



## Full wwPDB EM Validation Report ⓘ

Nov 3, 2024 – 01:43 AM EDT

PDB ID : 6UCB  
EMDB ID : EMD-20727  
Title : GluA2 in complex with its auxiliary subunit CNIH3 - with antagonist ZK200775, LBD, TMD, CNIH3, and lipids  
Authors : Nakagawa, T.  
Deposited on : 2019-09-15  
Resolution : 3.28 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>.

---

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

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

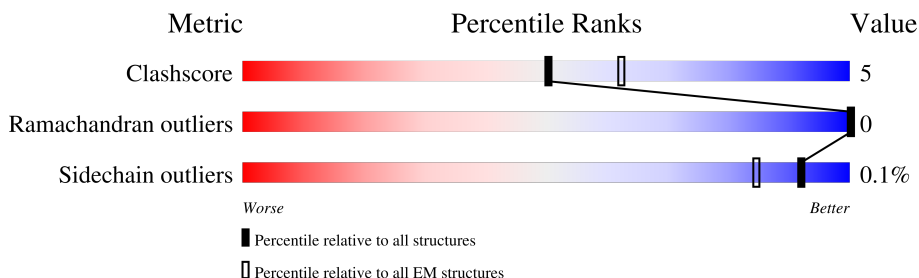
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.28 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	889	
1	B	889	
1	C	889	
1	D	889	
2	E	174	
2	F	174	
2	G	174	
2	H	174	

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 33286 atoms, of which 16656 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 Glutamate receptor 2.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	378	Total	C	H	N	O	S	0	0
			5781	1873	2890	471	529	18		
1	B	378	Total	C	H	N	O	S	0	0
			5778	1874	2888	471	527	18		
1	C	378	Total	C	H	N	O	S	0	0
			5781	1873	2890	471	529	18		
1	D	378	Total	C	H	N	O	S	0	0
			5778	1874	2888	471	527	18		

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	586	ARG	GLN	conflict	UNP P19491
A	848	ASP	-	expression tag	UNP P19491
A	849	TYR	-	expression tag	UNP P19491
A	850	LYS	-	expression tag	UNP P19491
A	851	ASP	-	expression tag	UNP P19491
A	852	ASP	-	expression tag	UNP P19491
A	853	ASP	-	expression tag	UNP P19491
A	854	ASP	-	expression tag	UNP P19491
A	855	LYS	-	expression tag	UNP P19491
A	856	GLU	-	expression tag	UNP P19491
A	857	GLY	-	expression tag	UNP P19491
A	858	TYR	-	expression tag	UNP P19491
A	859	ASN	-	expression tag	UNP P19491
A	860	VAL	-	expression tag	UNP P19491
A	861	TYR	-	expression tag	UNP P19491
A	862	GLY	-	expression tag	UNP P19491
A	863	ILE	-	expression tag	UNP P19491
A	864	GLU	-	expression tag	UNP P19491
A	865	SER	-	expression tag	UNP P19491
A	866	VAL	-	expression tag	UNP P19491
A	867	LYS	-	expression tag	UNP P19491
A	868	ILE	-	expression tag	UNP P19491

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
B	586	ARG	GLN	conflict	UNP P19491
B	848	ASP	-	expression tag	UNP P19491
B	849	TYR	-	expression tag	UNP P19491
B	850	LYS	-	expression tag	UNP P19491
B	851	ASP	-	expression tag	UNP P19491
B	852	ASP	-	expression tag	UNP P19491
B	853	ASP	-	expression tag	UNP P19491
B	854	ASP	-	expression tag	UNP P19491
B	855	LYS	-	expression tag	UNP P19491
B	856	GLU	-	expression tag	UNP P19491
B	857	GLY	-	expression tag	UNP P19491
B	858	TYR	-	expression tag	UNP P19491
B	859	ASN	-	expression tag	UNP P19491
B	860	VAL	-	expression tag	UNP P19491
B	861	TYR	-	expression tag	UNP P19491
B	862	GLY	-	expression tag	UNP P19491
B	863	ILE	-	expression tag	UNP P19491
B	864	GLU	-	expression tag	UNP P19491
B	865	SER	-	expression tag	UNP P19491
B	866	VAL	-	expression tag	UNP P19491
B	867	LYS	-	expression tag	UNP P19491
B	868	ILE	-	expression tag	UNP P19491
C	586	ARG	GLN	conflict	UNP P19491
C	848	ASP	-	expression tag	UNP P19491
C	849	TYR	-	expression tag	UNP P19491
C	850	LYS	-	expression tag	UNP P19491
C	851	ASP	-	expression tag	UNP P19491
C	852	ASP	-	expression tag	UNP P19491
C	853	ASP	-	expression tag	UNP P19491
C	854	ASP	-	expression tag	UNP P19491
C	855	LYS	-	expression tag	UNP P19491
C	856	GLU	-	expression tag	UNP P19491
C	857	GLY	-	expression tag	UNP P19491
C	858	TYR	-	expression tag	UNP P19491
C	859	ASN	-	expression tag	UNP P19491
C	860	VAL	-	expression tag	UNP P19491
C	861	TYR	-	expression tag	UNP P19491
C	862	GLY	-	expression tag	UNP P19491
C	863	ILE	-	expression tag	UNP P19491
C	864	GLU	-	expression tag	UNP P19491
C	865	SER	-	expression tag	UNP P19491
C	866	VAL	-	expression tag	UNP P19491

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
C	867	LYS	-	expression tag	UNP P19491
C	868	ILE	-	expression tag	UNP P19491
D	586	ARG	GLN	conflict	UNP P19491
D	848	ASP	-	expression tag	UNP P19491
D	849	TYR	-	expression tag	UNP P19491
D	850	LYS	-	expression tag	UNP P19491
D	851	ASP	-	expression tag	UNP P19491
D	852	ASP	-	expression tag	UNP P19491
D	853	ASP	-	expression tag	UNP P19491
D	854	ASP	-	expression tag	UNP P19491
D	855	LYS	-	expression tag	UNP P19491
D	856	GLU	-	expression tag	UNP P19491
D	857	GLY	-	expression tag	UNP P19491
D	858	TYR	-	expression tag	UNP P19491
D	859	ASN	-	expression tag	UNP P19491
D	860	VAL	-	expression tag	UNP P19491
D	861	TYR	-	expression tag	UNP P19491
D	862	GLY	-	expression tag	UNP P19491
D	863	ILE	-	expression tag	UNP P19491
D	864	GLU	-	expression tag	UNP P19491
D	865	SER	-	expression tag	UNP P19491
D	866	VAL	-	expression tag	UNP P19491
D	867	LYS	-	expression tag	UNP P19491
D	868	ILE	-	expression tag	UNP P19491

- Molecule 2 is a protein called Protein cornichon homolog 3.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	E	132	Total	C	H	N	O	S	0	0
			2121	741	1035	162	171	12		
2	F	134	Total	C	H	N	O	S	0	0
			2145	758	1033	166	176	12		
2	G	132	Total	C	H	N	O	S	0	0
			2121	741	1035	162	171	12		
2	H	134	Total	C	H	N	O	S	0	0
			2147	758	1035	166	176	12		

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	161	GLY	-	linker	UNP Q6ZWS4
E	162	GLY	-	linker	UNP Q6ZWS4

*Continued on next page...*

*Continued from previous page...*

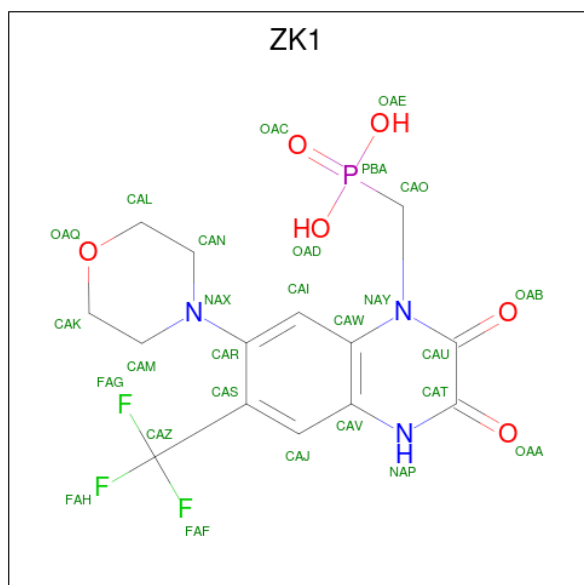
Chain	Residue	Modelled	Actual	Comment	Reference
E	163	ARG	-	linker	UNP Q6ZWS4
E	164	GLY	-	linker	UNP Q6ZWS4
E	165	GLY	-	linker	UNP Q6ZWS4
E	166	THR	-	expression tag	UNP Q6ZWS4
E	167	GLU	-	expression tag	UNP Q6ZWS4
E	168	THR	-	expression tag	UNP Q6ZWS4
E	169	SER	-	expression tag	UNP Q6ZWS4
E	170	GLN	-	expression tag	UNP Q6ZWS4
E	171	VAL	-	expression tag	UNP Q6ZWS4
E	172	ALA	-	expression tag	UNP Q6ZWS4
E	173	PRO	-	expression tag	UNP Q6ZWS4
E	174	ALA	-	expression tag	UNP Q6ZWS4
F	161	GLY	-	linker	UNP Q6ZWS4
F	162	GLY	-	linker	UNP Q6ZWS4
F	163	ARG	-	linker	UNP Q6ZWS4
F	164	GLY	-	linker	UNP Q6ZWS4
F	165	GLY	-	linker	UNP Q6ZWS4
F	166	THR	-	expression tag	UNP Q6ZWS4
F	167	GLU	-	expression tag	UNP Q6ZWS4
F	168	THR	-	expression tag	UNP Q6ZWS4
F	169	SER	-	expression tag	UNP Q6ZWS4
F	170	GLN	-	expression tag	UNP Q6ZWS4
F	171	VAL	-	expression tag	UNP Q6ZWS4
F	172	ALA	-	expression tag	UNP Q6ZWS4
F	173	PRO	-	expression tag	UNP Q6ZWS4
F	174	ALA	-	expression tag	UNP Q6ZWS4
G	161	GLY	-	linker	UNP Q6ZWS4
G	162	GLY	-	linker	UNP Q6ZWS4
G	163	ARG	-	linker	UNP Q6ZWS4
G	164	GLY	-	linker	UNP Q6ZWS4
G	165	GLY	-	linker	UNP Q6ZWS4
G	166	THR	-	expression tag	UNP Q6ZWS4
G	167	GLU	-	expression tag	UNP Q6ZWS4
G	168	THR	-	expression tag	UNP Q6ZWS4
G	169	SER	-	expression tag	UNP Q6ZWS4
G	170	GLN	-	expression tag	UNP Q6ZWS4
G	171	VAL	-	expression tag	UNP Q6ZWS4
G	172	ALA	-	expression tag	UNP Q6ZWS4
G	173	PRO	-	expression tag	UNP Q6ZWS4
G	174	ALA	-	expression tag	UNP Q6ZWS4
H	161	GLY	-	linker	UNP Q6ZWS4
H	162	GLY	-	linker	UNP Q6ZWS4

*Continued on next page...*

Continued from previous page...

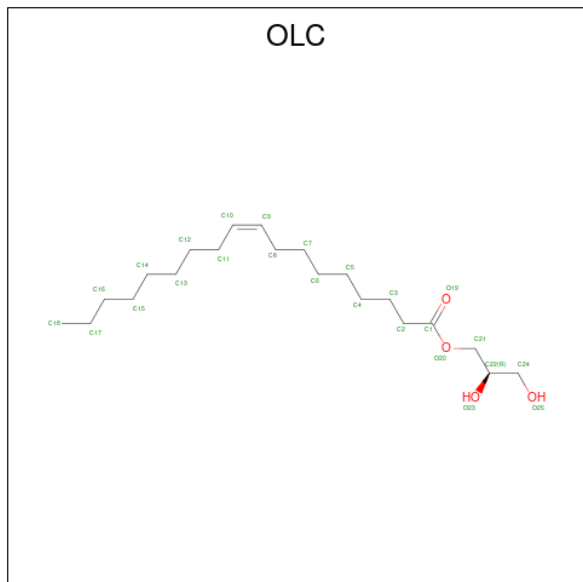
Chain	Residue	Modelled	Actual	Comment	Reference
H	163	ARG	-	linker	UNP Q6ZWS4
H	164	GLY	-	linker	UNP Q6ZWS4
H	165	GLY	-	linker	UNP Q6ZWS4
H	166	THR	-	expression tag	UNP Q6ZWS4
H	167	GLU	-	expression tag	UNP Q6ZWS4
H	168	THR	-	expression tag	UNP Q6ZWS4
H	169	SER	-	expression tag	UNP Q6ZWS4
H	170	GLN	-	expression tag	UNP Q6ZWS4
H	171	VAL	-	expression tag	UNP Q6ZWS4
H	172	ALA	-	expression tag	UNP Q6ZWS4
H	173	PRO	-	expression tag	UNP Q6ZWS4
H	174	ALA	-	expression tag	UNP Q6ZWS4

- Molecule 3 is {[7-morpholin-4-yl-2,3-dioxo-6-(trifluoromethyl)-3,4-dihydroquinoxalin-1(2H)-yl]methyl}phosphonic acid (three-letter code: ZK1) (formula: C<sub>14</sub>H<sub>15</sub>F<sub>3</sub>N<sub>3</sub>O<sub>6</sub>P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms							AltConf
3	A	1	Total	C	F	H	N	O	P	0
			40	14	3	13	3	6	1	
3	B	1	Total	C	F	H	N	O	P	0
			40	14	3	13	3	6	1	
3	C	1	Total	C	F	H	N	O	P	0
			40	14	3	13	3	6	1	
3	D	1	Total	C	F	H	N	O	P	0
			40	14	3	13	3	6	1	

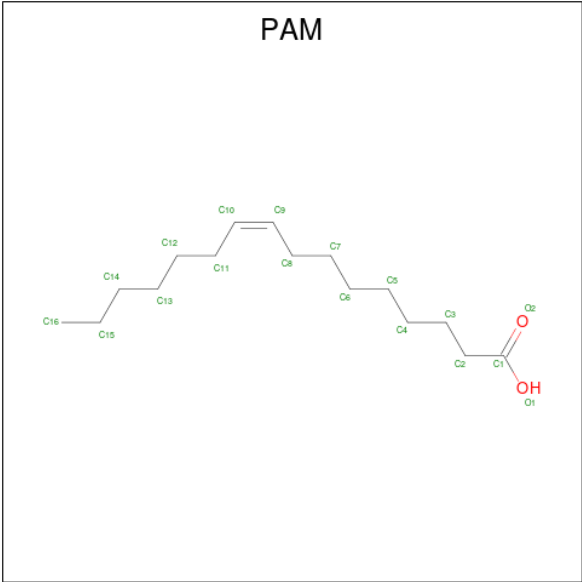
- Molecule 4 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (three-letter code: OLC) (formula:  $C_{21}H_{40}O_4$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	H	O	0
			65	21	40	4	
4	B	1	Total	C	H	O	0
			65	21	40	4	
4	B	1	Total	C	H	O	0
			65	21	40	4	
4	B	1	Total	C	H	O	0
			65	21	40	4	
4	C	1	Total	C	H	O	0
			65	21	40	4	
4	D	1	Total	C	H	O	0
			65	21	40	4	
4	D	1	Total	C	H	O	0
			65	21	40	4	
4	D	1	Total	C	H	O	0
			65	21	40	4	

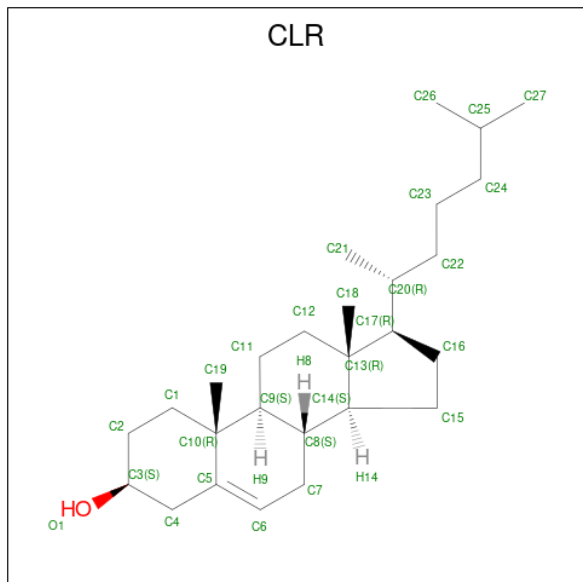
- Molecule 5 is PALMITOLEIC ACID (three-letter code: PAM) (formula:  $C_{16}H_{30}O_2$ ) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	H	O	0
			47	16	29	2	
5	A	1	Total	C	H	O	0
			47	16	29	2	
5	B	1	Total	C	H	O	0
			47	16	29	2	
5	B	1	Total	C	H	O	0
			47	16	29	2	
5	C	1	Total	C	H	O	0
			47	16	29	2	
5	C	1	Total	C	H	O	0
			47	16	29	2	
5	E	1	Total	C	H	O	0
			47	16	29	2	
5	F	1	Total	C	H	O	0
			47	16	29	2	
5	F	1	Total	C	H	O	0
			47	16	29	2	
5	G	1	Total	C	H	O	0
			47	16	29	2	
5	H	1	Total	C	H	O	0
			47	16	29	2	
5	H	1	Total	C	H	O	0
			47	16	29	2	
5	D	1	Total	C	H	O	0
			47	16	29	2	
5	D	1	Total	C	H	O	0
			47	16	29	2	

- Molecule 6 is CHOLESTEROL (three-letter code: CLR) (formula:  $C_{27}H_{46}O$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
6	B	1	Total	C	H	O	0
			74	27	46	1	
6	E	1	Total	C	H	O	0
			74	27	46	1	
6	G	1	Total	C	H	O	0
			74	27	46	1	
6	H	1	Total	C	H	O	0
			74	27	46	1	



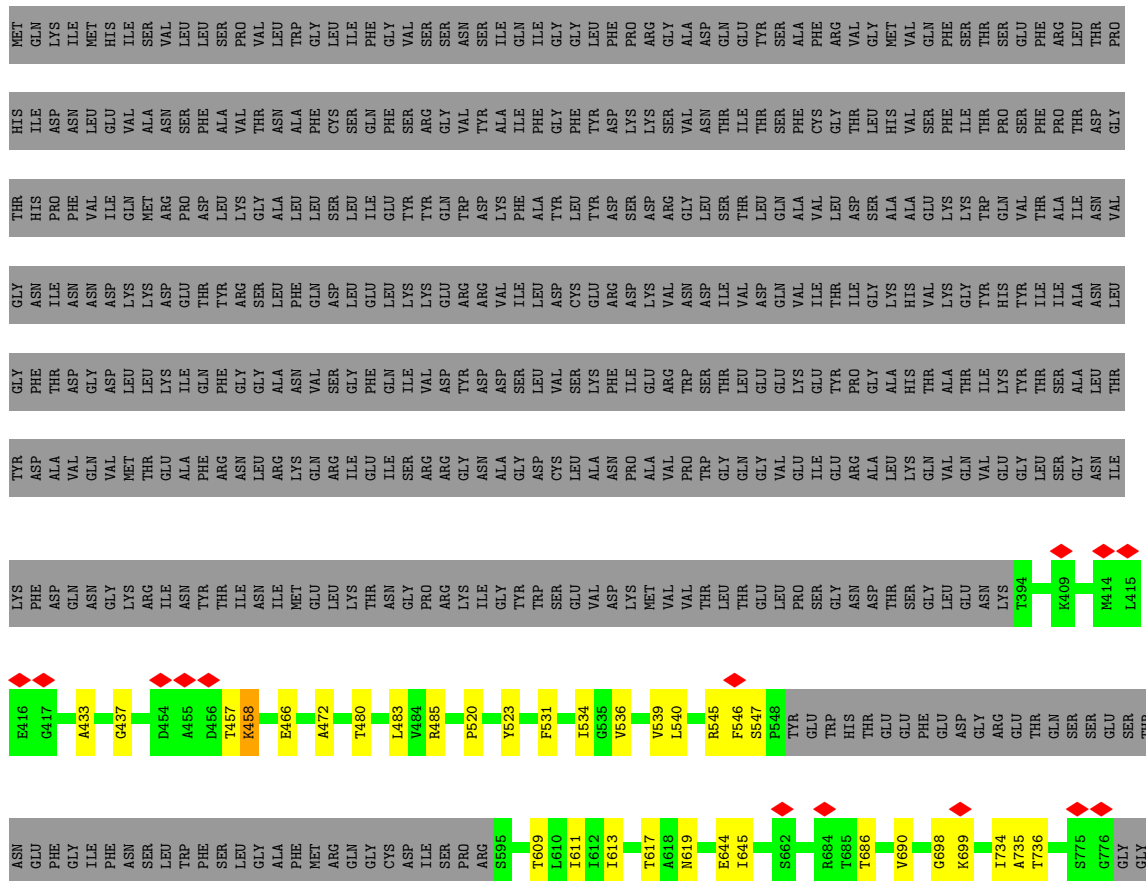
57%

ILE  
GLU  
SER  
VAL  
LYS  
ILE

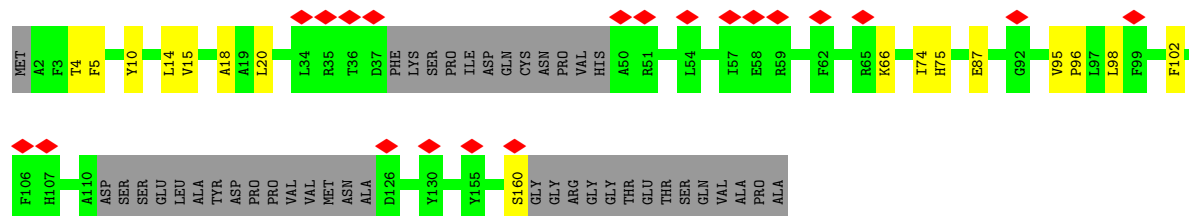
## 57%

GLY  
ASN  
ILE  
ASN  
ASN  
ASP

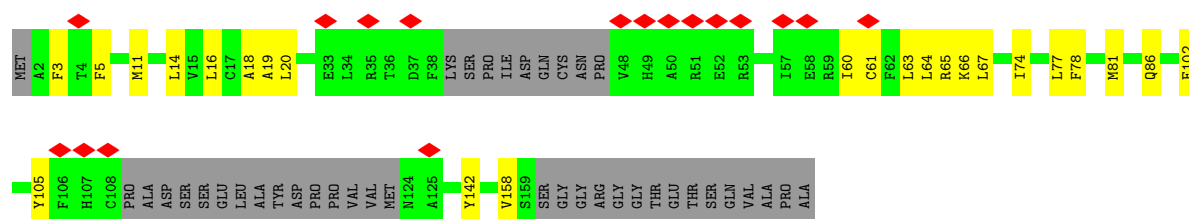
- Molecule 1: Glutamate receptor 2



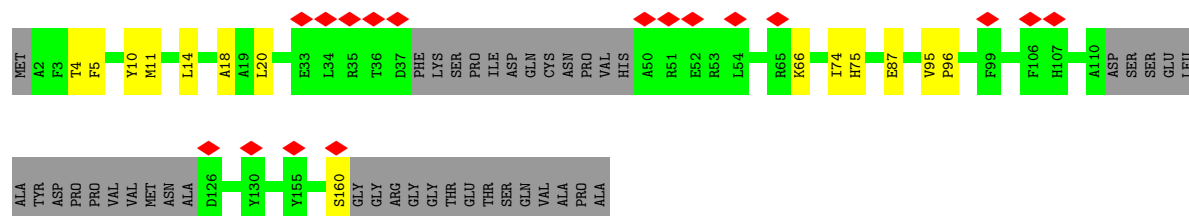
- Molecule 2: Protein cornichon homolog 3



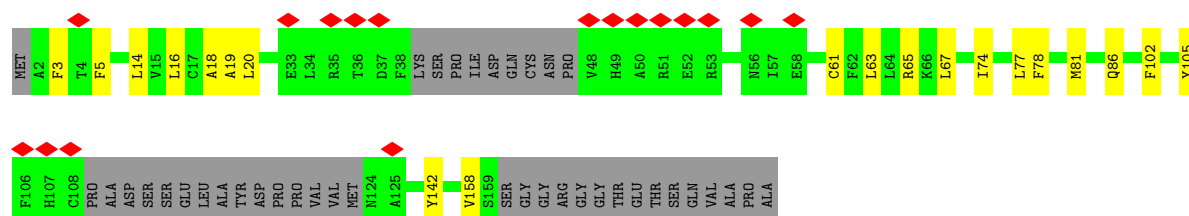
- Molecule 2: Protein cornichon homolog 3



- Molecule 2: Protein cornichon homolog 3



- Molecule 2: Protein cornichon homolog 3



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	111016	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	58.5	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.215	Depositor
Minimum map value	-0.122	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.027	Depositor
Map size (Å)	383.76, 383.76, 383.76	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.066, 1.066, 1.066	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: PAM, ZK1, CLR, OLC

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	0.28	0/2950	0.41	0/3990
1	B	0.28	0/2949	0.41	0/3988
1	C	0.28	0/2950	0.41	0/3990
1	D	0.28	0/2949	0.41	0/3988
2	E	0.27	0/1123	0.38	0/1527
2	F	0.28	0/1149	0.37	0/1561
2	G	0.27	0/1123	0.38	0/1527
2	H	0.28	0/1149	0.37	0/1561
All	All	0.28	0/16342	0.40	0/22132

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2891	2890	2898	35	0
1	B	2890	2888	2900	33	0
1	C	2891	2890	2898	34	0
1	D	2890	2888	2900	30	0
2	E	1086	1035	1047	12	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	1112	1033	1071	20	0
2	G	1086	1035	1047	13	0
2	H	1112	1035	1071	17	0
3	A	27	13	13	0	0
3	B	27	13	13	0	0
3	C	27	13	13	0	0
3	D	27	13	13	0	0
4	A	25	40	40	1	0
4	B	75	120	120	0	0
4	C	25	40	40	0	0
4	D	75	120	120	0	0
5	A	36	58	58	3	0
5	B	36	58	58	1	0
5	C	36	58	58	2	0
5	D	36	58	58	3	0
5	E	18	29	29	1	0
5	F	36	58	58	1	0
5	G	18	29	29	2	0
5	H	36	58	58	1	0
6	B	28	46	46	6	0
6	E	28	46	46	4	0
6	G	28	46	46	6	0
6	H	28	46	46	9	0
All	All	16630	16656	16794	181	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (181) 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)
6:H:203:CLR:H183	6:H:203:CLR:H212	1.48	0.95
6:B:907:CLR:H212	6:B:907:CLR:H183	1.52	0.88
1:B:539:VAL:HG21	1:C:803:LEU:HD12	1.54	0.87
1:A:803:LEU:HD12	1:D:539:VAL:HG21	1.55	0.86
6:G:202:CLR:H183	6:G:202:CLR:H212	1.57	0.83
2:G:14:LEU:HD23	6:G:202:CLR:H213	1.65	0.79
1:A:504:ILE:HD13	1:A:633:ILE:HD11	1.69	0.75
1:C:504:ILE:HD13	1:C:633:ILE:HD11	1.69	0.73
1:B:644:GLU:N	1:B:644:GLU:OE1	2.25	0.70
1:D:644:GLU:N	1:D:644:GLU:OE1	2.25	0.69

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:632:PRO:O	1:C:633:ILE:HG23	1.92	0.69
1:A:632:PRO:O	1:A:633:ILE:HG23	1.92	0.69
1:A:520:PRO:O	1:A:619:ASN:ND2	2.28	0.67
6:E:202:CLR:H212	6:E:202:CLR:H183	1.78	0.65
2:H:14:LEU:CD1	6:H:203:CLR:H213	2.25	0.65
1:C:520:PRO:O	1:C:619:ASN:ND2	2.28	0.65
6:B:907:CLR:H263	2:F:18:ALA:HB1	1.79	0.64
6:B:907:CLR:H213	2:F:14:LEU:HD13	1.80	0.63
1:D:433:ALA:O	1:D:437:GLY:N	2.31	0.63
6:B:907:CLR:H213	2:F:14:LEU:CD1	2.29	0.63
1:B:433:ALA:O	1:B:437:GLY:N	2.31	0.63
1:A:611:ILE:HG21	1:B:795:VAL:HG21	1.83	0.60
2:H:86:GLN:NE2	5:H:202:PAM:O2	2.33	0.60
1:C:614:SER:CB	1:D:617:THR:HG22	2.31	0.60
5:D:906:PAM:H61	5:D:906:PAM:H10	1.84	0.60
2:H:14:LEU:HD13	6:H:203:CLR:H213	1.83	0.60
2:F:86:GLN:NE2	5:F:202:PAM:O2	2.35	0.59
1:B:545:ARG:NH1	2:G:66:LYS:O	2.31	0.59
2:E:14:LEU:HD23	6:E:202:CLR:H213	1.85	0.59
1:D:520:PRO:O	1:D:619:ASN:ND2	2.35	0.58
1:B:520:PRO:O	1:B:619:ASN:ND2	2.36	0.58
2:G:14:LEU:CD2	6:G:202:CLR:H213	2.34	0.58
1:A:614:SER:CB	1:B:617:THR:HG22	2.34	0.57
1:A:684:ARG:NE	1:A:688:GLU:OE2	2.38	0.56
1:C:611:ILE:HG21	1:D:795:VAL:HG21	1.87	0.56
2:H:61:CYS:SG	2:H:65:ARG:NH1	2.79	0.56
2:F:61:CYS:SG	2:F:65:ARG:NH1	2.79	0.55
1:B:480:THR:O	1:B:485:ARG:NH1	2.39	0.55
1:D:480:THR:O	1:D:485:ARG:NH1	2.39	0.55
1:C:684:ARG:NE	1:C:688:GLU:OE2	2.38	0.55
1:A:452:ALA:N	1:A:461:ASN:OD1	2.40	0.55
1:C:524:GLU:OE2	2:H:5:PHE:N	2.40	0.54
2:G:18:ALA:CB	6:G:202:CLR:H263	2.38	0.54
1:C:452:ALA:N	1:C:461:ASN:OD1	2.40	0.54
1:A:524:GLU:OE2	2:F:5:PHE:N	2.40	0.54
1:C:521:LEU:HD12	1:C:525:ILE:HG21	1.90	0.54
1:D:801:GLY:HA3	5:D:906:PAM:H163	1.90	0.54
2:H:18:ALA:CB	6:H:203:CLR:H263	2.38	0.53
2:F:158:VAL:HG23	2:F:158:VAL:O	2.08	0.53
1:A:521:LEU:HD12	1:A:525:ILE:HG21	1.90	0.53
1:C:405:TYR:OH	1:C:707:THR:HG21	2.08	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:902:OLC:O25	5:A:903:PAM:O2	2.15	0.53
1:B:613:ILE:O	1:B:617:THR:HG23	2.09	0.53
1:D:613:ILE:O	1:D:617:THR:HG23	2.09	0.53
1:A:405:TYR:OH	1:A:707:THR:HG21	2.08	0.53
2:E:66:LYS:O	1:D:545:ARG:NH1	2.36	0.53
1:C:503:MET:HE1	1:C:690:VAL:HG22	1.91	0.53
2:E:18:ALA:CB	6:E:202:CLR:H263	2.39	0.53
2:H:158:VAL:O	2:H:158:VAL:HG23	2.09	0.52
1:C:456:ASP:OD2	1:C:457:THR:HG23	2.09	0.52
1:A:456:ASP:OD2	1:A:457:THR:HG23	2.09	0.52
6:B:907:CLR:H263	2:F:18:ALA:CB	2.39	0.52
6:H:203:CLR:H212	6:H:203:CLR:C18	2.32	0.51
2:H:77:LEU:HD21	2:H:81:MET:HE1	1.92	0.51
2:H:20:LEU:HD13	2:H:74:ILE:HD11	1.93	0.51
2:E:74:ILE:HG13	2:E:75:HIS:N	2.26	0.51
1:A:803:LEU:CD1	1:D:539:VAL:HG21	2.35	0.51
2:H:18:ALA:HB1	6:H:203:CLR:H263	1.91	0.51
1:A:600:ILE:HD11	1:B:806:ALA:HA	1.93	0.50
2:F:20:LEU:HD13	2:F:74:ILE:HD11	1.93	0.50
2:F:16:LEU:HD12	2:F:78:PHE:HE1	1.76	0.50
1:B:523:TYR:HB3	5:G:201:PAM:C5	2.42	0.50
1:B:611:ILE:HG21	1:C:795:VAL:HG21	1.94	0.49
2:G:18:ALA:HB1	6:G:202:CLR:H263	1.95	0.49
2:G:74:ILE:HG13	2:G:75:HIS:N	2.26	0.49
2:H:16:LEU:HD12	2:H:78:PHE:HE1	1.76	0.49
1:A:755:GLU:OE2	1:D:483:LEU:N	2.43	0.49
1:A:795:VAL:HG21	1:D:611:ILE:HG21	1.95	0.49
1:C:433:ALA:O	1:C:437:GLY:N	2.43	0.49
2:F:77:LEU:HD21	2:F:81:MET:HE1	1.93	0.49
1:A:521:LEU:HD21	1:A:526:TRP:CZ2	2.49	0.48
1:A:792:VAL:HG12	1:A:792:VAL:O	2.13	0.48
1:B:531:PHE:CD1	1:B:534:ILE:HD11	2.49	0.48
1:C:800:VAL:HG11	2:G:11:MET:HB3	1.95	0.48
1:D:531:PHE:CD1	1:D:534:ILE:HD11	2.49	0.48
1:C:630:VAL:O	1:C:630:VAL:HG23	2.13	0.48
1:C:502:ILE:O	1:C:709:ASN:ND2	2.46	0.48
1:A:502:ILE:O	1:A:709:ASN:ND2	2.46	0.48
1:B:801:GLY:HA3	5:B:906:PAM:H163	1.96	0.48
1:A:630:VAL:HG23	1:A:630:VAL:O	2.13	0.47
1:C:742:LEU:O	1:C:746:VAL:N	2.47	0.47
1:D:645:ILE:HG22	1:D:698:GLY:O	2.14	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:466:GLU:O	1:B:472:ALA:N	2.47	0.47
1:C:792:VAL:O	1:C:792:VAL:HG12	2.13	0.47
1:A:742:LEU:O	1:A:746:VAL:N	2.47	0.47
1:C:521:LEU:HD21	1:C:526:TRP:CZ2	2.49	0.47
5:A:903:PAM:H112	5:A:904:PAM:H161	1.96	0.47
1:A:503:MET:HE1	1:A:690:VAL:HG22	1.97	0.47
1:B:645:ILE:HG22	1:B:698:GLY:O	2.15	0.47
1:A:433:ALA:O	1:A:437:GLY:N	2.43	0.47
1:D:466:GLU:O	1:D:472:ALA:N	2.47	0.47
1:C:600:ILE:HD11	1:D:806:ALA:HA	1.96	0.47
5:A:903:PAM:C11	5:A:904:PAM:H161	2.45	0.46
6:H:203:CLR:H183	6:H:203:CLR:C21	2.32	0.46
1:C:646:ALA:N	1:C:699:LYS:O	2.49	0.46
2:G:95:VAL:N	2:G:96:PRO:CD	2.79	0.46
1:D:546:PHE:O	1:D:547:SER:OG	2.30	0.46
1:C:514:VAL:N	5:C:904:PAM:O1	2.49	0.46
2:E:95:VAL:N	2:E:96:PRO:CD	2.79	0.46
1:A:646:ALA:N	1:A:699:LYS:O	2.49	0.45
1:A:456:ASP:OD2	1:A:457:THR:N	2.49	0.45
1:C:456:ASP:OD2	1:C:457:THR:N	2.49	0.45
2:F:63:LEU:O	2:F:67:LEU:HD13	2.17	0.45
1:B:457:THR:O	1:B:458:LYS:HG3	2.16	0.45
2:H:63:LEU:O	2:H:67:LEU:HD13	2.17	0.45
1:D:457:THR:O	1:D:458:LYS:HG3	2.16	0.45
1:D:735:ALA:O	1:D:736:THR:OG1	2.32	0.45
2:F:20:LEU:HG	2:F:142:TYR:CD2	2.52	0.45
2:H:20:LEU:HG	2:H:142:TYR:CD2	2.52	0.45
1:B:735:ALA:O	1:B:736:THR:OG1	2.32	0.45
2:H:14:LEU:HD11	6:H:203:CLR:H213	1.97	0.44
2:H:19:ALA:HB2	1:D:807:MET:HE3	1.98	0.44
6:H:203:CLR:H41	5:D:906:PAM:H9	1.99	0.44
1:D:536:VAL:O	1:D:540:LEU:HD23	2.18	0.44
1:A:521:LEU:HD23	1:A:521:LEU:H	1.81	0.44
1:B:536:VAL:O	1:B:540:LEU:HD23	2.18	0.44
5:C:903:PAM:C11	5:C:904:PAM:H161	2.48	0.44
2:E:20:LEU:CD1	2:E:74:ILE:HD12	2.48	0.44
2:G:20:LEU:CD1	2:G:74:ILE:HD12	2.48	0.44
1:A:498:LEU:HD12	1:A:705:GLU:HG3	1.99	0.43
1:B:523:TYR:HB3	5:G:201:PAM:H51	1.99	0.43
1:C:498:LEU:HD12	1:C:705:GLU:HG3	1.99	0.43
1:C:521:LEU:H	1:C:521:LEU:HD23	1.81	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:539:VAL:HG21	1:C:803:LEU:CD1	2.35	0.43
1:A:502:ILE:HD12	1:A:633:ILE:HD12	2.00	0.43
6:B:907:CLR:H212	6:B:907:CLR:C18	2.35	0.43
1:A:519:ASP:N	1:A:520:PRO:CD	2.82	0.43
1:C:502:ILE:HD12	1:C:633:ILE:HD12	2.00	0.43
2:G:160:SER:O	2:G:160:SER:OG	2.31	0.43
1:A:600:ILE:HD11	1:B:806:ALA:CA	2.48	0.43
1:B:483:LEU:N	1:C:755:GLU:OE2	2.42	0.43
1:B:807:MET:HE1	2:F:16:LEU:HA	2.00	0.43
1:A:498:LEU:N	1:A:498:LEU:HD23	2.34	0.42
1:B:645:ILE:HG22	1:B:699:LYS:HA	2.01	0.42
1:C:498:LEU:HD23	1:C:498:LEU:N	2.34	0.42
1:C:819:ARG:O	1:C:824:ARG:N	2.47	0.42
6:G:202:CLR:H212	6:G:202:CLR:C18	2.40	0.42
1:A:545:ARG:NE	2:F:66:LYS:O	2.37	0.42
1:C:519:ASP:N	1:C:520:PRO:CD	2.82	0.42
1:D:645:ILE:HG22	1:D:699:LYS:HA	2.01	0.42
1:C:407:MET:O	1:C:422:GLU:N	2.51	0.42
1:D:686:THR:O	1:D:690:VAL:HG23	2.20	0.42
1:B:686:THR:O	1:B:690:VAL:HG23	2.19	0.42
5:E:201:PAM:C5	1:D:523:TYR:HB3	2.50	0.42
2:H:3:PHE:CG	1:D:789:LEU:HD22	2.54	0.42
2:E:160:SER:O	2:E:160:SER:OG	2.31	0.42
1:A:407:MET:O	1:A:422:GLU:N	2.51	0.42
1:B:546:PHE:O	1:B:547:SER:OG	2.30	0.41
1:B:789:LEU:HD22	2:F:3:PHE:CG	2.55	0.41
2:E:5:PHE:O	2:E:5:PHE:CG	2.73	0.41
2:E:4:THR:O	2:E:5:PHE:HB3	2.20	0.41
1:D:815:CYS:HG	1:D:816:TYR:HD1	1.67	0.41
1:A:500:ILE:N	1:A:728:ASP:OD1	2.54	0.41
1:B:609:THR:O	1:B:613:ILE:HD12	2.20	0.41
2:E:10:TYR:OH	2:E:87:GLU:OE2	2.39	0.41
1:A:506:LYS:NZ	1:A:718:CYS:O	2.42	0.41
2:F:60:ILE:O	2:F:64:LEU:HD13	2.21	0.41
2:G:5:PHE:O	2:G:5:PHE:CG	2.73	0.41
2:E:15:VAL:HG22	6:E:202:CLR:H222	2.02	0.41
2:F:102:PHE:HA	2:F:105:TYR:HD2	1.86	0.41
2:G:4:THR:O	2:G:5:PHE:HB3	2.20	0.41
2:H:102:PHE:HA	2:H:105:TYR:HD2	1.86	0.41
1:D:458:LYS:O	1:D:458:LYS:HD2	2.21	0.41
1:D:609:THR:O	1:D:613:ILE:HD12	2.20	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:458:LYS:O	1:B:458:LYS:HD2	2.21	0.41
1:B:800:VAL:HG21	2:F:11:MET:SD	2.61	0.41
2:E:98:LEU:HD21	2:E:102:PHE:CZ	2.56	0.41
1:D:734:ILE:HG22	1:D:735:ALA:N	2.36	0.41
1:B:734:ILE:HG22	1:B:735:ALA:N	2.36	0.40
1:B:807:MET:CE	2:F:19:ALA:HB2	2.51	0.40
2:G:10:TYR:OH	2:G:87:GLU:OE2	2.39	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	372/889 (42%)	352 (95%)	20 (5%)	0	100	100
1	B	372/889 (42%)	354 (95%)	18 (5%)	0	100	100
1	C	372/889 (42%)	351 (94%)	21 (6%)	0	100	100
1	D	372/889 (42%)	354 (95%)	18 (5%)	0	100	100
2	E	126/174 (72%)	118 (94%)	8 (6%)	0	100	100
2	F	128/174 (74%)	124 (97%)	4 (3%)	0	100	100
2	G	126/174 (72%)	118 (94%)	8 (6%)	0	100	100
2	H	128/174 (74%)	124 (97%)	4 (3%)	0	100	100
All	All	1996/4252 (47%)	1895 (95%)	101 (5%)	0	100	100

There are no Ramachandran outliers to report.

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

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

entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	302/761 (40%)	302 (100%)	0	100	100
1	B	302/761 (40%)	301 (100%)	1 (0%)	91	94
1	C	302/761 (40%)	302 (100%)	0	100	100
1	D	302/761 (40%)	301 (100%)	1 (0%)	91	94
2	E	111/153 (72%)	111 (100%)	0	100	100
2	F	114/153 (74%)	114 (100%)	0	100	100
2	G	111/153 (72%)	111 (100%)	0	100	100
2	H	114/153 (74%)	114 (100%)	0	100	100
All	All	1658/3656 (45%)	1656 (100%)	2 (0%)	92	96

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	458	LYS
1	D	458	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	791	ASN
1	C	791	ASN
2	F	27	HIS
2	F	56	ASN
2	F	94	ASN
2	H	27	HIS
2	H	56	ASN
2	H	94	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

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$
3	ZK1	B	901	-	29,29,29	3.71	12 (41%)	45,45,45	1.50	8 (17%)
4	OLC	D	904	-	24,24,24	1.47	4 (16%)	25,25,25	1.01	2 (8%)
4	OLC	B	902	-	24,24,24	1.40	3 (12%)	25,25,25	1.01	2 (8%)
5	PAM	B	905	-	17,17,17	0.85	0	17,17,17	0.67	0
5	PAM	C	903	-	17,17,17	0.83	0	17,17,17	0.74	0
4	OLC	B	903	-	24,24,24	1.43	4 (16%)	25,25,25	1.06	2 (8%)
5	PAM	A	903	-	17,17,17	0.88	0	17,17,17	0.70	0
5	PAM	H	201	-	17,17,17	0.83	0	17,17,17	0.72	0
6	CLR	G	202	-	31,31,31	1.14	3 (9%)	48,48,48	1.74	8 (16%)
5	PAM	B	906	-	17,17,17	0.79	0	17,17,17	0.72	0
6	CLR	H	203	-	31,31,31	1.11	3 (9%)	48,48,48	1.84	10 (20%)
4	OLC	C	902	-	24,24,24	1.42	4 (16%)	25,25,25	1.01	2 (8%)
3	ZK1	C	901	-	29,29,29	3.73	11 (37%)	45,45,45	1.47	7 (15%)
3	ZK1	A	901	-	29,29,29	3.73	11 (37%)	45,45,45	1.45	6 (13%)
5	PAM	C	904	-	17,17,17	0.86	0	17,17,17	0.77	0
4	OLC	A	902	-	24,24,24	1.42	4 (16%)	25,25,25	1.00	2 (8%)
6	CLR	B	907	-	31,31,31	1.10	4 (12%)	48,48,48	1.89	12 (25%)
5	PAM	D	905	-	17,17,17	0.87	0	17,17,17	0.66	0
5	PAM	D	906	-	17,17,17	0.80	0	17,17,17	0.74	0
4	OLC	D	903	-	24,24,24	1.37	4 (16%)	25,25,25	0.99	2 (8%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	ZK1	D	901	-	29,29,29	3.73	12 (41%)	45,45,45	1.49	8 (17%)
4	OLC	D	902	-	24,24,24	1.40	4 (16%)	25,25,25	1.01	2 (8%)
5	PAM	A	904	-	17,17,17	0.87	0	17,17,17	0.76	0
4	OLC	B	904	-	24,24,24	1.48	4 (16%)	25,25,25	1.01	2 (8%)
5	PAM	E	201	-	17,17,17	0.77	0	17,17,17	0.64	0
6	CLR	E	202	-	31,31,31	1.03	2 (6%)	48,48,48	1.64	7 (14%)
5	PAM	H	202	-	17,17,17	0.78	0	17,17,17	0.76	0
5	PAM	F	202	-	17,17,17	0.77	0	17,17,17	0.75	0
5	PAM	F	201	-	17,17,17	0.84	0	17,17,17	0.71	0
5	PAM	G	201	-	17,17,17	0.81	0	17,17,17	0.72	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
3	ZK1	B	901	-	-	7/13/23/23	0/3/3/3
4	OLC	D	904	-	-	12/24/24/24	-
4	OLC	B	902	-	-	10/24/24/24	-
5	PAM	B	905	-	-	8/15/15/15	-
5	PAM	C	903	-	-	7/15/15/15	-
4	OLC	B	903	-	-	11/24/24/24	-
5	PAM	A	903	-	-	8/15/15/15	-
5	PAM	H	201	-	-	5/15/15/15	-
6	CLR	G	202	-	-	3/10/68/68	0/4/4/4
5	PAM	B	906	-	-	6/15/15/15	-
6	CLR	H	203	-	-	7/10/68/68	0/4/4/4
4	OLC	C	902	-	-	15/24/24/24	-
3	ZK1	C	901	-	-	7/13/23/23	0/3/3/3
3	ZK1	A	901	-	-	7/13/23/23	0/3/3/3
5	PAM	C	904	-	-	9/15/15/15	-
4	OLC	A	902	-	-	14/24/24/24	-
6	CLR	B	907	-	-	6/10/68/68	0/4/4/4
5	PAM	D	905	-	-	8/15/15/15	-
5	PAM	D	906	-	-	8/15/15/15	-
4	OLC	D	903	-	-	17/24/24/24	-

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ZK1	D	901	-	-	4/13/23/23	0/3/3/3
4	OLC	D	902	-	-	14/24/24/24	-
5	PAM	A	904	-	-	9/15/15/15	-
4	OLC	B	904	-	-	10/24/24/24	-
5	PAM	E	201	-	-	8/15/15/15	-
6	CLR	E	202	-	-	2/10/68/68	0/4/4/4
5	PAM	H	202	-	-	9/15/15/15	-
5	PAM	F	202	-	-	8/15/15/15	-
5	PAM	F	201	-	-	6/15/15/15	-
5	PAM	G	201	-	-	10/15/15/15	-

All (89) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	901	ZK1	OAA-CAT	8.76	1.40	1.23
3	A	901	ZK1	OAA-CAT	8.75	1.40	1.23
3	C	901	ZK1	OAA-CAT	8.74	1.40	1.23
3	B	901	ZK1	OAA-CAT	8.73	1.40	1.23
3	C	901	ZK1	OAB-CAU	8.38	1.40	1.23
3	D	901	ZK1	OAB-CAU	8.38	1.40	1.23
3	A	901	ZK1	OAB-CAU	8.37	1.40	1.23
3	B	901	ZK1	OAB-CAU	8.36	1.40	1.23
3	A	901	ZK1	CAJ-CAV	7.33	1.51	1.39
3	D	901	ZK1	CAJ-CAV	7.32	1.51	1.39
3	C	901	ZK1	CAJ-CAV	7.27	1.51	1.39
3	B	901	ZK1	CAJ-CAV	7.26	1.51	1.39
3	C	901	ZK1	CAI-CAW	7.14	1.51	1.39
3	A	901	ZK1	CAI-CAW	7.02	1.51	1.39
3	D	901	ZK1	CAI-CAW	6.97	1.50	1.39
3	B	901	ZK1	CAI-CAW	6.95	1.50	1.39
3	C	901	ZK1	CAV-NAP	5.45	1.49	1.39
3	A	901	ZK1	CAV-NAP	5.38	1.49	1.39
3	B	901	ZK1	CAV-NAP	5.37	1.49	1.39
3	D	901	ZK1	CAV-NAP	5.37	1.49	1.39
3	C	901	ZK1	CAU-CAT	-5.30	1.45	1.53
3	A	901	ZK1	CAU-CAT	-5.29	1.45	1.53
3	D	901	ZK1	CAU-CAT	-5.28	1.45	1.53
3	B	901	ZK1	CAU-CAT	-5.22	1.46	1.53
3	B	901	ZK1	CAV-CAW	-5.00	1.35	1.40
3	D	901	ZK1	CAV-CAW	-4.92	1.35	1.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	901	ZK1	CAV-CAW	-4.87	1.35	1.40
3	C	901	ZK1	CAW-NAY	4.85	1.49	1.41
3	A	901	ZK1	CAW-NAY	4.83	1.49	1.41
3	A	901	ZK1	CAV-CAW	-4.82	1.35	1.40
3	D	901	ZK1	CAW-NAY	4.69	1.49	1.41
3	B	901	ZK1	CAW-NAY	4.58	1.49	1.41
3	D	901	ZK1	CAT-NAP	4.35	1.41	1.35
3	B	901	ZK1	CAT-NAP	4.31	1.41	1.35
3	A	901	ZK1	CAT-NAP	4.26	1.41	1.35
3	C	901	ZK1	CAT-NAP	4.20	1.41	1.35
4	B	903	OLC	C21-C22	3.43	1.62	1.51
4	B	904	OLC	C21-C22	3.39	1.62	1.51
4	A	902	OLC	C21-C22	3.37	1.62	1.51
4	C	902	OLC	C21-C22	3.35	1.62	1.51
4	D	904	OLC	C21-C22	3.35	1.62	1.51
4	D	902	OLC	C21-C22	3.34	1.62	1.51
4	D	903	OLC	C21-C22	3.28	1.62	1.51
4	B	902	OLC	C21-C22	3.25	1.62	1.51
6	H	203	CLR	C20-C17	3.22	1.59	1.54
6	G	202	CLR	C20-C17	3.20	1.59	1.54
6	B	907	CLR	C20-C17	3.19	1.59	1.54
6	B	907	CLR	C8-C9	2.62	1.58	1.53
6	G	202	CLR	C8-C9	2.52	1.58	1.53
6	H	203	CLR	C8-C9	2.50	1.58	1.53
4	D	902	OLC	C24-C22	2.44	1.61	1.51
4	B	902	OLC	C24-C22	2.44	1.61	1.51
4	C	902	OLC	C24-C22	2.37	1.60	1.51
4	B	903	OLC	C24-C22	2.37	1.60	1.51
6	E	202	CLR	C8-C9	2.36	1.58	1.53
4	D	904	OLC	C24-C22	2.36	1.60	1.51
4	B	904	OLC	C24-C22	2.35	1.60	1.51
4	B	903	OLC	O20-C1	2.34	1.40	1.33
4	A	902	OLC	C24-C22	2.32	1.60	1.51
4	D	903	OLC	C24-C22	2.32	1.60	1.51
4	B	903	OLC	C2-C1	2.30	1.57	1.50
4	B	904	OLC	C2-C1	2.29	1.57	1.50
4	A	902	OLC	O20-C1	2.24	1.39	1.33
4	B	902	OLC	O20-C1	2.23	1.39	1.33
4	D	902	OLC	O20-C1	2.22	1.39	1.33
4	D	904	OLC	C2-C1	2.21	1.57	1.50
6	E	202	CLR	C20-C17	2.19	1.58	1.54
4	A	902	OLC	C2-C1	2.18	1.57	1.50

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	901	ZK1	PBA-CAO	2.18	1.86	1.81
3	A	901	ZK1	PBA-CAO	2.18	1.86	1.81
3	D	901	ZK1	PBA-CAO	2.18	1.86	1.81
4	B	904	OLC	O20-C1	2.17	1.39	1.33
3	B	901	ZK1	PBA-CAO	2.17	1.86	1.81
4	D	903	OLC	O20-C1	2.16	1.39	1.33
4	C	902	OLC	C2-C1	2.13	1.56	1.50
4	C	902	OLC	O20-C1	2.13	1.39	1.33
3	B	901	ZK1	CAU-NAY	2.10	1.41	1.38
4	D	902	OLC	C2-C1	2.10	1.56	1.50
6	B	907	CLR	C6-C5	2.10	1.37	1.33
4	D	904	OLC	O20-C1	2.09	1.39	1.33
3	D	901	ZK1	CAU-NAY	2.09	1.41	1.38
3	D	901	ZK1	CAR-NAX	2.08	1.45	1.41
6	G	202	CLR	C6-C5	2.07	1.37	1.33
4	D	903	OLC	C2-C1	2.06	1.56	1.50
6	B	907	CLR	C4-C3	2.06	1.55	1.52
6	H	203	CLR	C6-C5	2.06	1.37	1.33
3	C	901	ZK1	CAU-NAY	2.05	1.41	1.38
3	A	901	ZK1	CAU-NAY	2.04	1.41	1.38
3	B	901	ZK1	CAR-NAX	2.00	1.45	1.41

All (82) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	203	CLR	C17-C13-C14	5.84	106.80	100.10
6	G	202	CLR	C17-C13-C14	5.70	106.64	100.10
6	B	907	CLR	C17-C13-C14	5.66	106.59	100.10
6	E	202	CLR	C19-C10-C9	-5.22	105.81	111.66
6	G	202	CLR	C19-C10-C9	-4.84	106.23	111.66
6	E	202	CLR	C17-C13-C14	4.71	105.50	100.10
6	B	907	CLR	C19-C10-C5	4.49	115.24	108.38
6	H	203	CLR	C19-C10-C9	-4.01	107.16	111.66
6	H	203	CLR	C19-C10-C5	3.93	114.39	108.38
6	E	202	CLR	C11-C9-C10	3.88	117.87	113.08
6	G	202	CLR	C19-C10-C5	3.77	114.14	108.38
3	B	901	ZK1	CAV-NAP-CAT	-3.74	119.59	124.82
3	D	901	ZK1	CAV-NAP-CAT	-3.73	119.59	124.82
6	H	203	CLR	C11-C9-C10	3.70	117.65	113.08
3	A	901	ZK1	CAV-NAP-CAT	-3.68	119.67	124.82
3	C	901	ZK1	CAV-NAP-CAT	-3.68	119.67	124.82
6	B	907	CLR	C19-C10-C9	-3.64	107.57	111.66

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	907	CLR	C11-C9-C10	3.54	117.45	113.08
6	E	202	CLR	C19-C10-C5	3.50	113.73	108.38
3	B	901	ZK1	CAO-NAY-CAU	3.43	120.04	116.55
4	B	903	OLC	O20-C1-C2	3.42	122.27	111.83
6	G	202	CLR	C11-C9-C10	3.36	117.23	113.08
6	B	907	CLR	C10-C9-C8	-3.33	107.84	112.71
6	H	203	CLR	C10-C9-C8	-3.33	107.85	112.71
6	B	907	CLR	C7-C8-C9	-3.25	105.96	109.72
4	B	902	OLC	O20-C1-C2	3.25	121.74	111.83
6	B	907	CLR	C14-C8-C9	3.22	113.29	109.09
4	C	902	OLC	O20-C1-C2	3.20	121.58	111.83
4	A	902	OLC	O20-C1-C2	3.16	121.47	111.83
4	D	902	OLC	O20-C1-C2	3.16	121.47	111.83
4	D	904	OLC	O20-C1-C2	3.15	121.45	111.83
4	B	904	OLC	O20-C1-C2	3.15	121.45	111.83
4	D	903	OLC	O20-C1-C2	3.12	121.34	111.83
6	H	203	CLR	C12-C13-C14	-3.02	102.73	107.25
6	H	203	CLR	C14-C8-C9	3.00	113.01	109.09
6	H	203	CLR	C7-C8-C9	-2.99	106.27	109.72
6	B	907	CLR	C12-C13-C14	-2.96	102.82	107.25
3	D	901	ZK1	CAN-NAX-CAR	-2.92	109.26	116.19
6	G	202	CLR	C12-C13-C14	-2.90	102.90	107.25
6	B	907	CLR	C7-C8-C14	2.86	114.98	110.93
3	C	901	ZK1	CAW-NAY-CAU	-2.78	119.42	122.84
3	C	901	ZK1	CAN-NAX-CAR	-2.72	109.74	116.19
3	A	901	ZK1	CAN-NAX-CAR	-2.69	109.79	116.19
3	D	901	ZK1	CAW-NAY-CAU	-2.67	119.56	122.84
3	A	901	ZK1	CAW-NAY-CAU	-2.65	119.58	122.84
3	B	901	ZK1	CAW-NAY-CAU	-2.65	119.58	122.84
4	B	903	OLC	O20-C1-O19	-2.60	117.12	123.63
3	B	901	ZK1	CAN-NAX-CAR	-2.59	110.04	116.19
3	C	901	ZK1	CAT-CAU-NAY	2.55	120.18	117.41
3	D	901	ZK1	CAO-NAY-CAU	2.54	119.14	116.55
6	E	202	CLR	C14-C8-C9	2.53	112.39	109.09
4	C	902	OLC	O20-C1-O19	-2.52	117.33	123.63
4	B	904	OLC	O20-C1-O19	-2.52	117.33	123.63
6	H	203	CLR	C7-C8-C14	2.50	114.47	110.93
4	D	904	OLC	O20-C1-O19	-2.50	117.38	123.63
4	D	902	OLC	O20-C1-O19	-2.48	117.44	123.63
3	A	901	ZK1	CAT-CAU-NAY	2.47	120.09	117.41
6	E	202	CLR	C12-C13-C14	-2.46	103.56	107.25
4	A	902	OLC	O20-C1-O19	-2.46	117.49	123.63

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	903	OLC	O20-C1-O19	-2.45	117.50	123.63
6	E	202	CLR	C10-C9-C8	-2.44	109.15	112.71
6	G	202	CLR	C14-C8-C9	2.43	112.26	109.09
4	B	902	OLC	O20-C1-O19	-2.40	117.64	123.63
3	B	901	ZK1	CAV-CAW-NAY	2.38	120.71	118.01
6	B	907	CLR	C15-C14-C13	-2.38	101.05	103.84
6	B	907	CLR	C2-C3-C4	-2.37	106.96	110.29
3	B	901	ZK1	CAU-CAT-NAP	2.34	119.85	117.46
6	G	202	CLR	C10-C9-C8	-2.34	109.30	112.71
3	D	901	ZK1	CAT-CAU-NAY	2.29	119.90	117.41
3	D	901	ZK1	CAU-CAT-NAP	2.23	119.74	117.46
6	B	907	CLR	C3-C4-C5	2.23	115.60	112.05
3	D	901	ZK1	CAV-CAW-NAY	2.21	120.51	118.01
3	C	901	ZK1	CAM-NAX-CAR	-2.20	110.97	116.19
6	G	202	CLR	C15-C14-C13	-2.18	101.27	103.84
3	A	901	ZK1	CAM-NAX-CAR	-2.18	111.01	116.19
3	B	901	ZK1	CAM-NAX-CAR	-2.14	111.09	116.19
3	D	901	ZK1	CAM-NAX-CAR	-2.14	111.11	116.19
3	B	901	ZK1	CAT-CAU-NAY	2.12	119.72	117.41
3	C	901	ZK1	CAV-CAW-NAY	2.09	120.38	118.01
3	C	901	ZK1	CAU-CAT-NAP	2.08	119.58	117.46
3	A	901	ZK1	CAU-CAT-NAP	2.08	119.58	117.46
6	H	203	CLR	C15-C14-C13	-2.06	101.42	103.84

There are no chirality outliers.

All (255) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	901	ZK1	NAY-CAO-PBA-OAD
3	A	901	ZK1	NAY-CAO-PBA-OAE
3	B	901	ZK1	NAY-CAO-PBA-OAD
3	B	901	ZK1	NAY-CAO-PBA-OAE
3	C	901	ZK1	NAY-CAO-PBA-OAD
3	C	901	ZK1	NAY-CAO-PBA-OAE
4	A	902	OLC	O20-C21-C22-C24
4	A	902	OLC	O20-C21-C22-O23
4	B	902	OLC	C21-C22-C24-O25
4	B	903	OLC	C2-C1-O20-C21
4	B	903	OLC	O19-C1-O20-C21
4	B	904	OLC	O20-C21-C22-C24
4	B	904	OLC	O20-C21-C22-O23
4	C	902	OLC	C21-C22-C24-O25

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
4	C	902	OLC	O23-C22-C24-O25
4	D	903	OLC	C21-C22-C24-O25
4	D	904	OLC	O20-C21-C22-C24
4	D	904	OLC	O20-C21-C22-O23
4	D	902	OLC	O19-C1-O20-C21
4	D	902	OLC	C2-C1-O20-C21
5	D	905	PAM	C5-C6-C7-C8
4	D	902	OLC	C11-C10-C9-C8
4	D	904	OLC	C2-C1-O20-C21
4	D	904	OLC	O19-C1-O20-C21
6	B	907	CLR	C21-C20-C22-C23
6	B	907	CLR	C17-C20-C22-C23
6	G	202	CLR	C17-C20-C22-C23
4	D	903	OLC	C11-C10-C9-C8
5	C	903	PAM	C11-C10-C9-C8
5	F	202	PAM	C11-C10-C9-C8
4	B	904	OLC	C2-C1-O20-C21
5	B	905	PAM	C12-C13-C14-C15
4	B	904	OLC	C5-C6-C7-C8
5	B	905	PAM	C5-C6-C7-C8
4	D	904	OLC	C5-C6-C7-C8
4	B	903	OLC	O20-C21-C22-C24
4	D	902	OLC	O20-C21-C22-C24
4	B	904	OLC	O19-C1-O20-C21
5	H	202	PAM	C11-C10-C9-C8
5	A	903	PAM	C5-C6-C7-C8
6	H	203	CLR	C17-C20-C22-C23
6	G	202	CLR	C21-C20-C22-C23
6	H	203	CLR	C21-C20-C22-C23
5	G	201	PAM	C1-C2-C3-C4
4	C	902	OLC	C2-C1-O20-C21
5	C	904	PAM	C6-C7-C8-C9
5	D	905	PAM	C12-C13-C14-C15
5	E	201	PAM	C1-C2-C3-C4
4	D	903	OLC	C2-C1-O20-C21
5	F	201	PAM	C5-C6-C7-C8
4	C	902	OLC	O19-C1-O20-C21
4	B	903	OLC	O20-C21-C22-O23
4	C	902	OLC	O20-C21-C22-O23
4	D	902	OLC	O20-C21-C22-O23
4	D	902	OLC	C21-C22-C24-O25
4	A	902	OLC	C1-C2-C3-C4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
5	H	202	PAM	C11-C12-C13-C14
5	H	202	PAM	C5-C6-C7-C8
4	B	903	OLC	C11-C10-C9-C8
5	A	904	PAM	C12-C13-C14-C15
5	G	201	PAM	C11-C12-C13-C14
4	B	902	OLC	O23-C22-C24-O25
4	C	902	OLC	C4-C5-C6-C7
4	B	902	OLC	C1-C2-C3-C4
4	D	904	OLC	C2-C3-C4-C5
4	D	903	OLC	O19-C1-O20-C21
4	B	903	OLC	C13-C14-C15-C16
4	D	902	OLC	C3-C4-C5-C6
4	D	903	OLC	C2-C3-C4-C5
5	F	201	PAM	C3-C4-C5-C6
4	D	903	OLC	C13-C14-C15-C16
5	A	903	PAM	C2-C3-C4-C5
5	D	905	PAM	C3-C4-C5-C6
4	D	903	OLC	C3-C4-C5-C6
5	H	202	PAM	C12-C13-C14-C15
5	B	906	PAM	C3-C4-C5-C6
4	A	902	OLC	C12-C13-C14-C15
4	C	902	OLC	C12-C13-C14-C15
5	F	202	PAM	C6-C7-C8-C9
5	A	903	PAM	C11-C10-C9-C8
5	B	905	PAM	C11-C10-C9-C8
5	D	905	PAM	C11-C10-C9-C8
5	F	202	PAM	C5-C6-C7-C8
4	C	902	OLC	C13-C14-C15-C16
5	B	905	PAM	C1-C2-C3-C4
5	F	202	PAM	C11-C12-C13-C14
4	A	902	OLC	C13-C14-C15-C16
5	C	904	PAM	C12-C13-C14-C15
4	B	904	OLC	C11-C12-C13-C14
4	D	903	OLC	C4-C5-C6-C7
5	D	906	PAM	C3-C4-C5-C6
4	D	904	OLC	C11-C12-C13-C14
5	A	903	PAM	C7-C8-C9-C10
5	A	904	PAM	C3-C4-C5-C6
6	B	907	CLR	C13-C17-C20-C21
6	B	907	CLR	C20-C22-C23-C24
5	G	201	PAM	C2-C3-C4-C5
4	B	902	OLC	C6-C7-C8-C9

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
5	H	202	PAM	C6-C7-C8-C9
5	F	202	PAM	C1-C2-C3-C4
5	D	905	PAM	C1-C2-C3-C4
5	E	201	PAM	C12-C13-C14-C15
5	G	201	PAM	C4-C5-C6-C7
5	E	201	PAM	C5-C6-C7-C8
6	G	202	CLR	C22-C23-C24-C25
4	B	903	OLC	C12-C13-C14-C15
4	B	904	OLC	C2-C3-C4-C5
4	B	903	OLC	C2-C3-C4-C5
5	C	904	PAM	C4-C5-C6-C7
5	A	904	PAM	C2-C3-C4-C5
5	F	201	PAM	C12-C13-C14-C15
6	H	203	CLR	C20-C22-C23-C24
4	D	903	OLC	O23-C22-C24-O25
5	C	904	PAM	C3-C4-C5-C6
5	D	906	PAM	C7-C8-C9-C10
5	F	201	PAM	C10-C11-C12-C13
5	H	201	PAM	C10-C11-C12-C13
4	C	902	OLC	C5-C6-C7-C8
5	A	904	PAM	C4-C5-C6-C7
5	E	201	PAM	C11-C12-C13-C14
5	H	202	PAM	C1-C2-C3-C4
4	D	903	OLC	C10-C11-C12-C13
5	A	904	PAM	C6-C7-C8-C9
5	G	201	PAM	C6-C7-C8-C9
3	D	901	ZK1	CAI-CAR-NAX-CAN
3	A	901	ZK1	CAI-CAR-NAX-CAN
3	B	901	ZK1	CAI-CAR-NAX-CAN
3	C	901	ZK1	CAI-CAR-NAX-CAN
5	E	201	PAM	C2-C3-C4-C5
6	B	907	CLR	C16-C17-C20-C21
6	H	203	CLR	C13-C17-C20-C21
4	D	903	OLC	O20-C21-C22-O23
3	D	901	ZK1	CAI-CAR-NAX-CAM
5	C	903	PAM	C10-C11-C12-C13
5	A	903	PAM	C11-C12-C13-C14
4	D	903	OLC	C12-C13-C14-C15
5	C	904	PAM	C2-C3-C4-C5
4	B	904	OLC	C15-C16-C17-C18
5	C	904	PAM	C11-C12-C13-C14
5	D	906	PAM	C11-C10-C9-C8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
5	D	905	PAM	C7-C8-C9-C10
6	E	202	CLR	C17-C20-C22-C23
6	H	203	CLR	C22-C23-C24-C25
4	A	902	OLC	C2-C1-O20-C21
4	D	904	OLC	C14-C15-C16-C17
5	C	903	PAM	C11-C12-C13-C14
4	D	904	OLC	C15-C16-C17-C18
4	C	902	OLC	C7-C8-C9-C10
5	A	903	PAM	C13-C14-C15-C16
4	D	903	OLC	C5-C6-C7-C8
4	A	902	OLC	C3-C4-C5-C6
6	H	203	CLR	C16-C17-C20-C21
5	B	906	PAM	C11-C12-C13-C14
5	F	202	PAM	C12-C13-C14-C15
4	C	902	OLC	O20-C1-C2-C3
4	B	903	OLC	C5-C6-C7-C8
5	B	905	PAM	C2-C3-C4-C5
5	B	905	PAM	C7-C8-C9-C10
5	G	201	PAM	C5-C6-C7-C8
4	D	903	OLC	O20-C21-C22-C24
5	E	201	PAM	C6-C7-C8-C9
5	H	201	PAM	C6-C7-C8-C9
5	G	201	PAM	C11-C10-C9-C8
4	A	902	OLC	C7-C8-C9-C10
4	D	904	OLC	O23-C22-C24-O25
3	B	901	ZK1	NAY-CAO-PBA-OAC
3	C	901	ZK1	NAY-CAO-PBA-OAC
4	D	902	OLC	C12-C13-C14-C15
5	D	905	PAM	C2-C3-C4-C5
4	D	902	OLC	O20-C1-C2-C3
4	A	902	OLC	O19-C1-O20-C21
3	A	901	ZK1	CAI-CAR-NAX-CAM
3	C	901	ZK1	CAI-CAR-NAX-CAM
4	B	904	OLC	C14-C15-C16-C17
5	F	201	PAM	C2-C3-C4-C5
3	B	901	ZK1	CAI-CAR-NAX-CAM
4	A	902	OLC	C6-C7-C8-C9
4	D	903	OLC	C14-C15-C16-C17
5	B	905	PAM	C3-C4-C5-C6
5	H	201	PAM	C2-C3-C4-C5
6	B	907	CLR	C16-C17-C20-C22
4	C	902	OLC	C14-C15-C16-C17

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
5	E	201	PAM	C10-C11-C12-C13
5	A	903	PAM	C1-C2-C3-C4
5	B	906	PAM	C12-C13-C14-C15
5	A	903	PAM	C12-C13-C14-C15
4	A	902	OLC	C5-C6-C7-C8
5	C	903	PAM	C4-C5-C6-C7
3	D	901	ZK1	CAS-CAR-NAX-CAM
5	D	906	PAM	C1-C2-C3-C4
4	D	902	OLC	C5-C6-C7-C8
5	D	906	PAM	C9-C10-C11-C12
3	A	901	ZK1	CAS-CAR-NAX-CAN
3	B	901	ZK1	CAS-CAR-NAX-CAN
3	C	901	ZK1	CAS-CAR-NAX-CAN
3	D	901	ZK1	CAS-CAR-NAX-CAN
4	B	903	OLC	C9-C10-C11-C12
5	H	201	PAM	C5-C6-C7-C8
5	B	906	PAM	C1-C2-C3-C4
4	B	902	OLC	C14-C15-C16-C17
5	A	904	PAM	C11-C12-C13-C14
5	B	905	PAM	C9-C10-C11-C12
5	G	201	PAM	C12-C13-C14-C15
5	C	904	PAM	O2-C1-C2-C3
4	B	902	OLC	C3-C4-C5-C6
5	A	904	PAM	O2-C1-C2-C3
5	C	903	PAM	O2-C1-C2-C3
5	H	202	PAM	O1-C1-C2-C3
4	B	902	OLC	O20-C21-C22-C24
5	C	904	PAM	O1-C1-C2-C3
4	D	904	OLC	O20-C1-C2-C3
5	A	904	PAM	O1-C1-C2-C3
5	C	903	PAM	O1-C1-C2-C3
5	H	201	PAM	C12-C13-C14-C15
4	D	902	OLC	O23-C22-C24-O25
5	H	202	PAM	O2-C1-C2-C3
6	H	203	CLR	C16-C17-C20-C22
3	A	901	ZK1	NAY-CAO-PBA-OAC
4	D	903	OLC	C9-C10-C11-C12
5	F	201	PAM	C11-C10-C9-C8
5	F	202	PAM	O1-C1-C2-C3
5	F	202	PAM	O2-C1-C2-C3
4	B	904	OLC	C9-C10-C11-C12
5	C	903	PAM	C6-C7-C8-C9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
5	C	904	PAM	C9-C10-C11-C12
4	C	902	OLC	C11-C10-C9-C8
4	A	902	OLC	C15-C16-C17-C18
5	A	904	PAM	C9-C10-C11-C12
4	C	902	OLC	O19-C1-C2-C3
4	A	902	OLC	C4-C5-C6-C7
4	D	903	OLC	C7-C8-C9-C10
6	E	202	CLR	C21-C20-C22-C23
4	A	902	OLC	C14-C15-C16-C17
5	E	201	PAM	C7-C8-C9-C10
5	D	905	PAM	C9-C10-C11-C12
4	B	902	OLC	C11-C10-C9-C8
5	G	201	PAM	C7-C8-C9-C10
5	B	906	PAM	O2-C1-C2-C3
3	A	901	ZK1	CAS-CAR-NAX-CAM
3	C	901	ZK1	CAS-CAR-NAX-CAM
5	D	906	PAM	C2-C3-C4-C5
4	D	904	OLC	C9-C10-C11-C12
5	D	906	PAM	O1-C1-C2-C3
5	D	906	PAM	O2-C1-C2-C3
4	B	902	OLC	O19-C1-O20-C21
4	D	902	OLC	O19-C1-C2-C3
3	B	901	ZK1	CAS-CAR-NAX-CAM
5	H	202	PAM	C13-C14-C15-C16
4	B	903	OLC	C7-C8-C9-C10
5	B	906	PAM	O1-C1-C2-C3
4	D	902	OLC	C9-C10-C11-C12
4	C	902	OLC	O20-C21-C22-C24
4	D	902	OLC	C1-C2-C3-C4
4	B	902	OLC	C2-C1-O20-C21
5	G	201	PAM	C3-C4-C5-C6

There are no ring outliers.

15 monomers are involved in 38 short contacts:

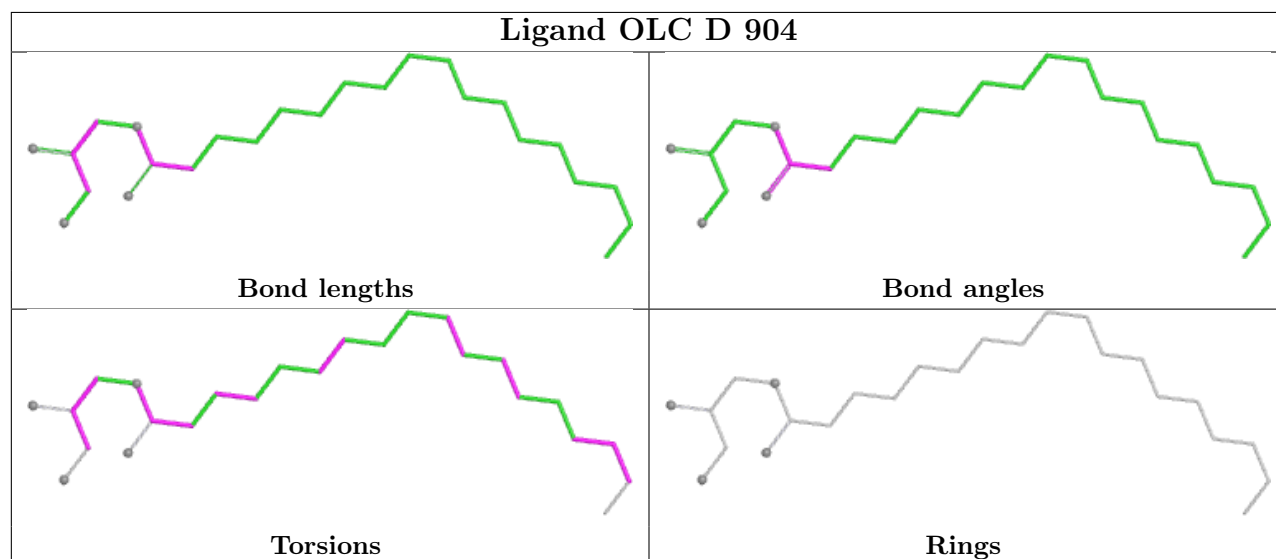
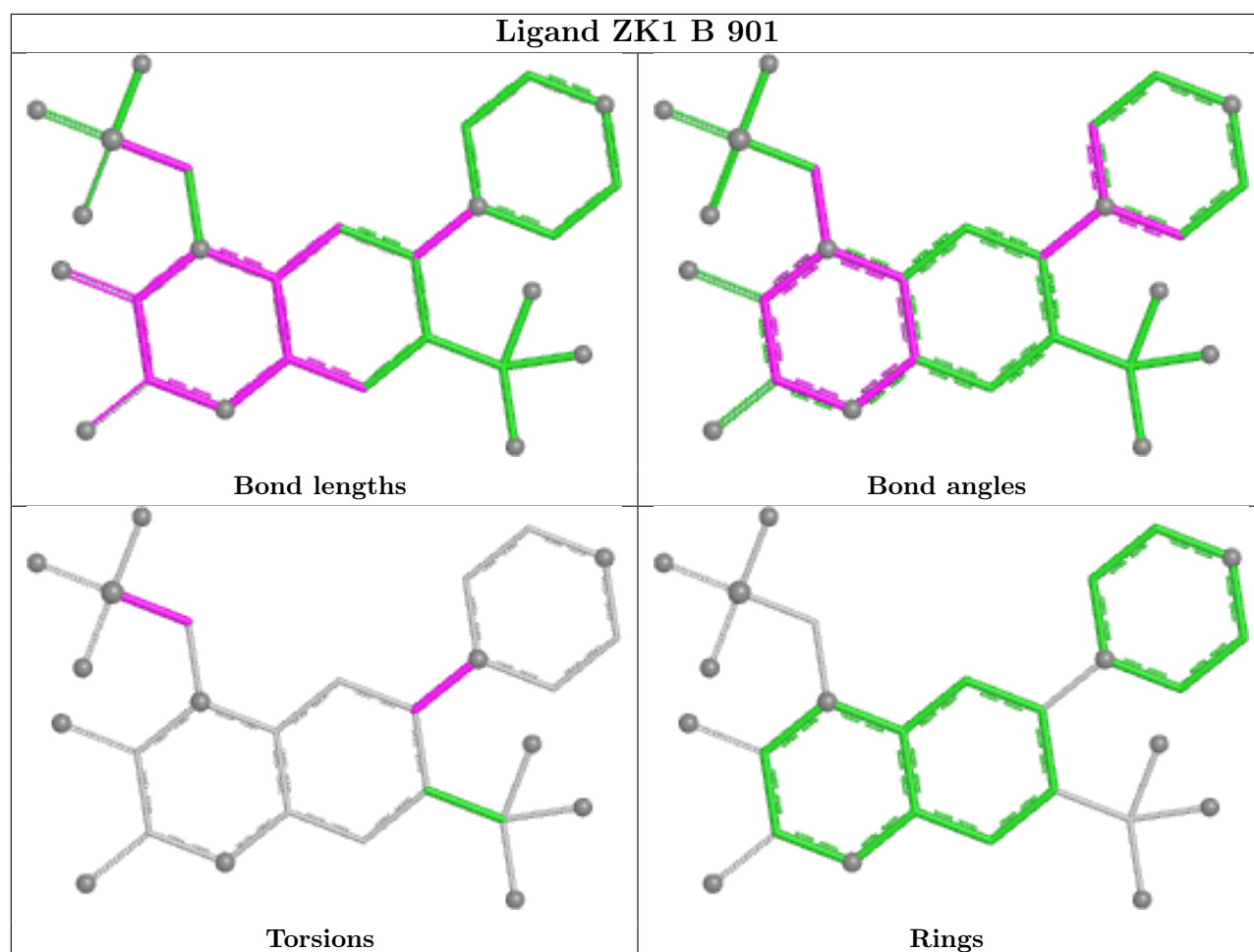
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	903	PAM	1	0
5	A	903	PAM	3	0
6	G	202	CLR	6	0
5	B	906	PAM	1	0
6	H	203	CLR	9	0
5	C	904	PAM	2	0

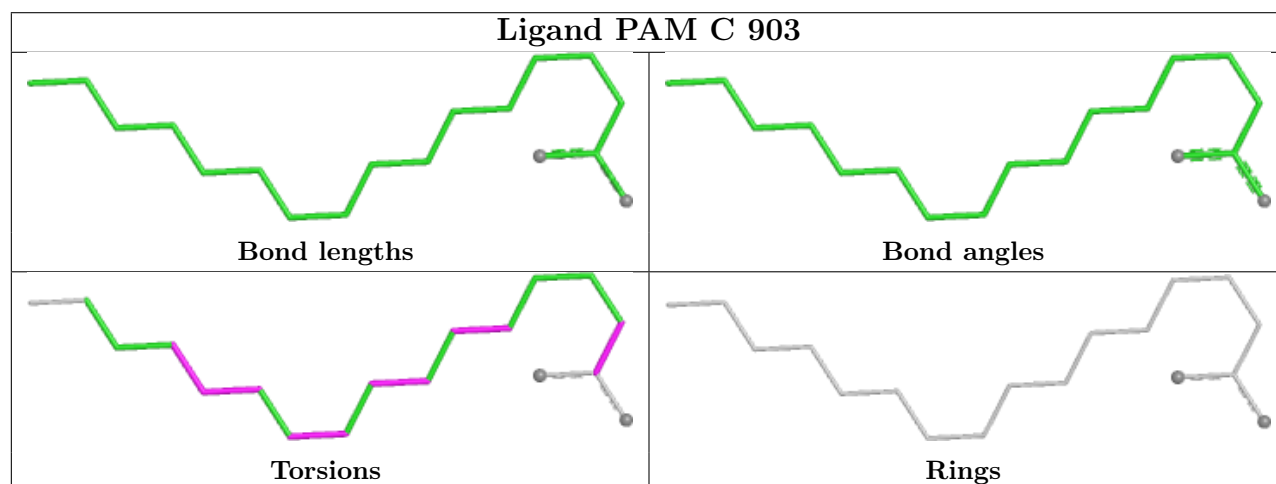
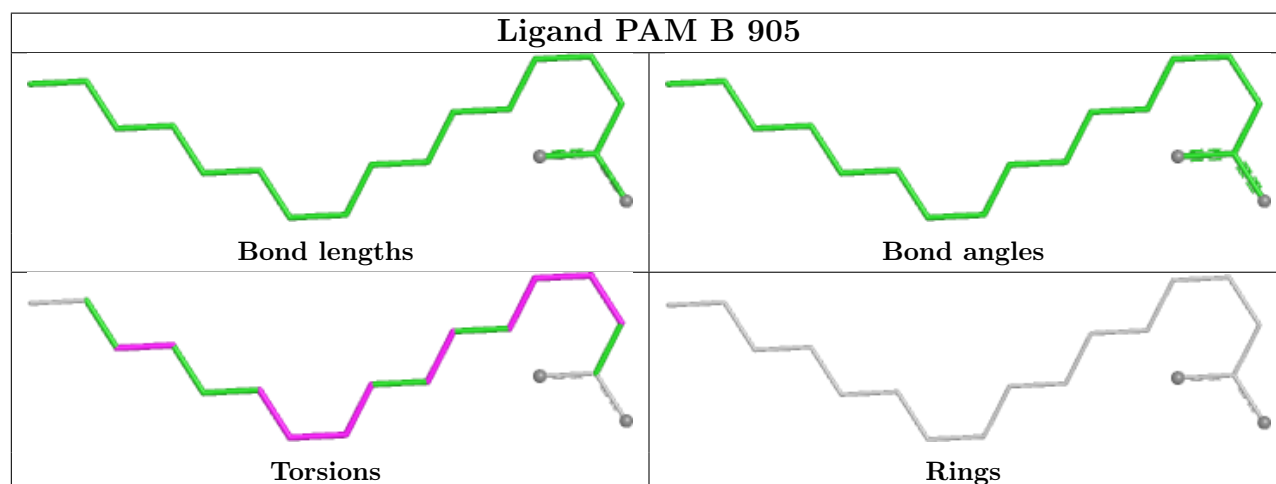
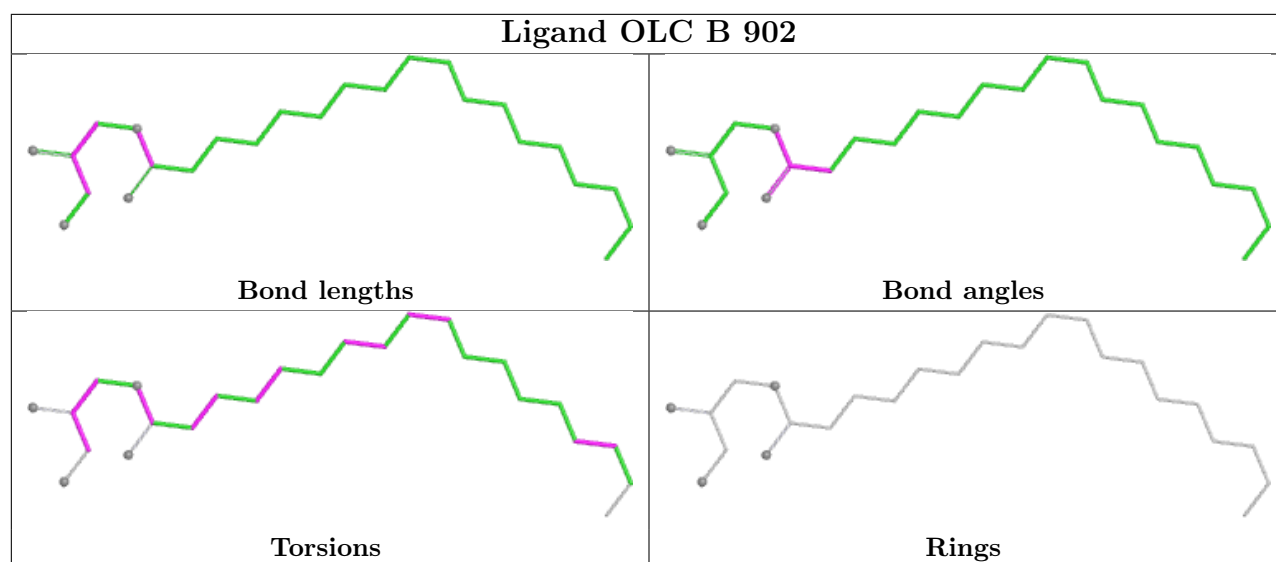
*Continued on next page...*

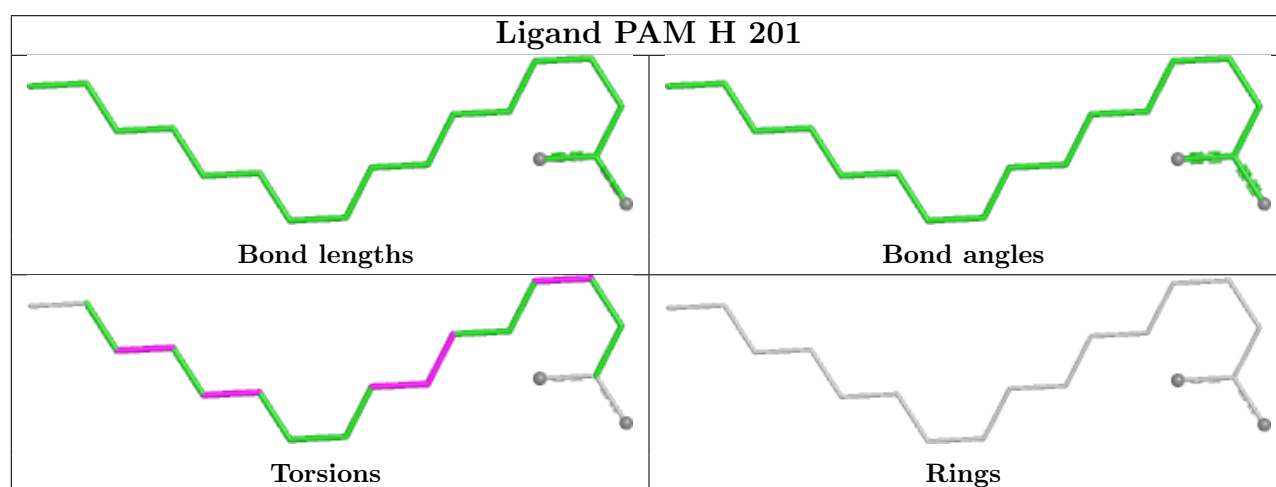
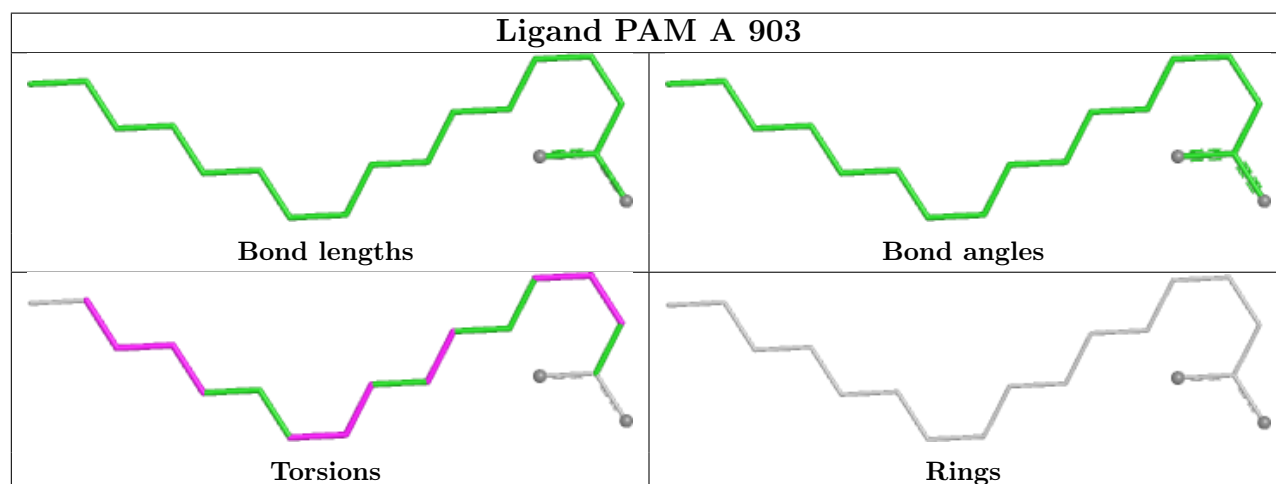
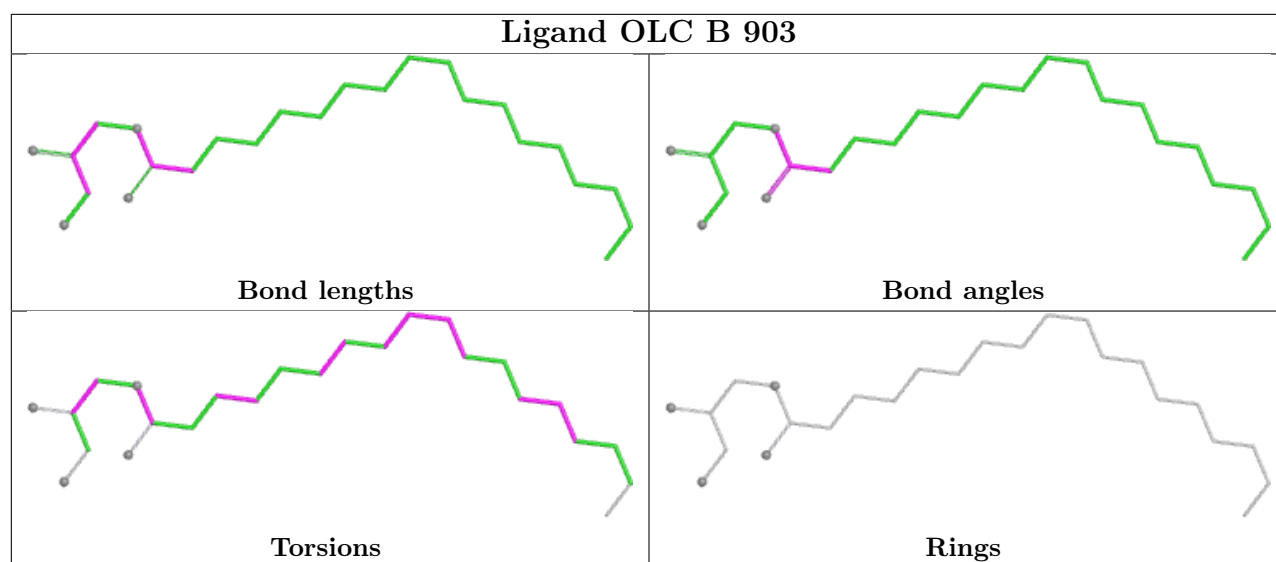
*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	902	OLC	1	0
6	B	907	CLR	6	0
5	D	906	PAM	3	0
5	A	904	PAM	2	0
5	E	201	PAM	1	0
6	E	202	CLR	4	0
5	H	202	PAM	1	0
5	F	202	PAM	1	0
5	G	201	PAM	2	0

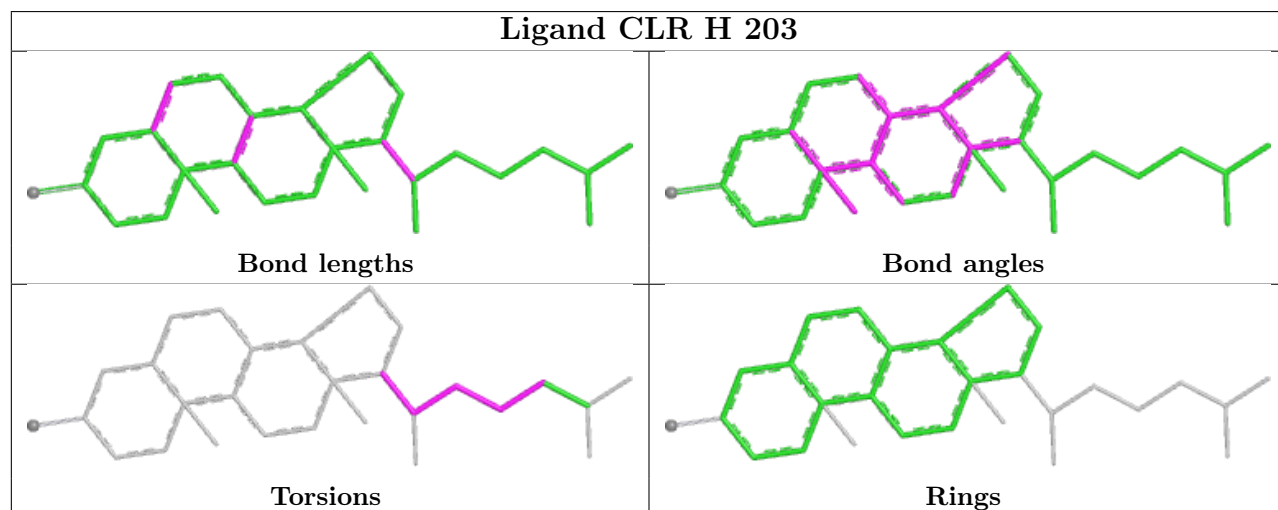
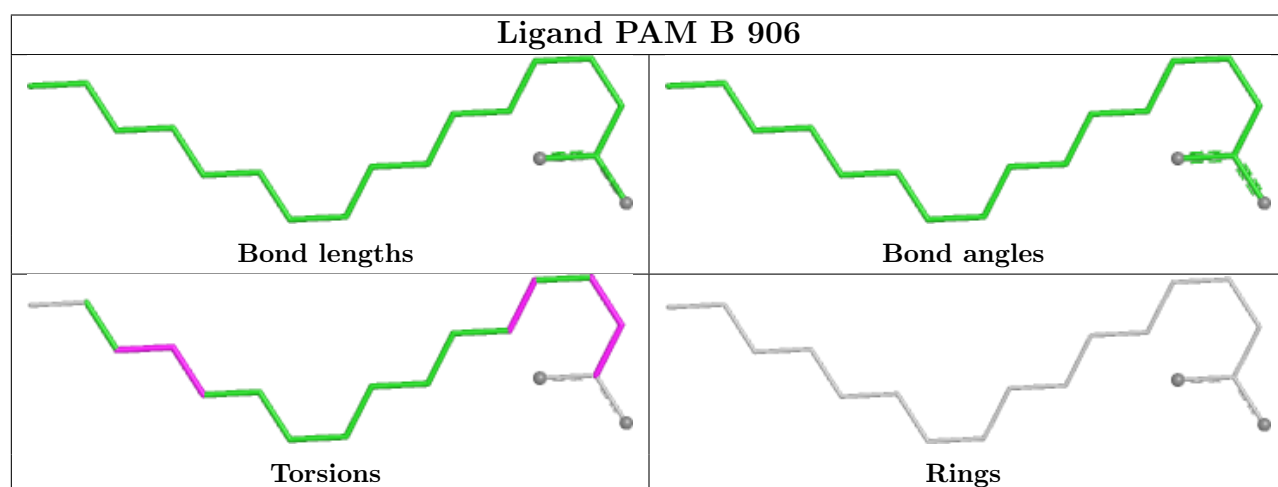
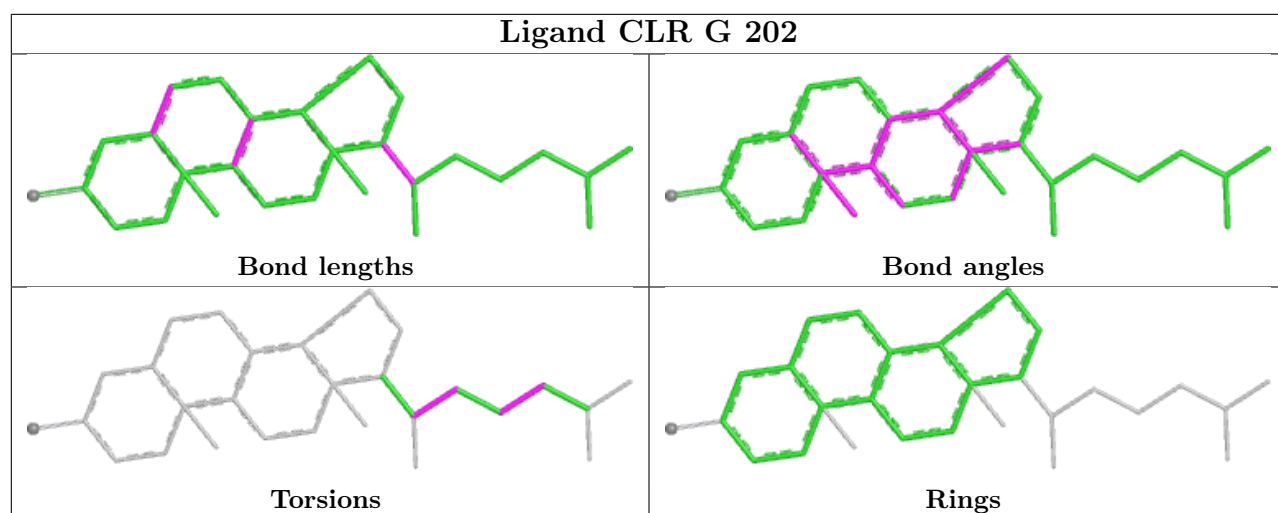
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

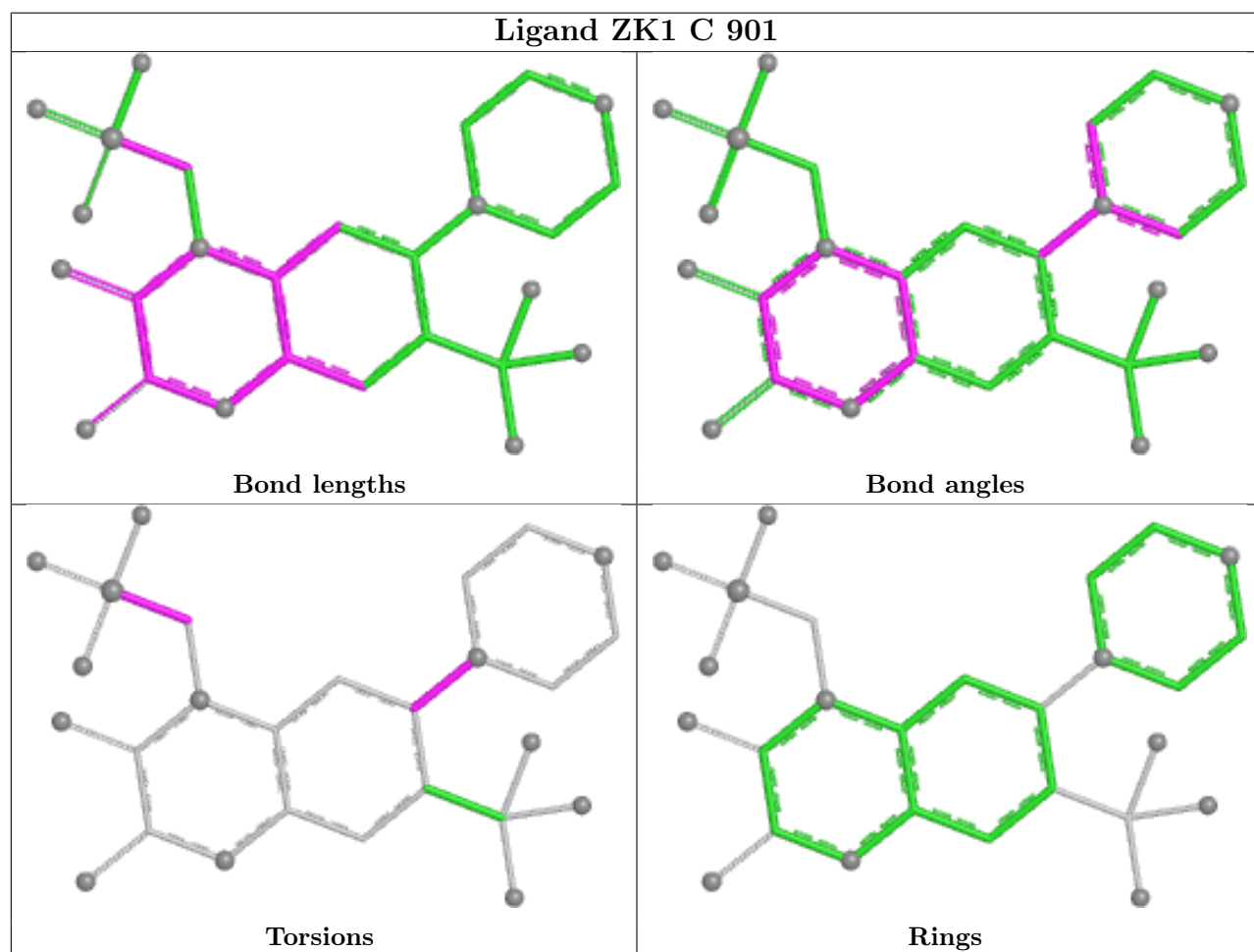
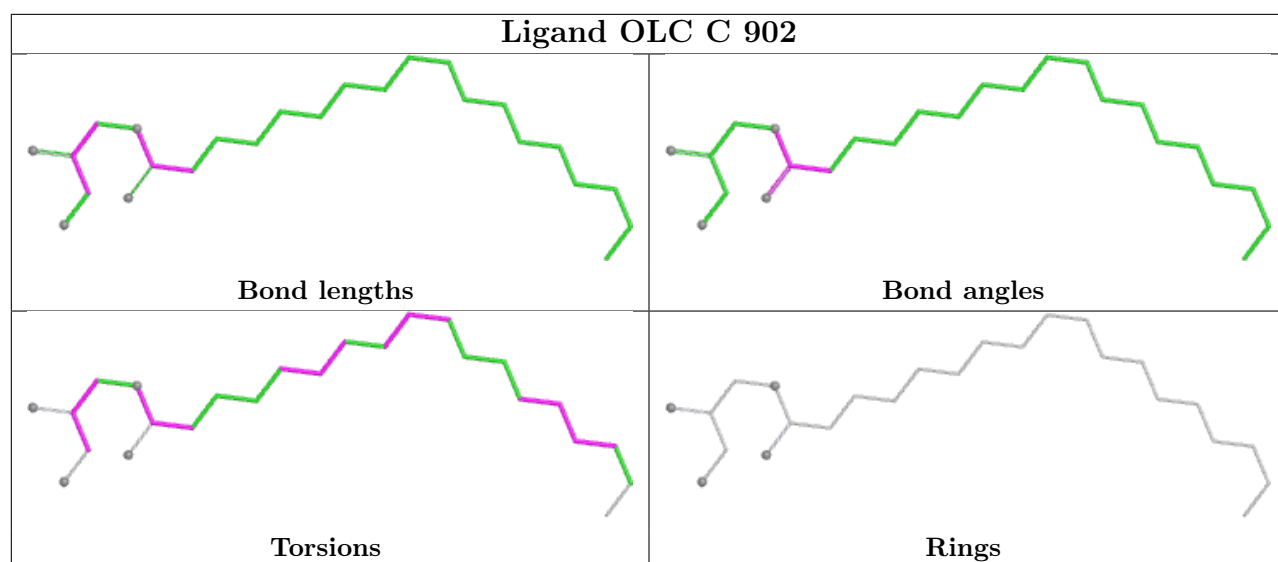


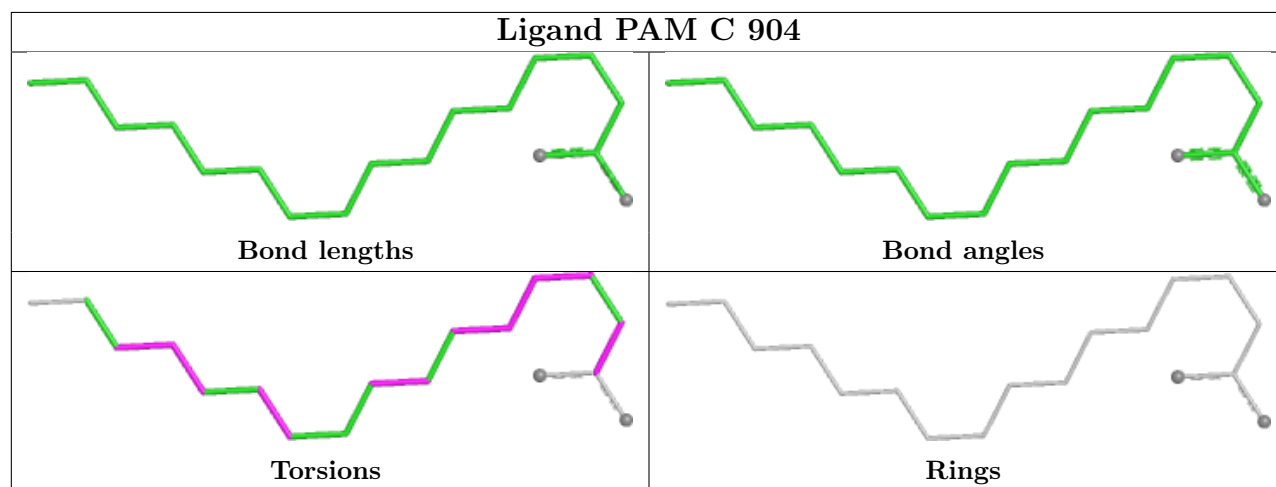
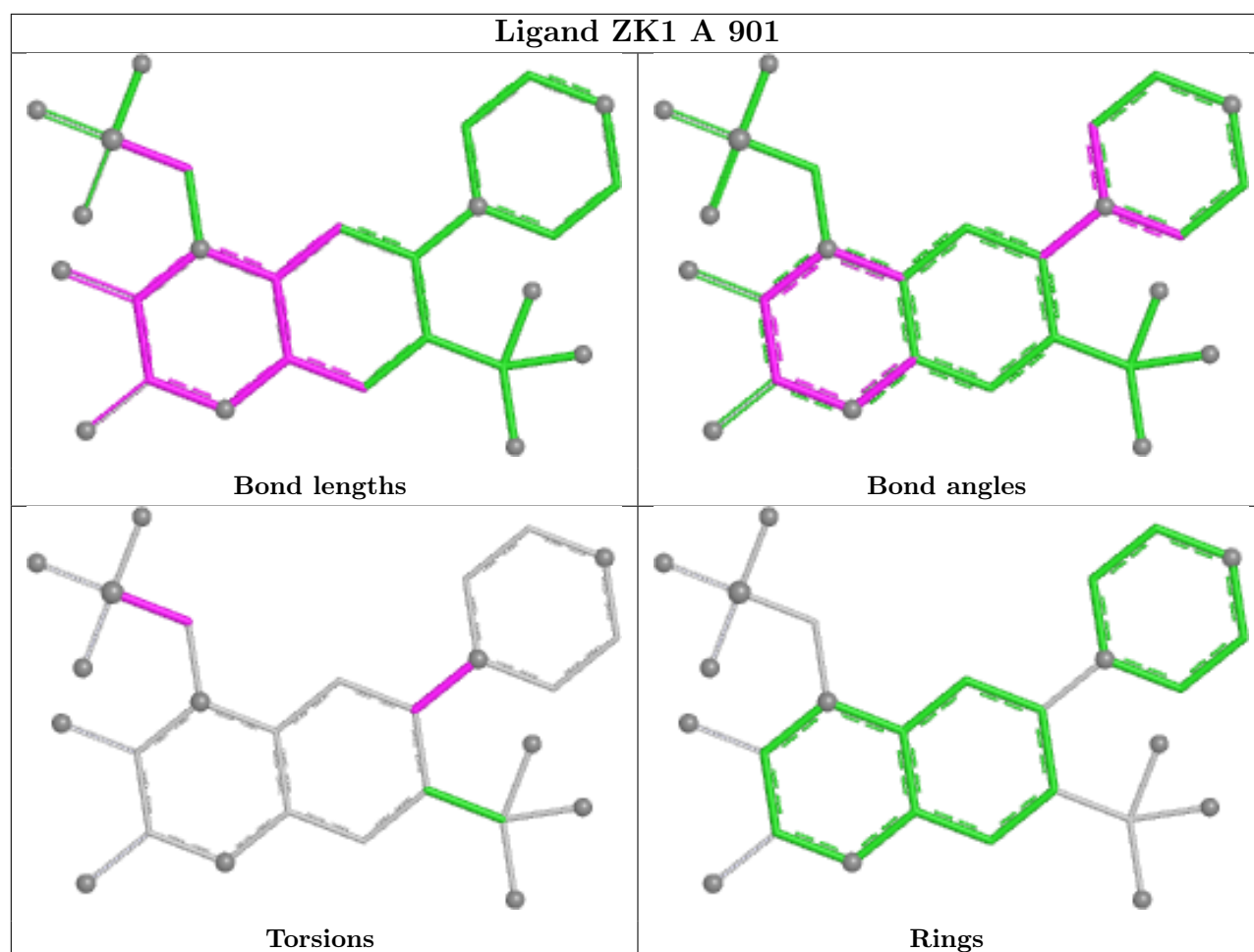


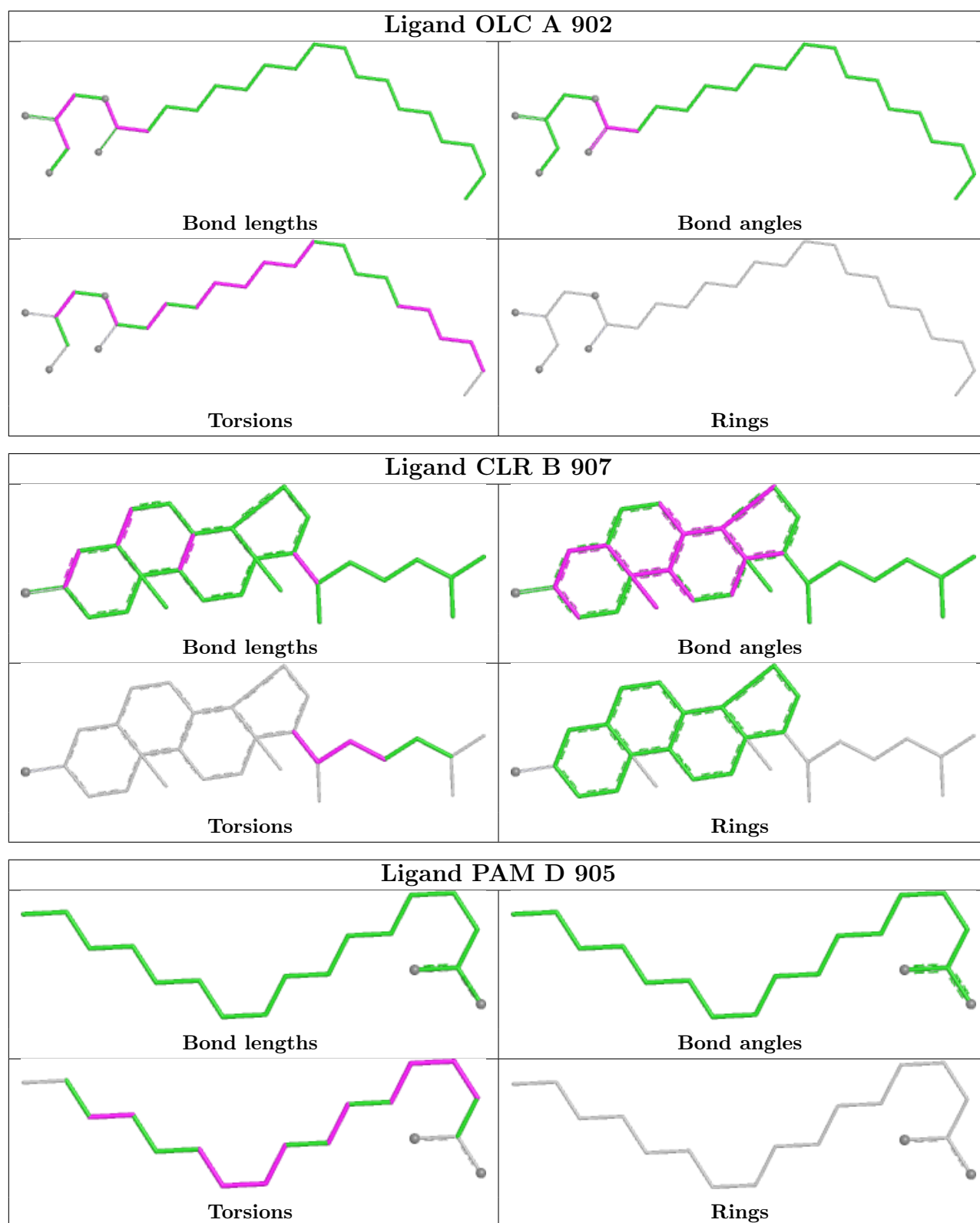


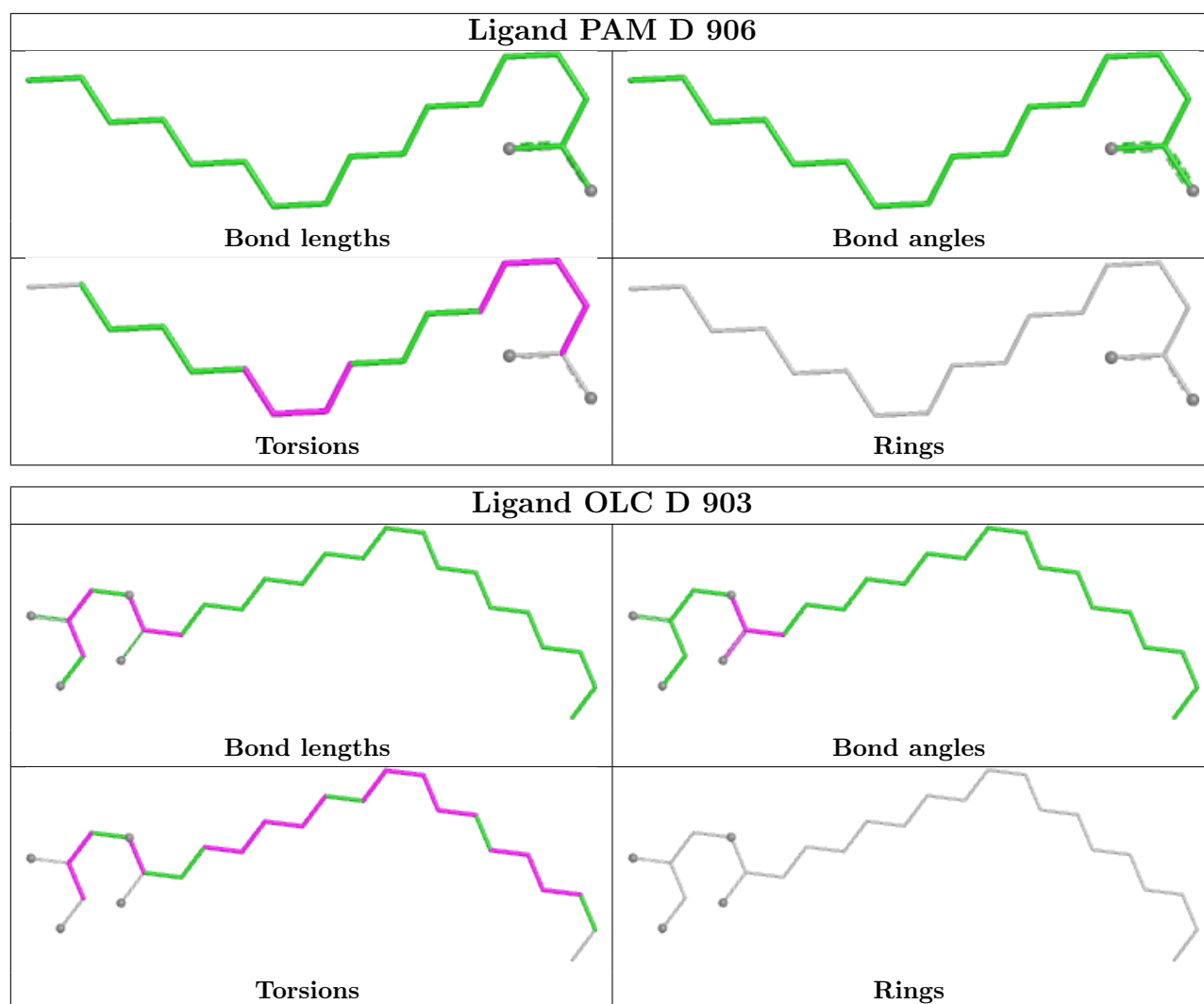


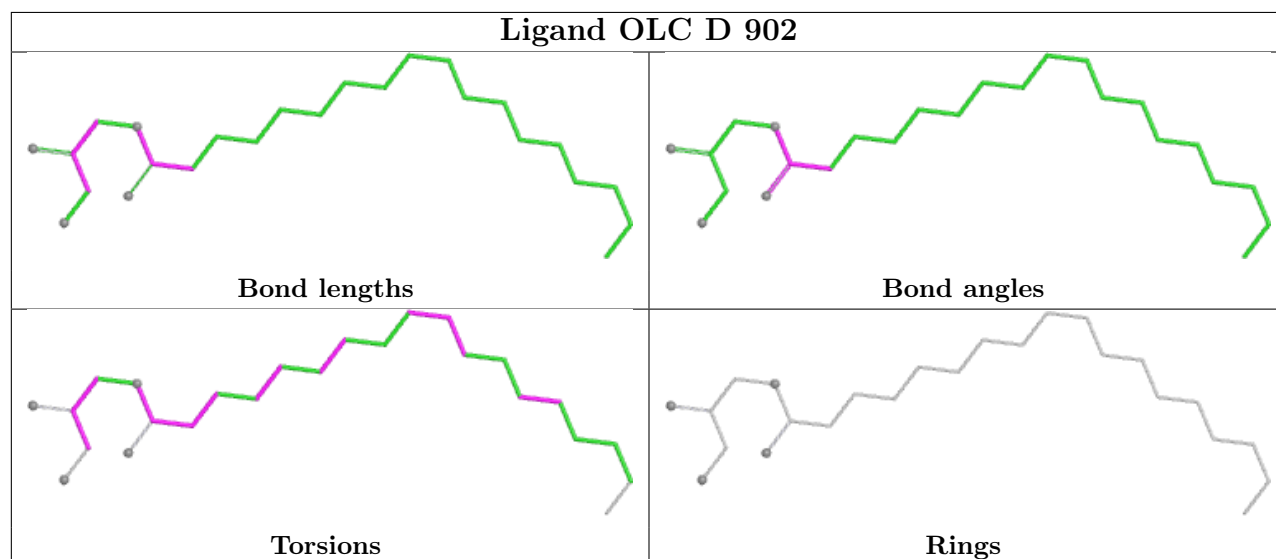
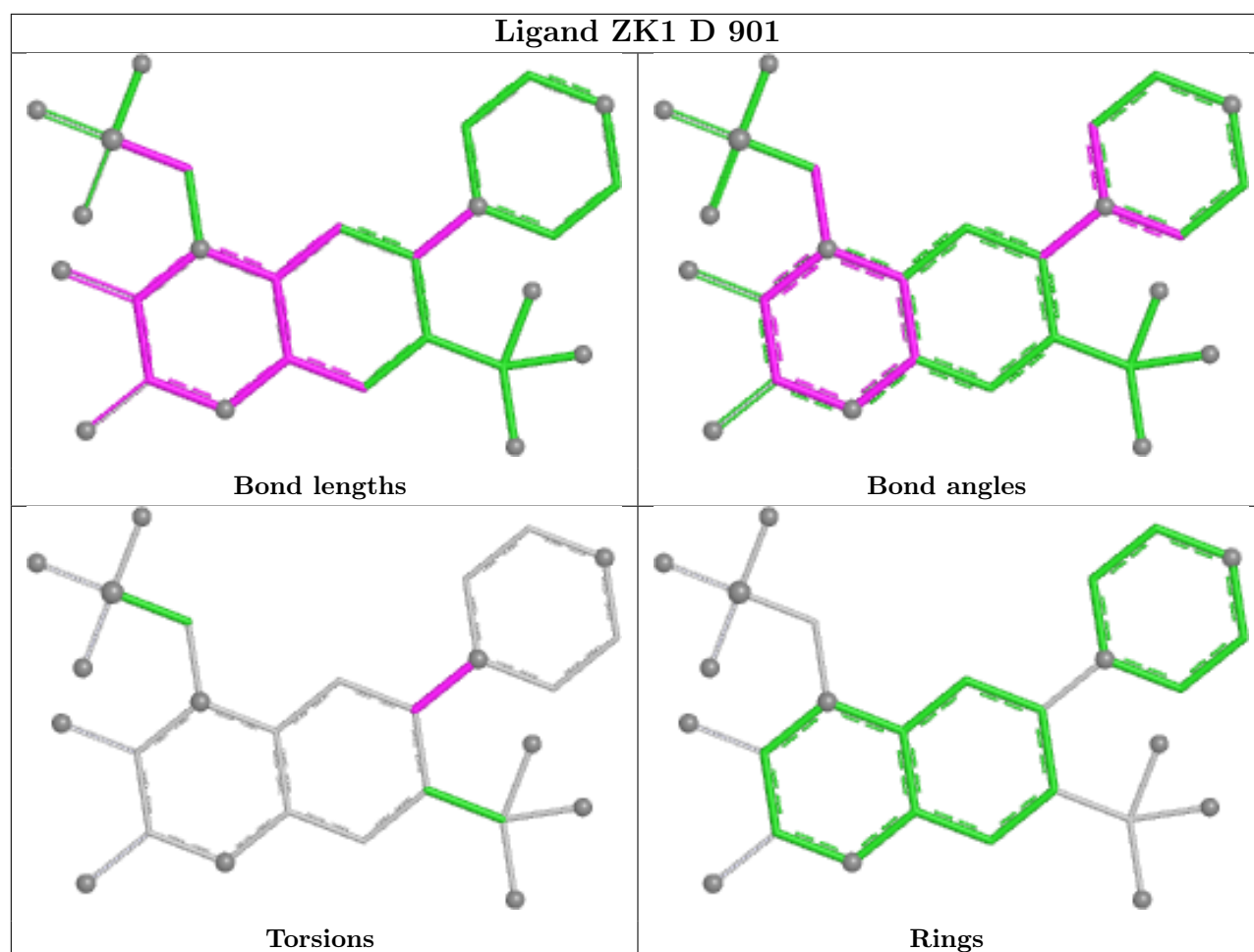


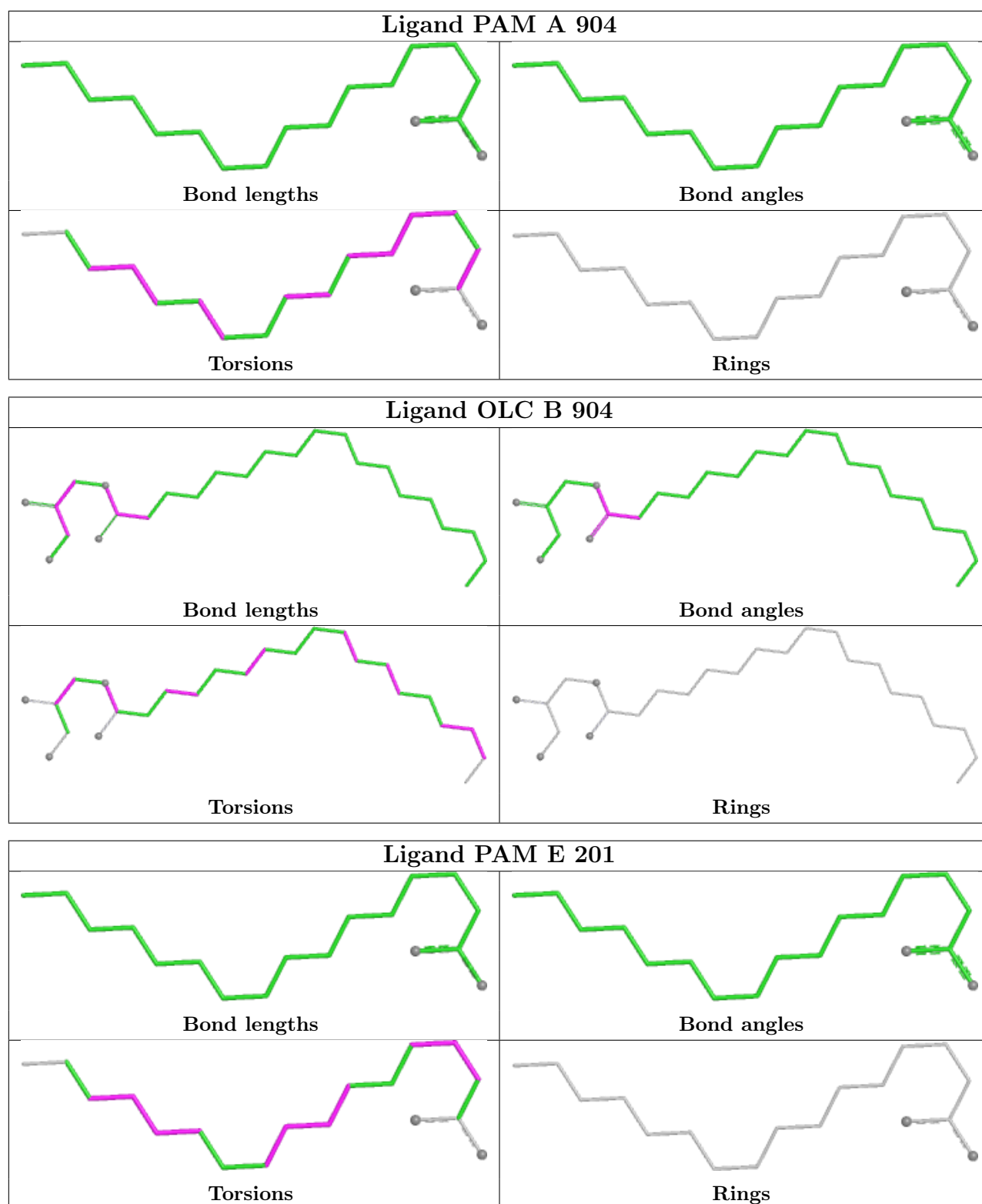


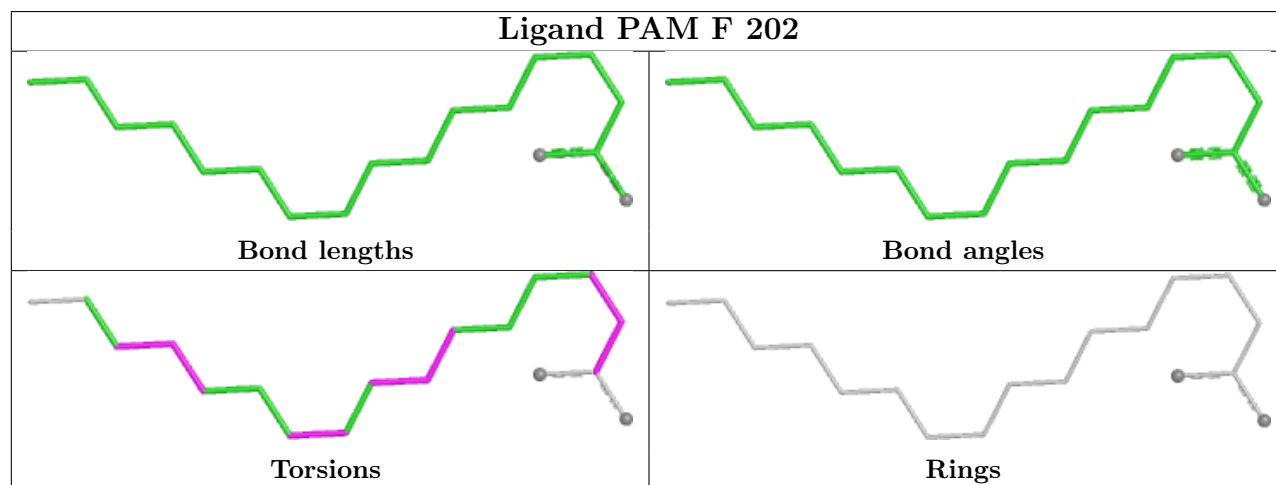
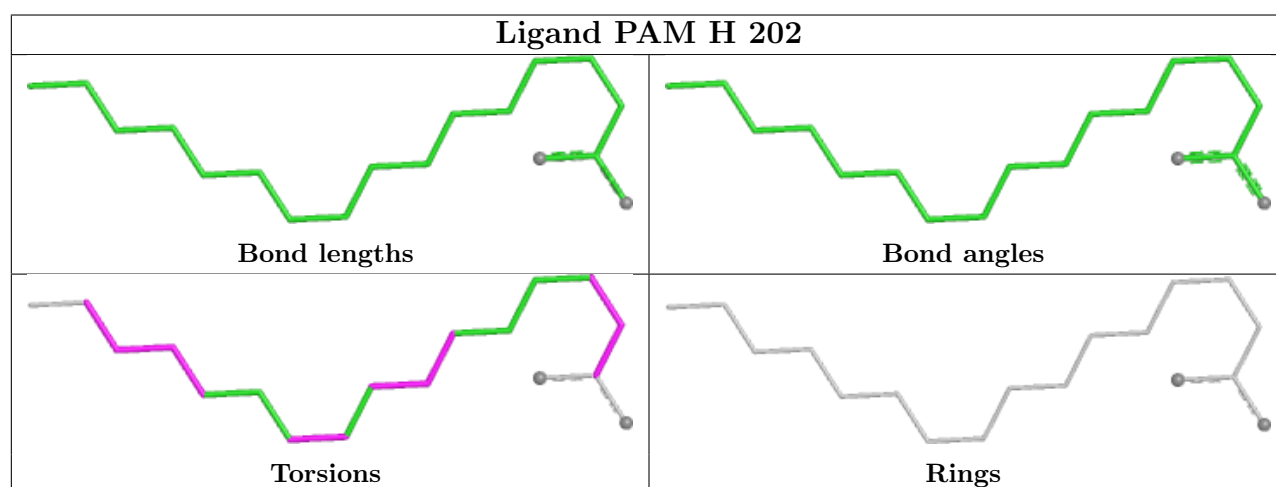
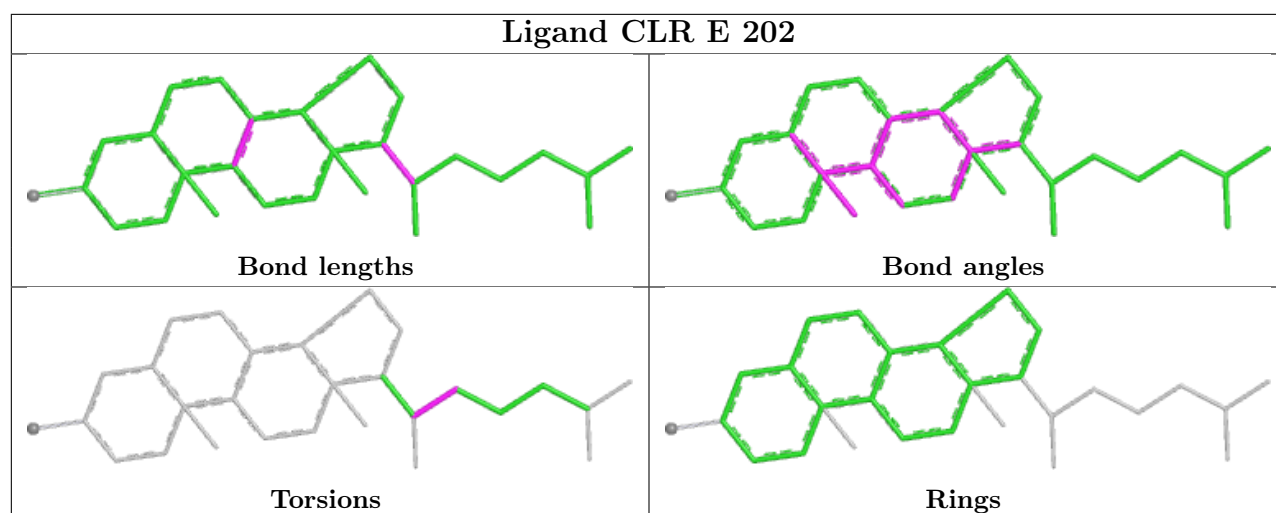




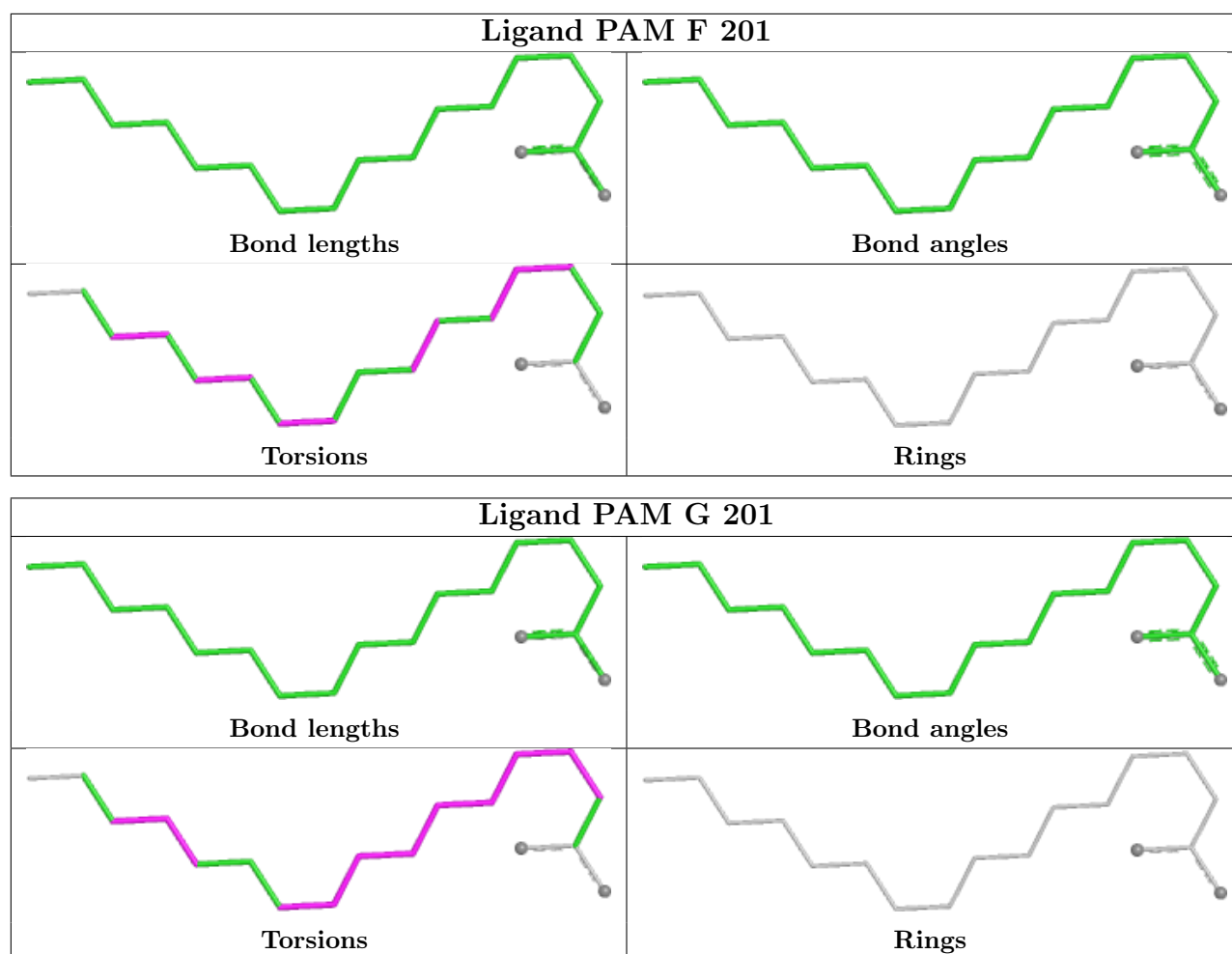












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

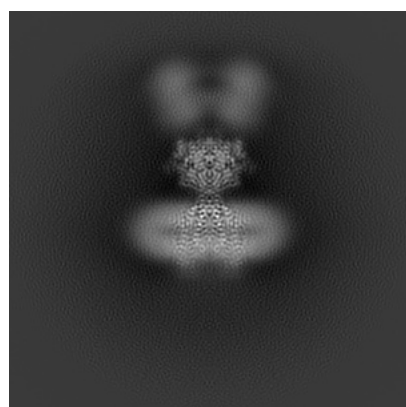
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20727. These allow visual inspection of the internal detail of the map and identification of artifacts.

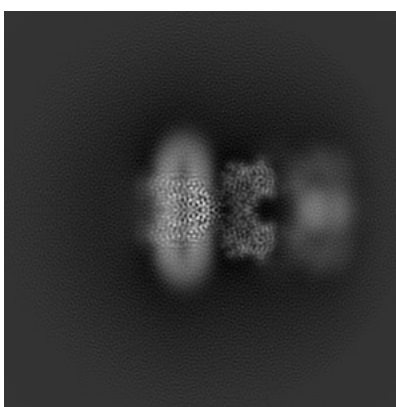
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

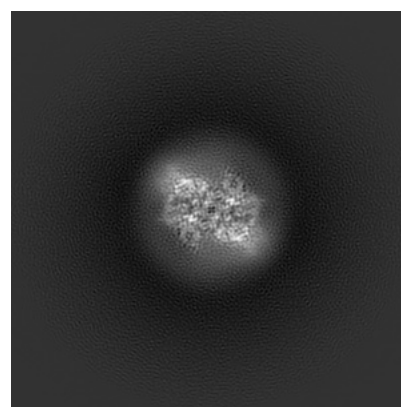
#### 6.1.1 Primary map



X



Y

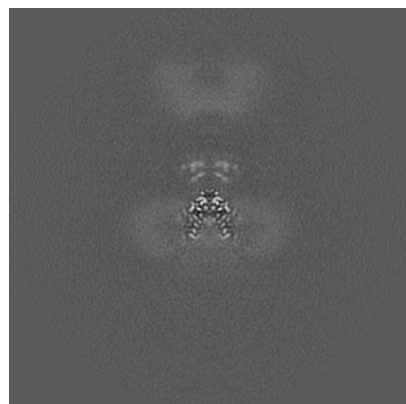


Z

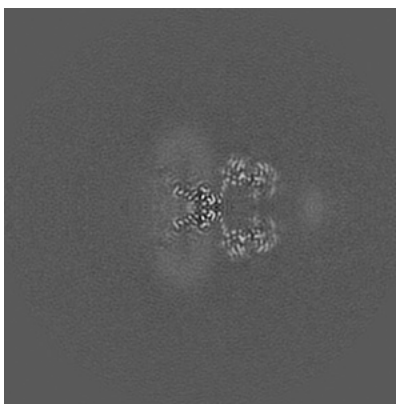
The images above show the map projected in three orthogonal directions.

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

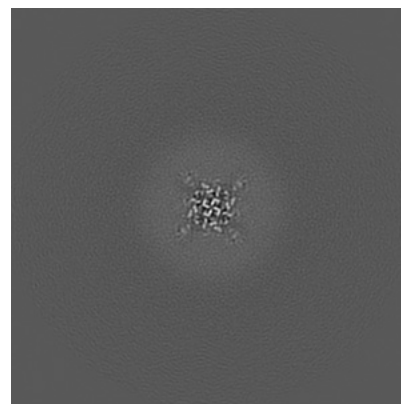
#### 6.2.1 Primary map



X Index: 180



Y Index: 180

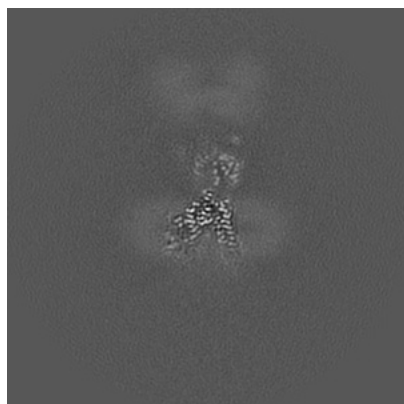


Z Index: 180

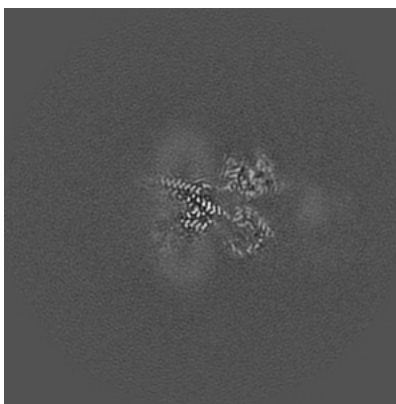
The images above show central slices of the map in three orthogonal directions.

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

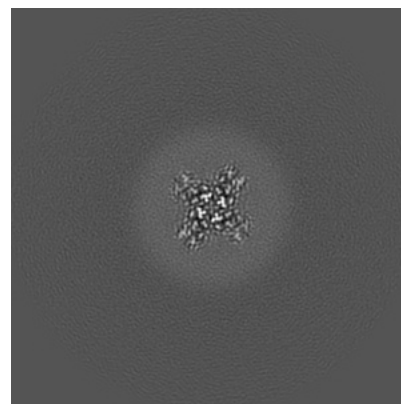
### 6.3.1 Primary map



X Index: 171



Y Index: 187

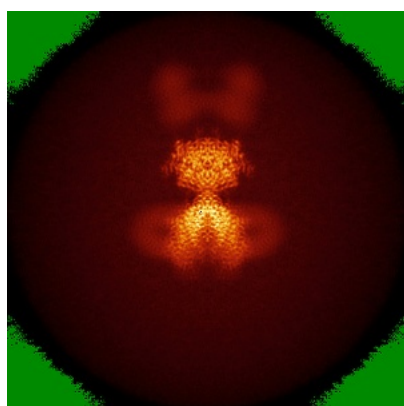


Z Index: 170

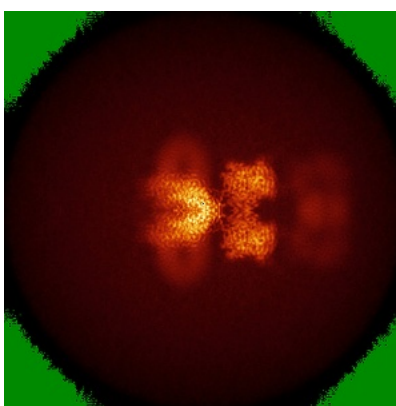
The images above show the largest variance slices of the map in three orthogonal directions.

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

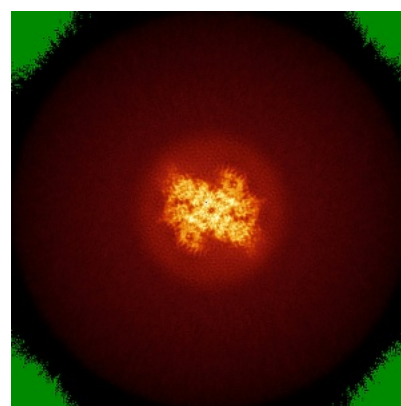
### 6.4.1 Primary map



X



Y

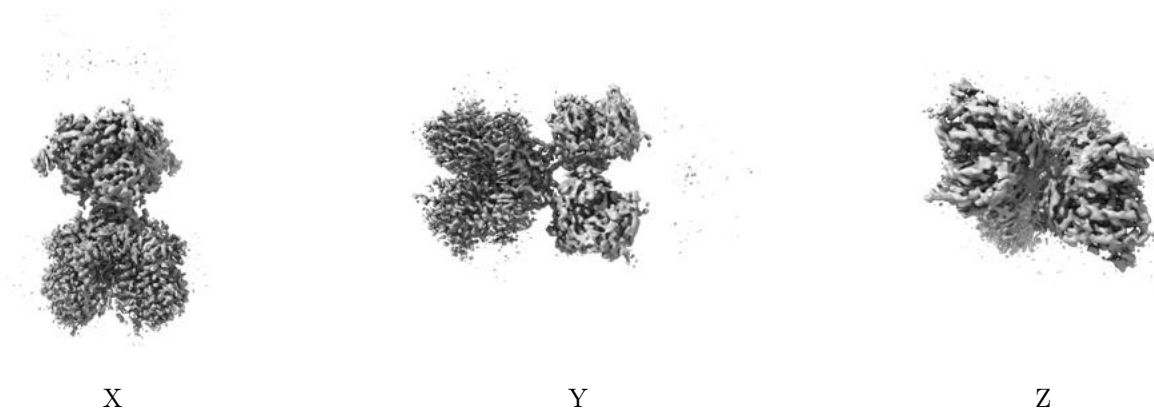


Z

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

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

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.027. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

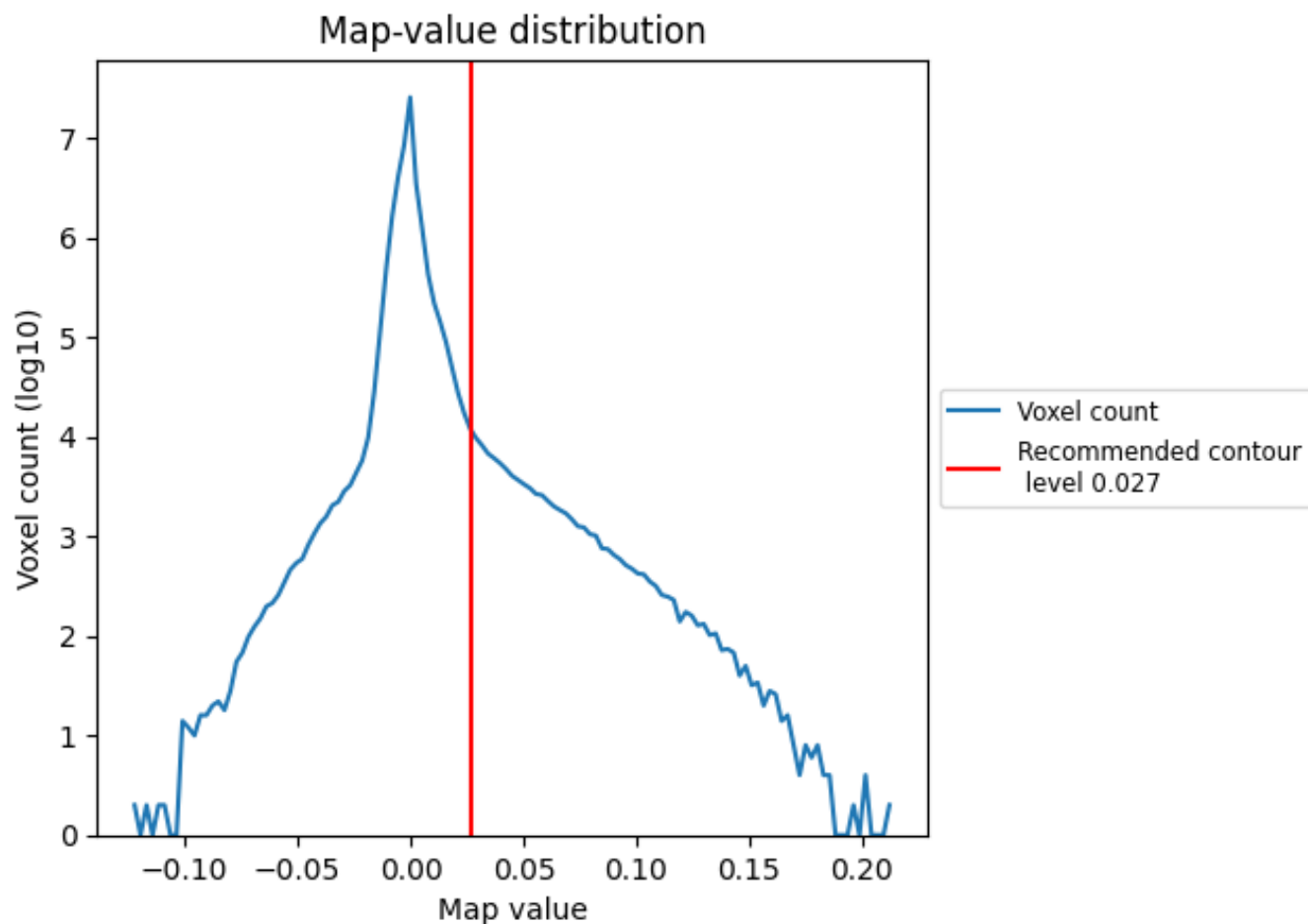
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

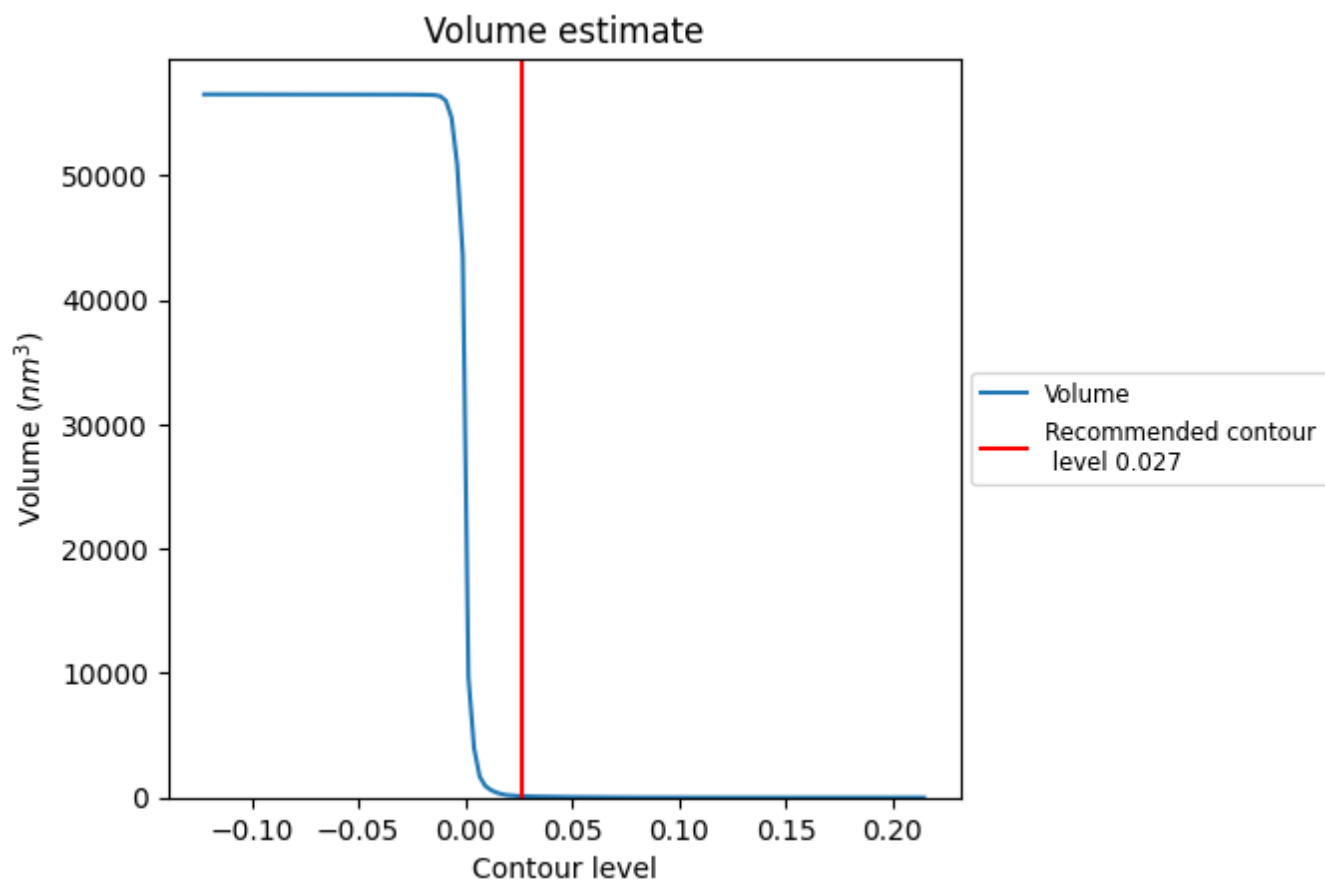
This section contains the results of statistical analysis of the map.

### 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.

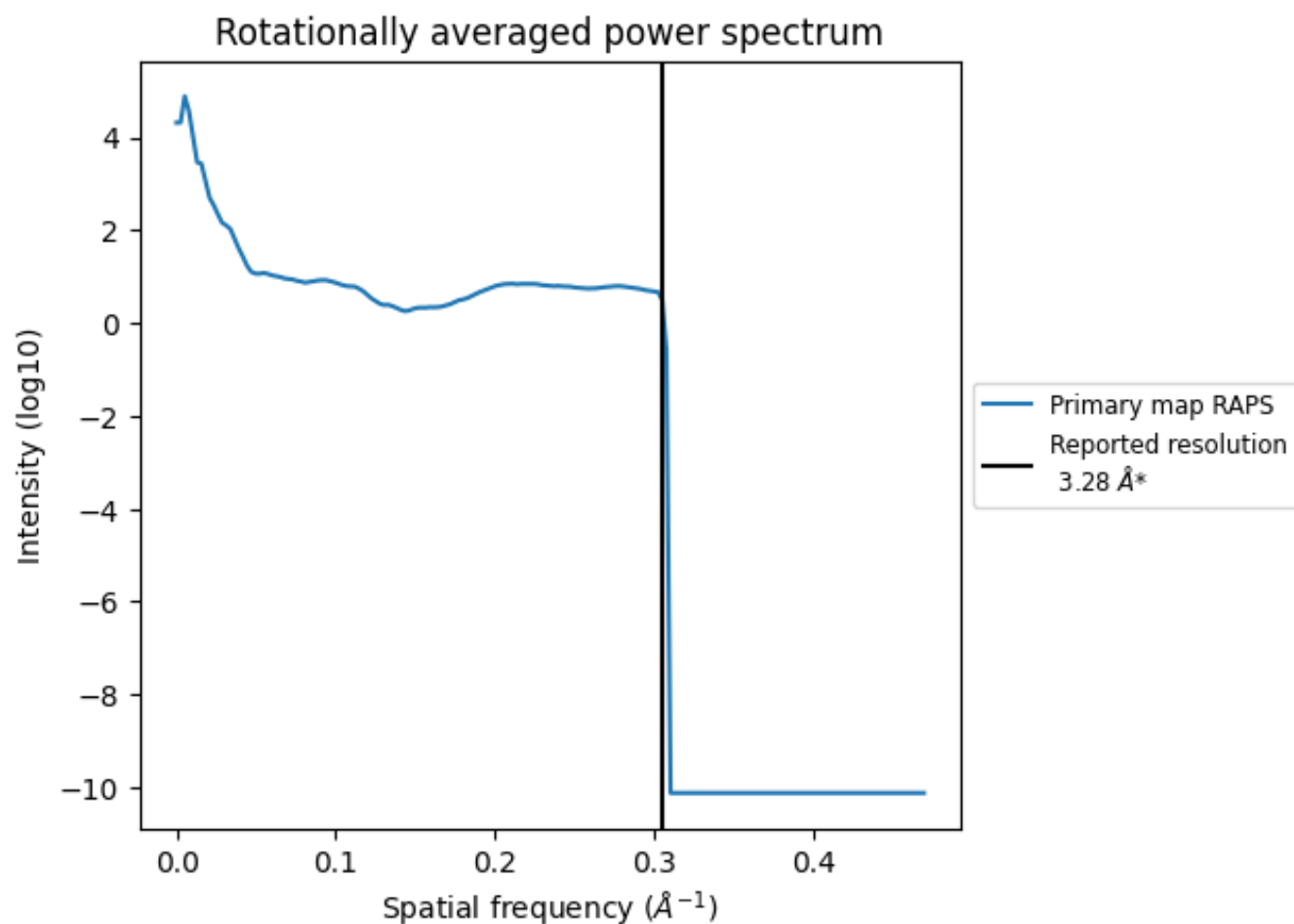
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 111 nm<sup>3</sup>; this corresponds to an approximate mass of 100 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 ⓘ

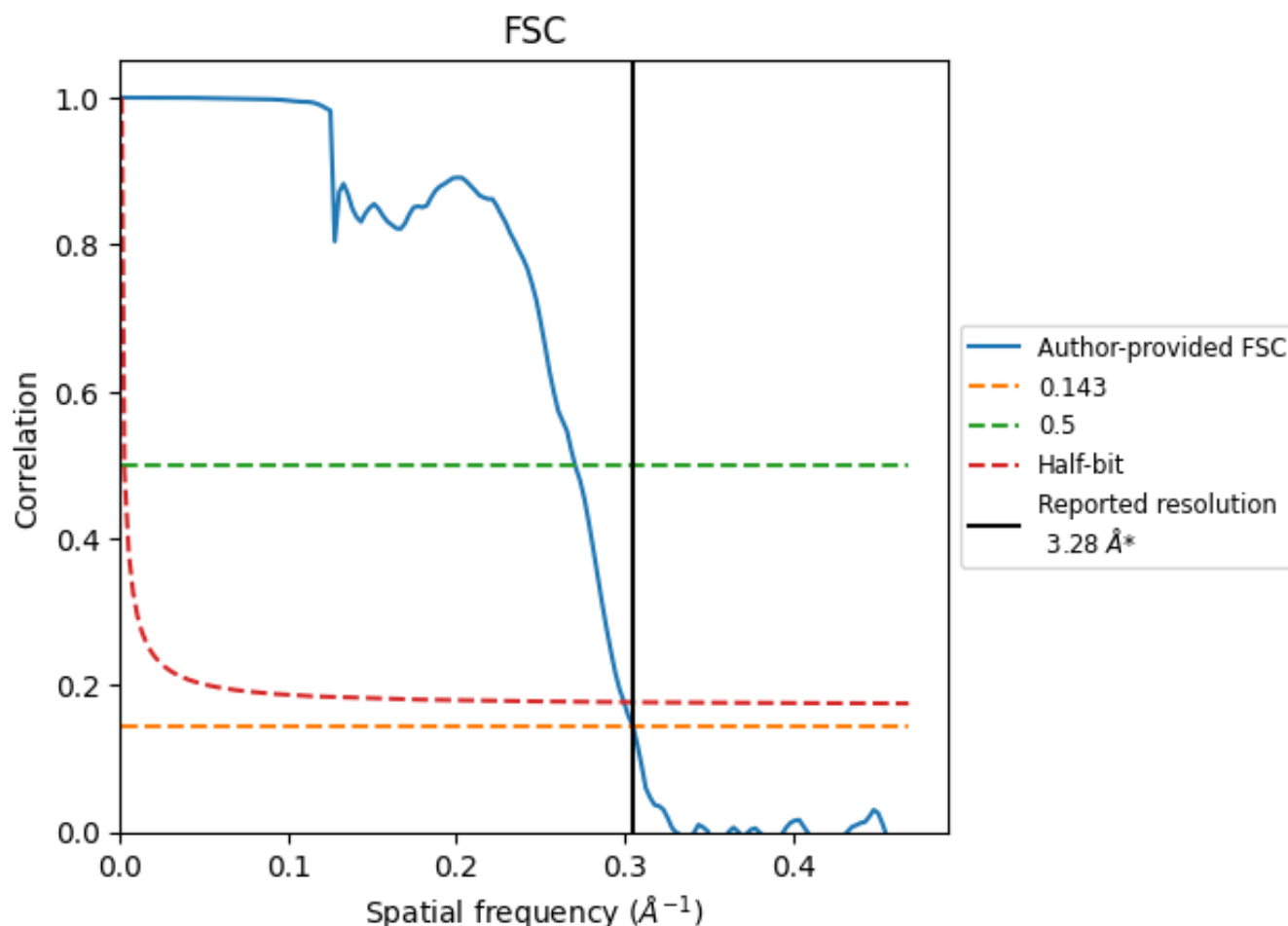


\*Reported resolution corresponds to spatial frequency of 0.305 Å<sup>-1</sup>

## 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 0.305 Å<sup>-1</sup>



## 8.2 Resolution estimates [i](#)

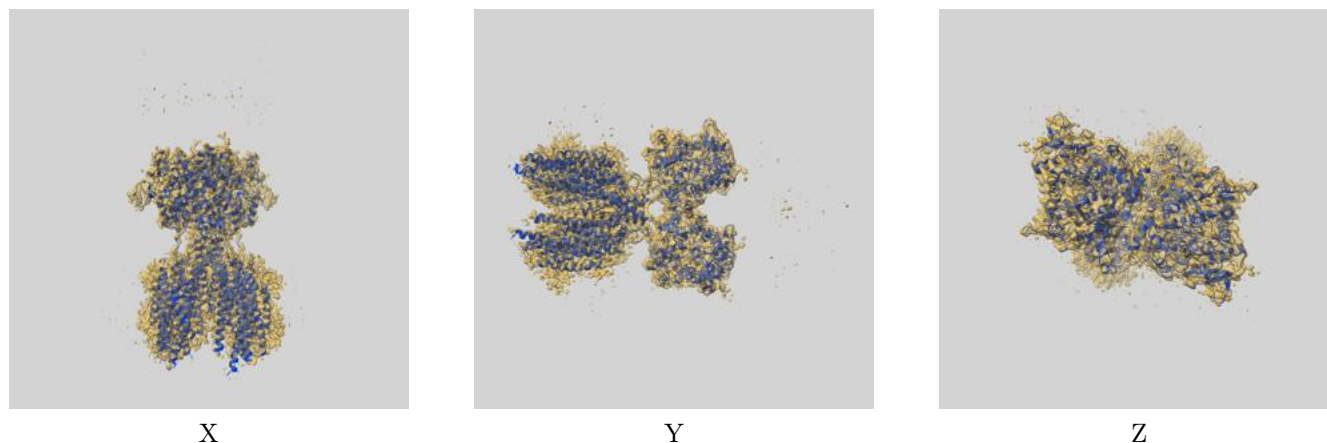
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.28	-	-
Author-provided FSC curve	3.28	3.70	3.34
Unmasked-calculated*	-	-	-

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

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

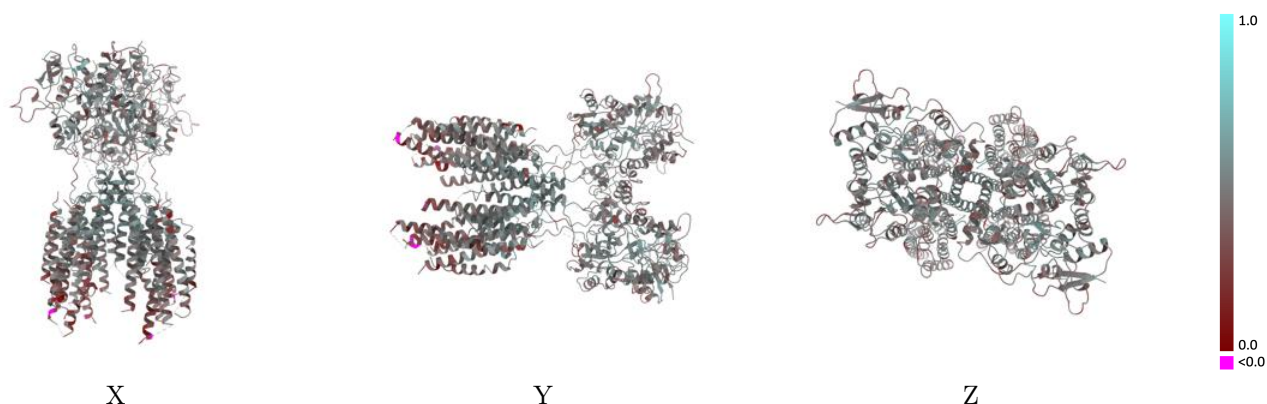
This section contains information regarding the fit between EMDB map EMD-20727 and PDB model 6UCB. Per-residue inclusion information can be found in section 3 on page 11.

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



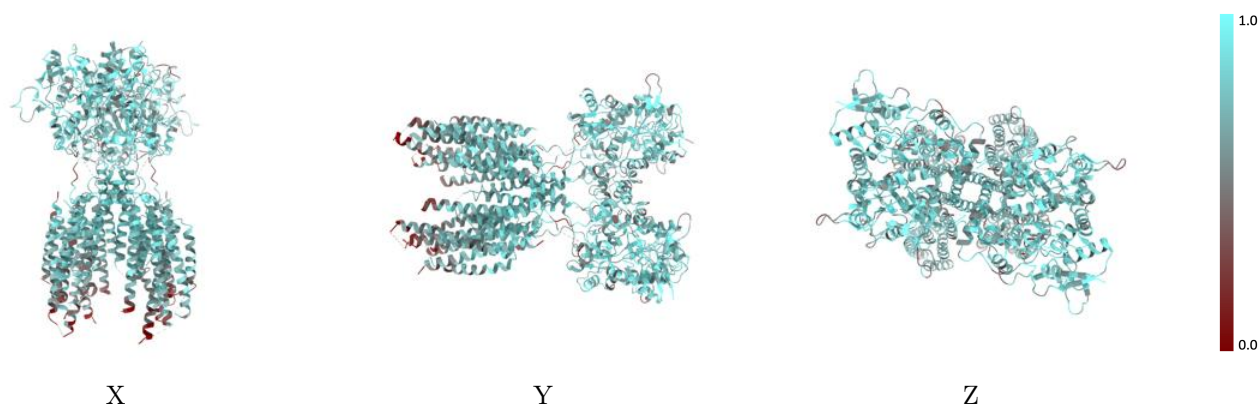
The images above show the 3D surface view of the map at the recommended contour level 0.027 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



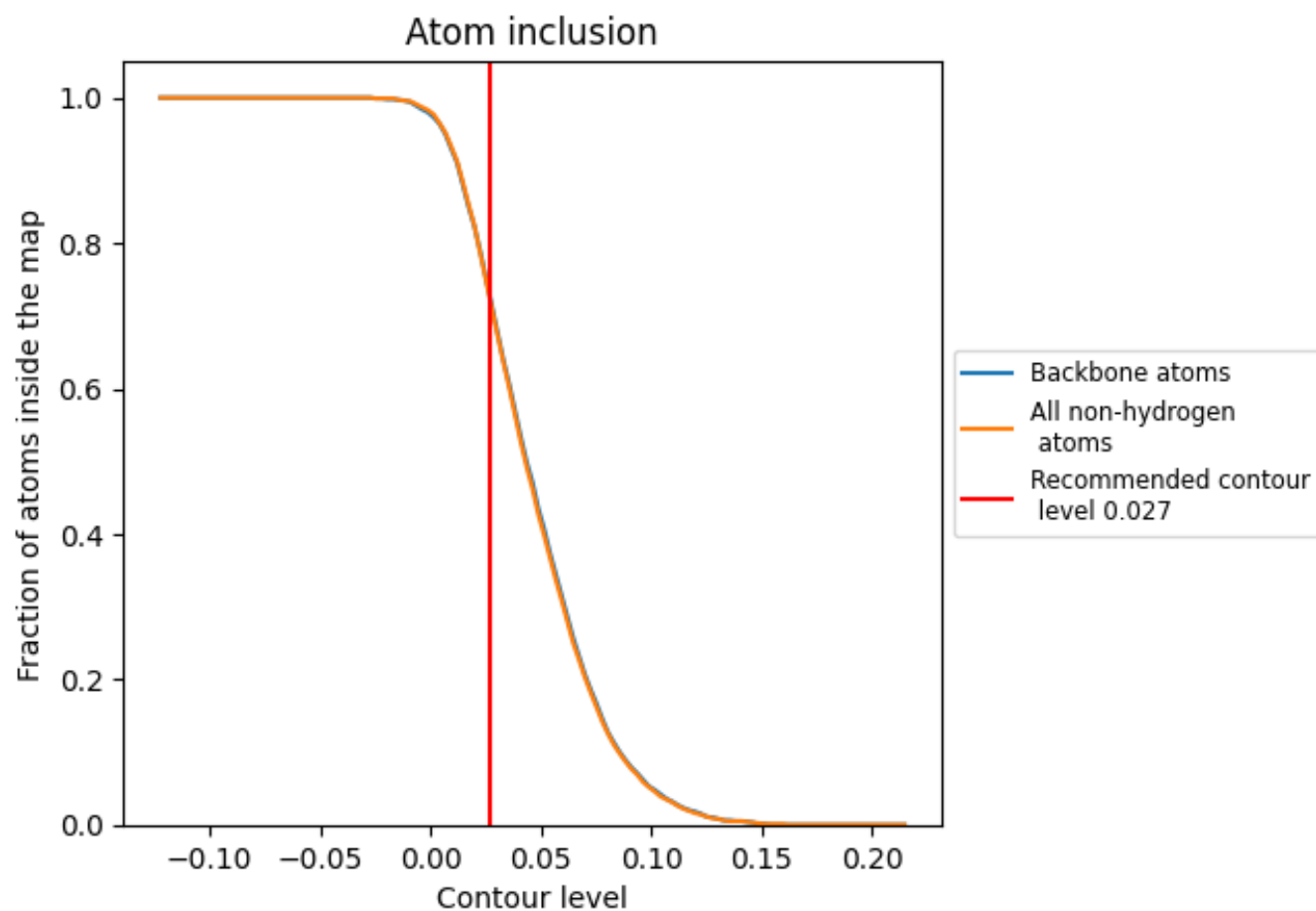
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.027).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 73% of all backbone atoms, 72% 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 (0.027) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.7220	<div><div></div></div> 0.4590
A	<div><div></div></div> 0.7580	<div><div></div></div> 0.4760
B	<div><div></div></div> 0.7570	<div><div></div></div> 0.4780
C	<div><div></div></div> 0.7580	<div><div></div></div> 0.4760
D	<div><div></div></div> 0.7570	<div><div></div></div> 0.4760
E	<div><div></div></div> 0.6390	<div><div></div></div> 0.3990
F	<div><div></div></div> 0.6780	<div><div></div></div> 0.4210
G	<div><div></div></div> 0.6430	<div><div></div></div> 0.4070
H	<div><div></div></div> 0.6740	<div><div></div></div> 0.4240

1.0

0.0

<0.0