
6	PUB	J	201	-	-	2/24/74/74	0/4/4/4
5	PEB	F	202	-	-	6/24/74/74	0/4/4/4
5	PEB	F	203	-	-	10/24/74/74	0/4/4/4
5	PEB	G	202	-	-	9/24/74/74	0/4/4/4
5	PEB	L	202	-	-	6/24/74/74	0/4/4/4
5	PEB	K	202	-	-	12/24/74/74	0/4/4/4
5	PEB	J	202	-	-	9/24/74/74	0/4/4/4

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	203	PEB	CHB-C4B	5.48	1.40	1.35
6	F	201	PUB	CHB-C1C	4.16	1.39	1.35
6	H	201	PUB	CHB-C1C	3.97	1.39	1.35
6	J	201	PUB	CHB-C1C	3.88	1.38	1.35
6	B	201	PUB	CHB-C1C	3.87	1.38	1.35
6	D	201	PUB	CHB-C1C	3.86	1.38	1.35
6	L	201	PUB	CHB-C1C	2.80	1.37	1.35
5	D	203	PEB	CHA-C4A	2.66	1.40	1.36
5	H	202	PEB	CHB-C4B	2.47	1.37	1.35
5	A	203	PEB	CHB-C4B	2.22	1.37	1.35
5	A	202	PEB	C1B-NB	-2.21	1.31	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	202	PEB	CHA-C1B	2.19	1.45	1.40
5	A	204	PEB	CHB-C4B	2.13	1.37	1.35
5	G	202	PEB	CHB-C4B	2.13	1.37	1.35
5	E	202	PEB	C1B-NB	-2.11	1.31	1.36
5	D	202	PEB	CHA-C1B	2.10	1.45	1.40
6	H	201	PUB	C2B-C1B	-2.07	1.38	1.41
5	L	202	PEB	CHA-C1B	2.06	1.45	1.40
5	E	202	PEB	CHA-C1B	2.05	1.45	1.40
6	J	201	PUB	C2B-C1B	-2.05	1.38	1.41
5	I	202	PEB	CHB-C4B	2.05	1.37	1.35
5	G	201	PEB	C1B-NB	-2.03	1.32	1.36
5	I	201	PEB	CHA-C1B	2.03	1.45	1.40
6	D	201	PUB	C2B-C1B	-2.02	1.38	1.41
5	B	202	PEB	C1B-NB	-2.01	1.32	1.36
5	C	202	PEB	CHB-C4B	2.01	1.37	1.35
5	E	201	PEB	C1B-NB	-2.00	1.32	1.36
5	K	201	PEB	C1B-NB	-2.00	1.32	1.36

All (97) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	201	PUB	CHA-C4A-NA	-6.57	106.75	113.84
6	L	201	PUB	CHA-C4A-NA	-4.96	108.49	113.84
5	K	202	PEB	CHB-C4B-NB	-4.71	122.37	128.76
5	E	202	PEB	C1B-CHA-C4A	-4.52	118.08	127.25
5	E	202	PEB	CHB-C4B-NB	-4.31	122.91	128.76
5	C	202	PEB	CHC-C1D-ND	4.30	118.47	113.84
5	A	202	PEB	CHB-C4B-NB	-4.12	123.17	128.76
6	J	201	PUB	CHA-C4A-NA	-4.08	109.44	113.84
6	F	201	PUB	CHA-C4A-NA	-3.99	109.54	113.84
5	A	201	PEB	CHB-C4B-NB	-3.97	123.37	128.76
5	H	202	PEB	CHB-C4B-NB	-3.94	123.41	128.76
6	D	201	PUB	CHA-C4A-NA	-3.92	109.61	113.84
5	E	202	PEB	CHA-C4A-NA	-3.87	120.80	125.63
6	H	201	PUB	CMA-C2A-C1A	3.73	129.02	121.21
5	I	201	PEB	CHB-C4B-NB	-3.68	123.77	128.76
5	D	203	PEB	C1A-NA-C4A	-3.33	109.23	113.41
5	E	201	PEB	CHB-C4B-NB	-3.31	124.27	128.76
5	G	202	PEB	CHB-C4B-NB	-3.30	124.29	128.76
5	C	202	PEB	CHB-C4B-NB	-3.30	124.29	128.76
6	H	201	PUB	CHA-C4A-NA	-3.27	110.31	113.84
5	K	201	PEB	CHB-C4B-NB	-3.27	124.32	128.76

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	202	PEB	CHB-C4B-NB	-3.27	124.32	128.76
5	H	203	PEB	CHB-C4B-NB	-3.25	124.36	128.76
5	A	204	PEB	CHB-C4B-NB	-3.24	124.37	128.76
6	H	201	PUB	CMA-C2A-C3A	-3.19	123.39	129.68
5	H	202	PEB	CHA-C1B-NB	-3.17	118.11	124.95
5	A	202	PEB	CHA-C4A-NA	-3.16	121.69	125.63
5	G	201	PEB	CHB-C4B-NB	-3.06	124.61	128.76
5	H	203	PEB	CHC-C1D-ND	-3.00	110.60	113.84
5	C	201	PEB	CMB-C2B-C1B	2.97	129.72	125.10
6	B	201	PUB	CHB-C1C-NC	-2.93	124.78	128.76
6	D	201	PUB	CHB-C1C-NC	-2.86	124.88	128.76
6	J	201	PUB	CHB-C1C-NC	-2.84	124.91	128.76
5	D	203	PEB	CHC-C1D-ND	-2.80	110.82	113.84
6	F	201	PUB	CHB-C1C-NC	-2.79	124.97	128.76
5	I	202	PEB	CHB-C4B-NB	-2.77	125.00	128.76
6	H	201	PUB	CHB-C1C-NC	-2.76	125.01	128.76
6	L	201	PUB	CMA-C2A-C1A	2.76	126.97	121.21
6	D	201	PUB	CMA-C2A-C1A	2.74	126.95	121.21
5	C	202	PEB	C1C-CHB-C4B	2.70	132.35	128.73
5	F	202	PEB	CHB-C4B-NB	-2.66	125.14	128.76
6	F	201	PUB	CMA-C2A-C1A	2.66	126.77	121.21
5	F	203	PEB	C1C-CHB-C4B	2.64	132.27	128.73
6	J	201	PUB	CMA-C2A-C1A	2.64	126.73	121.21
5	C	201	PEB	CHC-C1D-ND	-2.63	111.00	113.84
6	L	201	PUB	CHB-C1C-NC	-2.59	125.25	128.76
5	E	202	PEB	OA-C1A-C2A	2.59	128.23	126.17
5	C	201	PEB	OA-C1A-C2A	2.54	128.20	126.17
5	J	202	PEB	CMB-C2B-C1B	2.52	129.01	125.10
5	A	202	PEB	CHA-C1B-NB	-2.52	119.52	124.95
5	D	203	PEB	CHB-C4B-NB	-2.52	125.34	128.76
5	H	202	PEB	C1B-C2B-C3B	-2.50	103.64	106.48
5	J	202	PEB	C1A-NA-C4A	2.47	116.50	113.41
5	L	202	PEB	CHB-C4B-NB	-2.47	125.41	128.76
5	C	201	PEB	C1A-NA-C4A	2.44	116.47	113.41
5	E	202	PEB	C1A-NA-C4A	2.43	116.45	113.41
5	A	203	PEB	C1C-CHB-C4B	2.40	131.95	128.73
5	E	202	PEB	C1C-CHB-C4B	-2.40	125.51	128.73
5	B	202	PEB	CHA-C1B-NB	-2.40	119.76	124.95
5	L	203	PEB	C1C-CHB-C4B	2.39	131.93	128.73
5	I	201	PEB	OA-C1A-C2A	2.37	128.06	126.17
6	D	201	PUB	CMA-C2A-C3A	-2.37	125.02	129.68
6	L	201	PUB	CMA-C2A-C3A	-2.37	125.02	129.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	J	201	PUB	CMA-C2A-C3A	-2.35	125.06	129.68
5	B	202	PEB	C1B-CHA-C4A	2.34	132.01	127.25
6	F	201	PUB	CMA-C2A-C3A	-2.33	125.08	129.68
5	G	201	PEB	C2A-C3A-C4A	2.32	104.82	101.34
5	J	202	PEB	CHB-C4B-C3B	-2.31	120.07	125.40
5	C	202	PEB	C2A-C3A-C4A	2.30	104.78	101.34
5	D	202	PEB	CHB-C4B-NB	-2.26	125.69	128.76
5	E	201	PEB	CHA-C4A-NA	-2.20	122.89	125.63
5	D	202	PEB	C1A-NA-C4A	2.20	116.16	113.41
5	C	201	PEB	CHB-C4B-C3B	-2.19	120.34	125.40
5	J	202	PEB	OA-C1A-C2A	2.18	127.91	126.17
5	A	201	PEB	CHA-C1B-NB	-2.18	120.25	124.95
5	J	202	PEB	CHC-C1D-ND	-2.16	111.51	113.84
5	F	203	PEB	CHC-C1D-ND	-2.15	111.52	113.84
5	J	202	PEB	C1C-CHB-C4B	2.15	131.61	128.73
5	E	201	PEB	C2A-C3A-C4A	2.14	104.54	101.34
5	J	202	PEB	C2A-C3A-C4A	2.13	104.53	101.34
6	B	201	PUB	CMA-C2A-C3A	-2.13	125.49	129.68
5	K	202	PEB	C2A-C3A-C4A	2.12	104.51	101.34
5	I	201	PEB	C2A-C3A-C4A	2.12	104.51	101.34
5	L	202	PEB	C1A-NA-C4A	2.11	116.05	113.41
5	D	203	PEB	C1B-C2B-C3B	-2.11	104.08	106.48
5	F	202	PEB	C2A-C3A-C4A	2.11	104.49	101.34
5	B	202	PEB	C1A-NA-C4A	2.10	116.04	113.41
5	D	202	PEB	C2A-C3A-C4A	2.10	104.49	101.34
5	E	202	PEB	C2A-C3A-C4A	2.10	104.49	101.34
6	B	201	PUB	CMA-C2A-C1A	2.04	125.48	121.21
5	B	202	PEB	C2A-C3A-C4A	2.03	104.38	101.34
5	I	201	PEB	C1A-NA-C4A	2.03	115.95	113.41
5	F	202	PEB	C1A-NA-C4A	2.02	115.94	113.41
5	I	202	PEB	C2A-C3A-C4A	2.01	104.36	101.34
5	C	202	PEB	C1A-NA-C4A	2.01	115.92	113.41
5	A	202	PEB	O1C-CGC-CBC	-2.00	116.74	123.09
5	G	201	PEB	C1A-NA-C4A	2.00	115.91	113.41

There are no chirality outliers.

All (266) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	201	PEB	ND-C1D-CHC-C4C
5	A	201	PEB	NA-C4A-CHA-C1B
5	A	201	PEB	C3A-C4A-CHA-C1B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	A	202	PEB	NC-C1C-CHB-C4B
5	A	202	PEB	C2C-C1C-CHB-C4B
5	A	202	PEB	C2A-C3A-CAA-CBA
5	A	202	PEB	NA-C4A-CHA-C1B
5	A	202	PEB	C3A-C4A-CHA-C1B
5	A	202	PEB	NB-C1B-CHA-C4A
5	A	202	PEB	NB-C4B-CHB-C1C
5	A	203	PEB	NA-C4A-CHA-C1B
5	A	203	PEB	C3A-C4A-CHA-C1B
5	A	203	PEB	NB-C1B-CHA-C4A
5	A	203	PEB	C2B-C1B-CHA-C4A
5	A	204	PEB	C2D-C3D-CAD-CBD
5	A	204	PEB	C4D-C3D-CAD-CBD
5	A	204	PEB	C2A-C3A-CAA-CBA
5	A	204	PEB	C4A-C3A-CAA-CBA
5	A	204	PEB	NA-C4A-CHA-C1B
5	A	204	PEB	C3A-C4A-CHA-C1B
5	A	204	PEB	NB-C1B-CHA-C4A
5	A	204	PEB	C2B-C1B-CHA-C4A
5	B	202	PEB	C2A-C3A-CAA-CBA
5	B	202	PEB	NA-C4A-CHA-C1B
5	B	202	PEB	C3A-C4A-CHA-C1B
5	B	202	PEB	NB-C1B-CHA-C4A
5	B	202	PEB	C2B-C1B-CHA-C4A
5	C	201	PEB	NA-C4A-CHA-C1B
5	C	201	PEB	C3A-C4A-CHA-C1B
5	C	201	PEB	NB-C1B-CHA-C4A
5	C	201	PEB	C2B-C1B-CHA-C4A
5	C	202	PEB	NC-C1C-CHB-C4B
5	C	202	PEB	NB-C1B-CHA-C4A
5	C	202	PEB	C2B-C1B-CHA-C4A
5	D	202	PEB	NA-C4A-CHA-C1B
5	D	202	PEB	NB-C1B-CHA-C4A
5	D	202	PEB	C2B-C1B-CHA-C4A
5	D	203	PEB	NC-C1C-CHB-C4B
5	D	203	PEB	C2C-C1C-CHB-C4B
5	D	203	PEB	NB-C1B-CHA-C4A
5	D	203	PEB	C2B-C1B-CHA-C4A
5	D	203	PEB	NB-C4B-CHB-C1C
5	D	203	PEB	C3B-C4B-CHB-C1C
5	E	201	PEB	NA-C4A-CHA-C1B
5	E	201	PEB	C3A-C4A-CHA-C1B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	E	201	PEB	NB-C1B-CHA-C4A
5	E	201	PEB	C2B-C1B-CHA-C4A
5	E	202	PEB	NC-C1C-CHB-C4B
5	E	202	PEB	C2C-C1C-CHB-C4B
5	E	202	PEB	NB-C1B-CHA-C4A
5	E	202	PEB	C2B-C1B-CHA-C4A
5	F	202	PEB	NA-C4A-CHA-C1B
5	F	202	PEB	C3A-C4A-CHA-C1B
5	F	202	PEB	NB-C1B-CHA-C4A
5	F	202	PEB	C2B-C1B-CHA-C4A
5	F	203	PEB	C2A-C3A-CAA-CBA
5	F	203	PEB	C4A-C3A-CAA-CBA
5	F	203	PEB	NA-C4A-CHA-C1B
5	F	203	PEB	C3A-C4A-CHA-C1B
5	F	203	PEB	NB-C1B-CHA-C4A
5	F	203	PEB	C2B-C1B-CHA-C4A
5	G	201	PEB	C2A-C3A-CAA-CBA
5	G	201	PEB	C4A-C3A-CAA-CBA
5	G	201	PEB	NA-C4A-CHA-C1B
5	G	201	PEB	C3A-C4A-CHA-C1B
5	G	201	PEB	NB-C1B-CHA-C4A
5	G	201	PEB	C2B-C1B-CHA-C4A
5	G	202	PEB	NA-C4A-CHA-C1B
5	G	202	PEB	C3A-C4A-CHA-C1B
5	G	202	PEB	NB-C1B-CHA-C4A
5	G	202	PEB	C2B-C1B-CHA-C4A
5	H	202	PEB	NC-C1C-CHB-C4B
5	H	202	PEB	C2C-C1C-CHB-C4B
5	H	202	PEB	NA-C4A-CHA-C1B
5	H	202	PEB	NB-C1B-CHA-C4A
5	H	202	PEB	C2B-C1B-CHA-C4A
5	H	202	PEB	NB-C4B-CHB-C1C
5	H	202	PEB	C3B-C4B-CHB-C1C
5	H	203	PEB	C2C-CAC-CBC-CGC
5	H	203	PEB	C2A-C3A-CAA-CBA
5	H	203	PEB	C4A-C3A-CAA-CBA
5	H	203	PEB	C3A-C4A-CHA-C1B
5	H	203	PEB	NB-C1B-CHA-C4A
5	H	203	PEB	C2B-C1B-CHA-C4A
5	I	201	PEB	NA-C4A-CHA-C1B
5	I	201	PEB	C3A-C4A-CHA-C1B
5	I	201	PEB	NB-C1B-CHA-C4A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	I	201	PEB	C2B-C1B-CHA-C4A
5	I	202	PEB	NB-C1B-CHA-C4A
5	I	202	PEB	C2B-C1B-CHA-C4A
5	J	202	PEB	C2A-C3A-CAA-CBA
5	J	202	PEB	NA-C4A-CHA-C1B
5	J	202	PEB	C3A-C4A-CHA-C1B
5	J	202	PEB	NB-C1B-CHA-C4A
5	J	202	PEB	C2B-C1B-CHA-C4A
5	K	201	PEB	NA-C4A-CHA-C1B
5	K	201	PEB	C3A-C4A-CHA-C1B
5	K	201	PEB	NB-C1B-CHA-C4A
5	K	201	PEB	C2B-C1B-CHA-C4A
5	K	202	PEB	NC-C1C-CHB-C4B
5	K	202	PEB	C2C-C1C-CHB-C4B
5	K	202	PEB	NA-C4A-CHA-C1B
5	K	202	PEB	C3A-C4A-CHA-C1B
5	K	202	PEB	NB-C1B-CHA-C4A
5	K	202	PEB	C2B-C1B-CHA-C4A
5	K	202	PEB	NB-C4B-CHB-C1C
5	K	202	PEB	C3B-C4B-CHB-C1C
5	L	202	PEB	NA-C4A-CHA-C1B
5	L	202	PEB	C3A-C4A-CHA-C1B
5	L	202	PEB	NB-C1B-CHA-C4A
5	L	202	PEB	C2B-C1B-CHA-C4A
5	L	203	PEB	C2A-C3A-CAA-CBA
5	L	203	PEB	C4A-C3A-CAA-CBA
5	L	203	PEB	NA-C4A-CHA-C1B
5	L	203	PEB	C3A-C4A-CHA-C1B
5	L	203	PEB	NB-C1B-CHA-C4A
5	L	203	PEB	C2B-C1B-CHA-C4A
5	L	203	PEB	C3B-CAB-CBB-CGB
6	B	201	PUB	C2B-C3B-CAB-CBB
6	B	201	PUB	C4B-C3B-CAB-CBB
6	D	201	PUB	C2A-C3A-CAA-CBA
6	F	201	PUB	C2A-C3A-CAA-CBA
6	H	201	PUB	NA-C4A-CHA-C1B
6	L	201	PUB	C2A-C3A-CAA-CBA
6	L	201	PUB	C4A-C3A-CAA-CBA
6	D	201	PUB	C4A-C3A-CAA-CBA
6	F	201	PUB	C4A-C3A-CAA-CBA
5	A	204	PEB	C3B-CAB-CBB-CGB
5	F	203	PEB	C3B-CAB-CBB-CGB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	A	202	PEB	C2B-C1B-CHA-C4A
5	C	202	PEB	NB-C4B-CHB-C1C
5	C	202	PEB	C2C-CAC-CBC-CGC
5	F	203	PEB	C2C-CAC-CBC-CGC
5	A	201	PEB	NB-C1B-CHA-C4A
5	A	201	PEB	C3B-CAB-CBB-CGB
5	H	203	PEB	C3B-CAB-CBB-CGB
5	A	201	PEB	C2B-C1B-CHA-C4A
5	A	202	PEB	C3B-C4B-CHB-C1C
5	C	202	PEB	C4D-C3D-CAD-CBD
5	I	201	PEB	C2A-C3A-CAA-CBA
5	C	202	PEB	C4B-C3B-CAB-CBB
5	A	201	PEB	C2C-CAC-CBC-CGC
5	C	202	PEB	C2B-C3B-CAB-CBB
5	A	202	PEB	C4A-C3A-CAA-CBA
6	D	201	PUB	C2B-C3B-CAB-CBB
6	F	201	PUB	C2B-C3B-CAB-CBB
6	H	201	PUB	C2B-C3B-CAB-CBB
6	F	201	PUB	C4B-C3B-CAB-CBB
6	H	201	PUB	C4B-C3B-CAB-CBB
5	A	201	PEB	C2D-C1D-CHC-C4C
6	H	201	PUB	C3A-C4A-CHA-C1B
6	B	201	PUB	NA-C4A-CHA-C1B
5	A	203	PEB	C2A-C3A-CAA-CBA
5	K	201	PEB	C2A-C3A-CAA-CBA
5	I	201	PEB	C3B-CAB-CBB-CGB
5	D	202	PEB	C2C-CAC-CBC-CGC
6	L	201	PUB	C2B-C3B-CAB-CBB
6	D	201	PUB	C4B-C3B-CAB-CBB
5	D	203	PEB	CAC-CBC-CGC-O2C
5	G	202	PEB	C3B-CAB-CBB-CGB
5	C	202	PEB	C3B-C4B-CHB-C1C
5	I	201	PEB	CAC-CBC-CGC-O2C
5	I	201	PEB	CAC-CBC-CGC-O1C
5	F	203	PEB	CAC-CBC-CGC-O2C
5	C	201	PEB	CAC-CBC-CGC-O1C
5	G	202	PEB	CAB-CBB-CGB-O1B
5	C	201	PEB	CAB-CBB-CGB-O1B
5	D	202	PEB	CAC-CBC-CGC-O2C
5	E	201	PEB	CAC-CBC-CGC-O1C
5	G	201	PEB	CAB-CBB-CGB-O1B
5	L	203	PEB	C2C-CAC-CBC-CGC

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	A	204	PEB	CAC-CBC-CGC-O2C
5	B	202	PEB	CAB-CBB-CGB-O2B
5	G	201	PEB	CAC-CBC-CGC-O1C
5	H	203	PEB	CAC-CBC-CGC-O1C
5	K	202	PEB	CAB-CBB-CGB-O2B
5	F	203	PEB	CAC-CBC-CGC-O1C
5	C	201	PEB	CAC-CBC-CGC-O2C
5	D	203	PEB	CAB-CBB-CGB-O2B
5	G	201	PEB	CAB-CBB-CGB-O2B
5	G	202	PEB	CAC-CBC-CGC-O2C
5	H	203	PEB	CAC-CBC-CGC-O2C
5	A	202	PEB	CAC-CBC-CGC-O2C
5	C	201	PEB	CAB-CBB-CGB-O2B
5	D	203	PEB	CAC-CBC-CGC-O1C
5	L	202	PEB	CAC-CBC-CGC-O1C
5	A	203	PEB	CAB-CBB-CGB-O1B
5	I	202	PEB	CAB-CBB-CGB-O2B
5	J	202	PEB	CAC-CBC-CGC-O1C
5	K	202	PEB	CAB-CBB-CGB-O1B
5	A	202	PEB	CAC-CBC-CGC-O1C
5	C	202	PEB	CAB-CBB-CGB-O2B
5	E	201	PEB	CAB-CBB-CGB-O1B
5	E	202	PEB	CAC-CBC-CGC-O1C
5	E	202	PEB	CAC-CBC-CGC-O2C
5	E	202	PEB	CAB-CBB-CGB-O1B
5	F	202	PEB	CAC-CBC-CGC-O1C
5	G	201	PEB	CAC-CBC-CGC-O2C
5	K	201	PEB	CAC-CBC-CGC-O2C
5	A	202	PEB	CAB-CBB-CGB-O1B
5	G	202	PEB	CAB-CBB-CGB-O2B
5	H	202	PEB	CAC-CBC-CGC-O1C
5	K	202	PEB	CAC-CBC-CGC-O1C
5	K	202	PEB	CAC-CBC-CGC-O2C
5	A	203	PEB	CAC-CBC-CGC-O2C
5	A	204	PEB	CAC-CBC-CGC-O1C
5	B	202	PEB	CAC-CBC-CGC-O1C
5	E	201	PEB	CAC-CBC-CGC-O2C
5	A	203	PEB	CAC-CBC-CGC-O1C
5	K	201	PEB	CAC-CBC-CGC-O1C
6	B	201	PUB	CAB-CBB-CGB-O2B
6	H	201	PUB	CAB-CBB-CGB-O2B
6	L	201	PUB	CAB-CBB-CGB-O2B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	G	202	PEB	CAC-CBC-CGC-O1C
6	F	201	PUB	CAB-CBB-CGB-O2B
6	J	201	PUB	CAB-CBB-CGB-O2B
5	B	202	PEB	CAB-CBB-CGB-O1B
5	C	202	PEB	CAB-CBB-CGB-O1B
5	E	202	PEB	CAB-CBB-CGB-O2B
5	I	202	PEB	CAB-CBB-CGB-O1B
6	D	201	PUB	CAB-CBB-CGB-O2B
5	D	202	PEB	C3A-C4A-CHA-C1B
5	A	203	PEB	CAB-CBB-CGB-O2B
5	B	202	PEB	CAC-CBC-CGC-O2C
5	D	203	PEB	CAB-CBB-CGB-O1B
5	E	201	PEB	CAB-CBB-CGB-O2B
6	H	201	PUB	CAB-CBB-CGB-O1B
5	A	204	PEB	C2C-CAC-CBC-CGC
5	A	202	PEB	CAB-CBB-CGB-O2B
6	L	201	PUB	CAC-CBC-CGC-O2C
6	L	201	PUB	CAB-CBB-CGB-O1B
5	D	202	PEB	CAC-CBC-CGC-O1C
5	K	201	PEB	CAB-CBB-CGB-O1B
5	H	202	PEB	CAC-CBC-CGC-O2C
5	F	202	PEB	CAC-CBC-CGC-O2C
5	J	202	PEB	CAC-CBC-CGC-O2C
6	B	201	PUB	CAB-CBB-CGB-O1B
5	I	201	PEB	CAB-CBB-CGB-O2B
6	D	201	PUB	CAC-CBC-CGC-O2C
5	J	202	PEB	CAB-CBB-CGB-O2B
5	L	202	PEB	CAC-CBC-CGC-O2C
6	H	201	PUB	CAC-CBC-CGC-O2C
6	F	201	PUB	CAB-CBB-CGB-O1B
6	B	201	PUB	CAC-CBC-CGC-O2C
6	D	201	PUB	CAB-CBB-CGB-O1B
6	F	201	PUB	CAC-CBC-CGC-O2C
5	L	203	PEB	CAC-CBC-CGC-O2C
6	D	201	PUB	CAC-CBC-CGC-O1C
6	J	201	PUB	CAB-CBB-CGB-O1B
5	I	202	PEB	CAC-CBC-CGC-O2C
5	L	203	PEB	CAC-CBC-CGC-O1C
5	J	202	PEB	CAB-CBB-CGB-O1B
6	L	201	PUB	CAC-CBC-CGC-O1C
6	L	201	PUB	C4B-C3B-CAB-CBB
5	I	201	PEB	CAB-CBB-CGB-O1B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	I	202	PEB	CAC-CBC-CGC-O1C
5	C	202	PEB	CAC-CBC-CGC-O1C
6	F	201	PUB	CAC-CBC-CGC-O1C
5	C	202	PEB	CAC-CBC-CGC-O2C
6	B	201	PUB	CAC-CBC-CGC-O1C
5	D	202	PEB	CAB-CBB-CGB-O2B
6	H	201	PUB	CAC-CBC-CGC-O1C
5	K	201	PEB	CAB-CBB-CGB-O2B
6	B	201	PUB	C3A-C4A-CHA-C1B
5	D	202	PEB	CAB-CBB-CGB-O1B
5	I	201	PEB	C2B-C3B-CAB-CBB

There are no ring outliers.

30 monomers are involved in 124 short contacts:

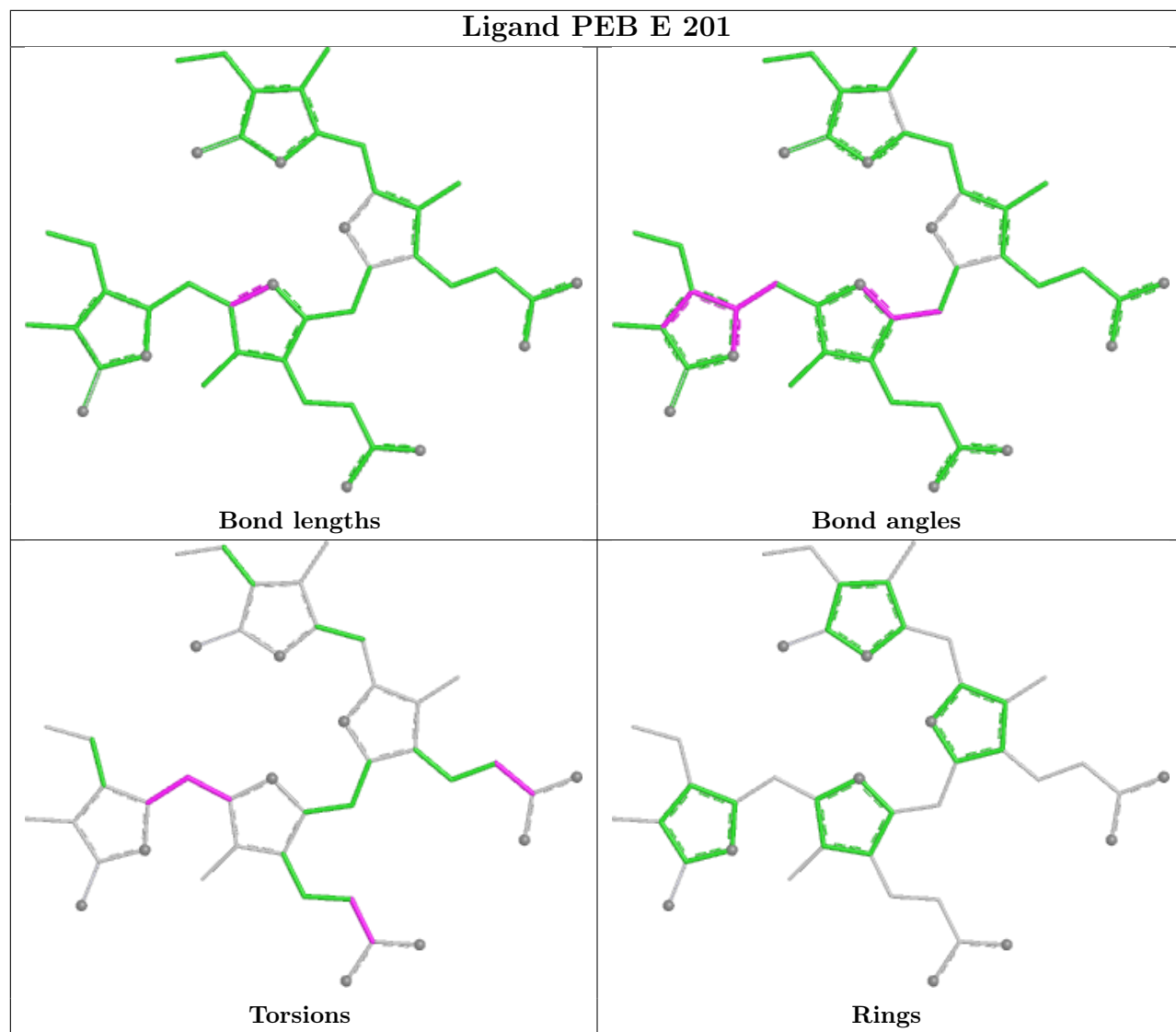
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	201	PEB	8	0
5	A	204	PEB	1	0
6	L	201	PUB	3	0
5	A	201	PEB	3	0
6	F	201	PUB	3	0
6	D	201	PUB	1	0
5	B	202	PEB	3	0
5	G	201	PEB	8	0
5	K	201	PEB	9	0
5	D	202	PEB	1	0
5	I	202	PEB	1	0
5	H	202	PEB	5	0
5	L	203	PEB	3	0
5	A	202	PEB	6	0
6	H	201	PUB	1	0
5	C	201	PEB	12	0
5	D	203	PEB	2	0
5	H	203	PEB	8	0
5	I	201	PEB	10	0
5	A	203	PEB	1	0
5	C	202	PEB	7	0
5	E	202	PEB	5	0
6	B	201	PUB	2	0
6	J	201	PUB	1	0
5	F	202	PEB	4	0
5	F	203	PEB	6	0

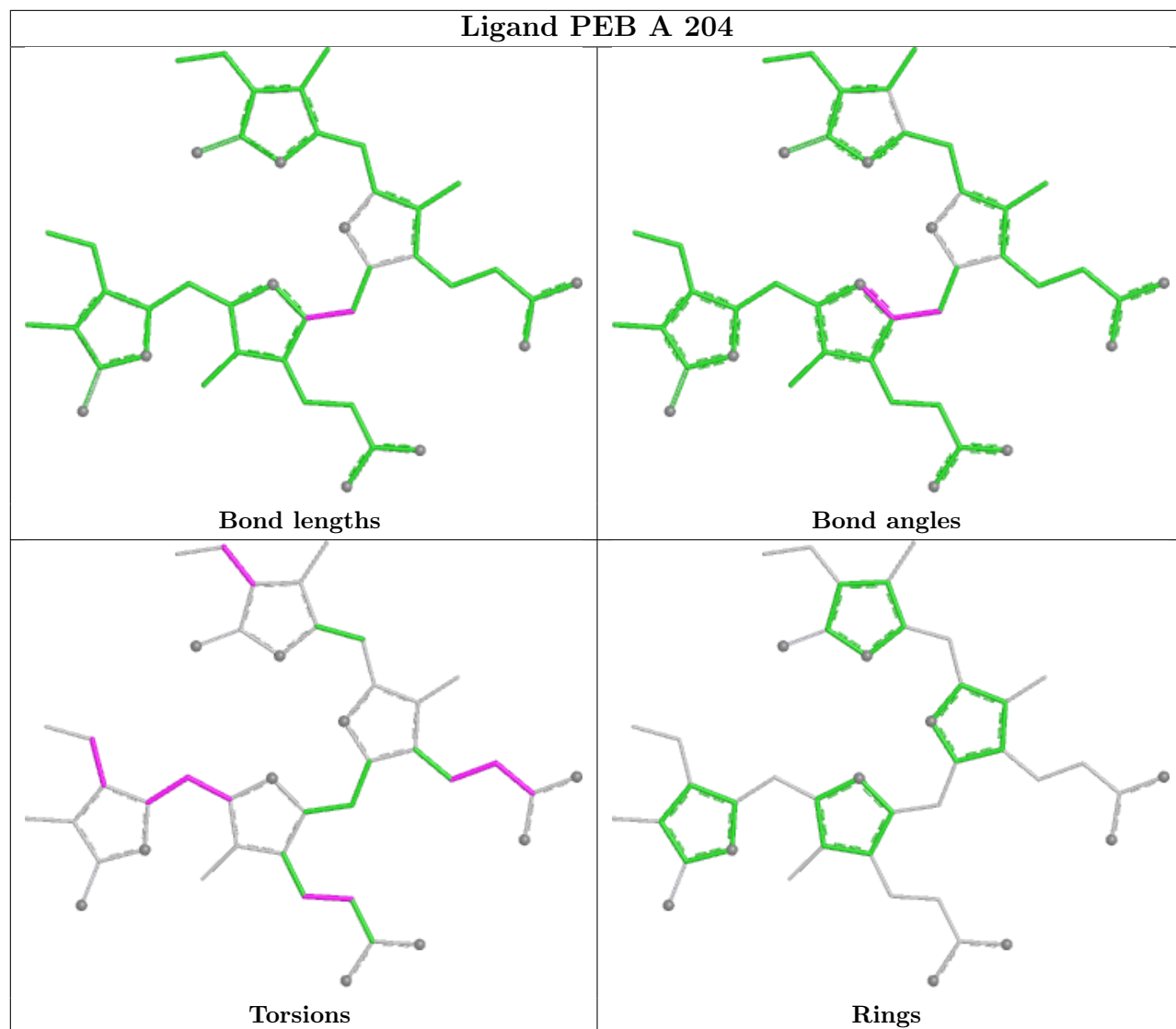
Continued on next page...

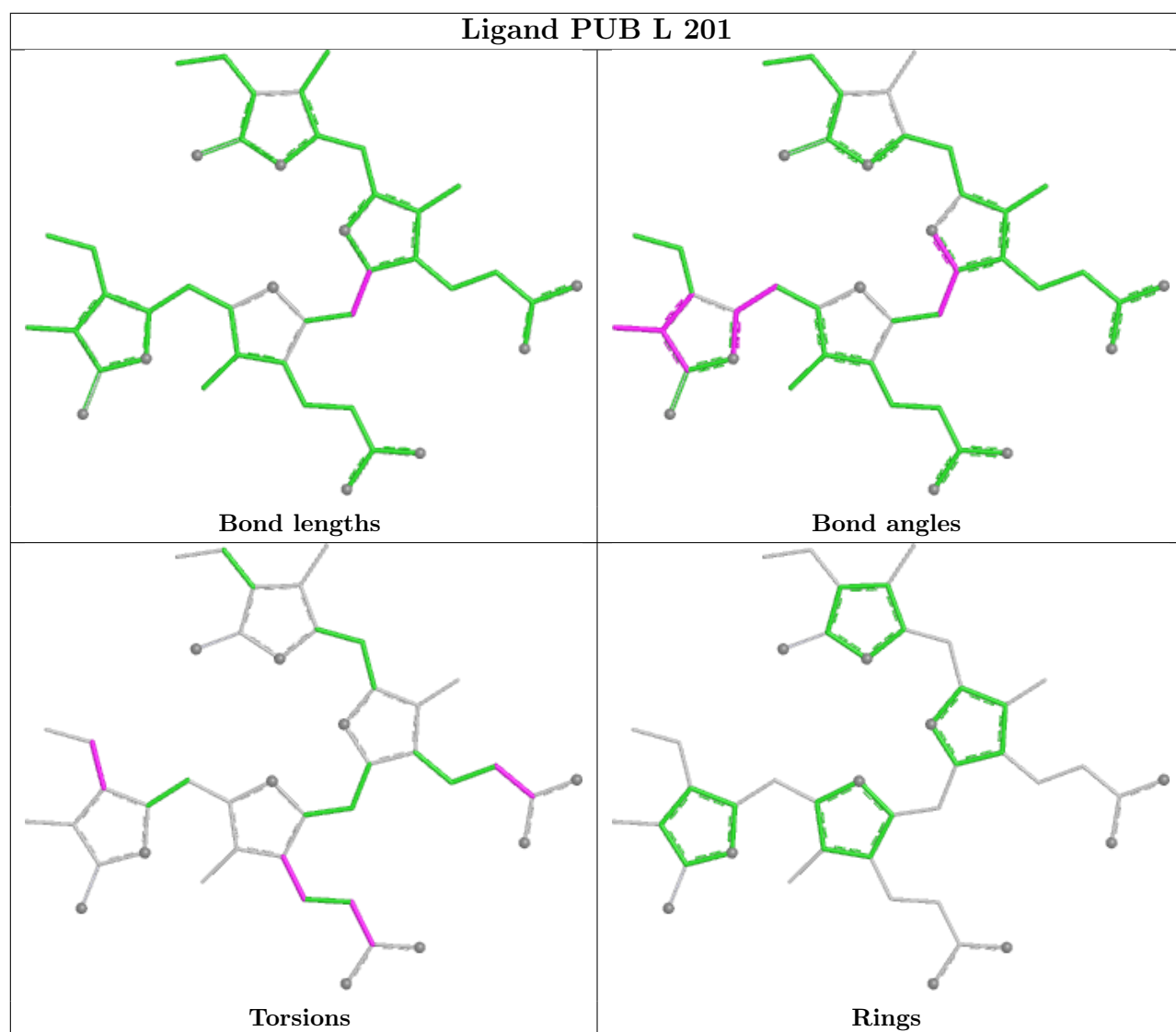
Continued from previous page...

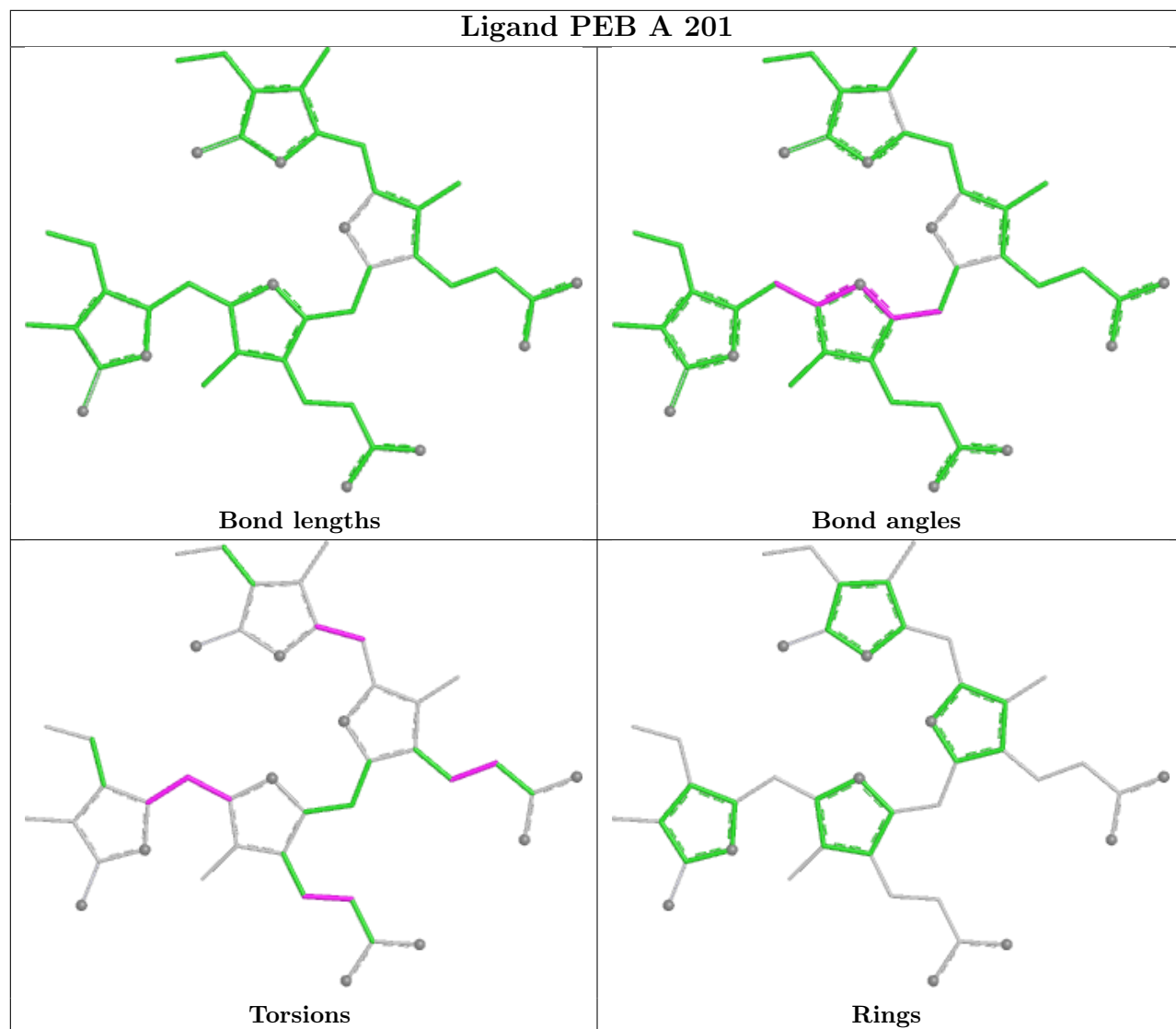
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	G	202	PEB	1	0
5	L	202	PEB	2	0
5	K	202	PEB	5	0
5	J	202	PEB	2	0

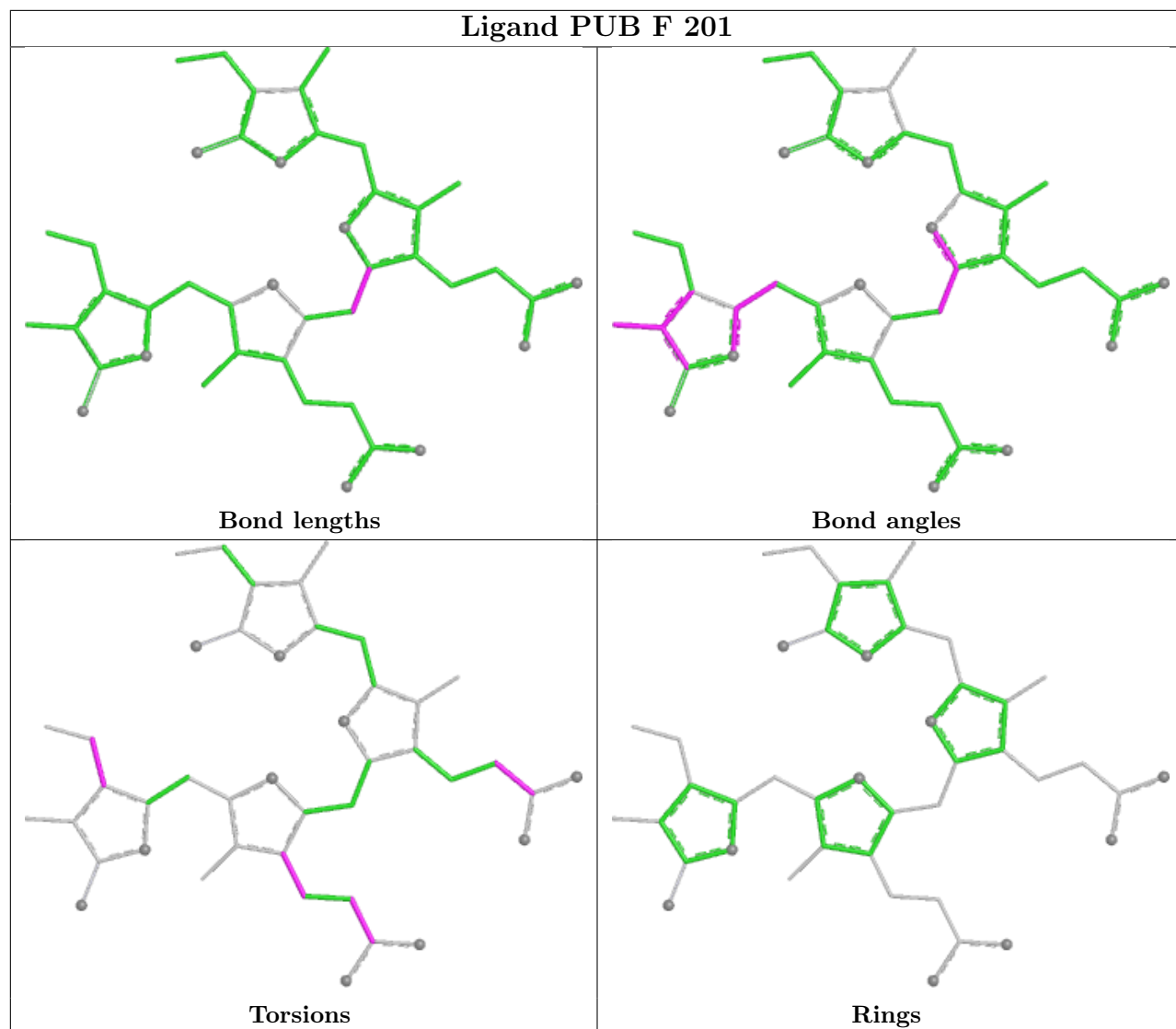
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

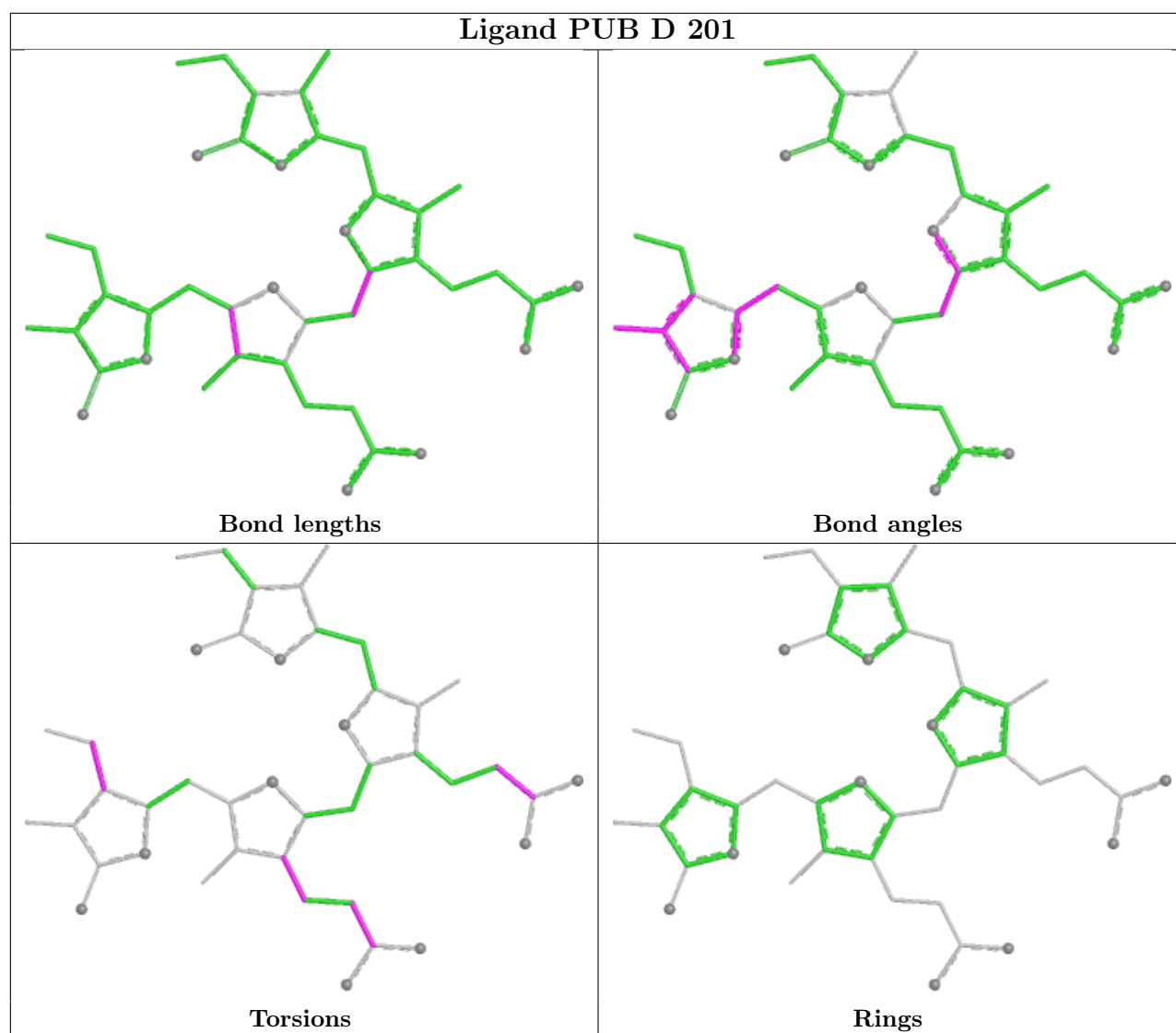


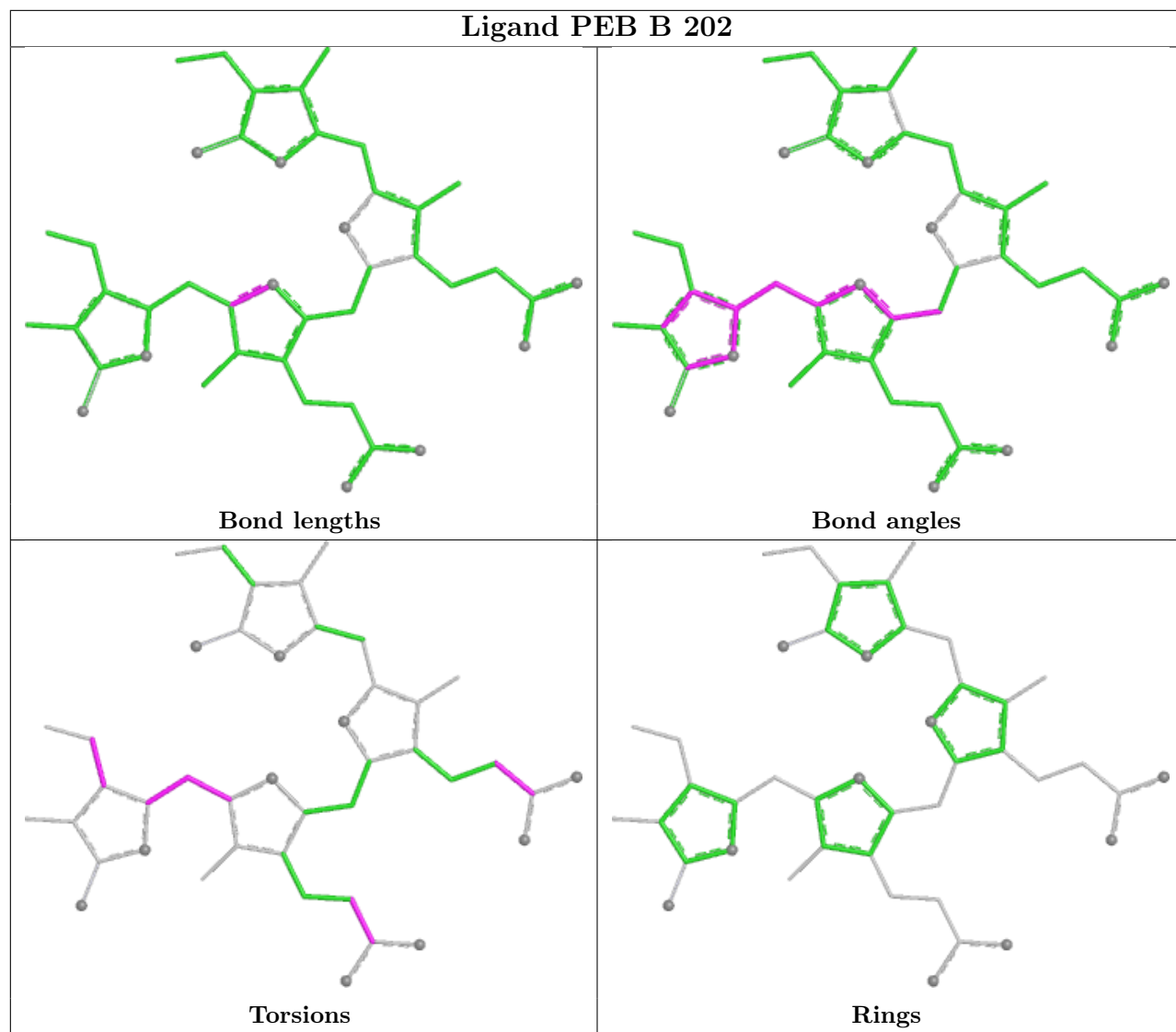


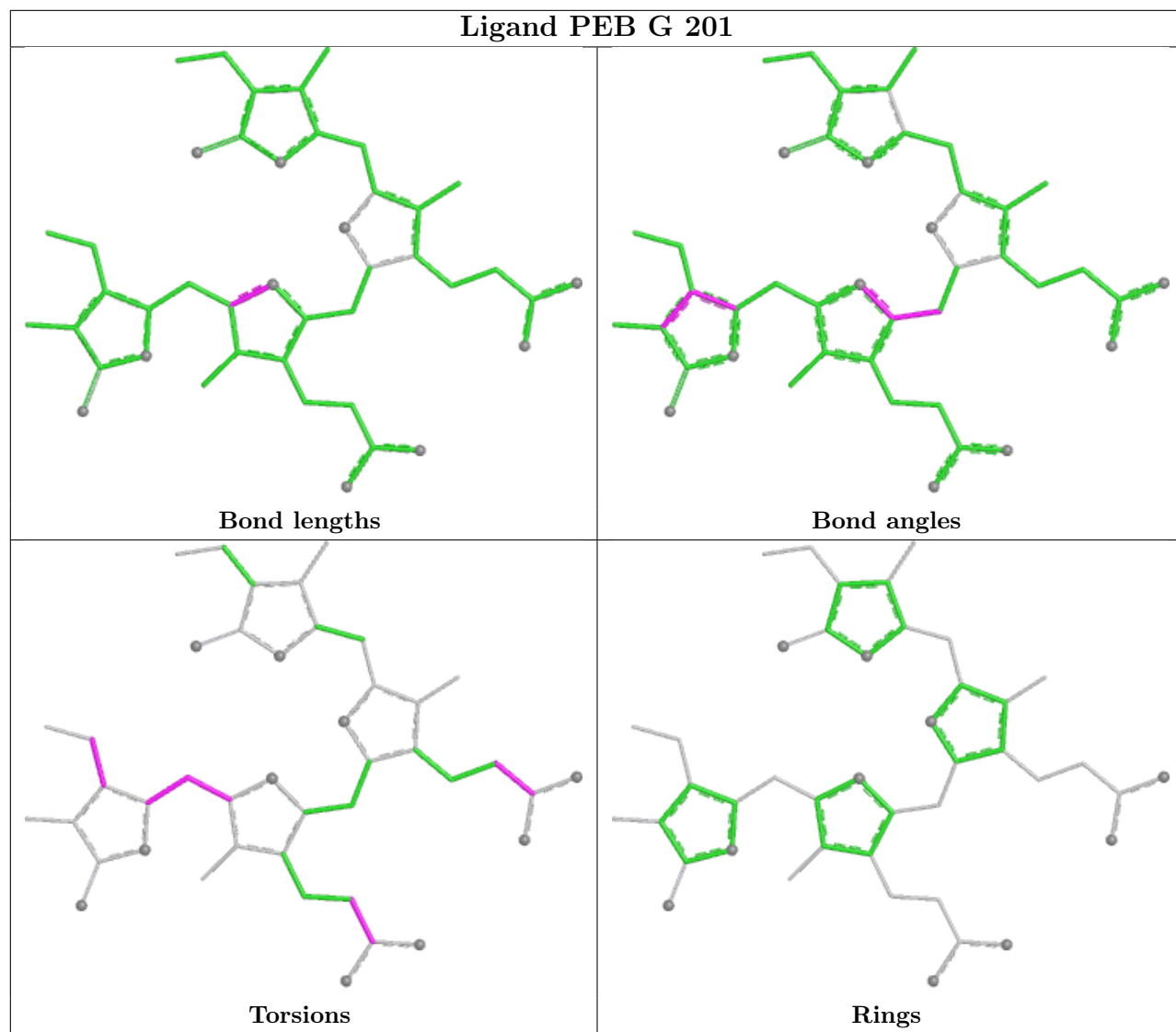


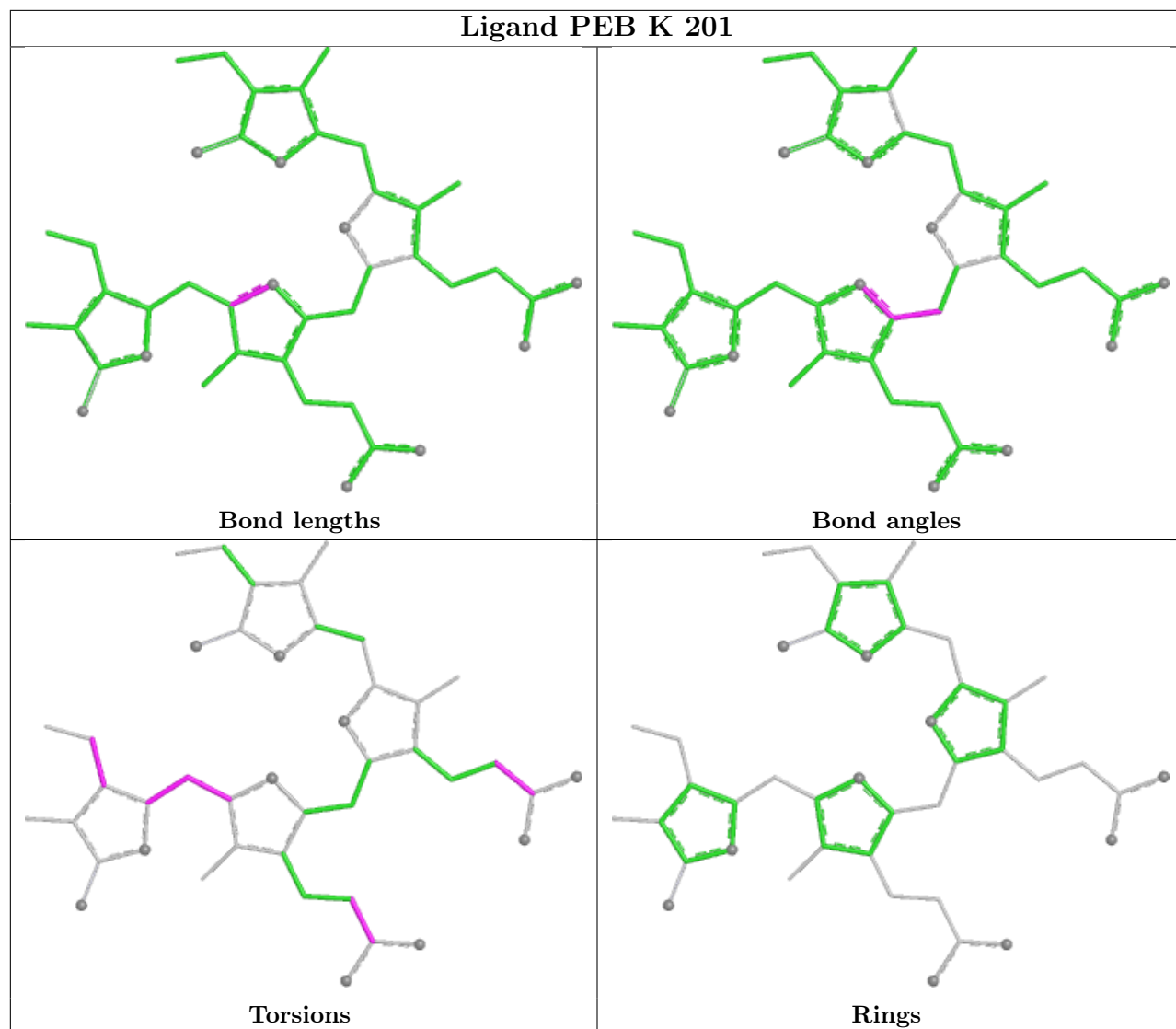


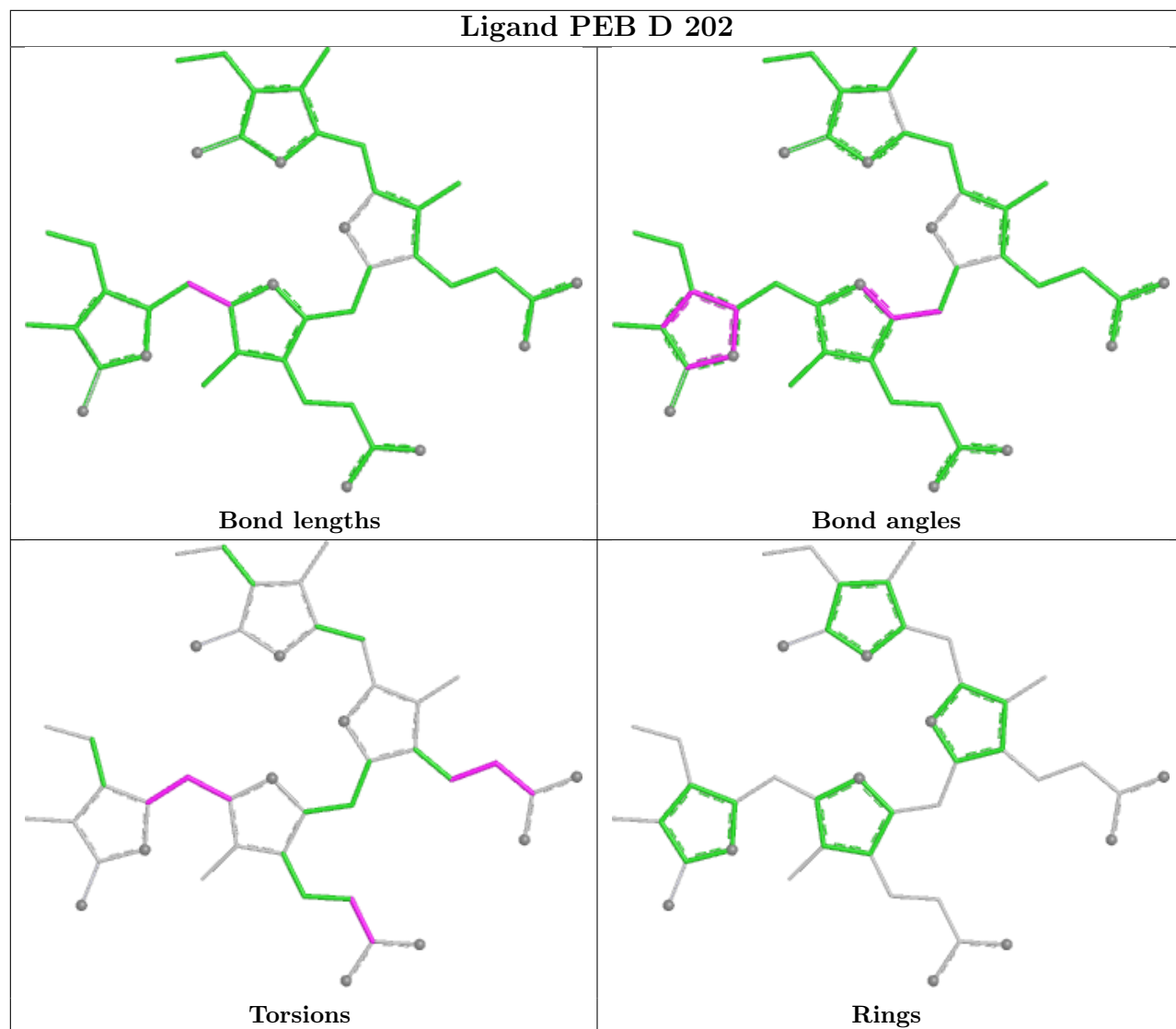




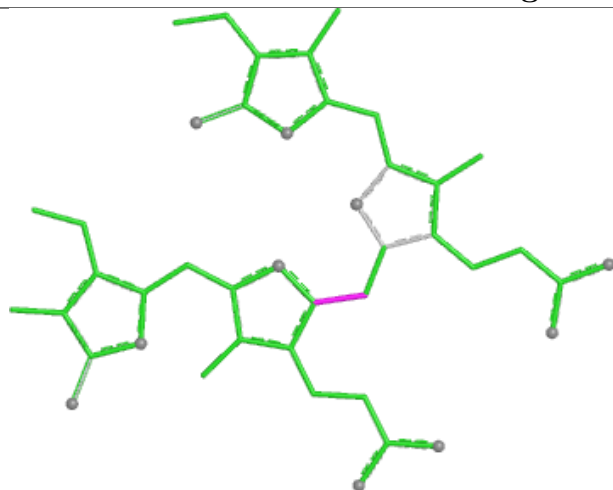




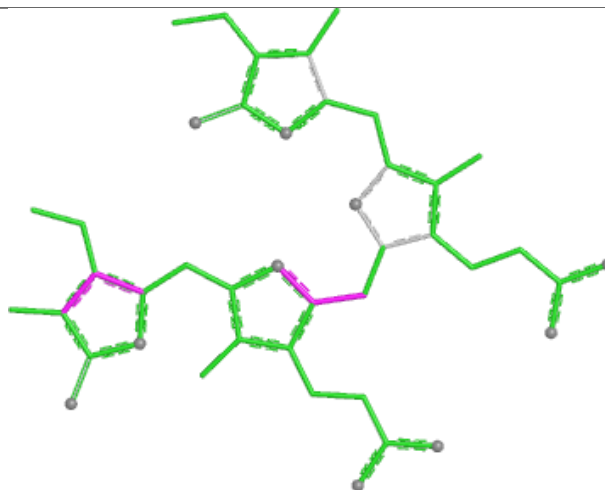




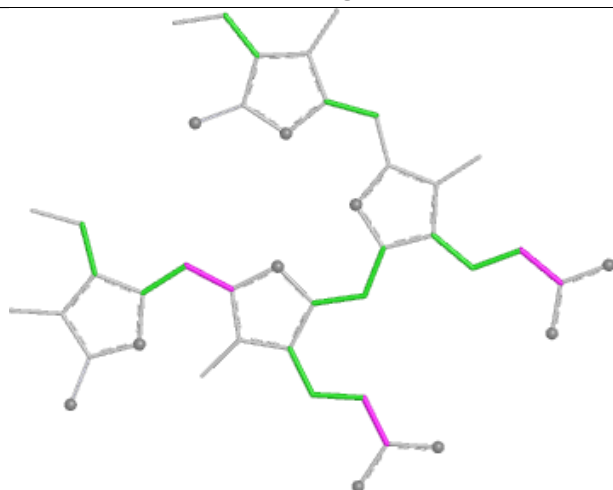
Ligand PEB I 202



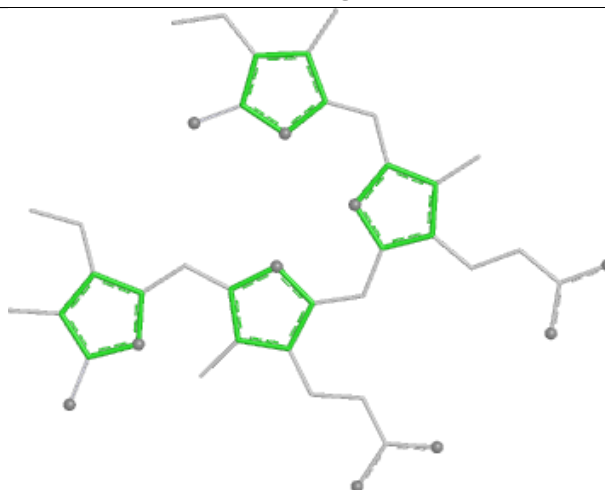
Bond lengths



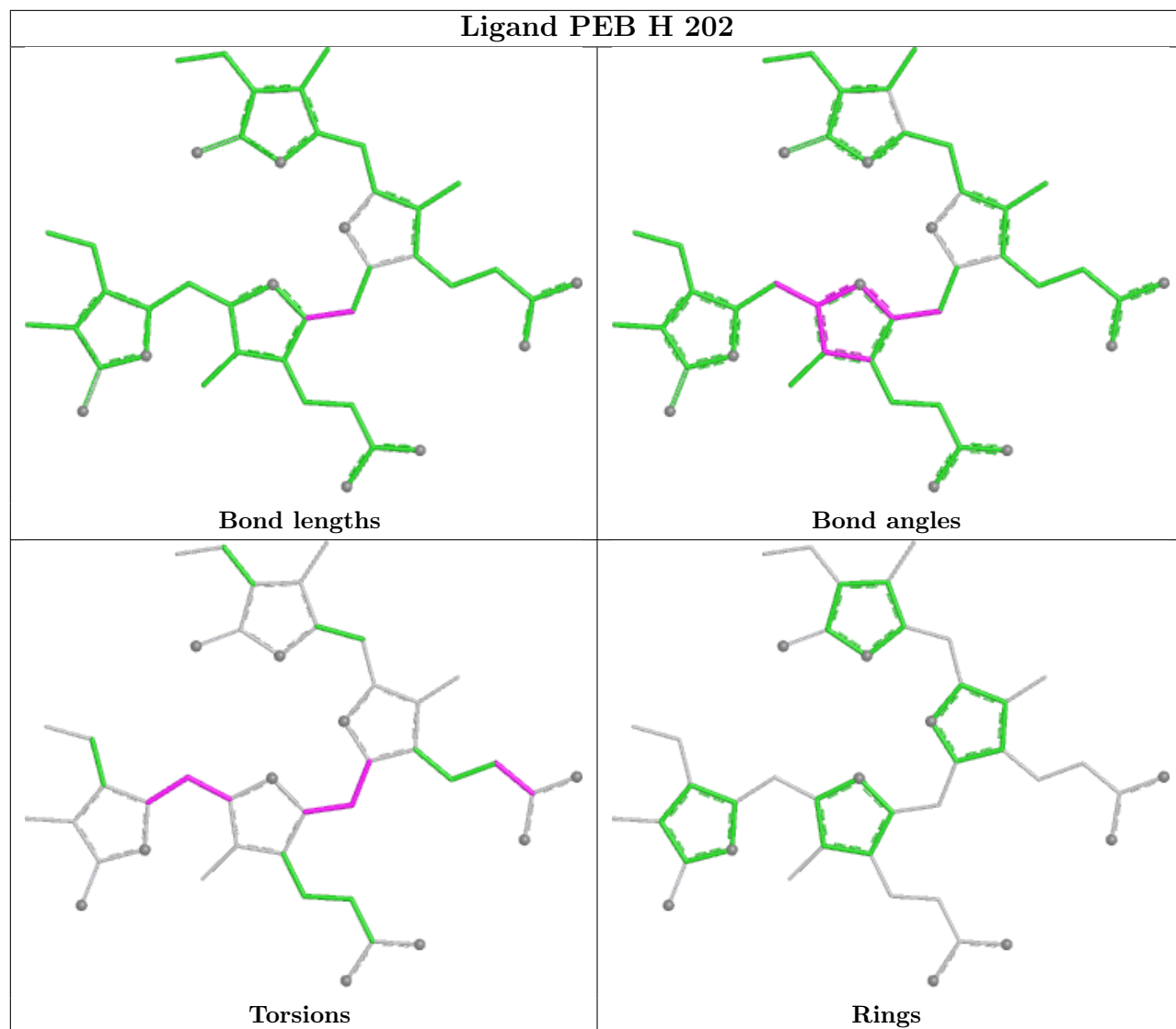
Bond angles

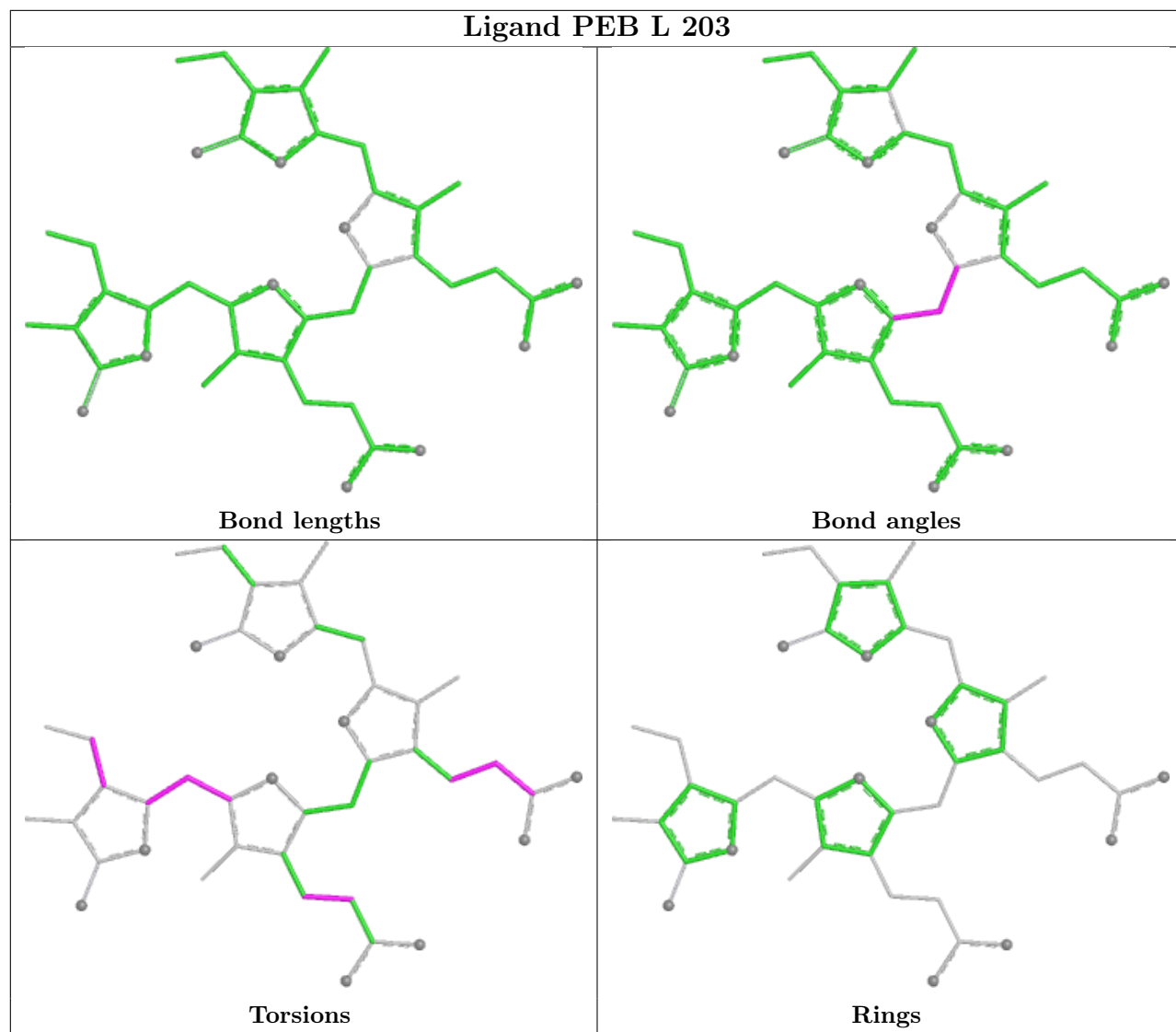


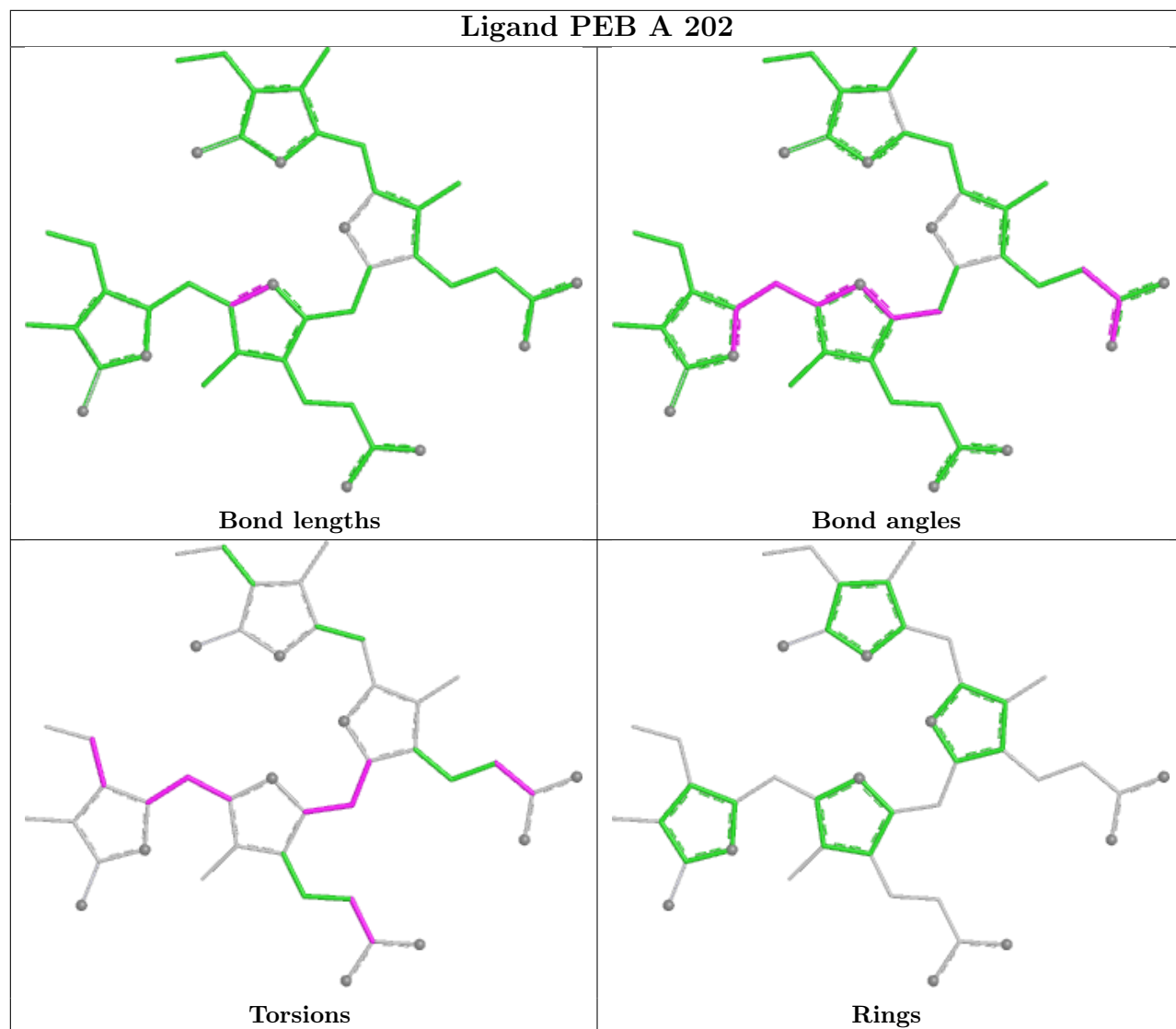
Torsions

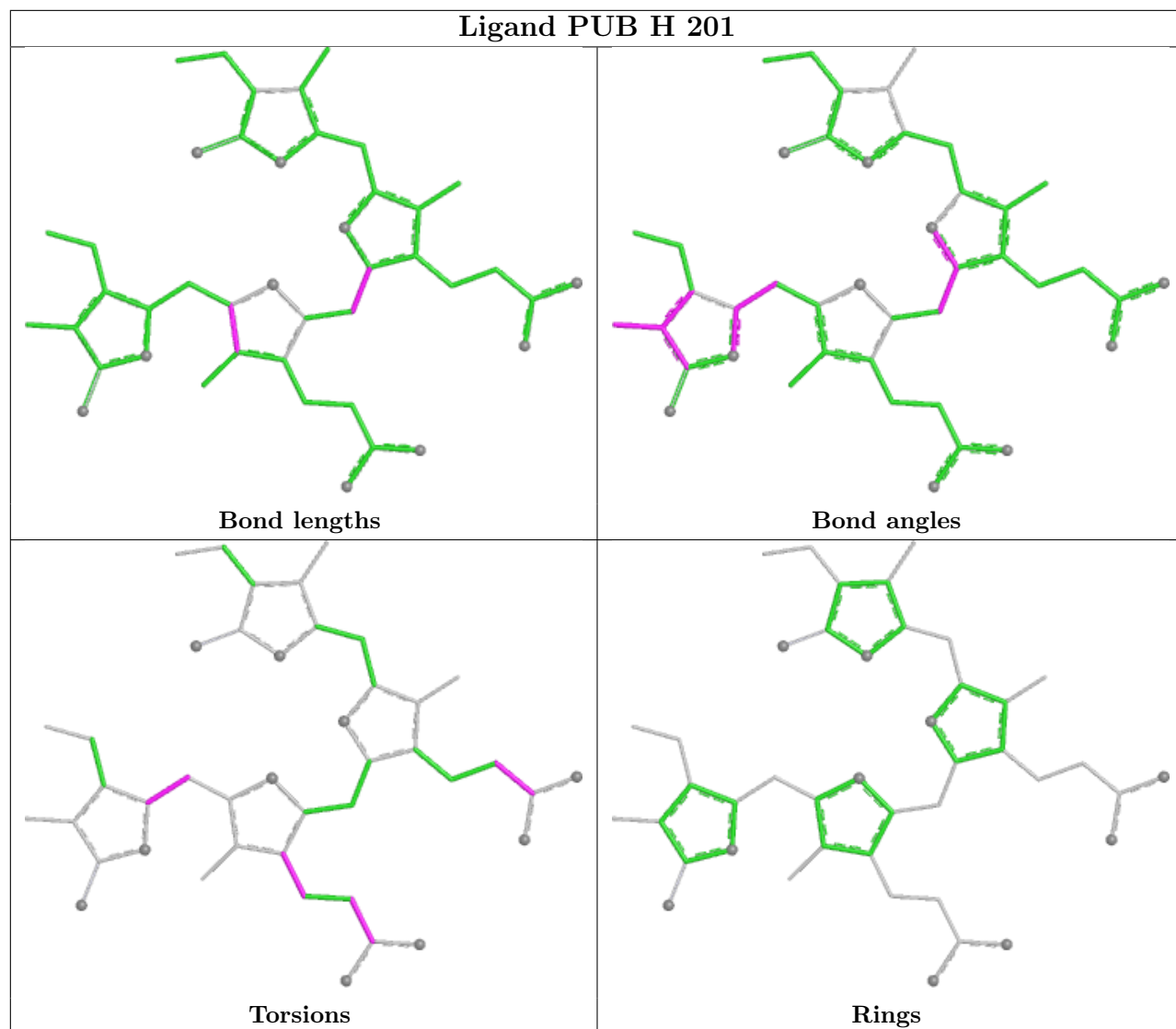


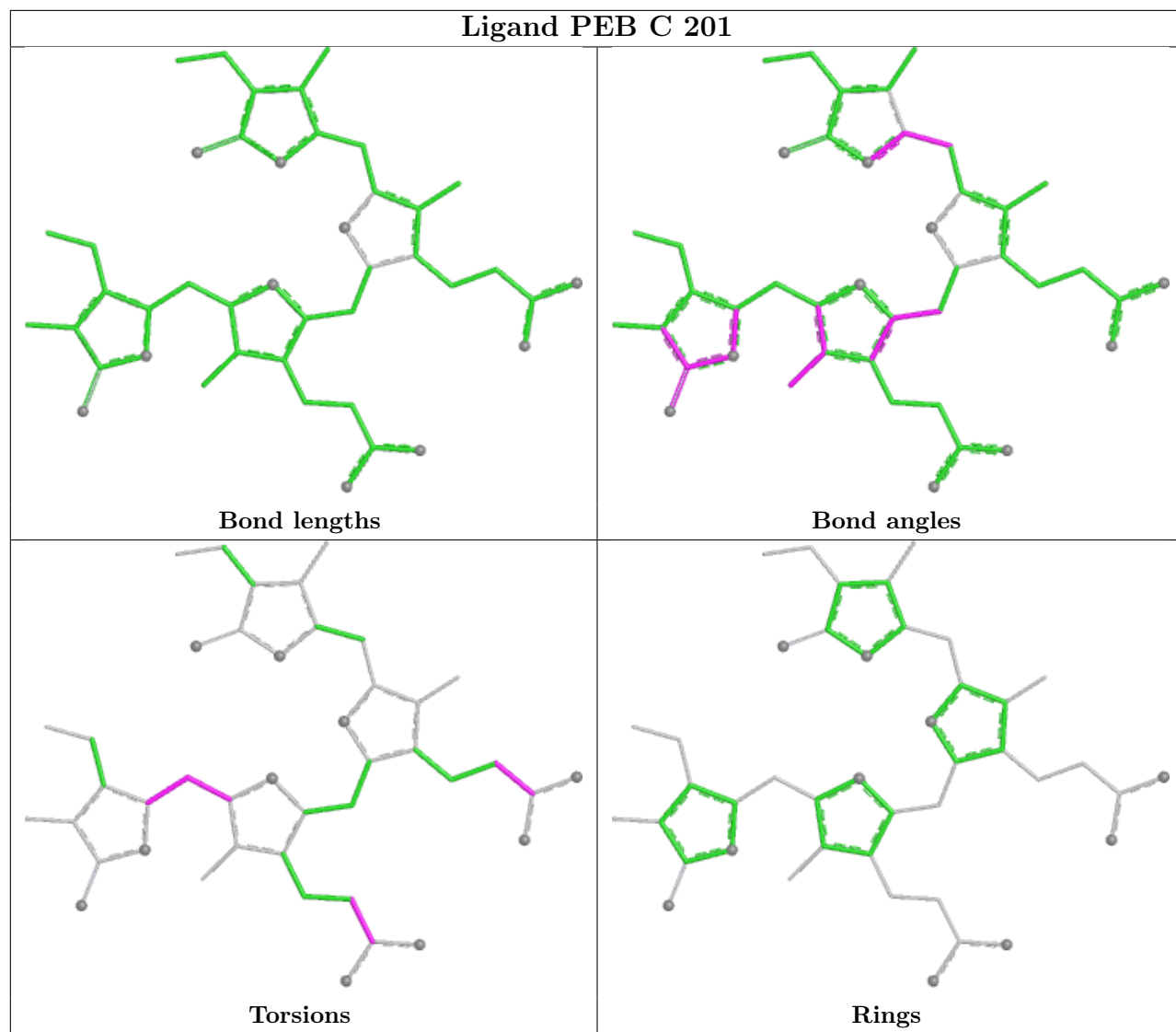
Rings

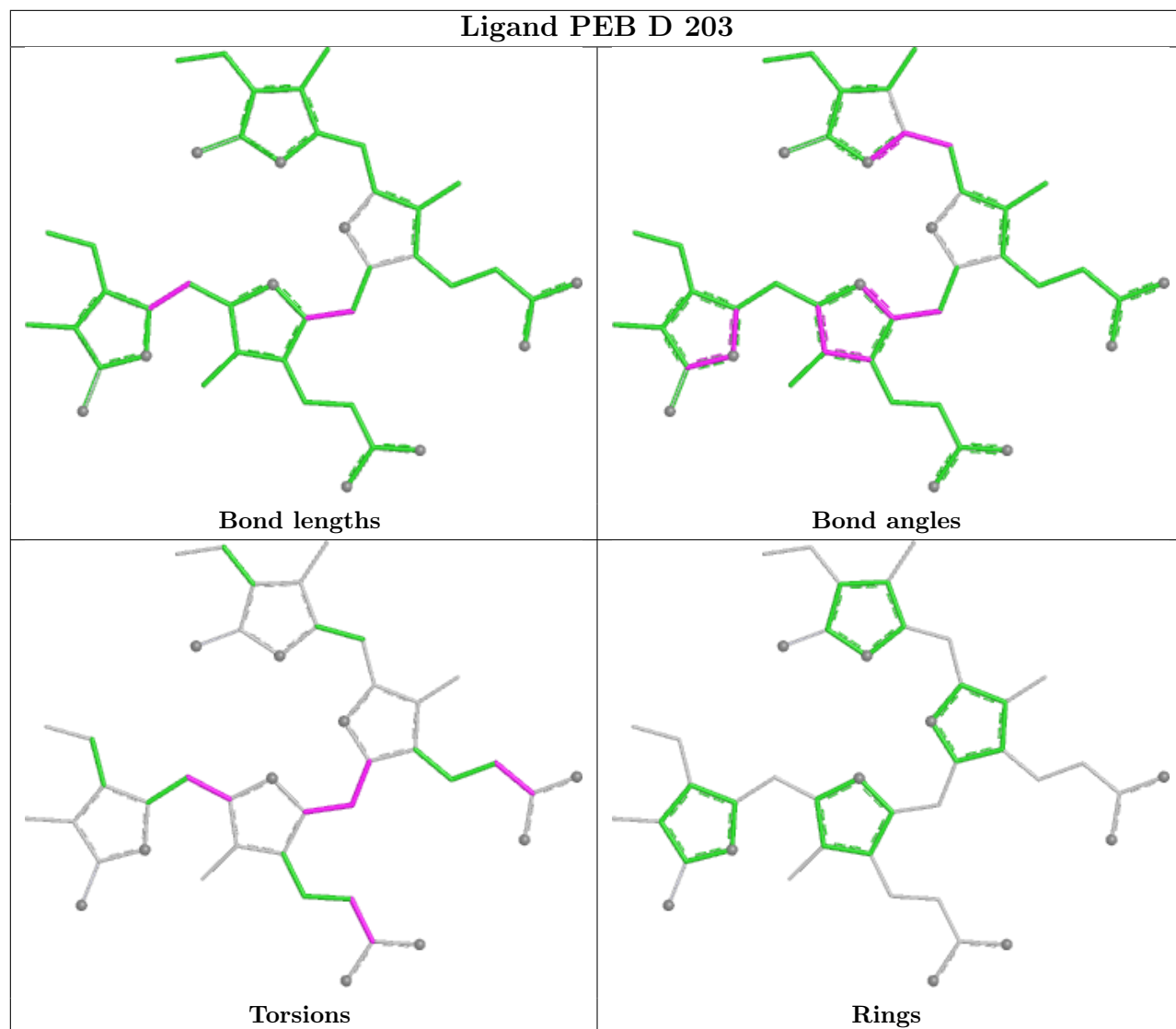


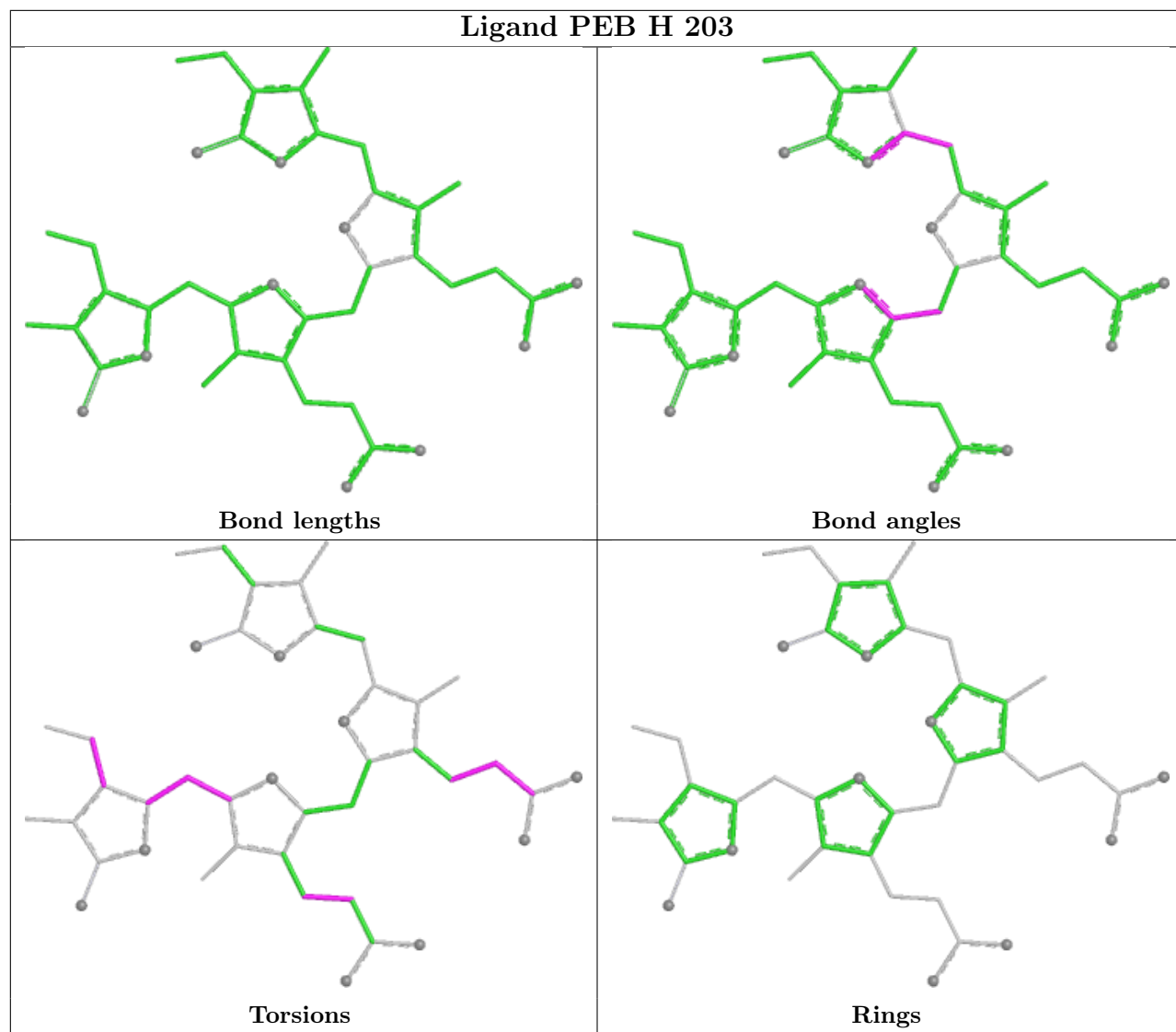


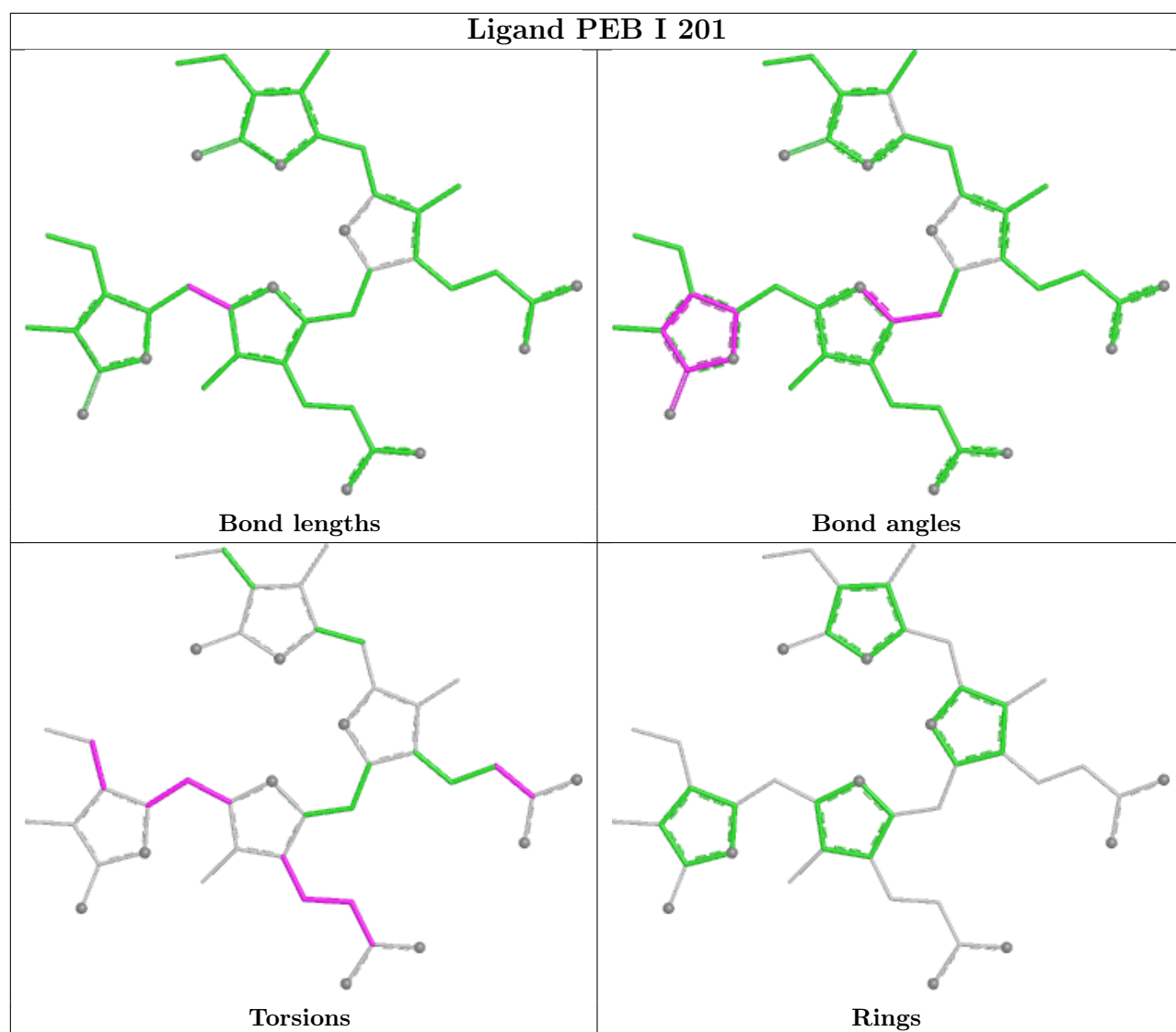


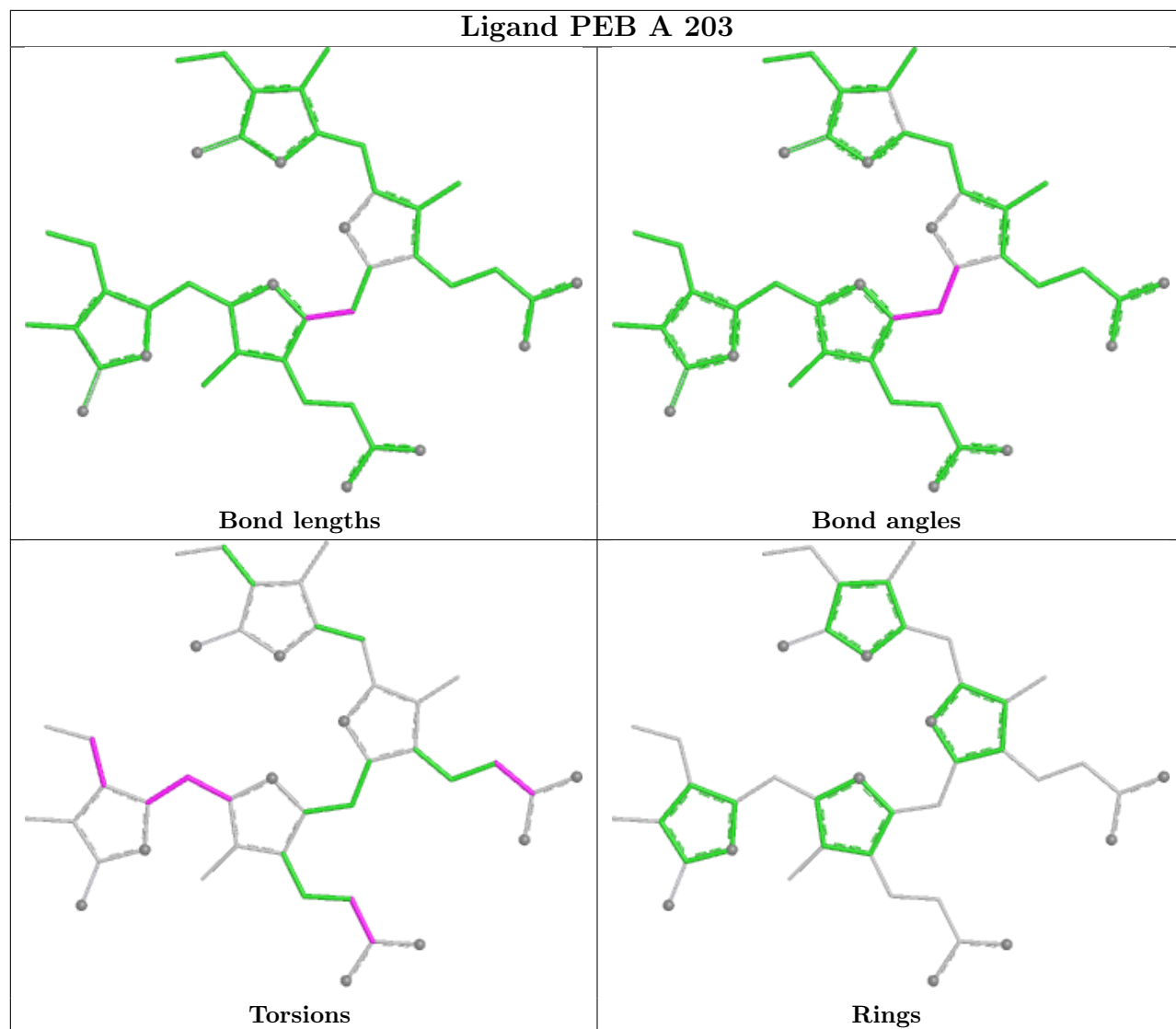


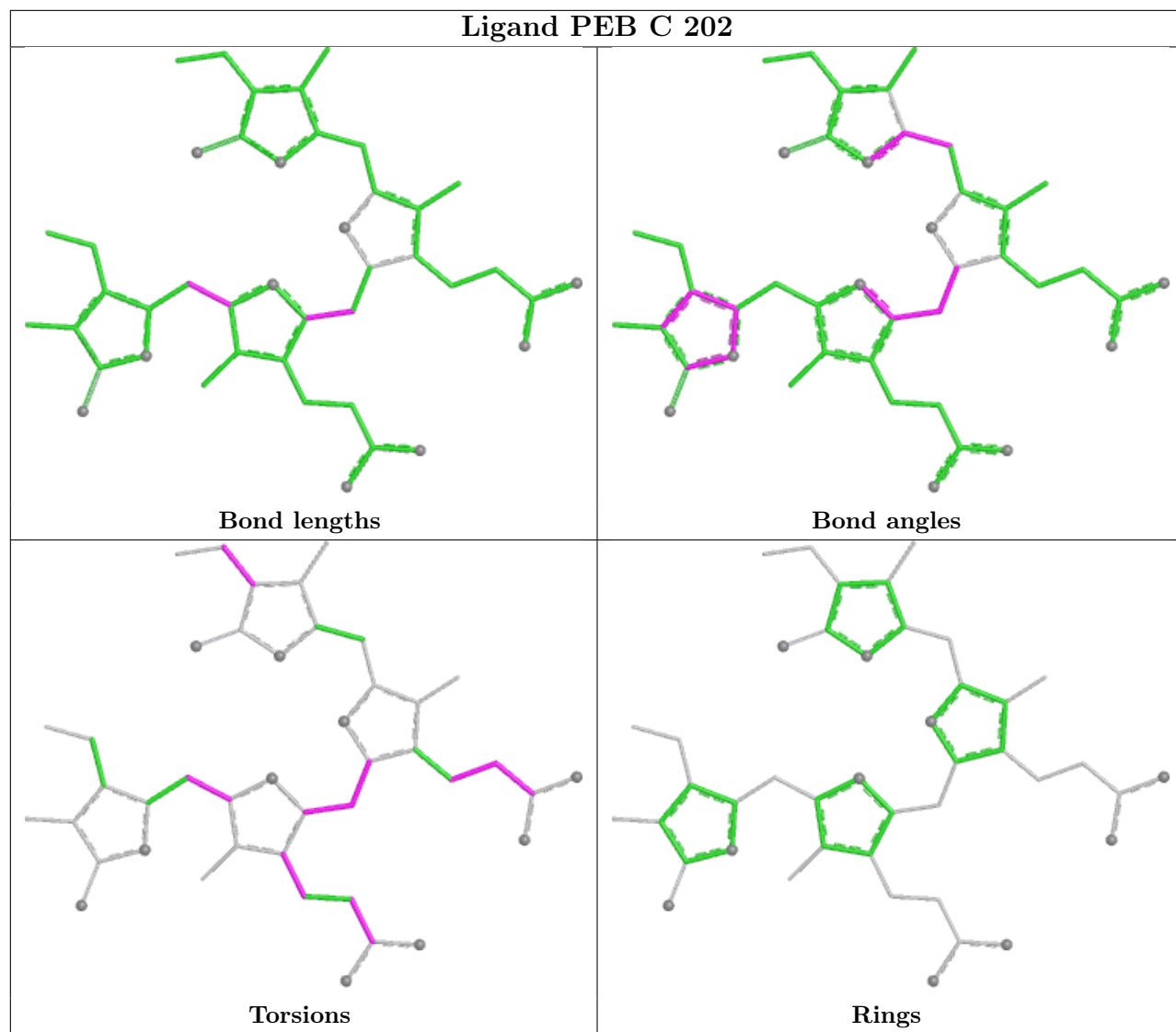


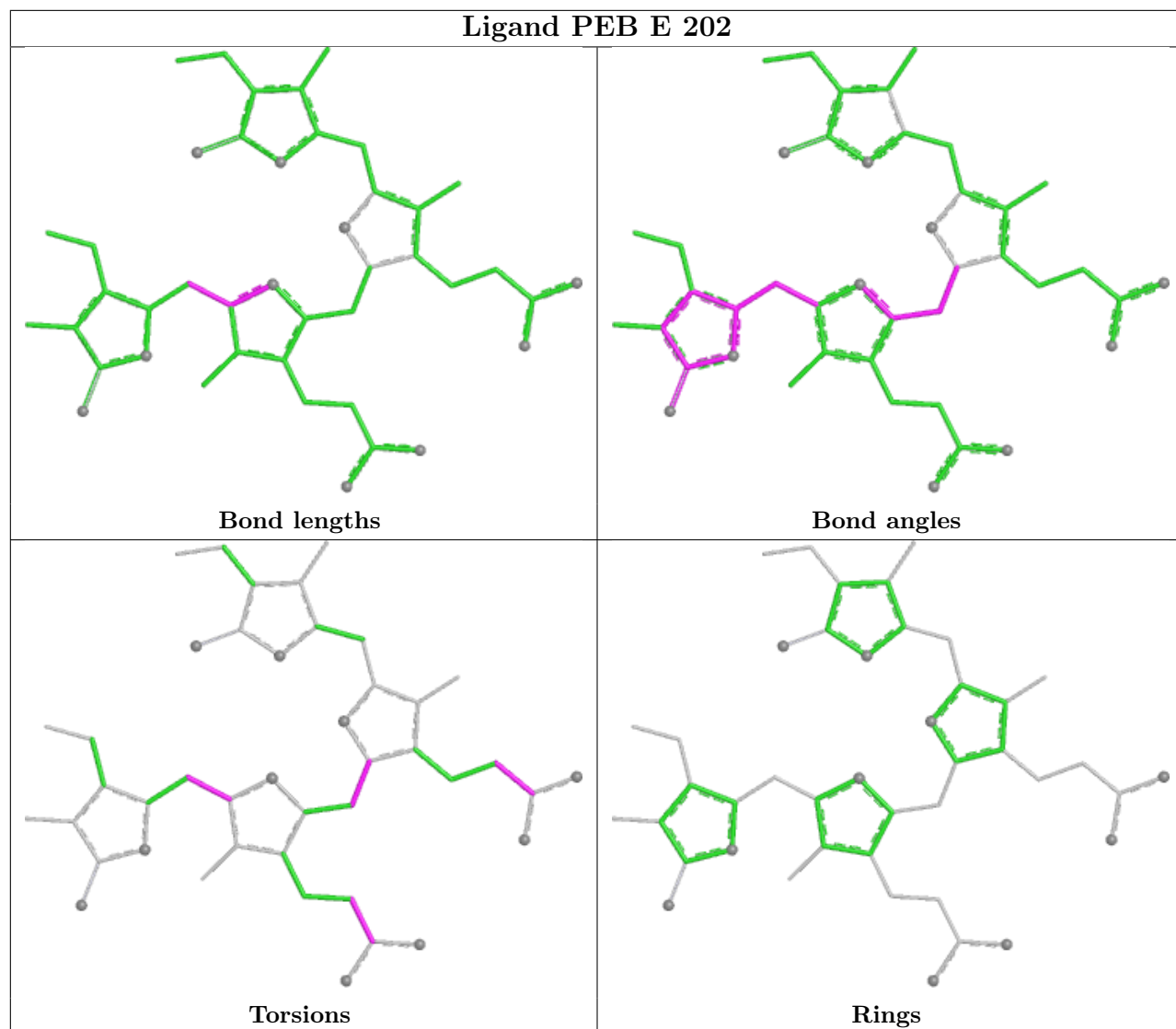


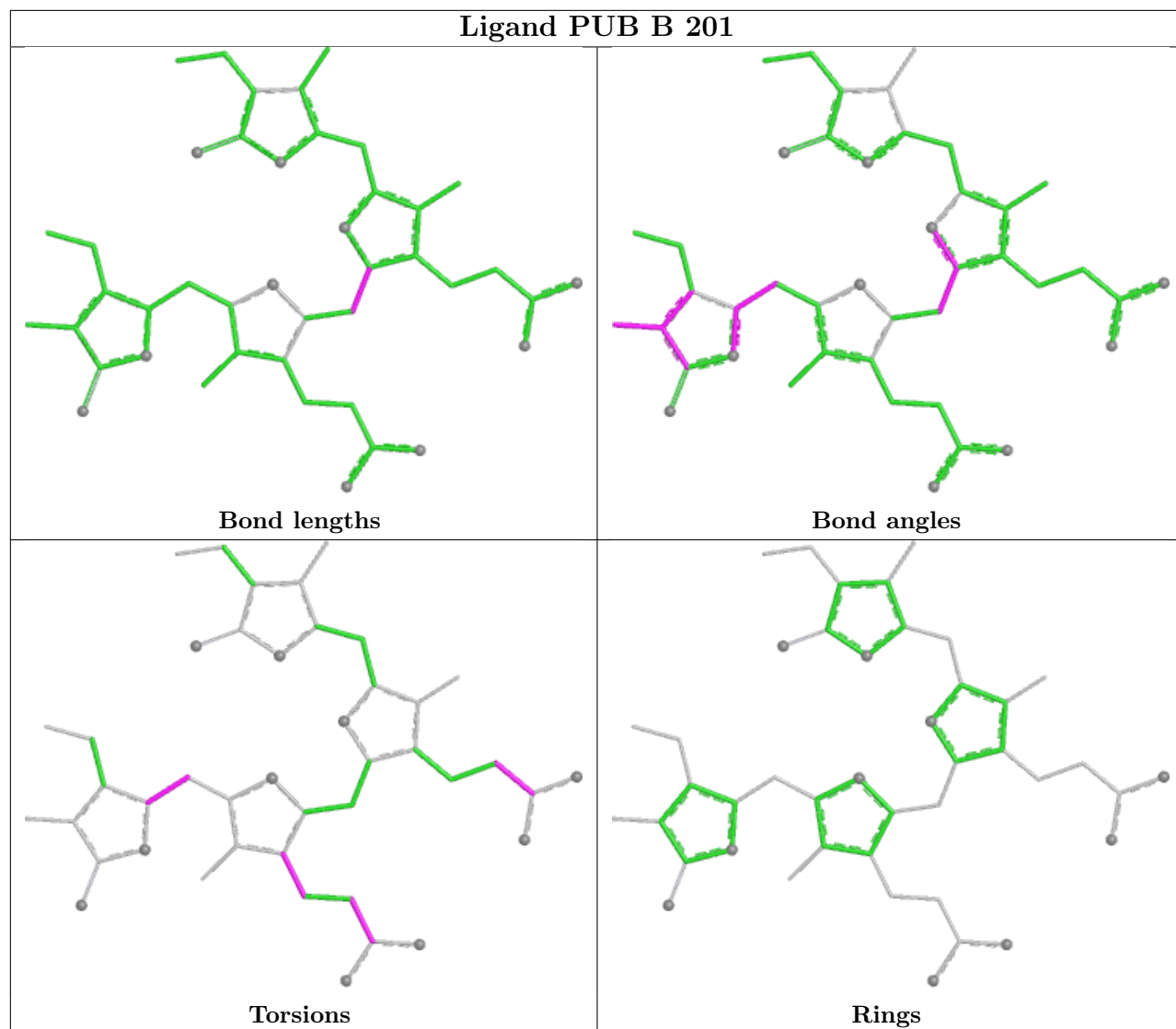


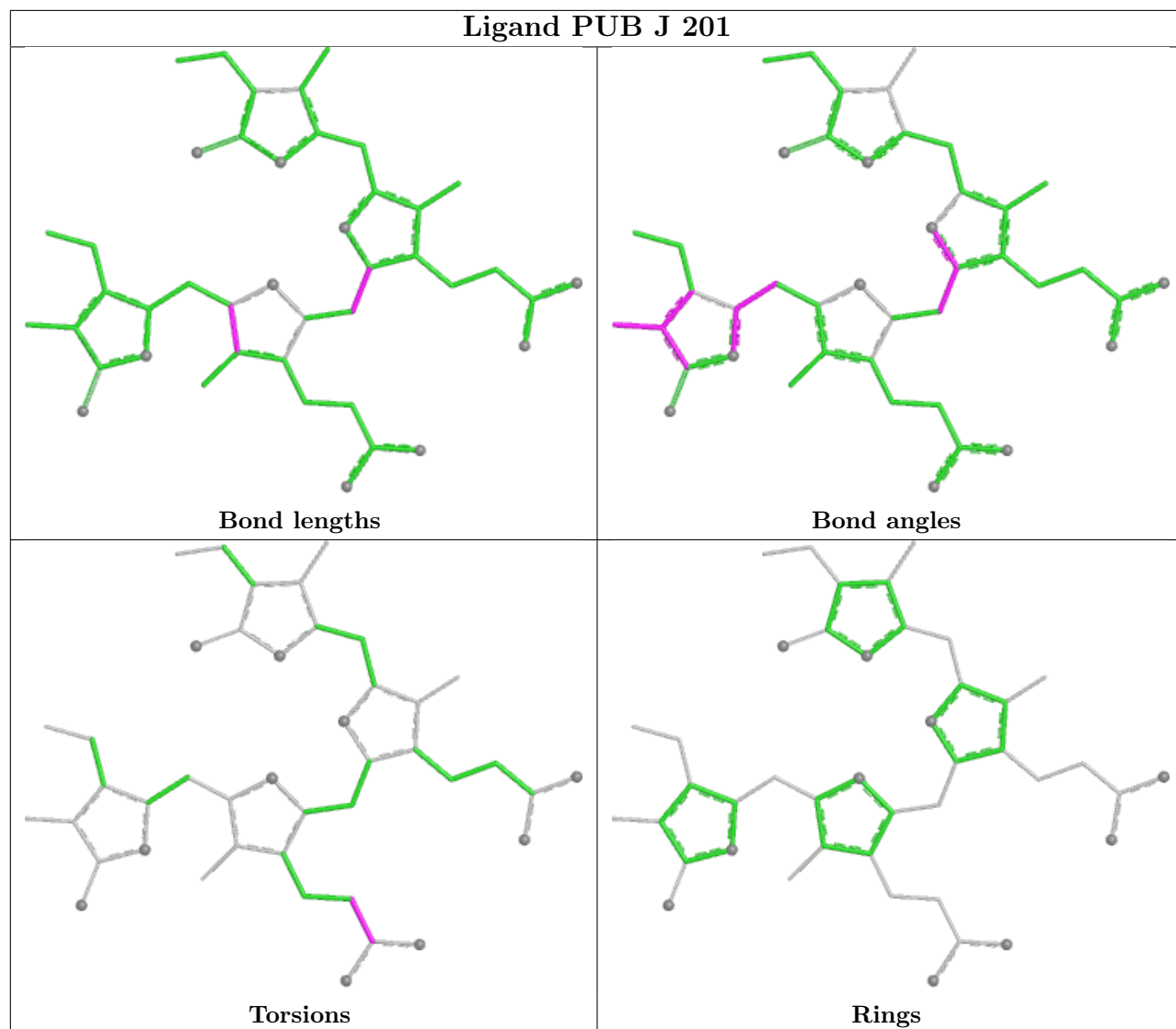


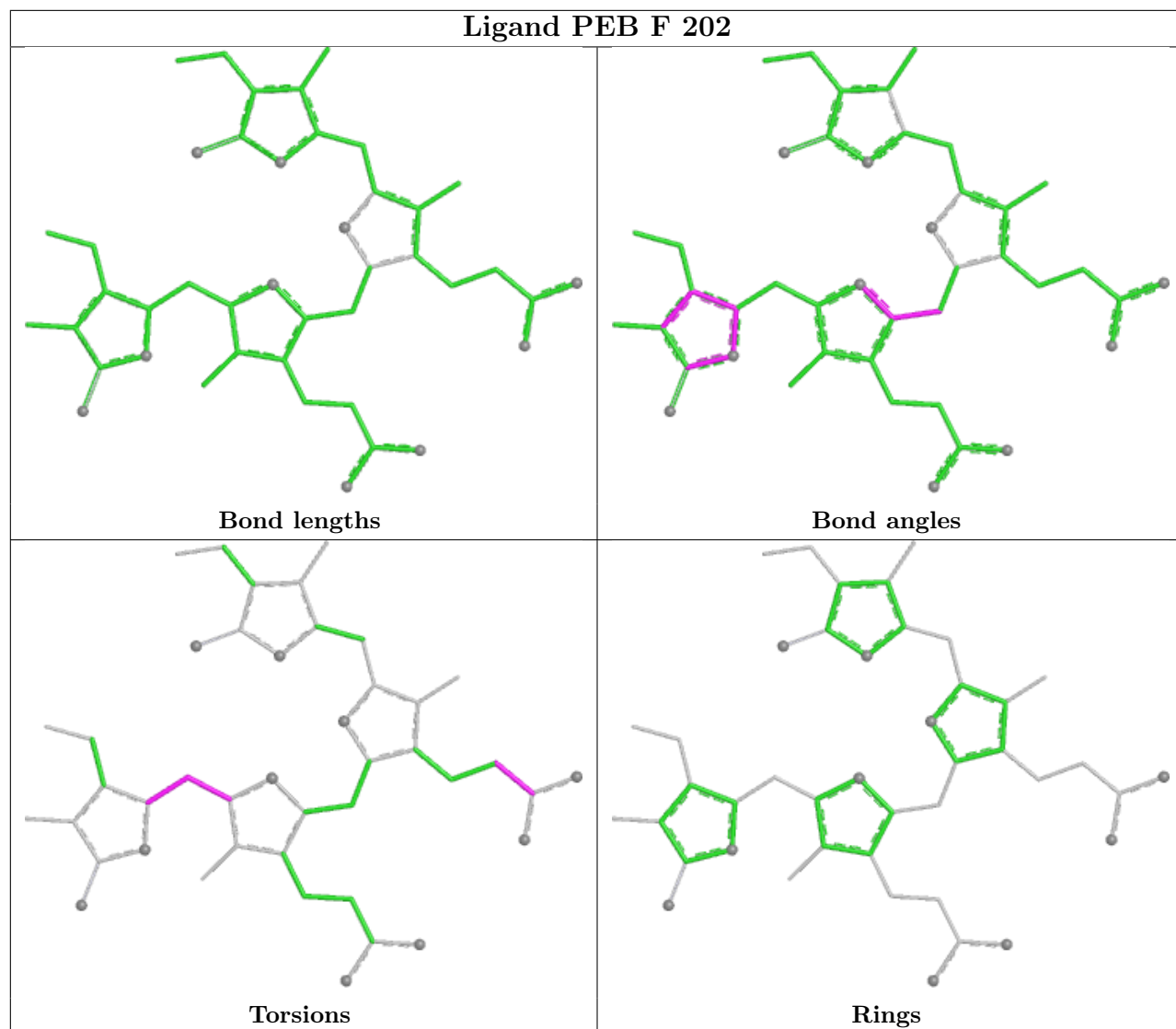


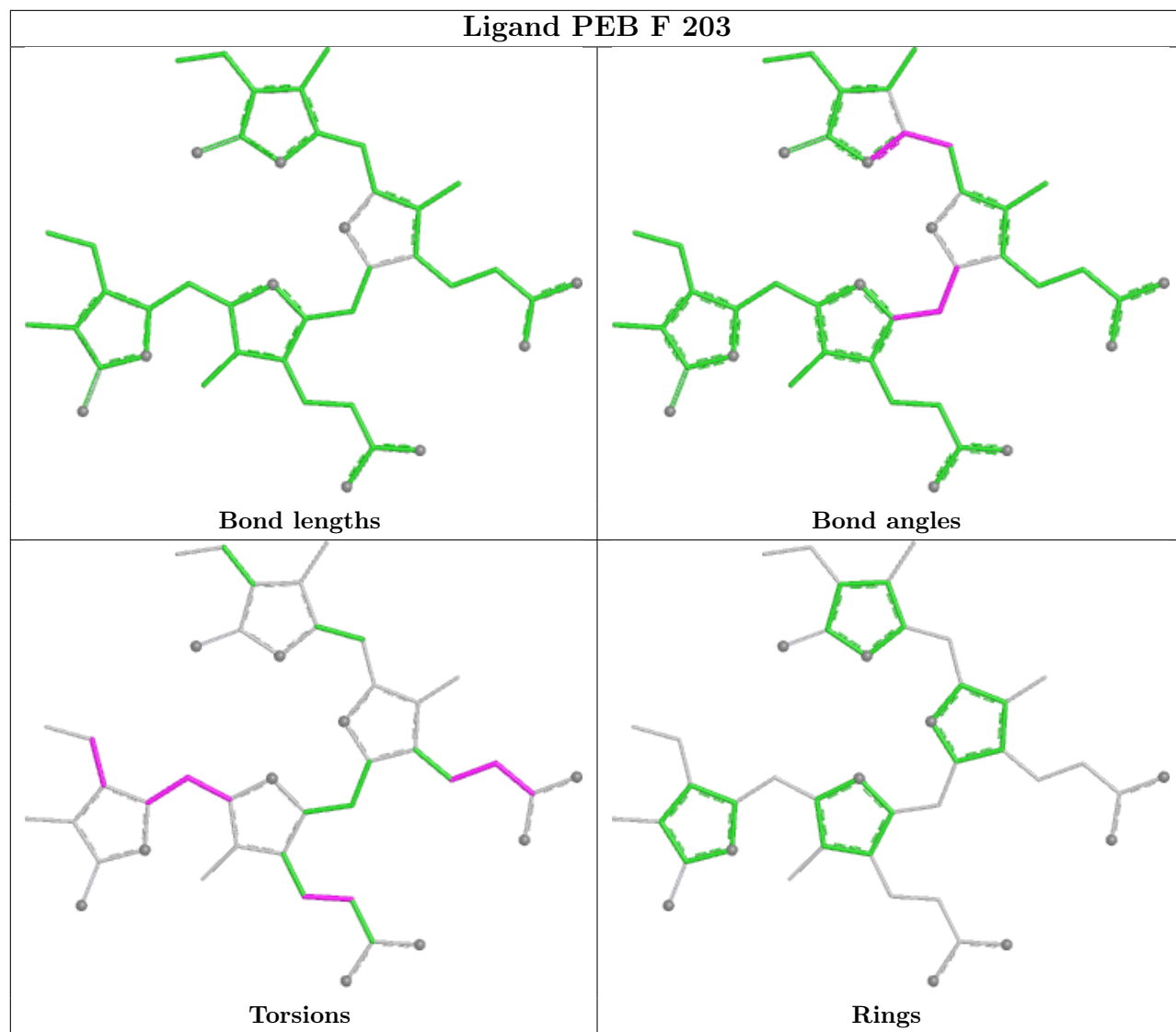


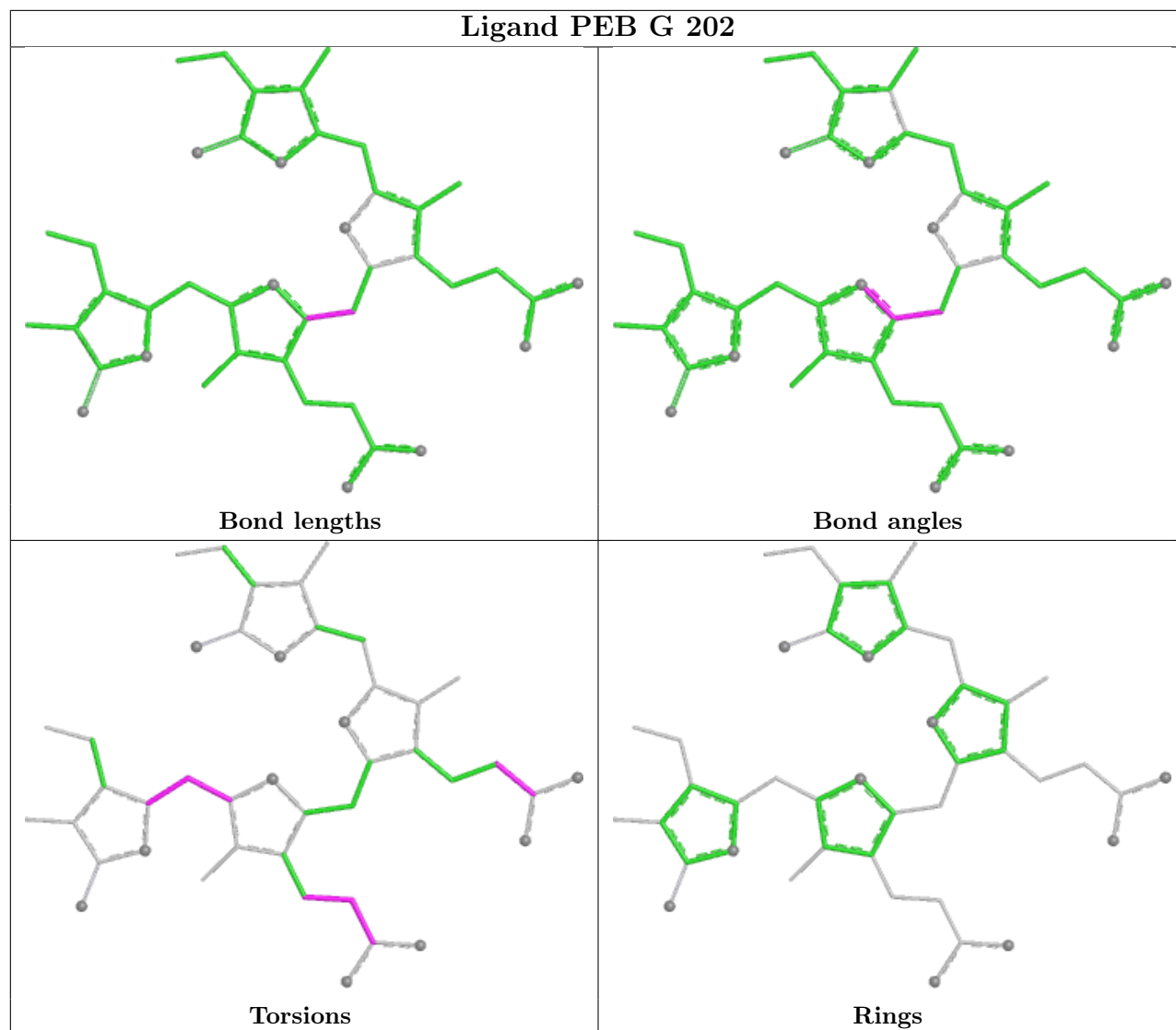


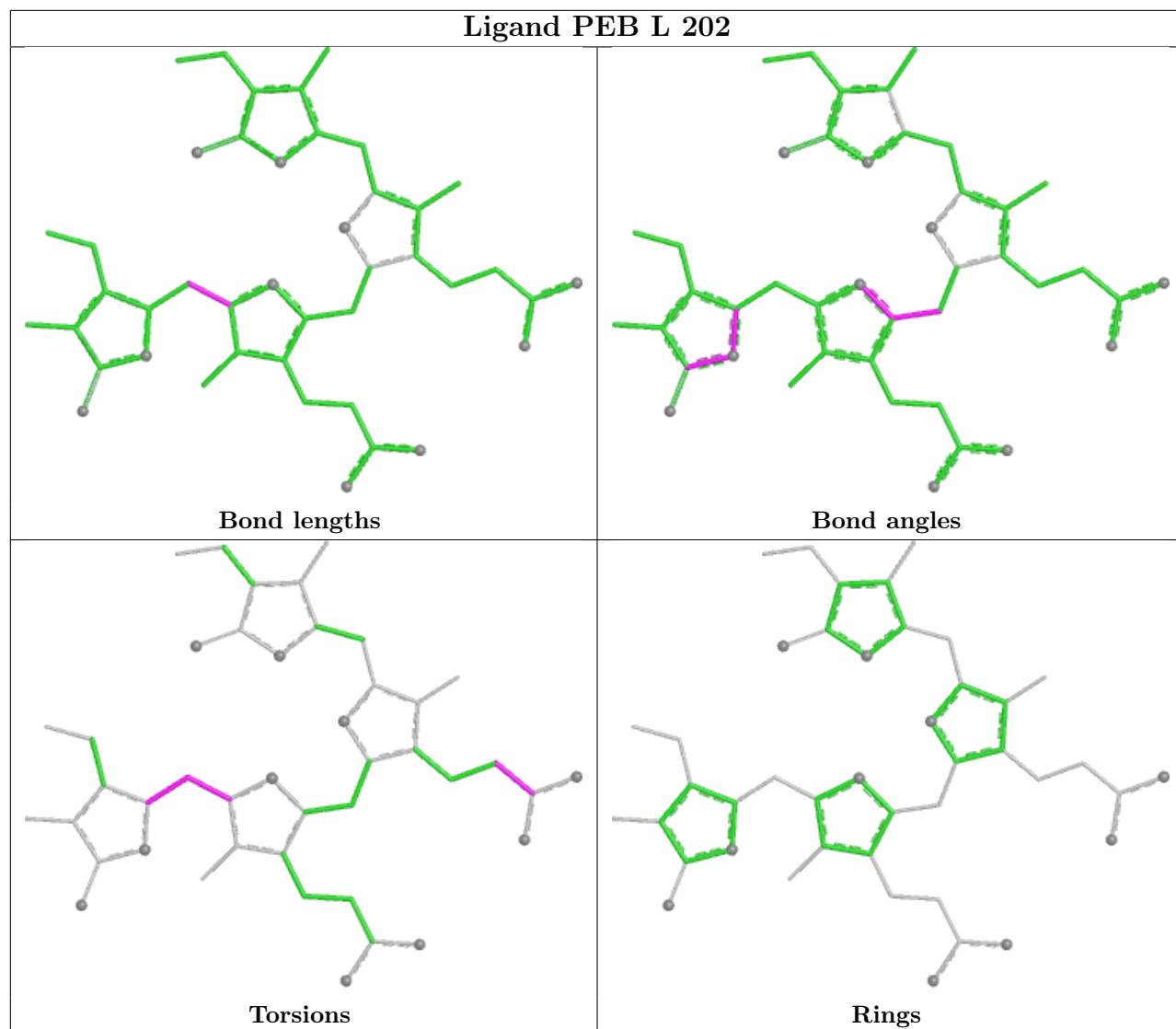


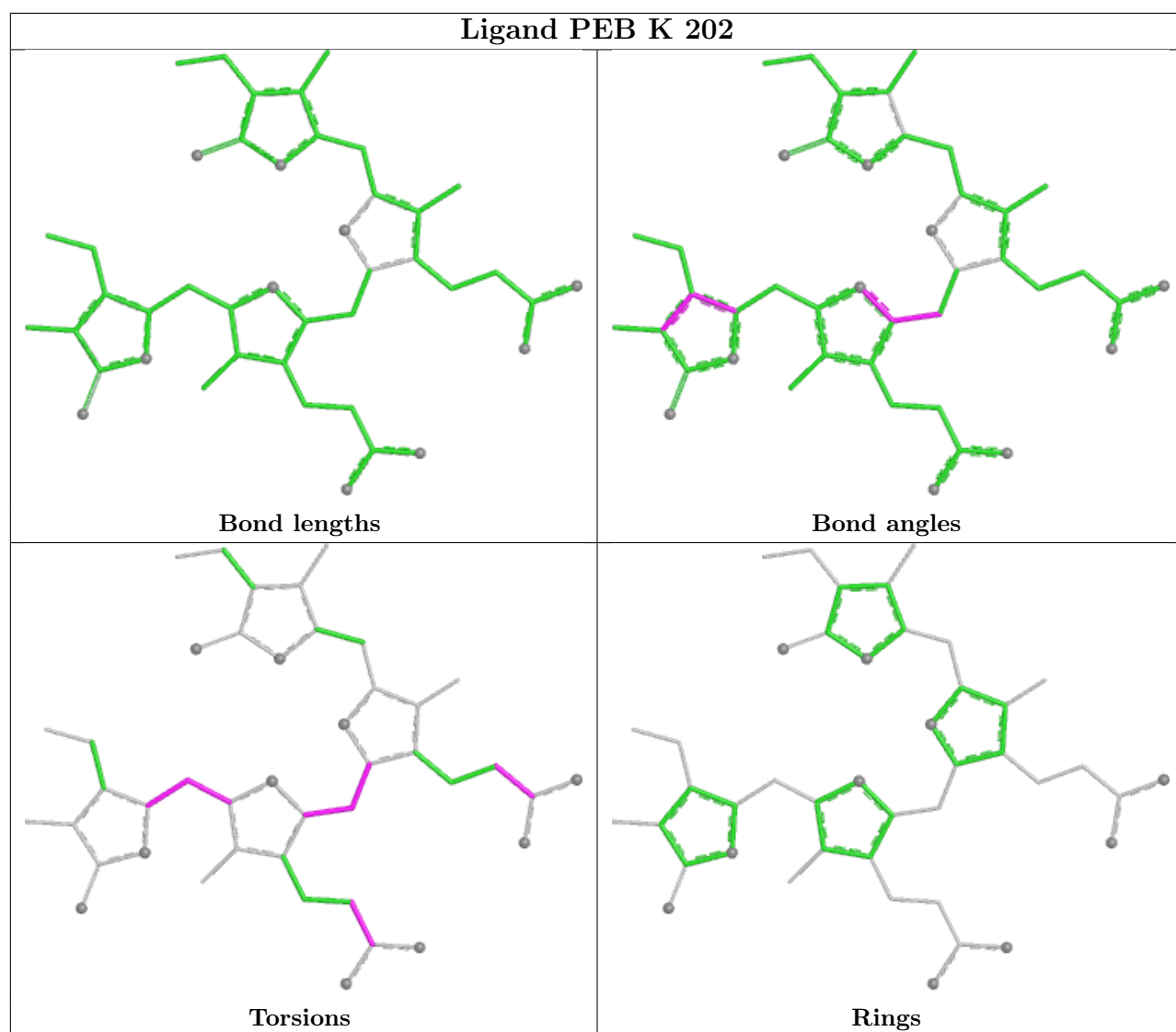


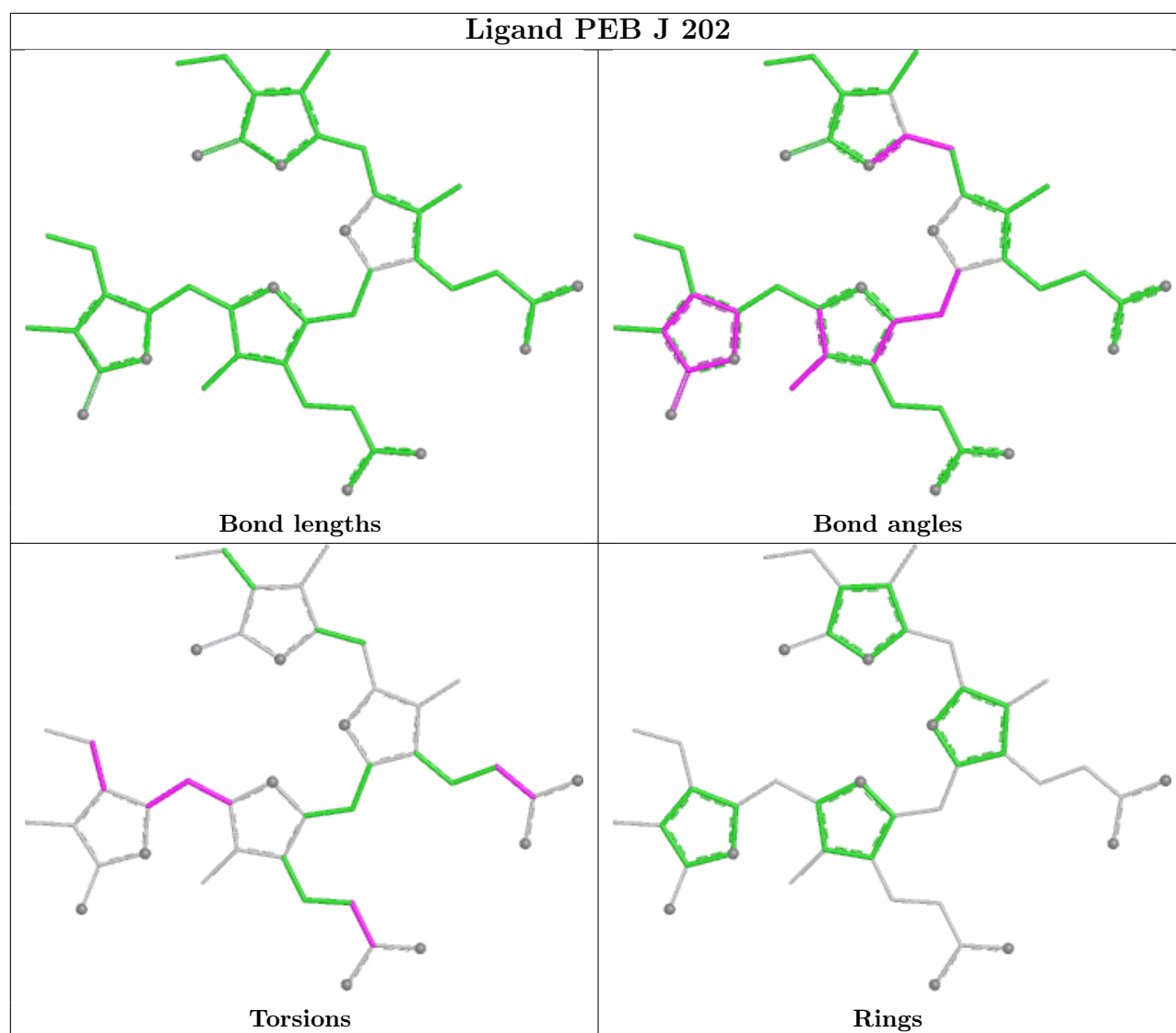












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

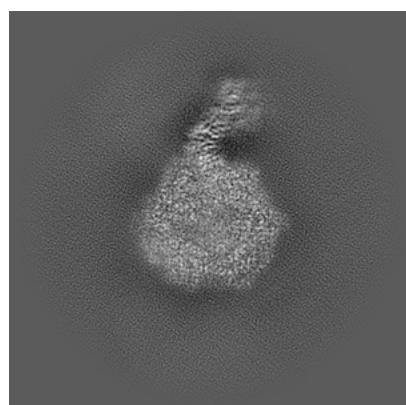
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-70157. These allow visual inspection of the internal detail of the map and identification of artifacts.

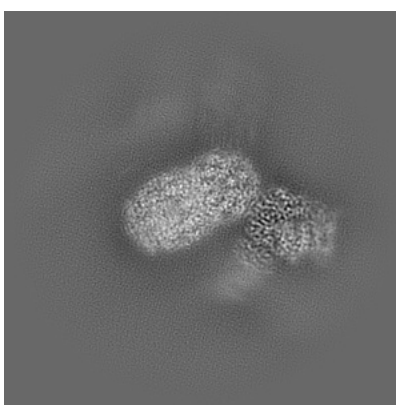
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

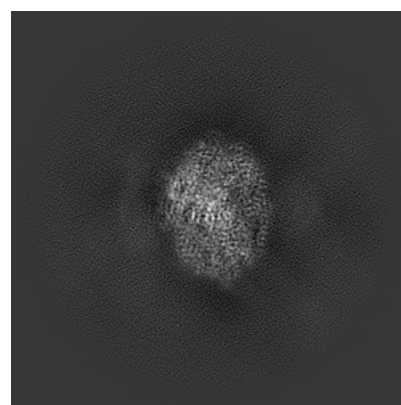
6.1.1 Primary map



X



Y

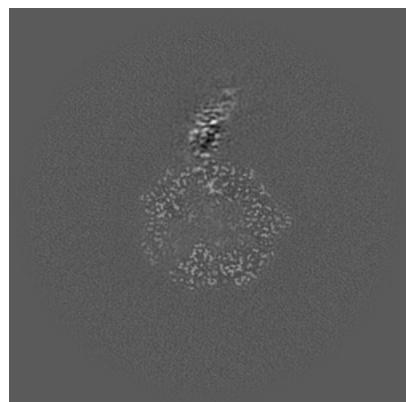


Z

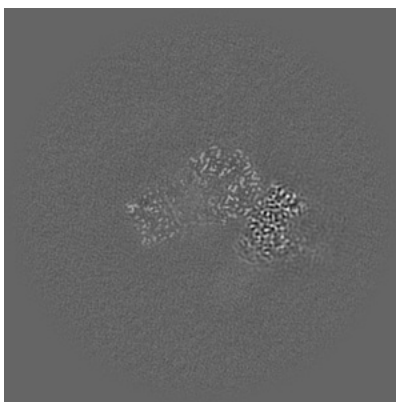
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

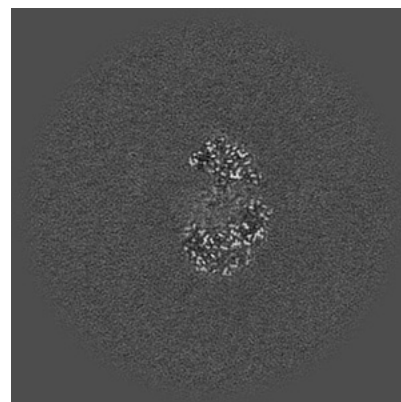
6.2.1 Primary map



X Index: 180



Y Index: 180

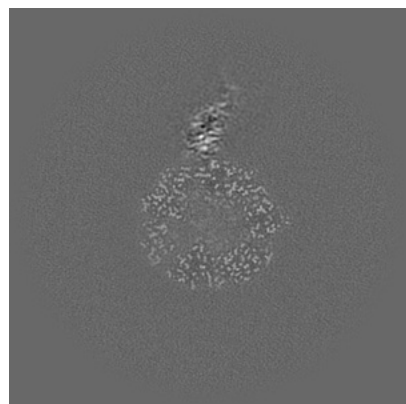


Z Index: 180

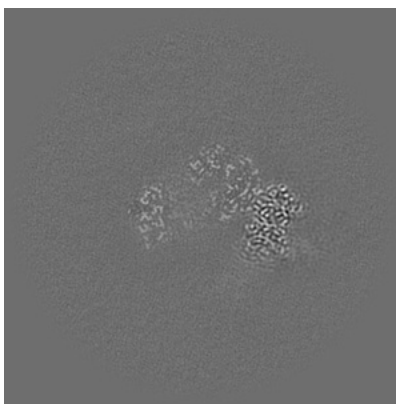
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

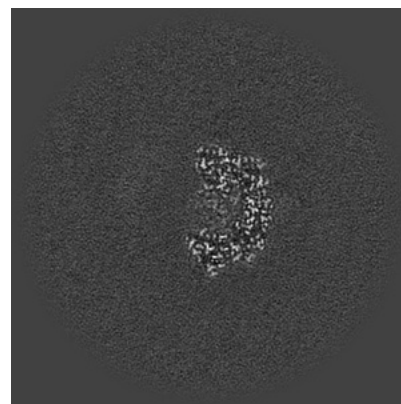
6.3.1 Primary map



X Index: 182



Y Index: 177

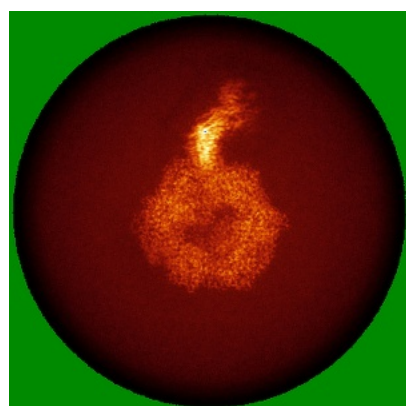


Z Index: 187

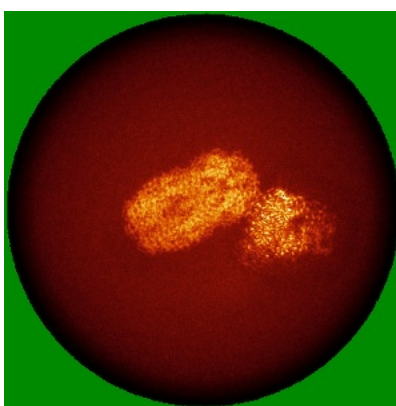
The images above show the largest variance slices of the map in three orthogonal directions.

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

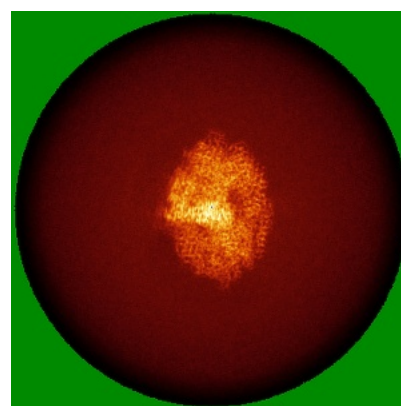
6.4.1 Primary map



X



Y

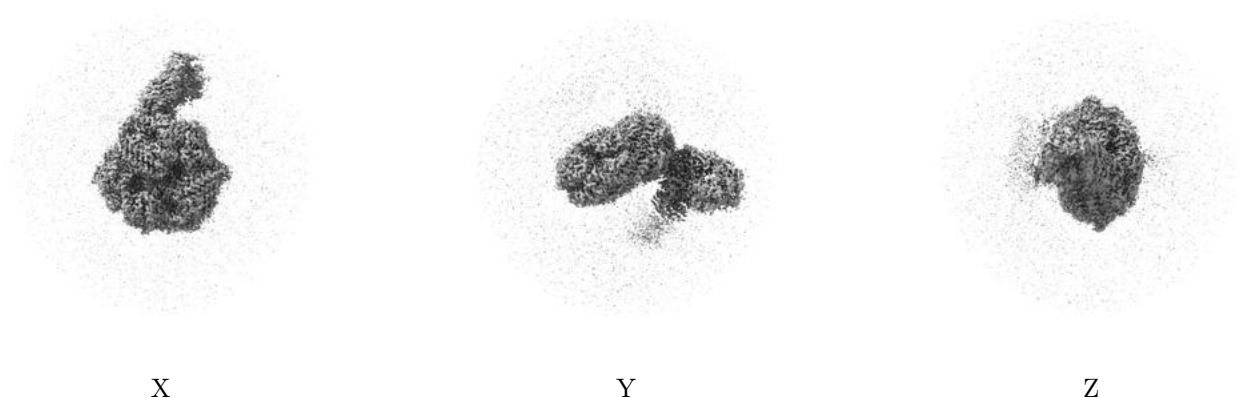


Z

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 3.7. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

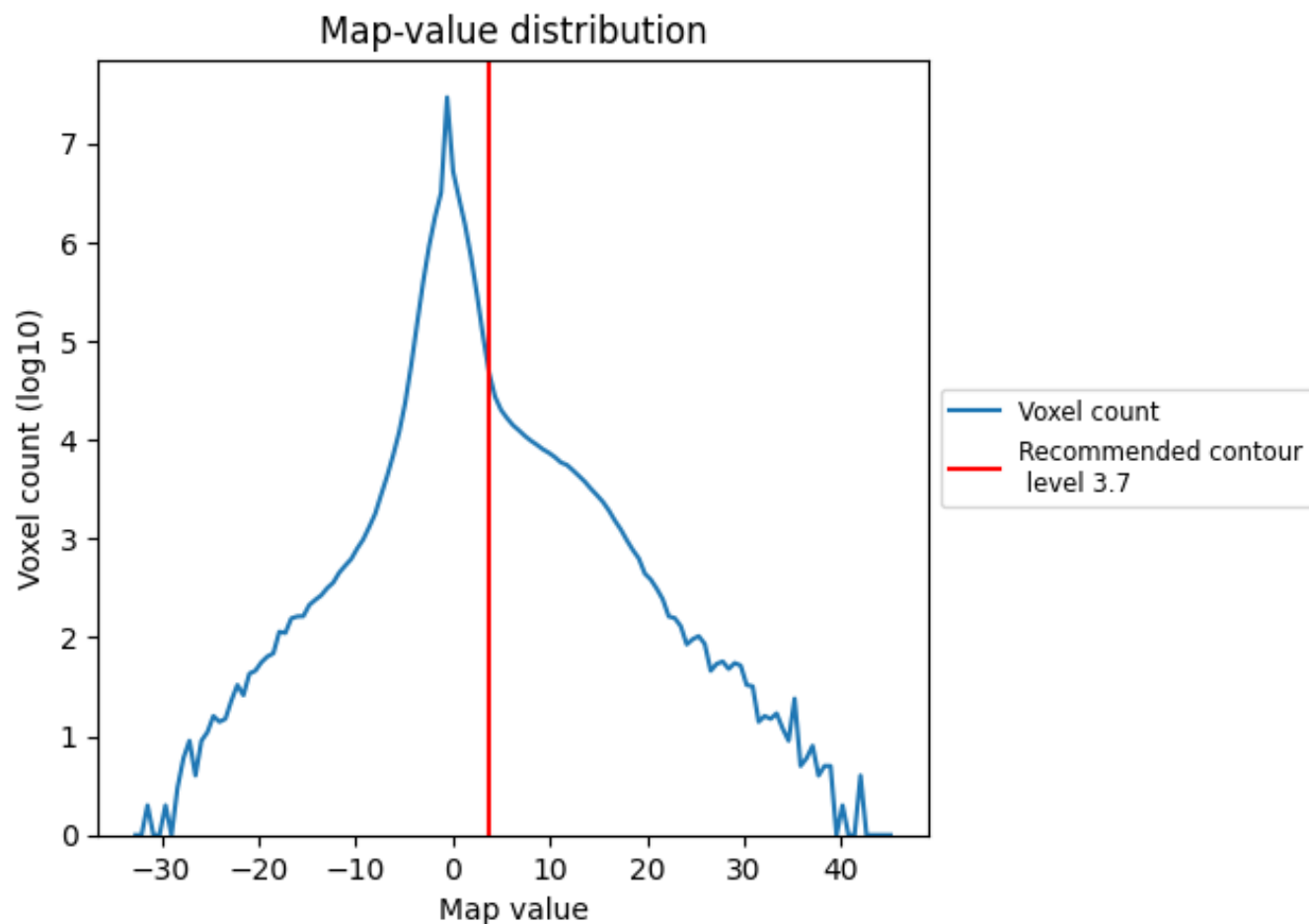
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

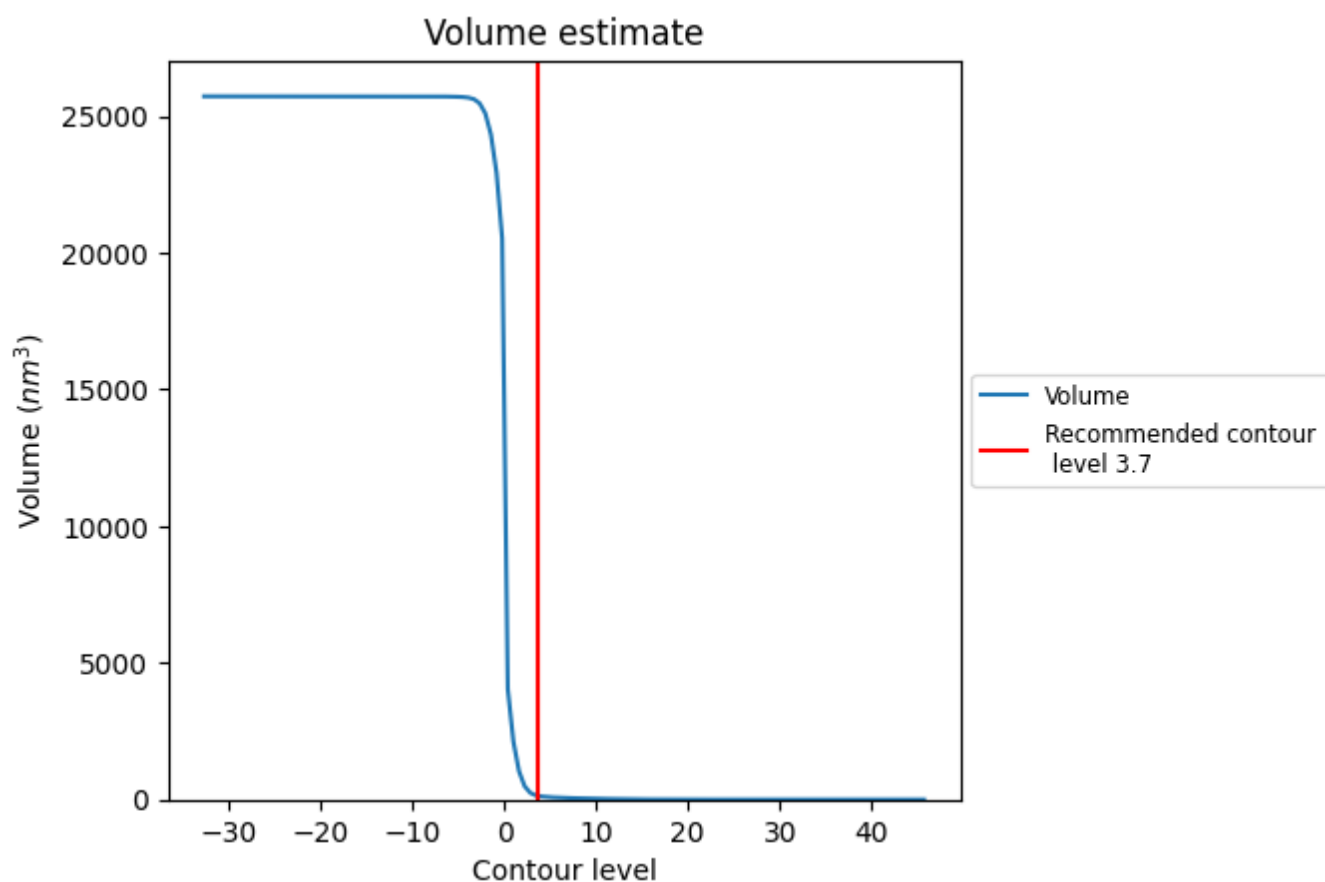
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

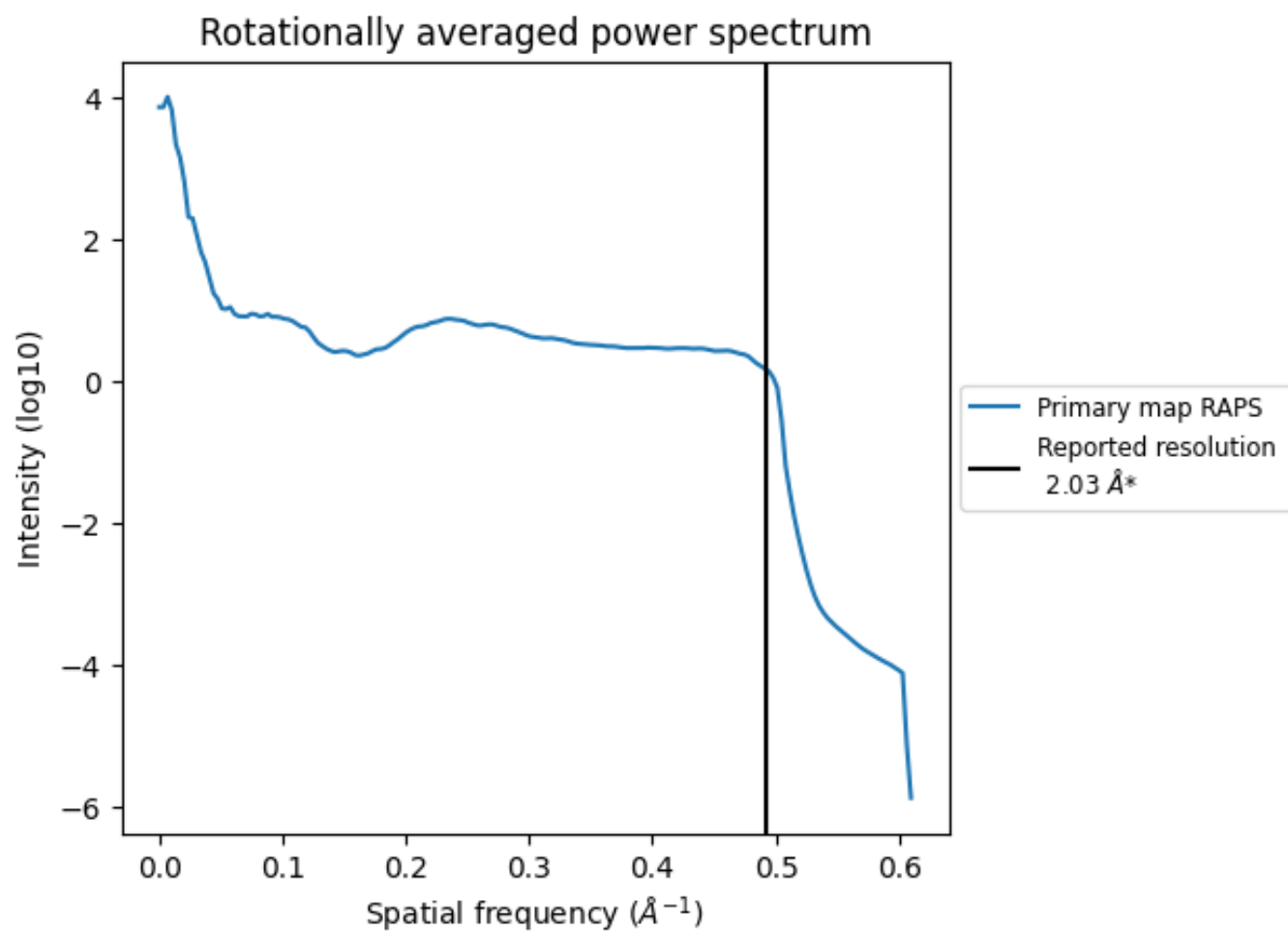
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 135 nm³; this corresponds to an approximate mass of 122 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.493 Å⁻¹

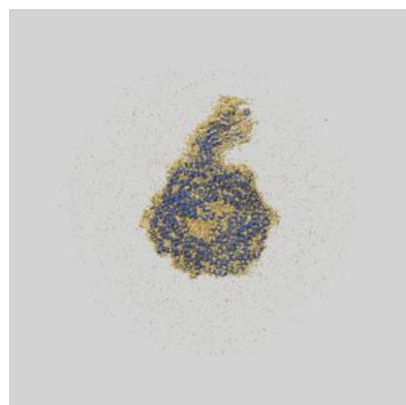
8 Fourier-Shell correlation ⓘ

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

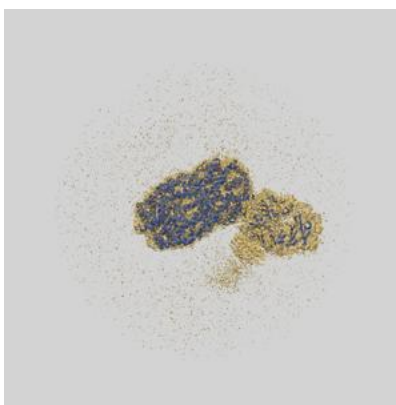
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-70157 and PDB model 9O62. Per-residue inclusion information can be found in [section 3](#) on [page 11](#).

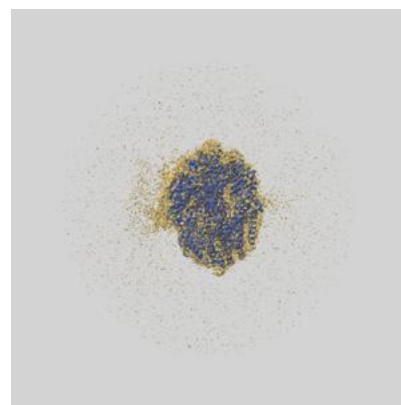
9.1 Map-model overlay [i](#)



X



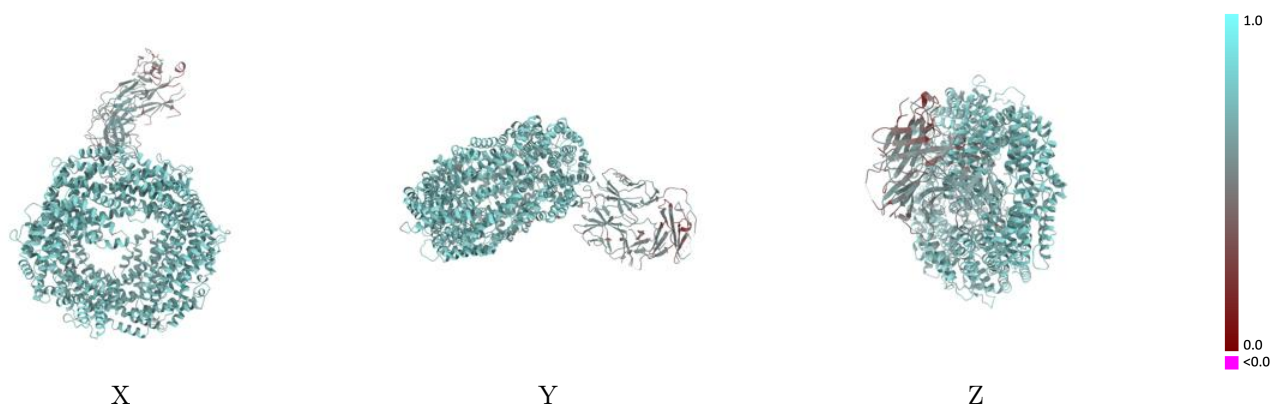
Y



Z

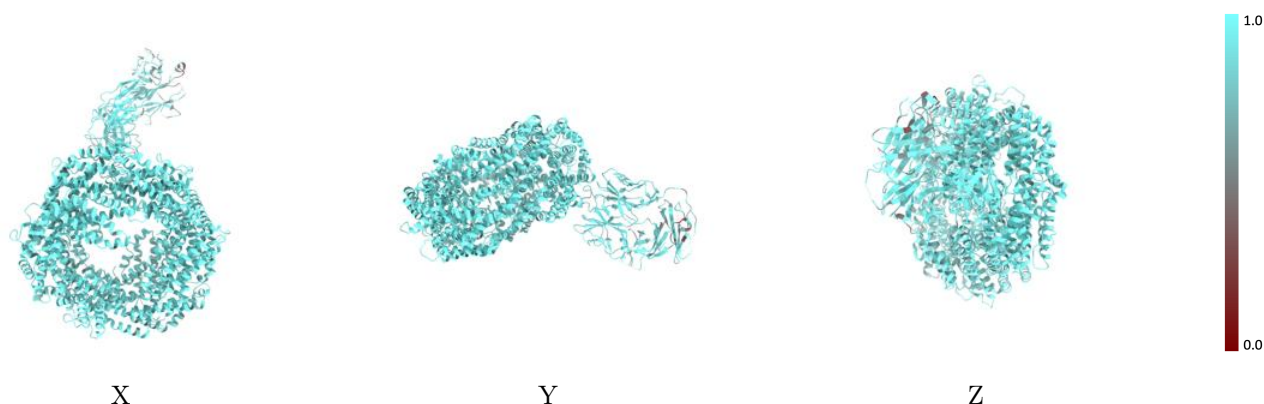
The images above show the 3D surface view of the map at the recommended contour level 3.7 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



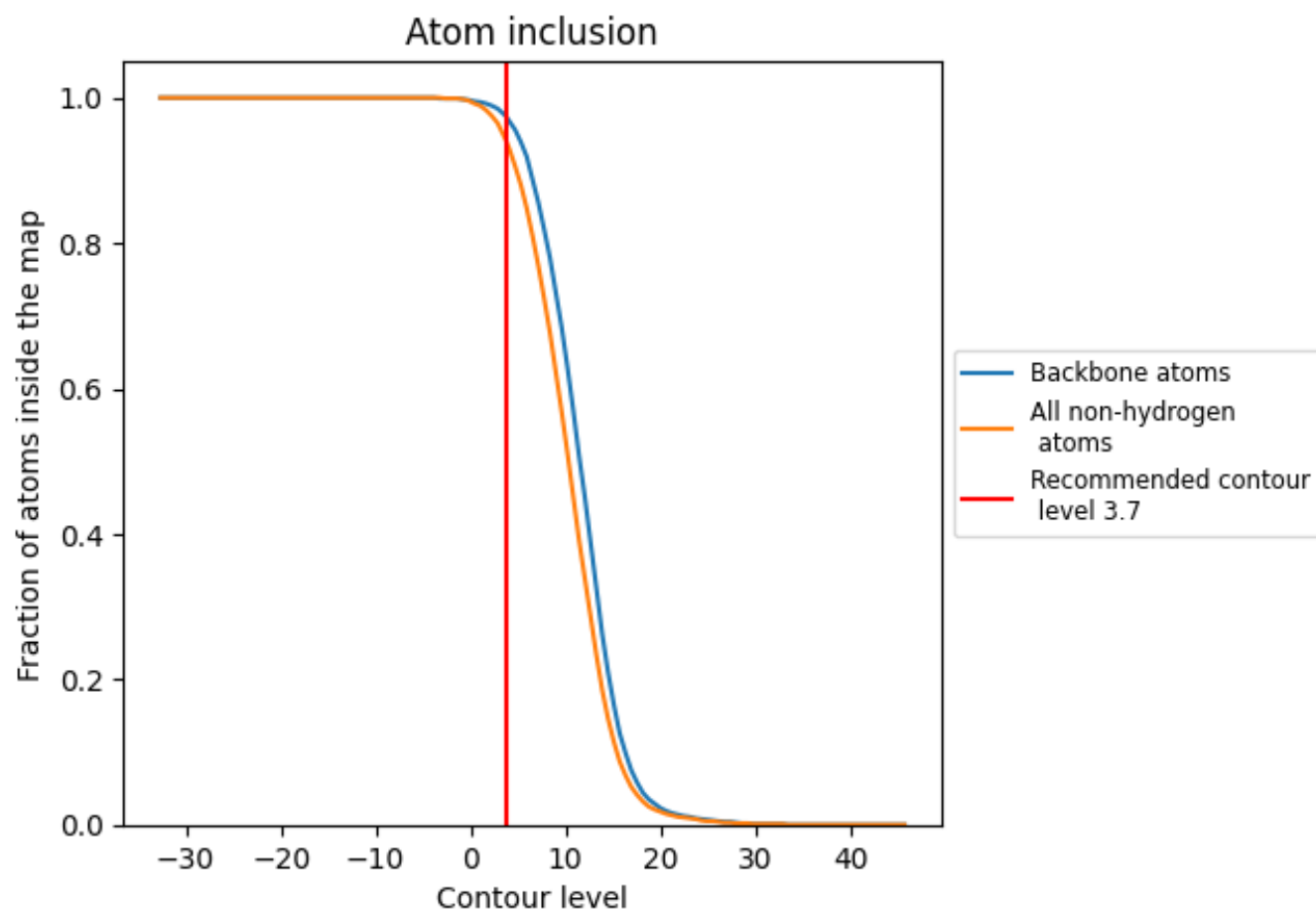
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (3.7).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% 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 (3.7) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.9420	<div></div> 0.6910
A	<div></div> 0.9480	<div></div> 0.7210
B	<div></div> 0.9590	<div></div> 0.7200
C	<div></div> 0.9550	<div></div> 0.7220
D	<div></div> 0.9560	<div></div> 0.7190
E	<div></div> 0.9710	<div></div> 0.7330
F	<div></div> 0.9630	<div></div> 0.7260
G	<div></div> 0.9240	<div></div> 0.7110
H	<div></div> 0.9530	<div></div> 0.7160
I	<div></div> 0.9750	<div></div> 0.7320
J	<div></div> 0.9670	<div></div> 0.7310
K	<div></div> 0.9690	<div></div> 0.7240
L	<div></div> 0.9570	<div></div> 0.7220
a	<div></div> 0.8570	<div></div> 0.5190
b	<div></div> 0.8490	<div></div> 0.5050

1.0

0.0

<0.0