wwPDB EM Validation Summary Report (i)

Nov 5, 2024 – 03:13 AM EST

PDB ID	:	8SS2
EMDB ID	:	EMD-40741
Title	:	Structure of AMPA receptor GluA2 complex with auxiliary subunits TARP gamma-5 and cornichon-2 bound to competitive antagonist ZK and channel blocker spermidine (closed state)
Authors	:	Gangwar, S.P.; Yen, L.Y.; Yelshanskaya, M.V.; Sobolevsky, A.I.
Deposited on	:	2023-05-08
Resolution	:	3.58 Å(reported)

This is a wwPDB EM Validation Summary 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 (i) 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 (i)) were used in the production of this report:

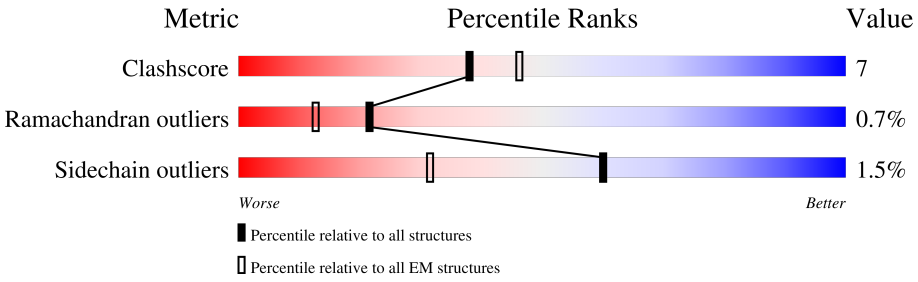
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA,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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.58 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	1026	8% 79% 15% • 5%
1	B	1026	• 63% 13% 24%
1	C	1026	8% 80% 15% • 5%
1	D	1026	• 63% 13% 24%
2	E	160	28% 70% 15% •• 12%
2	F	160	28% 71% 14% •• 12%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	CLR	A	1105	X	-	-	-
5	CLR	C	1105	X	-	-	-
6	AJP	A	1106	X	-	X	-
6	AJP	C	1106	X	-	X	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 31146 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 Glutamate receptor 2, Voltage-dependent calcium channel gamma-5 subunit chimera.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	978	Total	C	N	O	S	0	0
			7714	4982	1270	1422	40		
1	B	783	Total	C	N	O	S	0	0
			6177	3969	1022	1156	30		
1	C	978	Total	C	N	O	S	0	0
			7714	4982	1270	1422	40		
1	D	783	Total	C	N	O	S	0	0
			6177	3969	1022	1156	30		

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	241	GLU	ASN	conflict	UNP P19491
A	382	LEU	VAL	conflict	UNP P19491
A	?	-	LEU	deletion	UNP P19491
A	?	-	THR	deletion	UNP P19491
A	?	-	GLU	deletion	UNP P19491
A	?	-	LEU	deletion	UNP P19491
A	?	-	PRO	deletion	UNP P19491
A	?	-	SER	deletion	UNP P19491
A	384	GLU	GLY	conflict	UNP P19491
A	385	ASP	ASN	conflict	UNP P19491
A	392	GLN	ASN	conflict	UNP P19491
A	754	SER	ASN	conflict	UNP P19491
A	758	VAL	LEU	conflict	UNP P19491
A	827	GLY	-	linker	UNP P19491
A	828	THR	-	linker	UNP P19491
A	829	GLY	-	linker	UNP P19491
A	830	SER	-	linker	UNP P19491
A	831	ALA	-	linker	UNP P19491
B	241	GLU	ASN	conflict	UNP P19491
B	382	LEU	VAL	conflict	UNP P19491
B	?	-	LEU	deletion	UNP P19491

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	THR	deletion	UNP P19491
B	?	-	GLU	deletion	UNP P19491
B	?	-	LEU	deletion	UNP P19491
B	?	-	PRO	deletion	UNP P19491
B	?	-	SER	deletion	UNP P19491
B	384	GLU	GLY	conflict	UNP P19491
B	385	ASP	ASN	conflict	UNP P19491
B	392	GLN	ASN	conflict	UNP P19491
B	754	SER	ASN	conflict	UNP P19491
B	758	VAL	LEU	conflict	UNP P19491
B	827	GLY	-	linker	UNP P19491
B	828	THR	-	linker	UNP P19491
B	829	GLY	-	linker	UNP P19491
B	830	SER	-	linker	UNP P19491
B	831	ALA	-	linker	UNP P19491
C	241	GLU	ASN	conflict	UNP P19491
C	382	LEU	VAL	conflict	UNP P19491
C	?	-	LEU	deletion	UNP P19491
C	?	-	THR	deletion	UNP P19491
C	?	-	GLU	deletion	UNP P19491
C	?	-	LEU	deletion	UNP P19491
C	?	-	PRO	deletion	UNP P19491
C	?	-	SER	deletion	UNP P19491
C	384	GLU	GLY	conflict	UNP P19491
C	385	ASP	ASN	conflict	UNP P19491
C	392	GLN	ASN	conflict	UNP P19491
C	754	SER	ASN	conflict	UNP P19491
C	758	VAL	LEU	conflict	UNP P19491
C	827	GLY	-	linker	UNP P19491
C	828	THR	-	linker	UNP P19491
C	829	GLY	-	linker	UNP P19491
C	830	SER	-	linker	UNP P19491
C	831	ALA	-	linker	UNP P19491
D	241	GLU	ASN	conflict	UNP P19491
D	382	LEU	VAL	conflict	UNP P19491
D	?	-	LEU	deletion	UNP P19491
D	?	-	THR	deletion	UNP P19491
D	?	-	GLU	deletion	UNP P19491
D	?	-	LEU	deletion	UNP P19491
D	?	-	PRO	deletion	UNP P19491
D	?	-	SER	deletion	UNP P19491
D	384	GLU	GLY	conflict	UNP P19491

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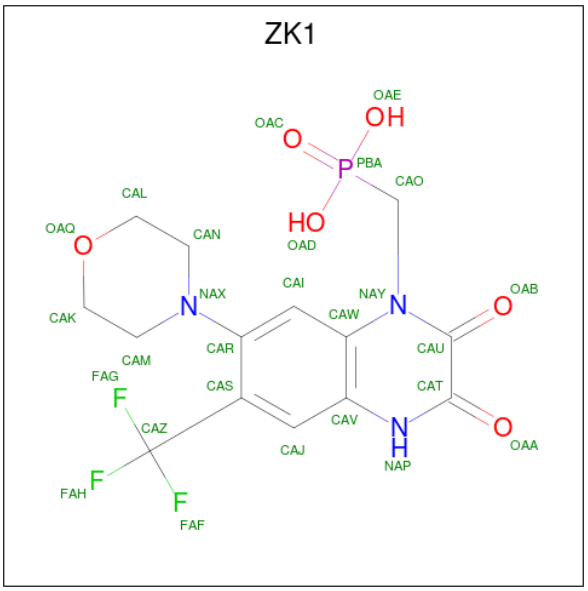
Chain	Residue	Modelled	Actual	Comment	Reference
D	385	ASP	ASN	conflict	UNP P19491
D	392	GLN	ASN	conflict	UNP P19491
D	754	SER	ASN	conflict	UNP P19491
D	758	VAL	LEU	conflict	UNP P19491
D	827	GLY	-	linker	UNP P19491
D	828	THR	-	linker	UNP P19491
D	829	GLY	-	linker	UNP P19491
D	830	SER	-	linker	UNP P19491
D	831	ALA	-	linker	UNP P19491

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	140	Total	C	N	O	S	0	0
			1166	787	175	191	13		
2	F	140	Total	C	N	O	S	0	0
			1166	787	175	191	13		

- 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: $C_{14}H_{15}F_3N_3O_6P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
3	A	1	Total	C	F	N	O	P	0
			27	14	3	3	6	1	
3	B	1	Total	C	F	N	O	P	0
			27	14	3	3	6	1	

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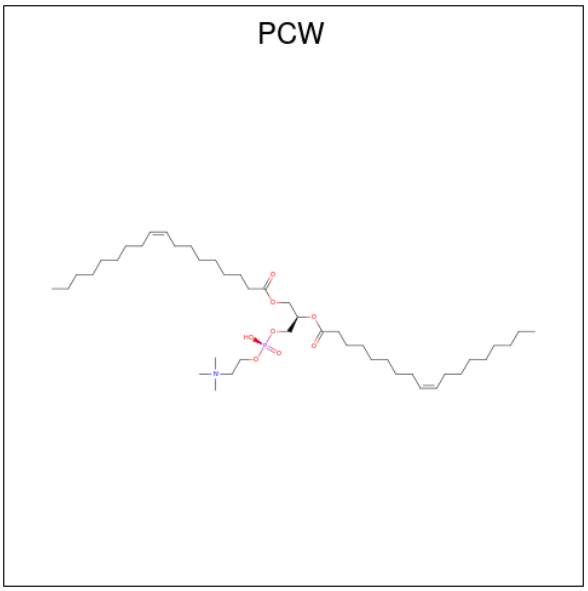
Mol	Chain	Residues	Atoms						AltConf
3	C	1	Total	C	F	N	O	P	0
			27	14	3	3	6	1	
3	D	1	Total	C	F	N	O	P	0
			27	14	3	3	6	1	

- Molecule 4 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PCW) (formula: $C_{44}H_{85}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			40	30	1	8	1	
4	A	1	Total	C	N	O	P	0
			43	33	1	8	1	
4	A	1	Total	C				0
			11	11				
4	A	1	Total	C	N	O	P	0
			51	41	1	8	1	
4	A	1	Total	C				0
			11	11				
4	A	1	Total	C	N	O	P	0
			39	29	1	8	1	
4	A	1	Total	C				0
			11	11				
4	B	1	Total	C	N	O	P	0
			43	33	1	8	1	
4	B	1	Total	C	N	O	P	0
			32	22	1	8	1	

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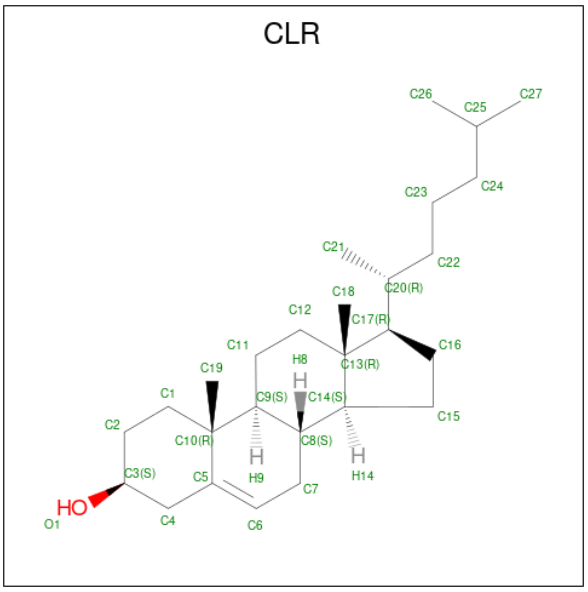
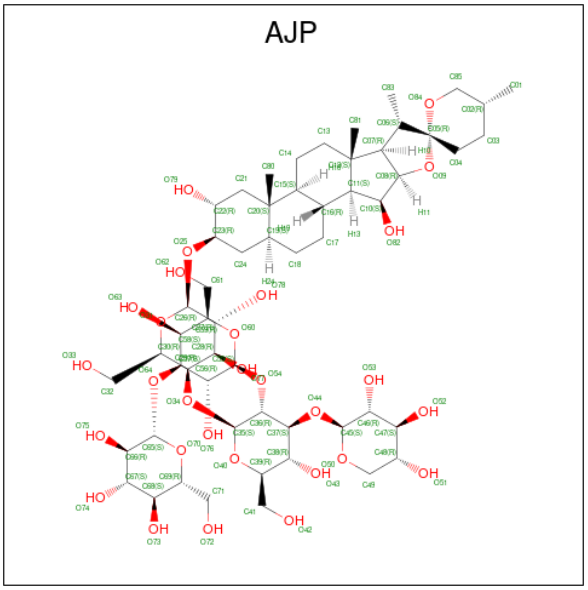
Mol	Chain	Residues	Atoms					AltConf
4	B	1	Total	C	N	O	P	0
			41	31	1	8	1	
4	B	1	Total	C				0
			11	11				
4	C	1	Total	C	N	O	P	0
			40	30	1	8	1	
4	C	1	Total	C	N	O	P	0
			43	33	1	8	1	
4	C	1	Total	C				0
			11	11				
4	C	1	Total	C	N	O	P	0
			51	41	1	8	1	
4	C	1	Total	C				0
			11	11				
4	C	1	Total	C	N	O	P	0
			39	29	1	8	1	
4	C	1	Total	C				0
			11	11				
4	D	1	Total	C	N	O	P	0
			43	33	1	8	1	
4	D	1	Total	C	N	O	P	0
			32	22	1	8	1	
4	D	1	Total	C	N	O	P	0
			41	31	1	8	1	
4	D	1	Total	C				0
			11	11				
4	E	1	Total	C				0
			11	11				
4	E	1	Total	C	N	O	P	0
			43	33	1	8	1	
4	F	1	Total	C				0
			11	11				
4	F	1	Total	C	N	O	P	0
			43	33	1	8	1	

- Molecule 5 is CHOLESTEROL (three-letter code: CLR) (formula: $C_{27}H_{46}O$).



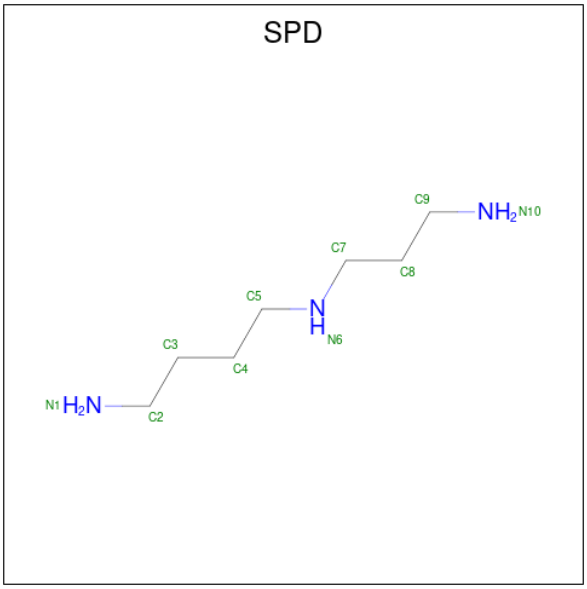
Mol	Chain	Residues	Atoms	AltConf
5	A	1	Total C O 28 27 1	0
5	C	1	Total C O 28 27 1	0

- Molecule 6 is Digitonin (three-letter code: AJP) (formula: $C_{56}H_{92}O_{29}$).



Mol	Chain	Residues	Atoms	AltConf
6	A	1	Total C O 42 33 9	0
6	C	1	Total C O 42 33 9	0

- Molecule 7 is SPERMIDINE (three-letter code: SPD) (formula: $C_7H_{19}N_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	N	
7	A	1	10	7	3	0

3 Residue-property plots (i)

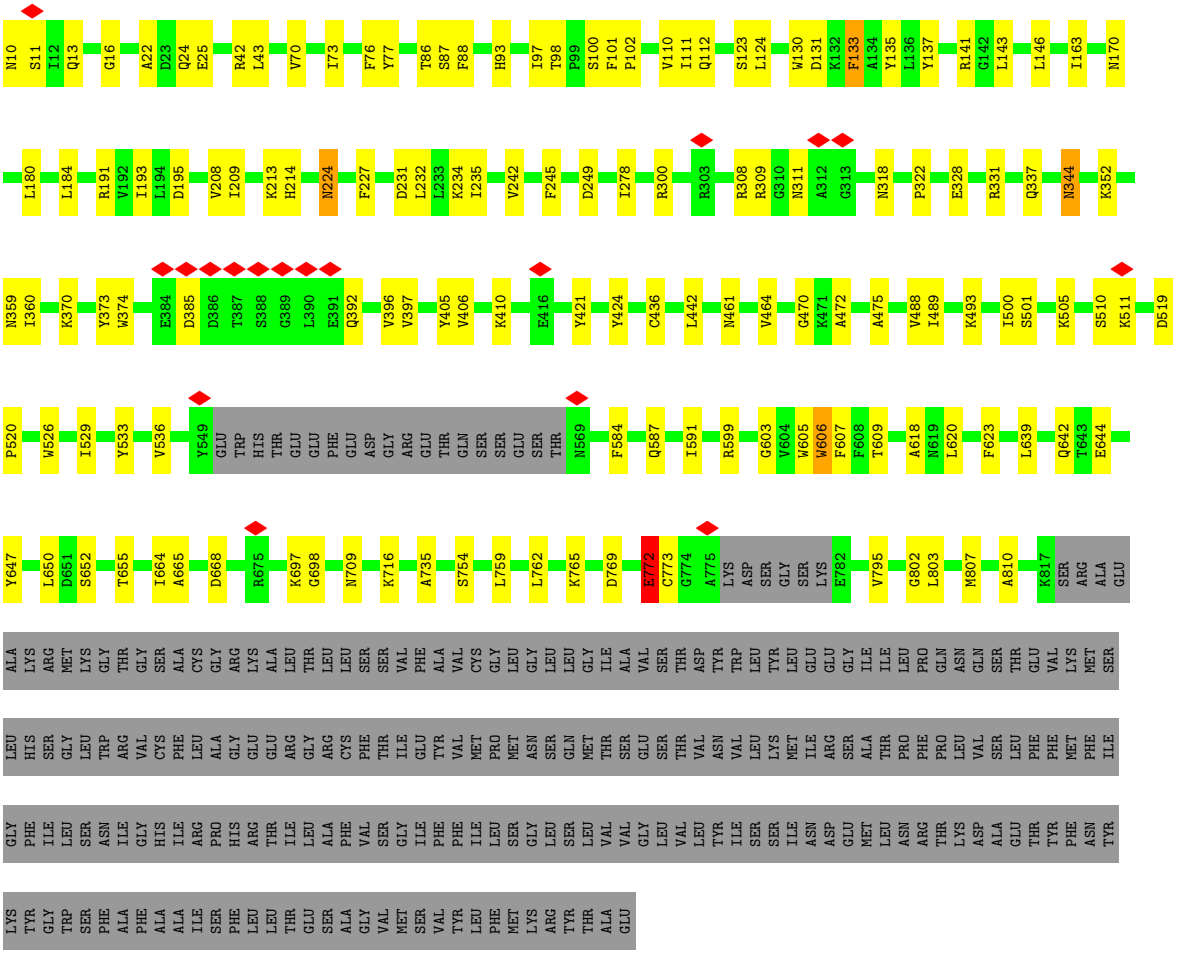
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: Glutamate receptor 2, Voltage-dependent calcium channel gamma-5 subunit chimera

Chain A:

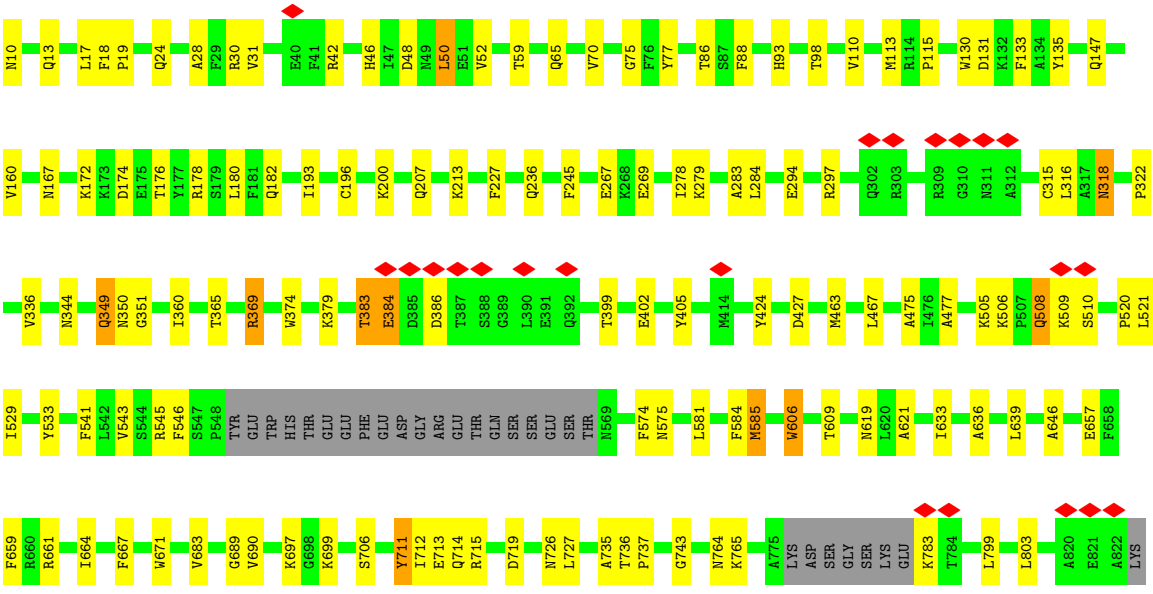
• Molecule 1: Glutamate receptor 2, Voltage-dependent calcium channel gamma-5 subunit chimera

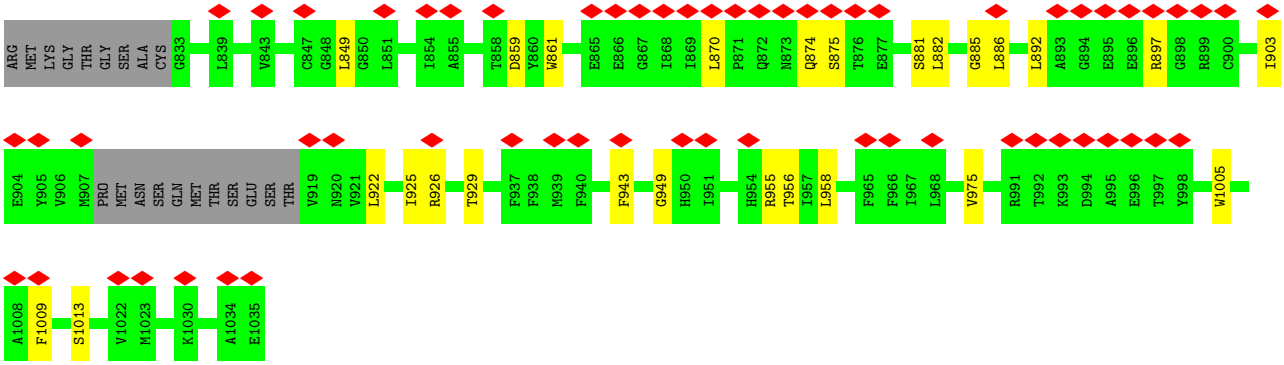
Chain B:



• Molecule 1: Glutamate receptor 2, Voltage-dependent calcium channel gamma-5 subunit chimera

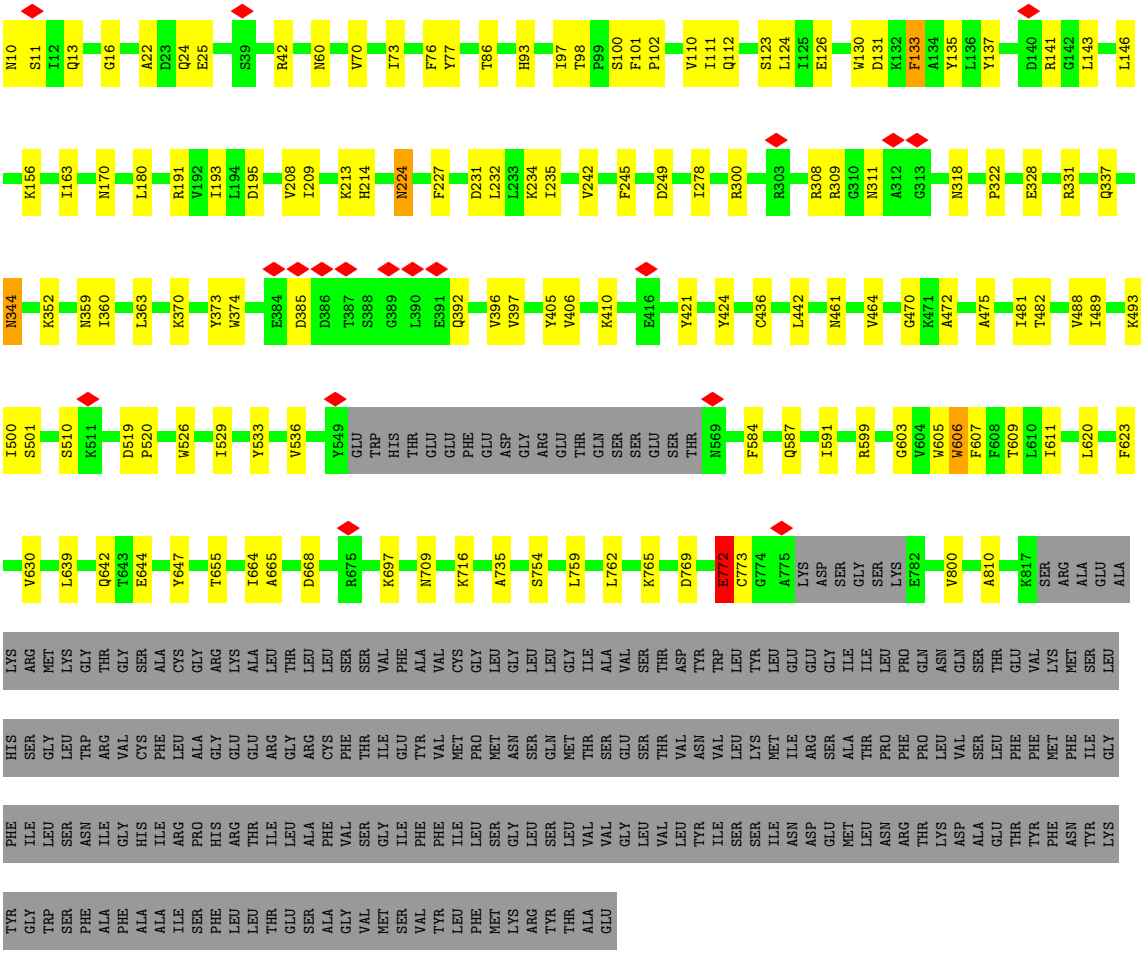
Chain C:





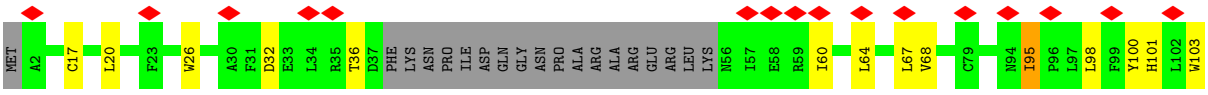
• Molecule 1: Glutamate receptor 2, Voltage-dependent calcium channel gamma-5 subunit chimera

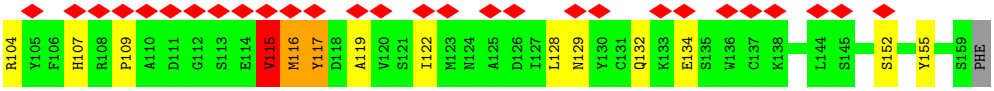
Chain D:



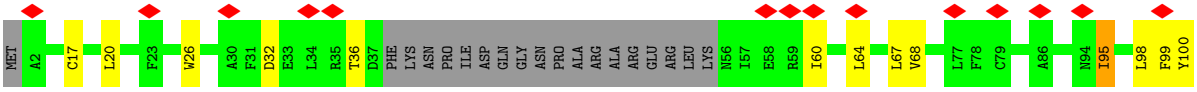
• Molecule 2: Protein cornichon homolog 2

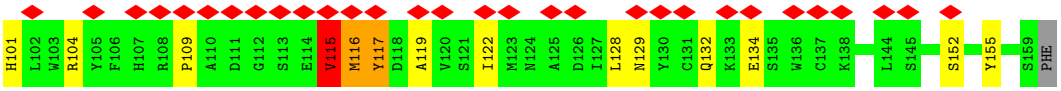
Chain E:





• Molecule 2: Protein cornichon homolog 2





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	55275	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 ($e^-/Å^2$)	58	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.107	Depositor
Minimum map value	-0.718	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.025	Depositor
Recommended contour level	0.13	Depositor
Map size (Å)	345.28, 345.28, 345.28	wwPDB
Map dimensions	416, 416, 416	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PCW, AJP, CLR, SPD, ZK1

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	0.58	3/7880 (0.0%)	0.68	2/10648 (0.0%)
1	B	0.58	1/6308 (0.0%)	0.67	3/8523 (0.0%)
1	C	0.58	3/7880 (0.0%)	0.68	2/10648 (0.0%)
1	D	0.58	1/6308 (0.0%)	0.67	3/8523 (0.0%)
2	E	0.37	0/1203	0.68	2/1636 (0.1%)
2	F	0.37	0/1203	0.68	2/1636 (0.1%)
All	All	0.57	8/30782 (0.0%)	0.68	14/41614 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	7
1	B	0	7
1	C	0	7
1	D	0	7
2	E	0	4
2	F	0	4
All	All	0	36

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	130	TRP	CB-CG	-5.45	1.40	1.50
1	A	130	TRP	CB-CG	-5.41	1.40	1.50
1	C	402	GLU	C-N	-5.25	1.22	1.34
1	A	402	GLU	C-N	-5.22	1.22	1.34
1	A	606	TRP	CB-CG	-5.05	1.41	1.50

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	762	LEU	CA-CB-CG	6.26	129.69	115.30
1	B	762	LEU	CA-CB-CG	6.24	129.66	115.30
1	C	50	LEU	CA-CB-CG	6.02	129.14	115.30
1	A	50	LEU	CA-CB-CG	6.01	129.13	115.30
1	D	232	LEU	CB-CG-CD2	-5.96	100.86	111.00

There are no chirality outliers.

5 of 36 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	267	GLU	Peptide
1	A	318	ASN	Peptide
1	A	383	THR	Peptide
1	A	506	LYS	Peptide
1	A	546	PHE	Peptide

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	7714	0	7731	97	0
1	B	6177	0	6164	90	0
1	C	7714	0	7731	89	0
1	D	6177	0	6164	85	0
2	E	1166	0	1152	16	0
2	F	1166	0	1152	16	0
3	A	27	0	13	0	0
3	B	27	0	13	0	0
3	C	27	0	13	1	0
3	D	27	0	13	0	0
4	A	206	0	282	8	0
4	B	127	0	161	3	0
4	C	206	0	282	5	0
4	D	127	0	161	5	0
4	E	54	0	73	2	0
4	F	54	0	73	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	28	0	37	4	0
5	C	28	0	37	3	0
6	A	42	0	0	33	0
6	C	42	0	0	36	0
7	A	10	0	19	2	0
All	All	31146	0	31271	451	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 7.

The worst 5 of 451 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:C:1106:AJP:C19	6:C:1106:AJP:C24	1.77	1.61
6:A:1106:AJP:C14	6:A:1106:AJP:C15	1.79	1.60
6:C:1106:AJP:C15	6:C:1106:AJP:C14	1.79	1.59
6:C:1106:AJP:C18	6:C:1106:AJP:C17	1.81	1.58
5:A:1105:CLR:C15	5:A:1105:CLR:C16	1.77	1.58

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	968/1026 (94%)	813 (84%)	148 (15%)	7 (1%)	19 53
1	B	777/1026 (76%)	654 (84%)	120 (15%)	3 (0%)	30 62
1	C	968/1026 (94%)	812 (84%)	149 (15%)	7 (1%)	19 53
1	D	777/1026 (76%)	654 (84%)	120 (15%)	3 (0%)	30 62
2	E	136/160 (85%)	119 (88%)	14 (10%)	3 (2%)	5 32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	F	136/160 (85%)	119 (88%)	14 (10%)	3 (2%)	5 32
All	All	3762/4424 (85%)	3171 (84%)	565 (15%)	26 (1%)	21 53

5 of 26 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	350	ASN
1	C	350	ASN
1	A	349	GLN
1	A	384	GLU
1	B	773	CYS

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	834/877 (95%)	820 (98%)	14 (2%)	56 76
1	B	668/877 (76%)	659 (99%)	9 (1%)	65 82
1	C	834/877 (95%)	821 (98%)	13 (2%)	58 77
1	D	668/877 (76%)	659 (99%)	9 (1%)	65 82
2	E	126/143 (88%)	124 (98%)	2 (2%)	58 77
2	F	126/143 (88%)	124 (98%)	2 (2%)	58 77
All	All	3256/3794 (86%)	3207 (98%)	49 (2%)	60 79

5 of 49 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	318	ASN
1	C	897	ARG
1	C	344	ASN
1	C	585	MET
1	D	224	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 51 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	726	ASN
1	D	224	ASN
2	F	129	ASN
1	C	764	ASN
1	D	24	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

35 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	A	1101	-	29,29,29	3.50	10 (34%)	45,45,45	1.74	9 (20%)
4	PCW	A	1103	-	42,42,53	1.27	5 (11%)	48,50,61	1.04	3 (6%)
4	PCW	C	1103	-	42,42,53	1.27	5 (11%)	48,50,61	1.06	3 (6%)
4	PCW	C	1109	-	38,38,53	1.31	5 (13%)	44,46,61	1.19	3 (6%)
4	PCW	A	1108	-	10,10,53	0.83	0	9,9,61	0.33	0
5	CLR	C	1105	-	31,31,31	9.43	22 (70%)	48,48,48	3.79	25 (52%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	PCW	D	1104	-	40,40,53	1.27	4 (10%)	46,48,61	1.22	3 (6%)
4	PCW	C	1104	-	10,10,53	0.82	0	9,9,61	0.38	0
4	PCW	B	1105	-	10,10,53	0.82	0	9,9,61	0.35	0
4	PCW	C	1102	-	39,39,53	1.26	4 (10%)	45,47,61	1.08	3 (6%)
4	PCW	E	201	-	10,10,53	0.80	0	9,9,61	0.34	0
4	PCW	F	202	-	42,42,53	1.27	4 (9%)	48,50,61	1.10	3 (6%)
4	PCW	B	1102	-	42,42,53	1.21	3 (7%)	48,50,61	1.14	3 (6%)
4	PCW	D	1102	-	42,42,53	1.22	3 (7%)	48,50,61	1.12	3 (6%)
6	AJP	A	1106	-	48,48,95	18.69	38 (79%)	72,78,149	3.60	40 (55%)
4	PCW	B	1103	-	31,31,53	1.28	2 (6%)	37,39,61	1.24	2 (5%)
4	PCW	C	1107	-	50,50,53	1.17	4 (8%)	56,58,61	1.07	4 (7%)
3	ZK1	C	1101	-	29,29,29	3.53	10 (34%)	45,45,45	1.76	9 (20%)
4	PCW	B	1104	-	40,40,53	1.27	4 (10%)	46,48,61	1.23	3 (6%)
4	PCW	A	1107	-	50,50,53	1.17	4 (8%)	56,58,61	1.06	4 (7%)
4	PCW	C	1110	-	10,10,53	0.83	0	9,9,61	0.39	0
7	SPD	A	1111	-	9,9,9	0.39	0	8,8,8	0.89	0
4	PCW	D	1105	-	10,10,53	0.82	0	9,9,61	0.35	0
5	CLR	A	1105	-	31,31,31	9.41	22 (70%)	48,48,48	3.95	24 (50%)
4	PCW	F	201	-	10,10,53	0.80	0	9,9,61	0.33	0
4	PCW	E	202	-	42,42,53	1.27	4 (9%)	48,50,61	1.09	3 (6%)
4	PCW	C	1108	-	10,10,53	0.83	0	9,9,61	0.32	0
4	PCW	A	1109	-	38,38,53	1.30	4 (10%)	44,46,61	1.18	4 (9%)
6	AJP	C	1106	-	48,48,95	18.94	40 (83%)	72,78,149	3.54	39 (54%)
4	PCW	A	1102	-	39,39,53	1.26	4 (10%)	45,47,61	1.08	3 (6%)
3	ZK1	D	1101	-	29,29,29	3.42	9 (31%)	45,45,45	1.91	11 (24%)
4	PCW	A	1104	-	10,10,53	0.82	0	9,9,61	0.38	0
3	ZK1	B	1101	-	29,29,29	3.42	9 (31%)	45,45,45	1.93	10 (22%)
4	PCW	D	1103	-	31,31,53	1.29	2 (6%)	37,39,61	1.37	2 (5%)
4	PCW	A	1110	-	10,10,53	0.82	0	9,9,61	0.39	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	A	1101	-	-	4/13/23/23	0/3/3/3
4	PCW	A	1103	-	-	26/46/46/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PCW	C	1103	-	-	32/46/46/57	-
4	PCW	C	1109	-	-	28/42/42/57	-
5	CLR	C	1105	-	2/2/10/11	7/10/68/68	0/4/4/4
4	PCW	A	1108	-	-	3/8/8/57	-
4	PCW	D	1104	-	-	24/44/44/57	-
4	PCW	C	1104	-	-	2/8/8/57	-
4	PCW	B	1105	-	-	5/8/8/57	-
4	PCW	C	1102	-	-	19/43/43/57	-
4	PCW	E	201	-	-	4/8/8/57	-
4	PCW	F	202	-	-	25/46/46/57	-
4	PCW	B	1102	-	-	28/46/46/57	-
4	PCW	D	1102	-	-	29/46/46/57	-
6	AJP	A	1106	-	12/12/18/38	0/6/117/220	0/7/7/11
4	PCW	B	1103	-	-	18/34/34/57	-
4	PCW	C	1107	-	-	25/54/54/57	-
3	ZK1	C	1101	-	-	5/13/23/23	0/3/3/3
4	PCW	B	1104	-	-	23/44/44/57	-
4	PCW	A	1107	-	-	26/54/54/57	-
4	PCW	C	1110	-	-	4/8/8/57	-
7	SPD	A	1111	-	-	3/7/7/7	-
4	PCW	D	1105	-	-	5/8/8/57	-
5	CLR	A	1105	-	2/2/10/11	6/10/68/68	0/4/4/4
4	PCW	F	201	-	-	4/8/8/57	-
4	PCW	E	202	-	-	24/46/46/57	-
4	PCW	C	1108	-	-	3/8/8/57	-
4	PCW	A	1109	-	-	27/42/42/57	-
6	AJP	C	1106	-	12/12/18/38	0/6/117/220	0/7/7/11
4	PCW	A	1102	-	-	18/43/43/57	-
3	ZK1	D	1101	-	-	5/13/23/23	0/3/3/3
4	PCW	A	1104	-	-	1/8/8/57	-
3	ZK1	B	1101	-	-	4/13/23/23	0/3/3/3
4	PCW	D	1103	-	-	18/34/34/57	-
4	PCW	A	1110	-	-	5/8/8/57	-

The worst 5 of 221 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	1106	AJP	O78-C27	-54.22	0.08	1.43
6	A	1106	AJP	O78-C27	-51.45	0.15	1.43
6	A	1106	AJP	O25-C23	-51.28	0.49	1.44
6	C	1106	AJP	O25-C23	-51.06	0.50	1.44
6	C	1106	AJP	C07-C08	41.66	2.22	1.53

The worst 5 of 216 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	1105	CLR	C18-C13-C17	-12.88	88.31	111.68
5	C	1105	CLR	C18-C13-C17	-11.67	90.52	111.68
6	A	1106	AJP	C04-C05-C06	10.38	134.46	115.66
6	C	1106	AJP	C04-C05-C06	10.25	134.22	115.66
6	A	1106	AJP	O78-C27-C28	9.43	129.29	110.05

5 of 28 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	1105	CLR	C9
5	A	1105	CLR	C17
5	C	1105	CLR	C9
5	C	1105	CLR	C17
6	A	1106	AJP	C05

5 of 460 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1102	PCW	C32-C31-O2-C2
4	A	1102	PCW	C4-O4P-P-O1P
4	A	1102	PCW	C4-O4P-P-O3P
4	A	1103	PCW	C1-O3P-P-O1P
4	A	1103	PCW	C1-O3P-P-O2P

There are no ring outliers.

17 monomers are involved in 101 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1103	PCW	4	0
4	C	1103	PCW	3	0
4	C	1109	PCW	1	0
5	C	1105	CLR	3	0
4	B	1102	PCW	3	0

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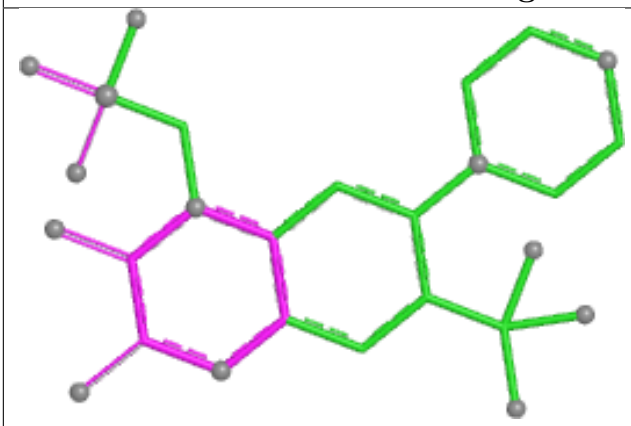
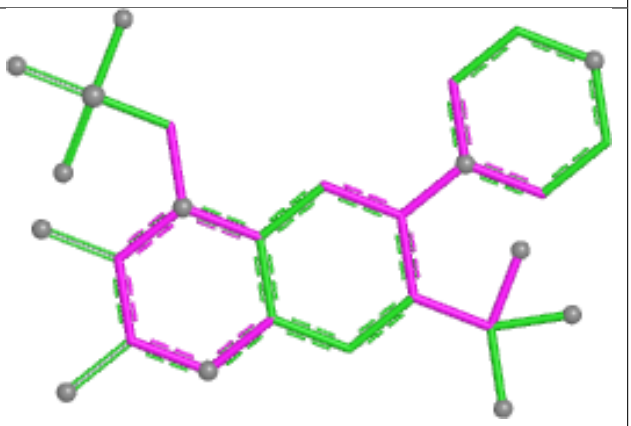
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1102	PCW	3	0
6	A	1106	AJP	33	0
4	C	1107	PCW	1	0
3	C	1101	ZK1	1	0
4	A	1107	PCW	1	0
7	A	1111	SPD	2	0
5	A	1105	CLR	4	0
4	E	202	PCW	2	0
4	A	1109	PCW	2	0
6	C	1106	AJP	36	0
4	A	1104	PCW	1	0
4	D	1103	PCW	2	0

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 then 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.

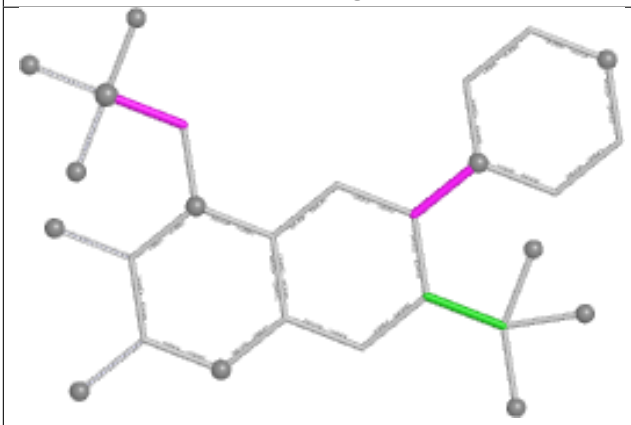
Ligand ZK1 A 1101



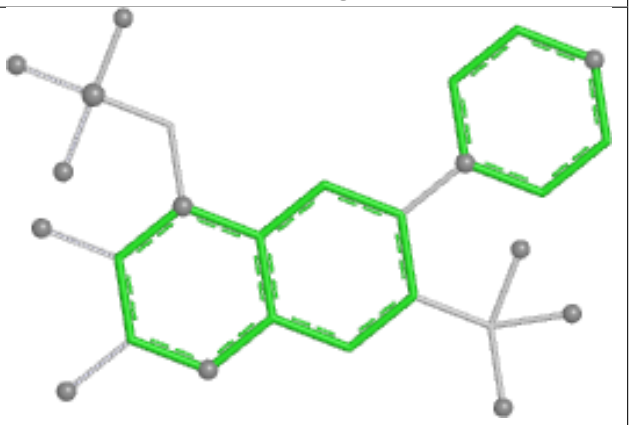
Bond lengths



Bond angles

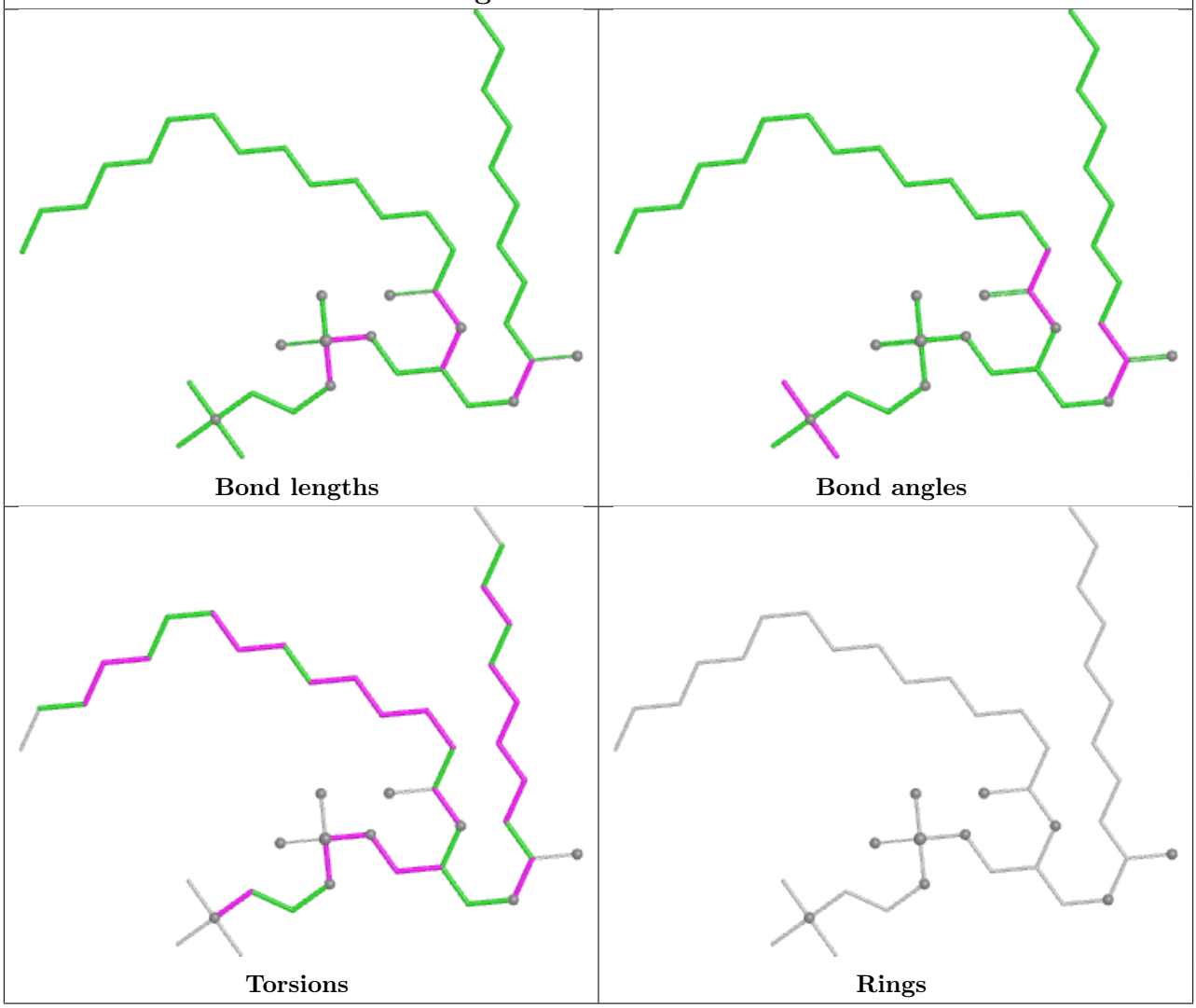


Torsions

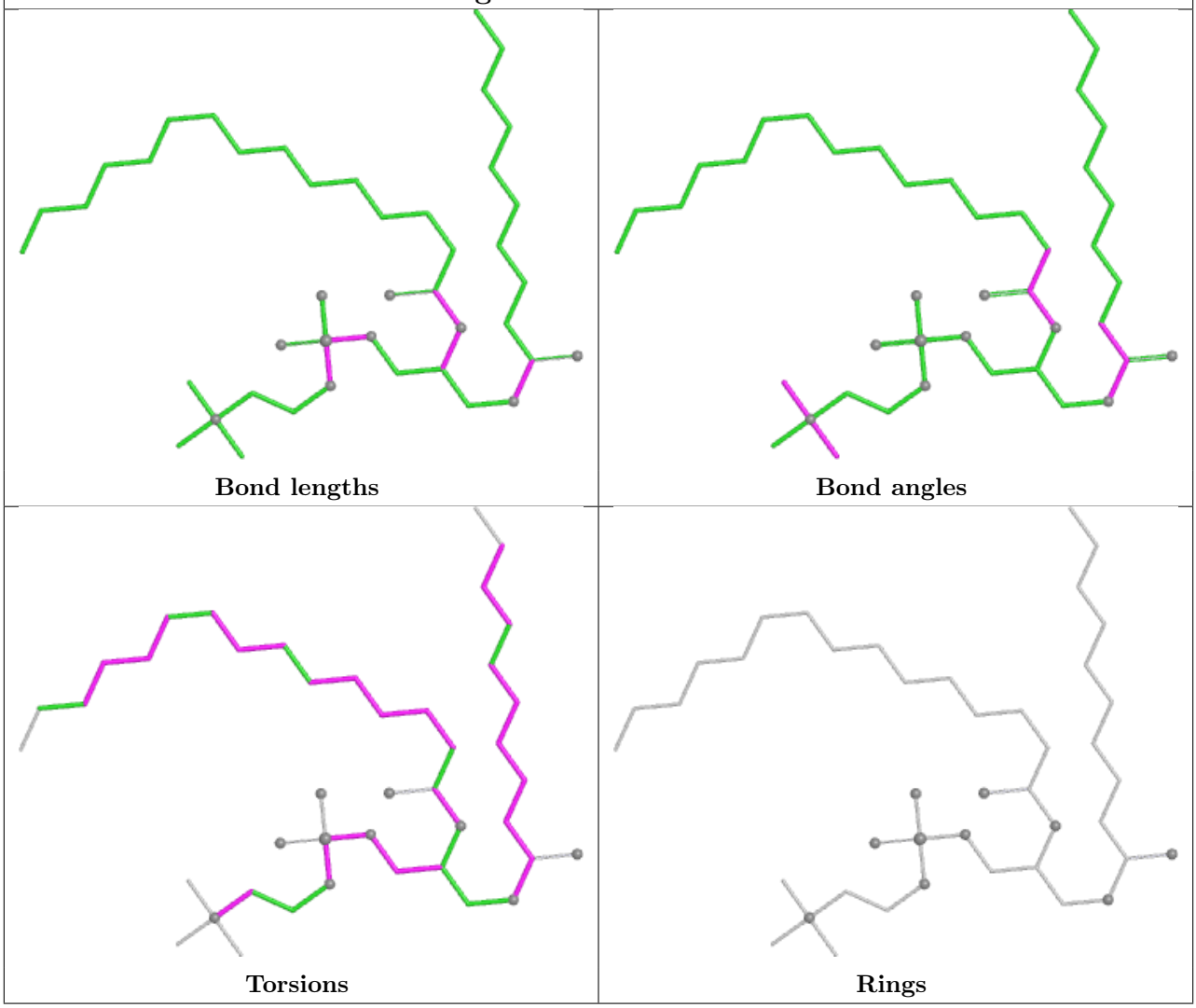


Rings

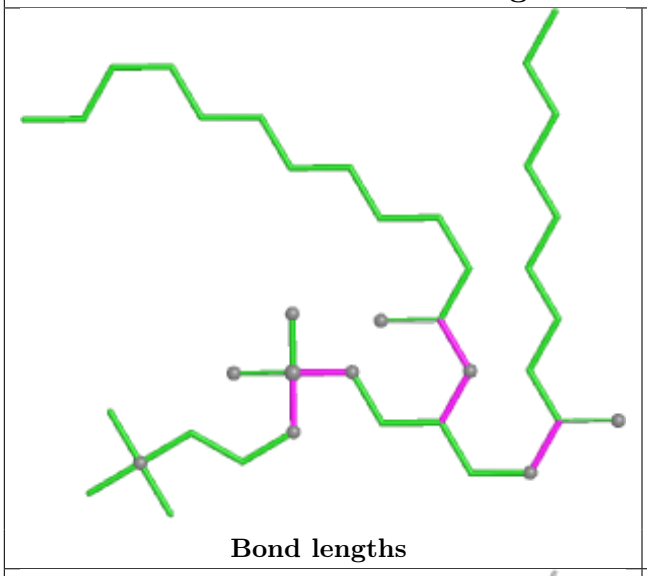
Ligand PCW A 1103



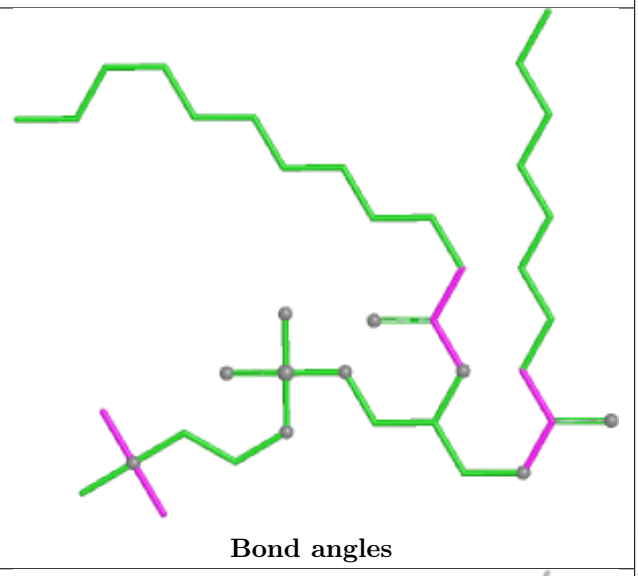
Ligand PCW C 1103



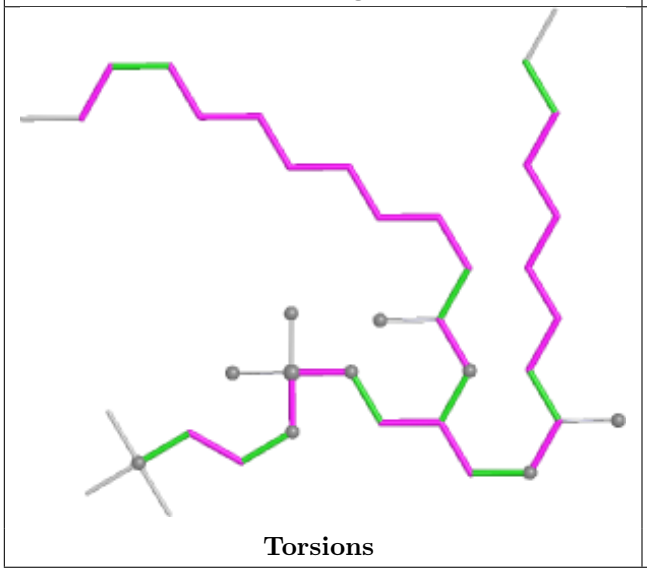
Ligand PCW C 1109



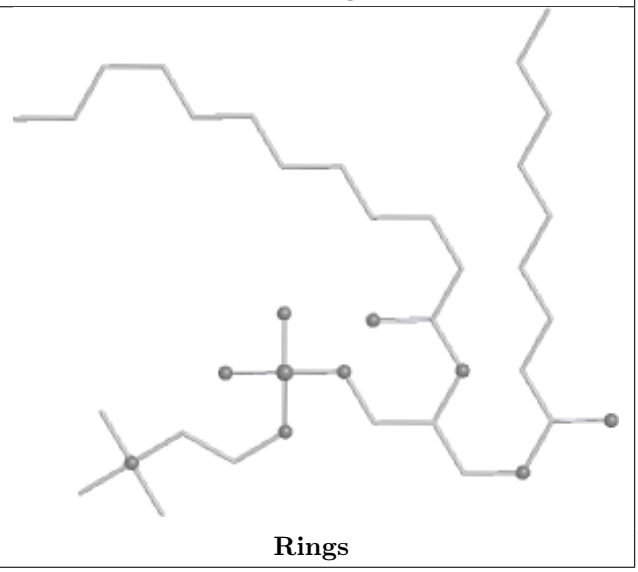
Bond lengths



Bond angles



Torsions



Rings

Ligand PCW A 1108

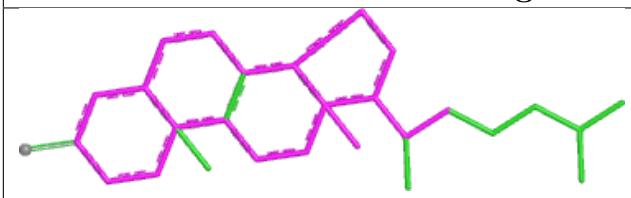
Bond lengths

Bond angles

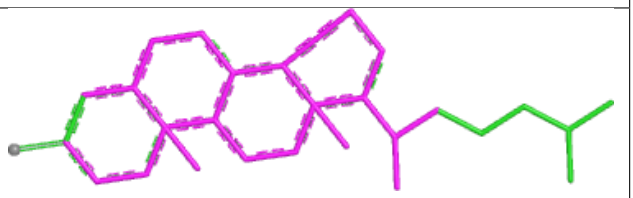
Torsions

Rings

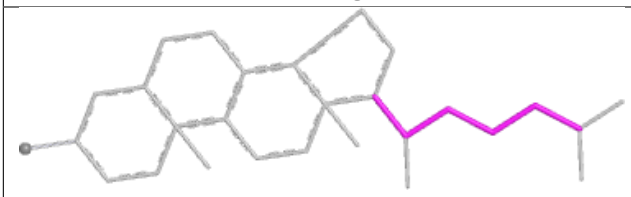
Ligand CLR C 1105



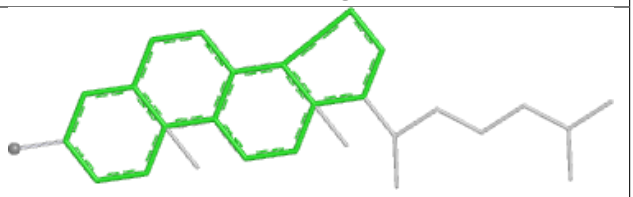
Bond lengths



Bond angles

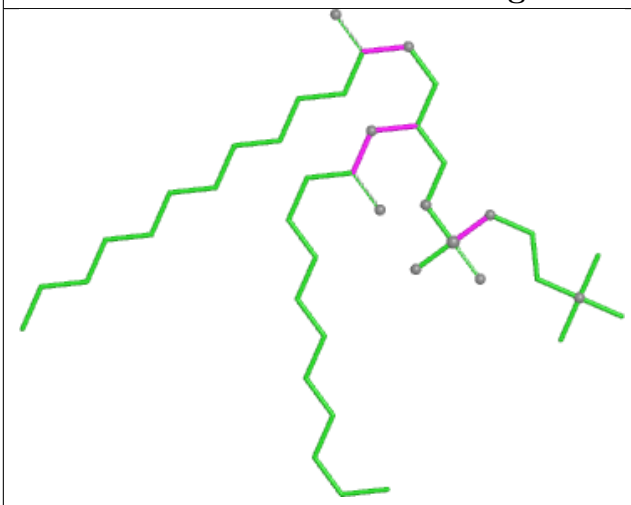


Torsions

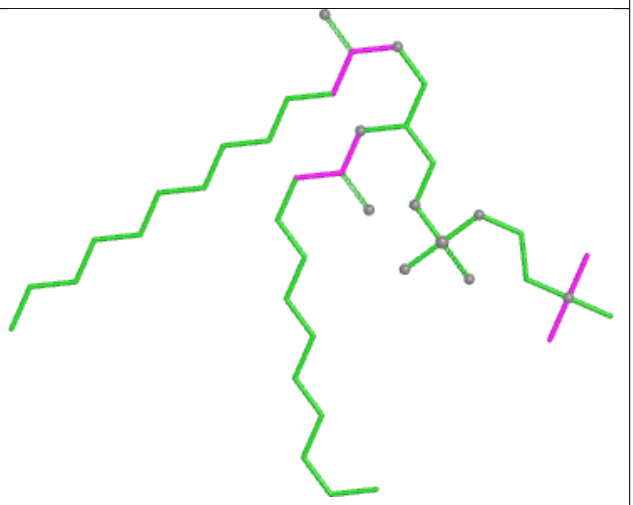


Rings

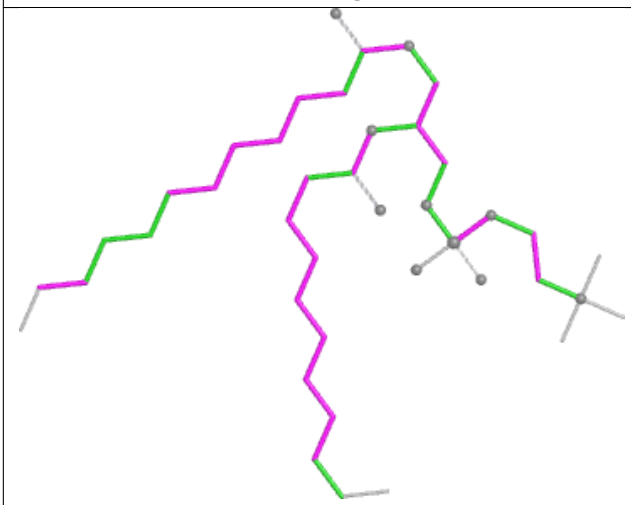
Ligand PCW D 1104



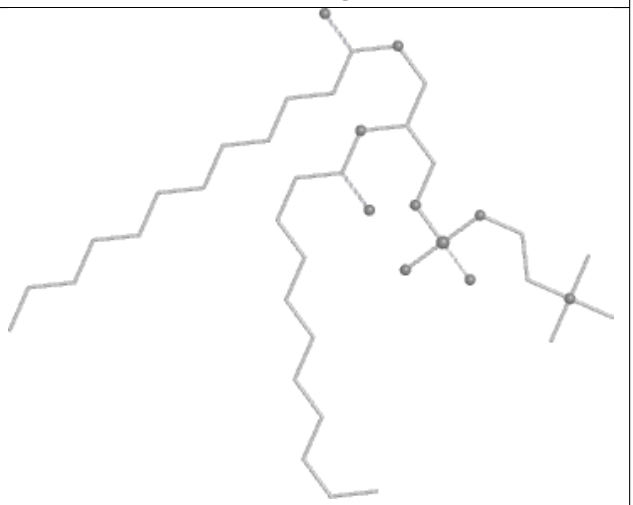
Bond lengths



Bond angles

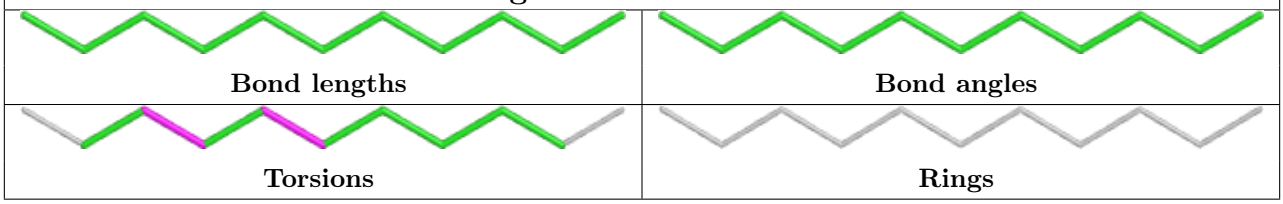


Torsions

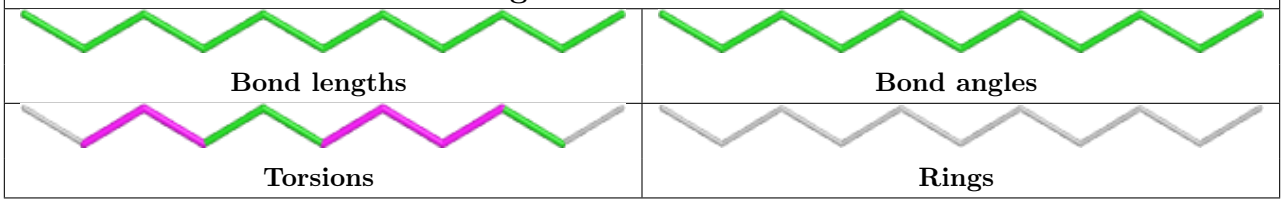


Rings

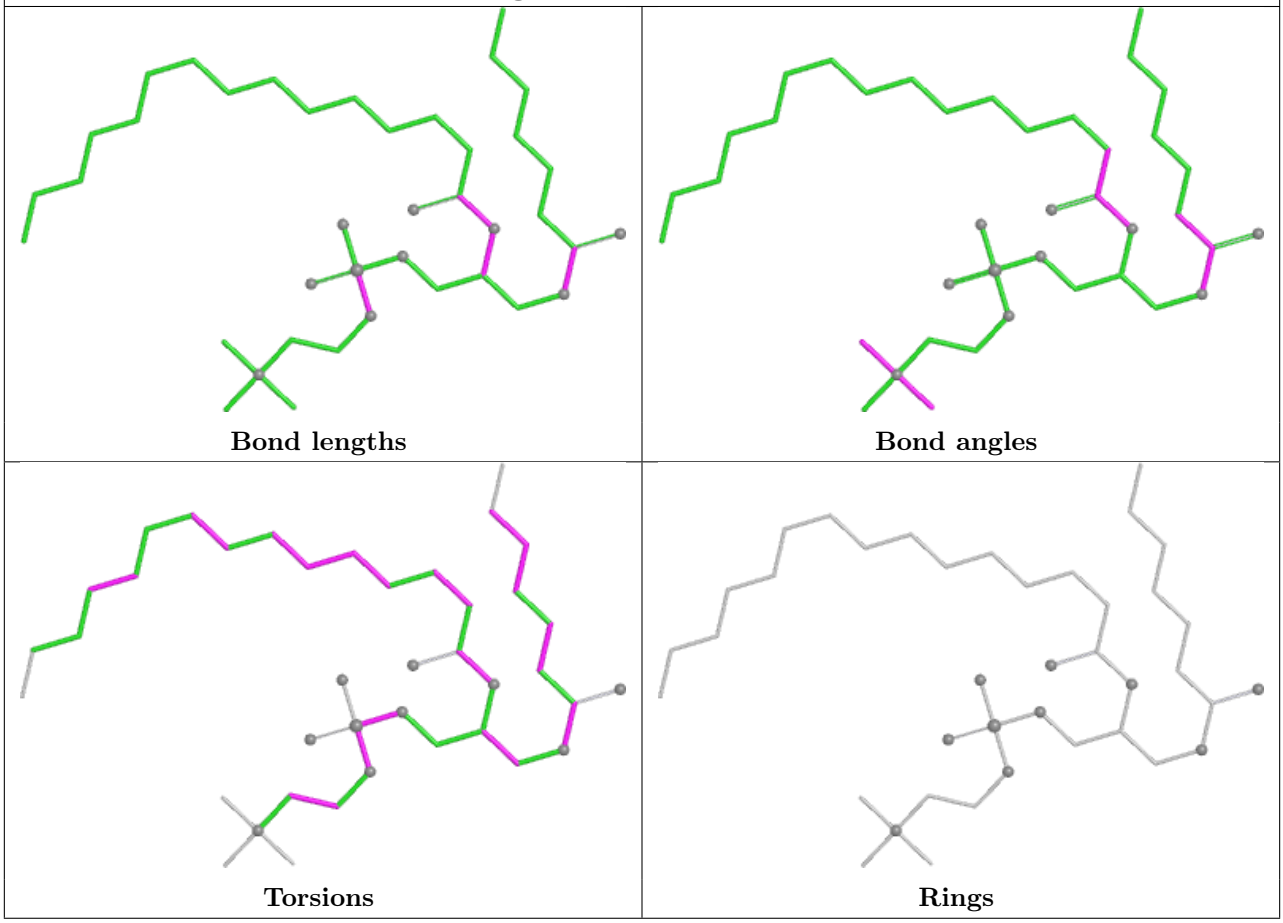
Ligand PCW C 1104



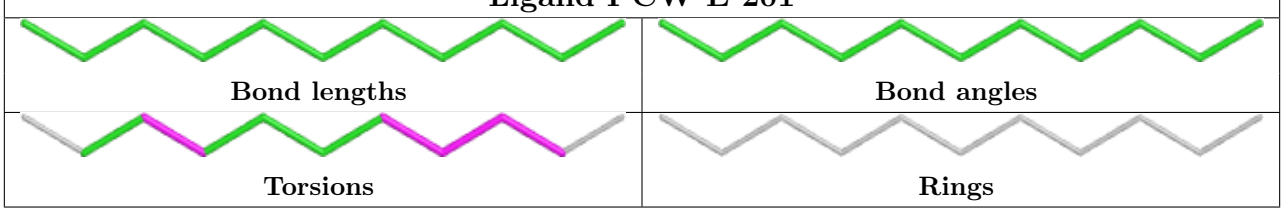
Ligand PCW B 1105



Ligand PCW C 1102

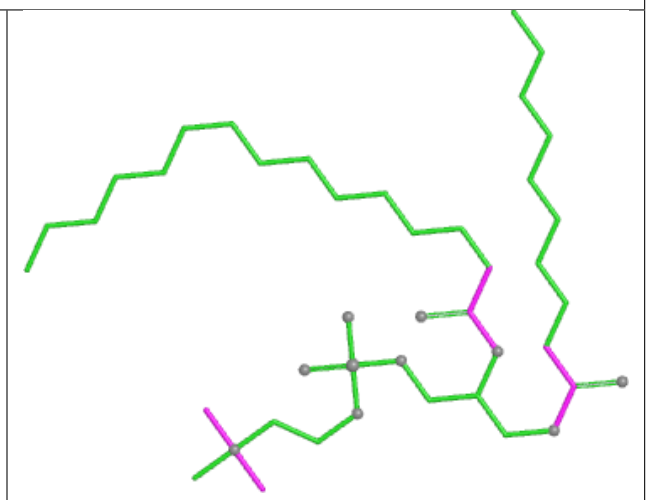


Ligand PCW E 201

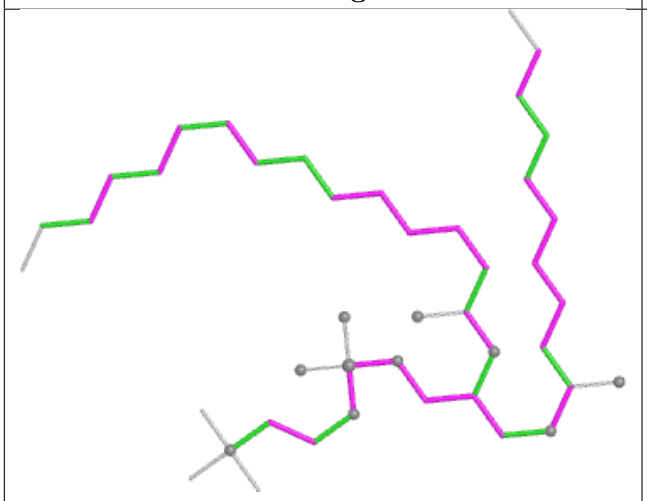


Ligand PCW F 202

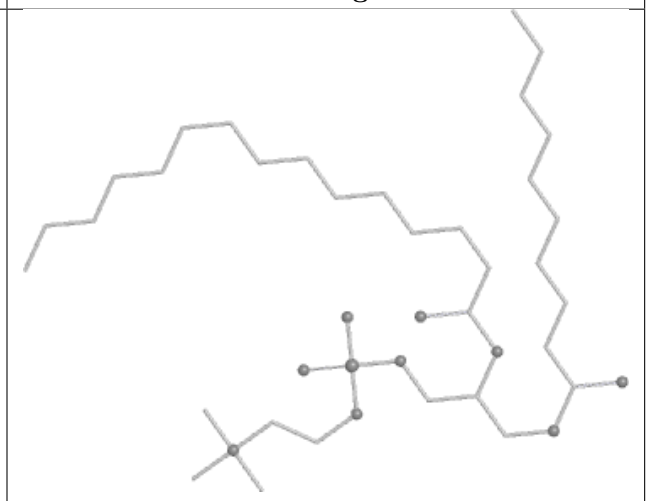
Bond lengths



Bond angles

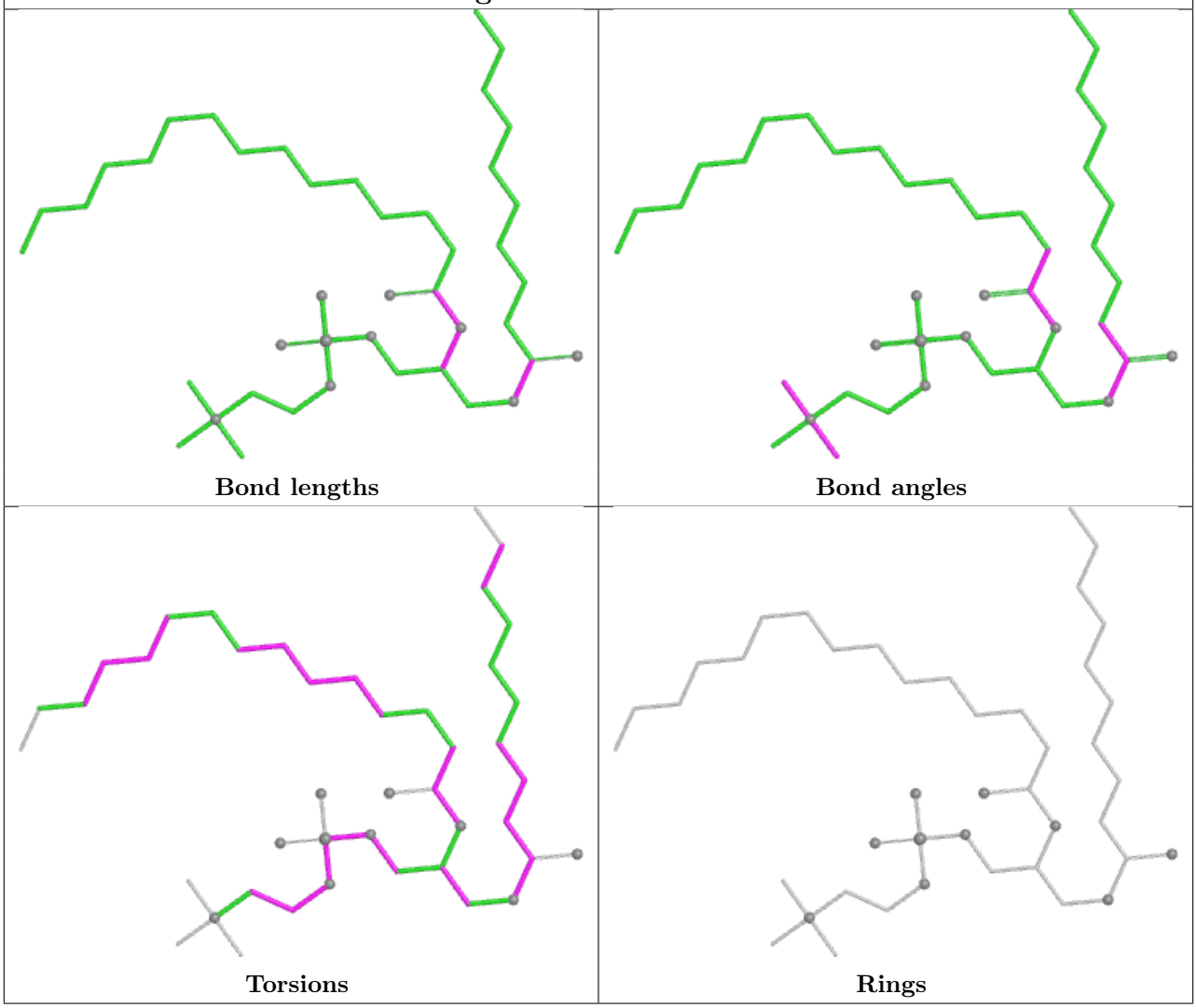


Torsions

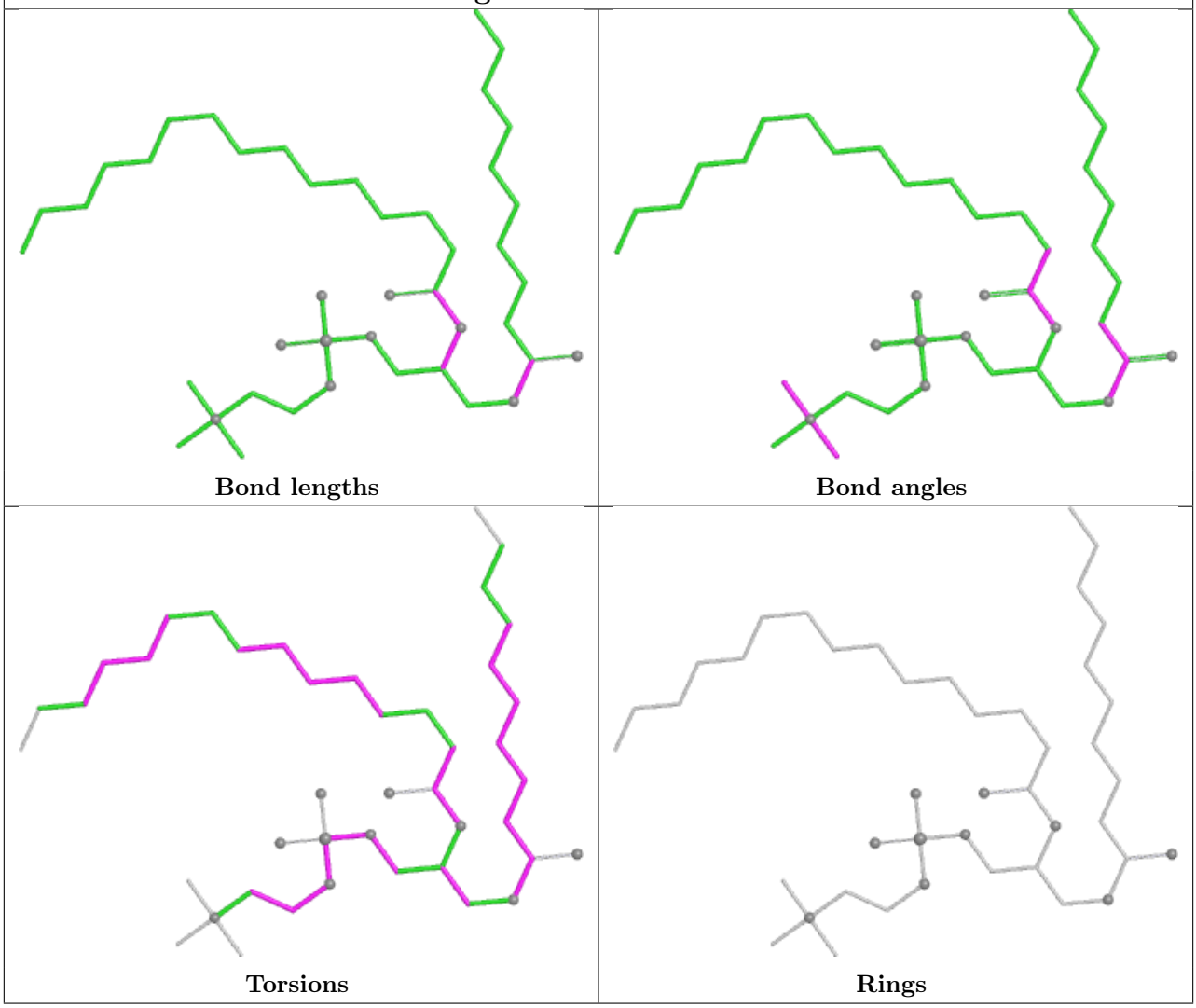


Rings

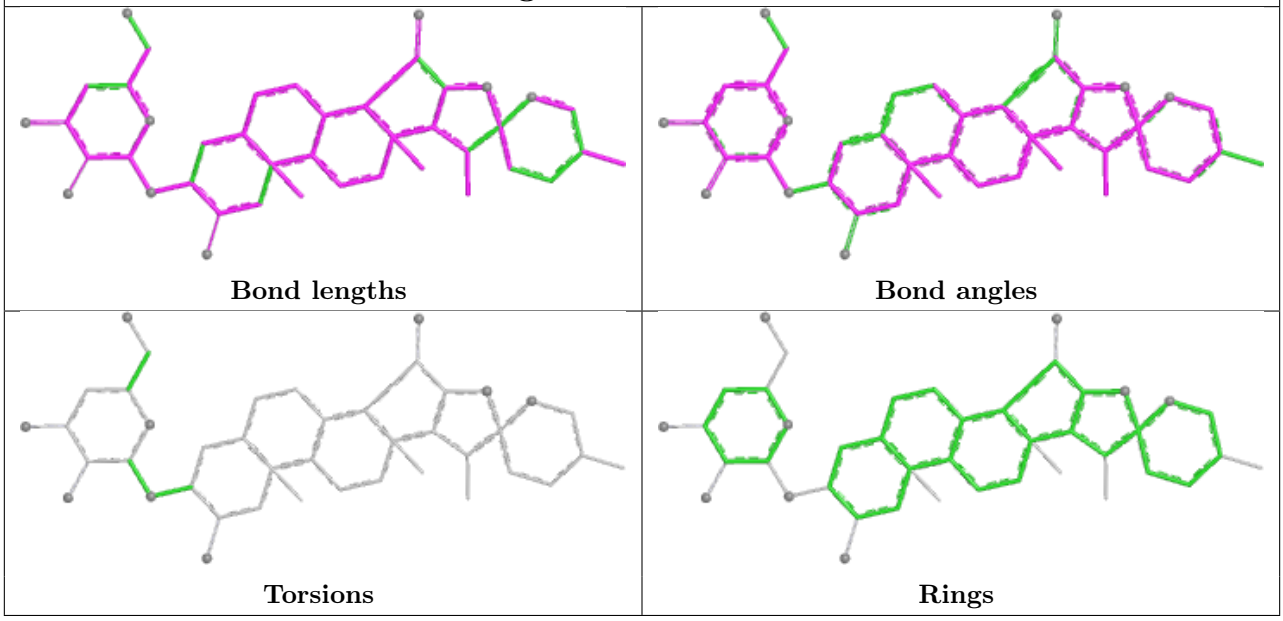
Ligand PCW B 1102



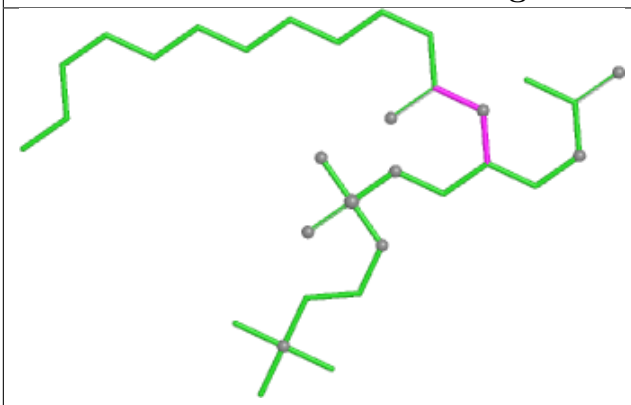
Ligand PCW D 1102



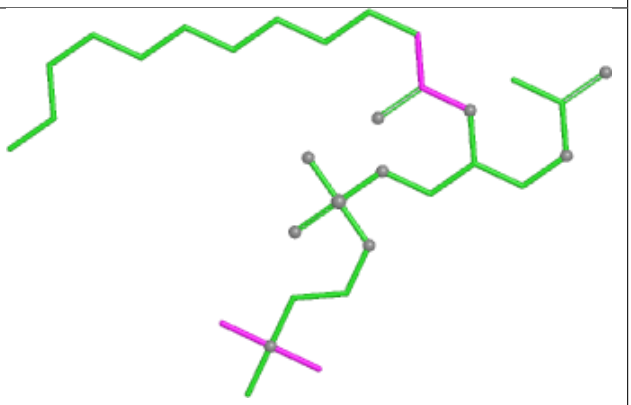
Ligand AJP A 1106



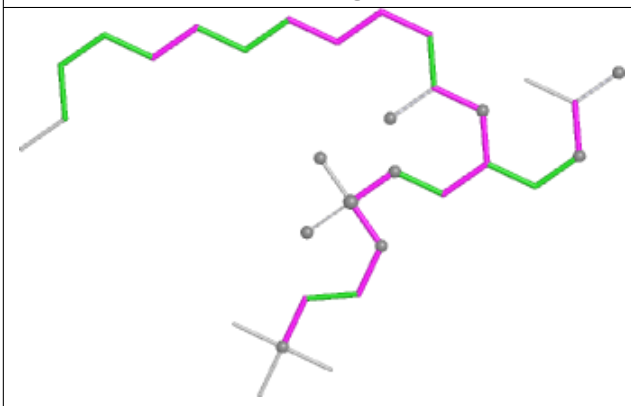
Ligand PCW B 1103



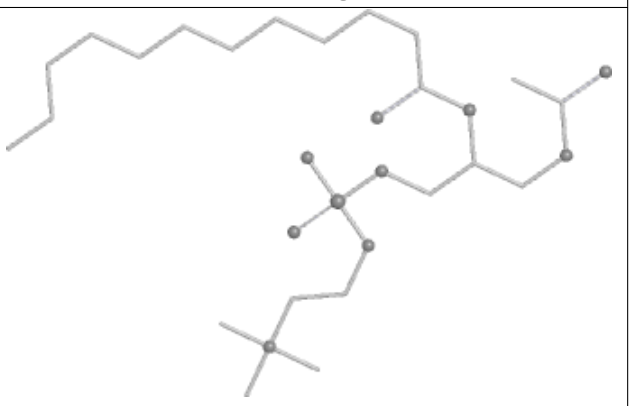
Bond lengths



Bond angles

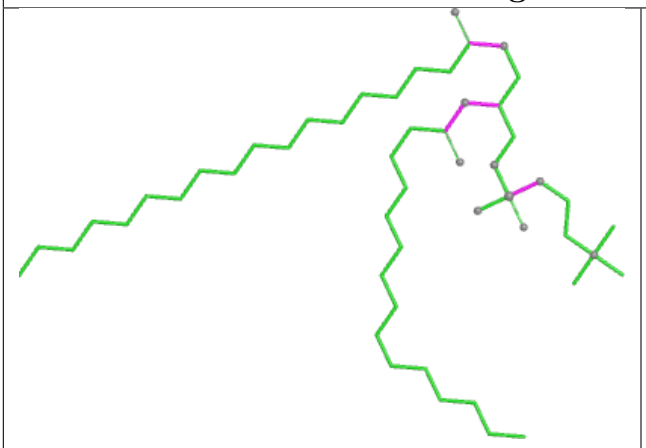


Torsions

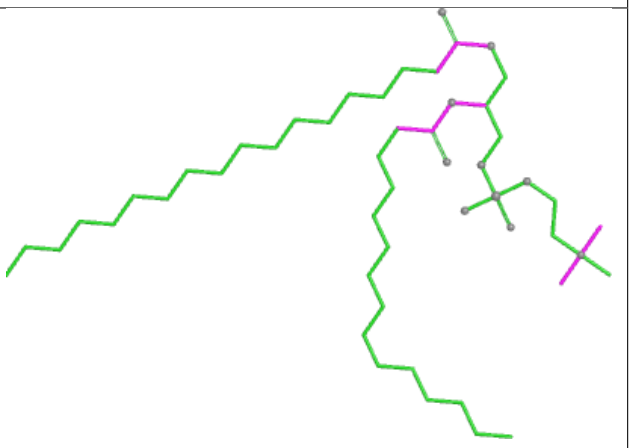


Rings

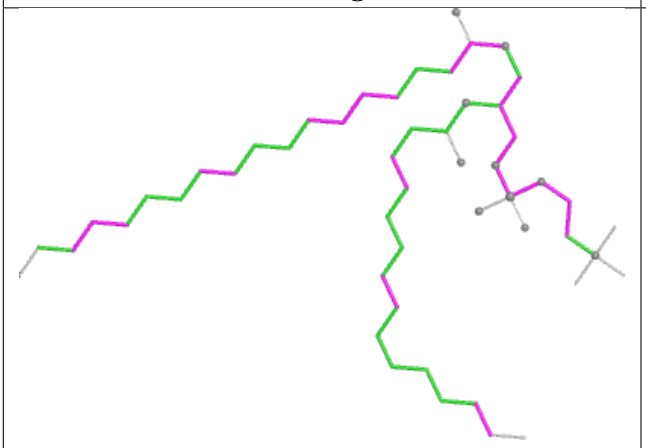
Ligand PCW C 1107



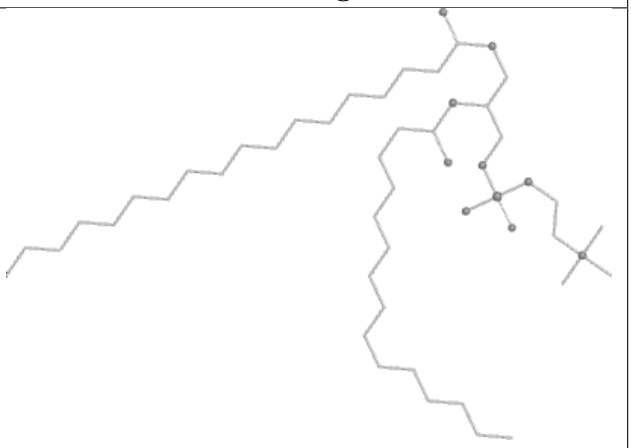
Bond lengths



Bond angles

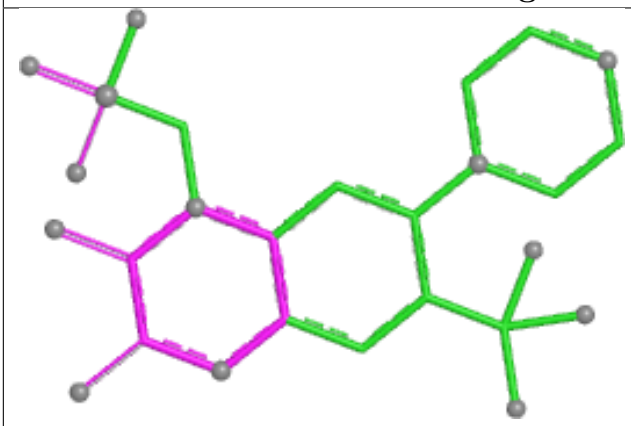


Torsions

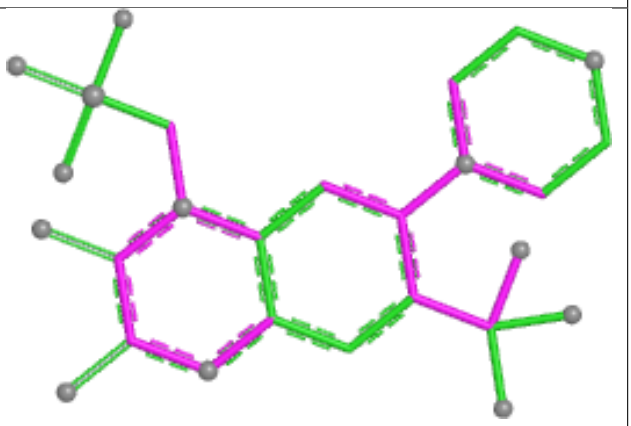


Rings

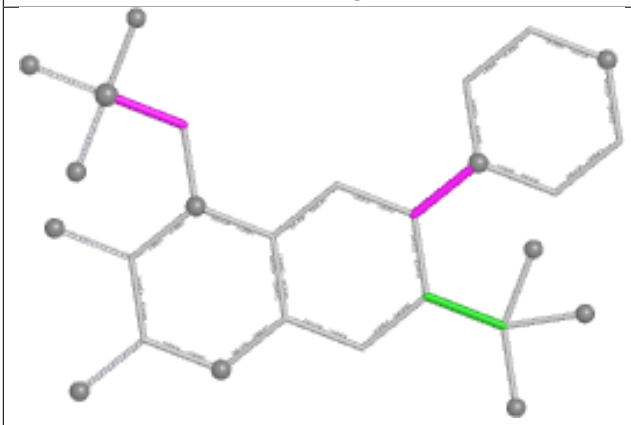
Ligand ZK1 C 1101



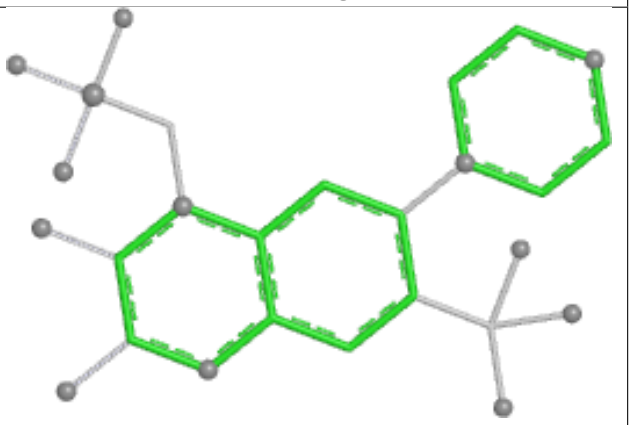
Bond lengths



Bond angles

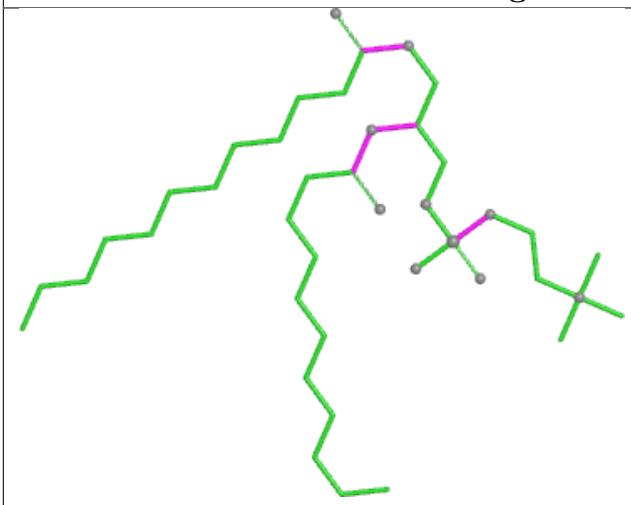


Torsions

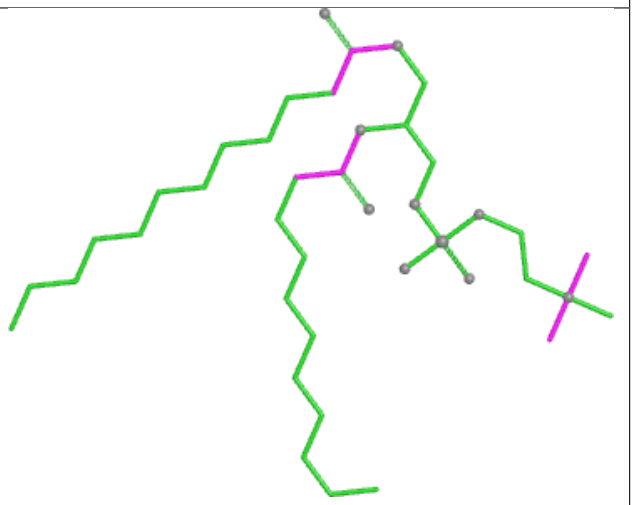


Rings

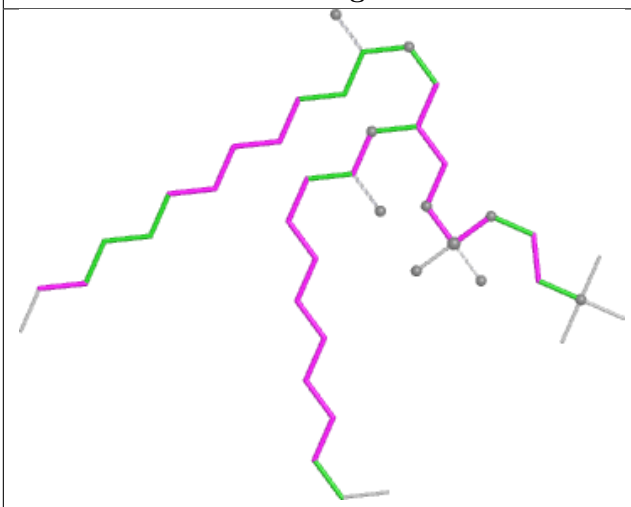
Ligand PCW B 1104



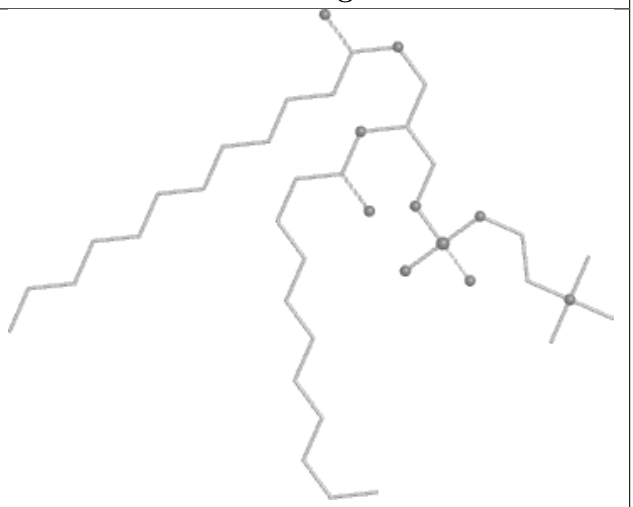
Bond lengths



Bond angles

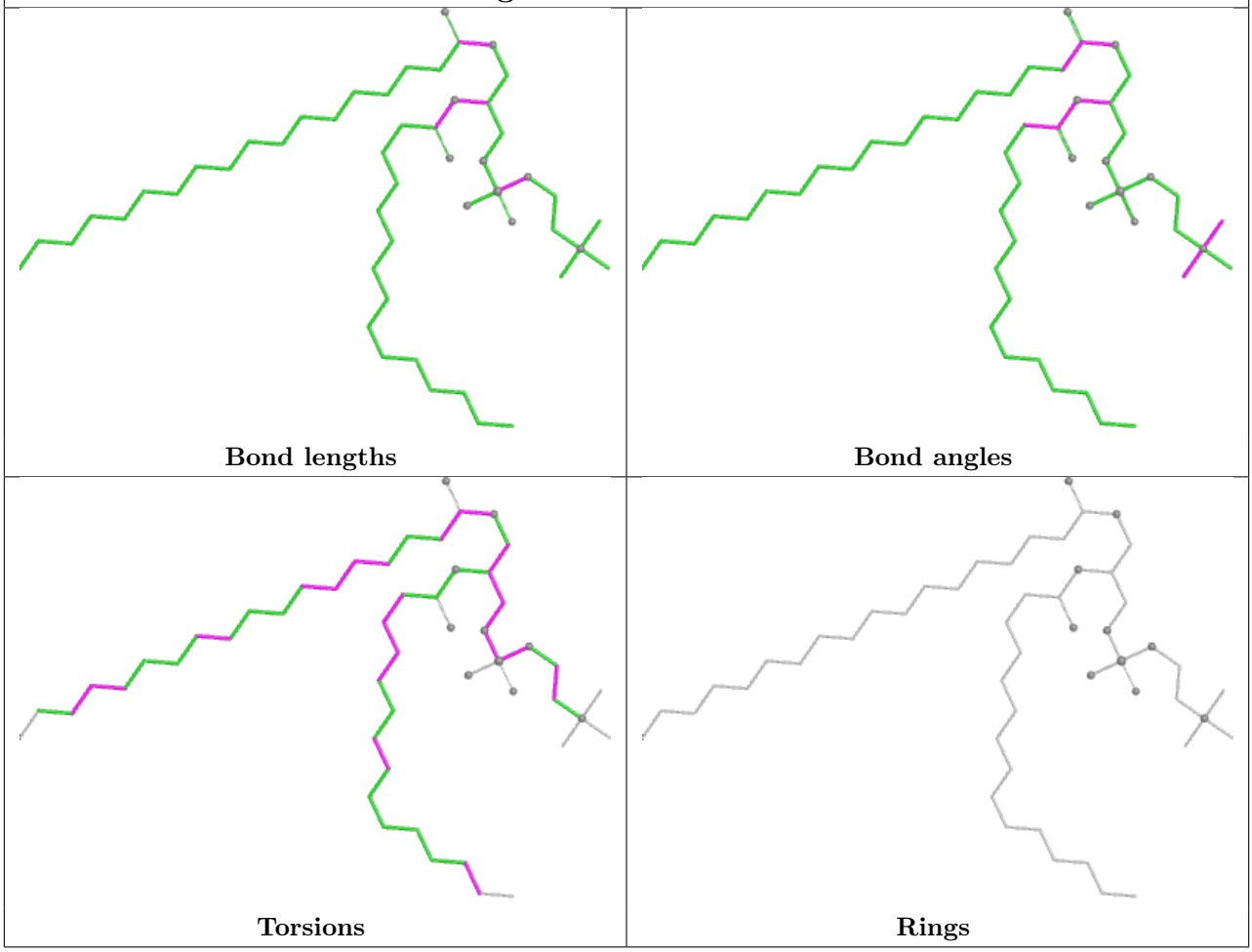


Torsions

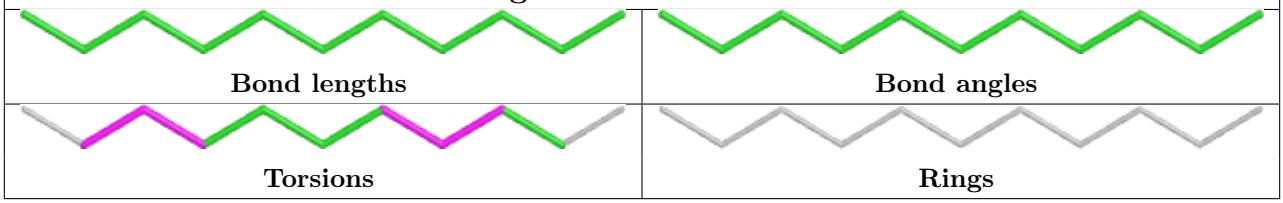


Rings

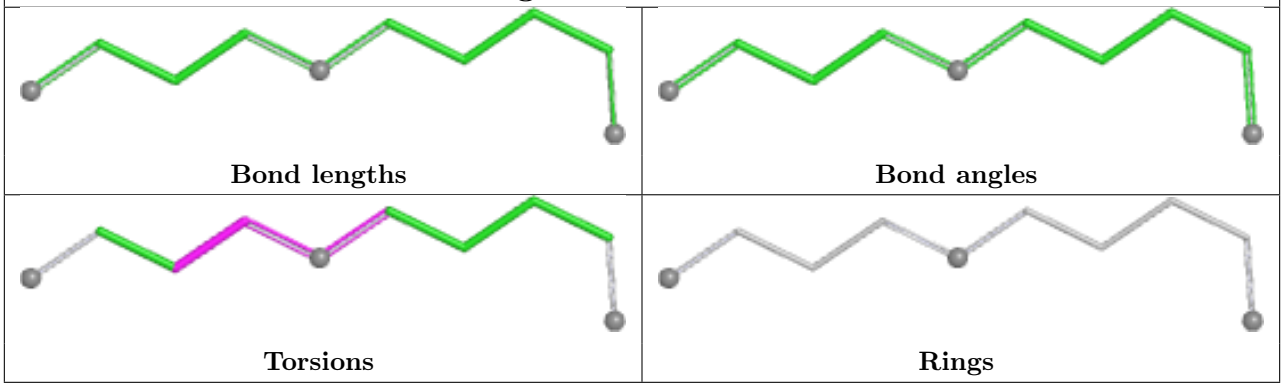
Ligand PCW A 1107

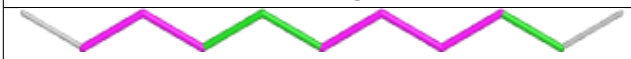


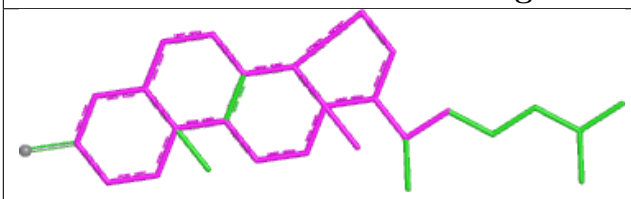
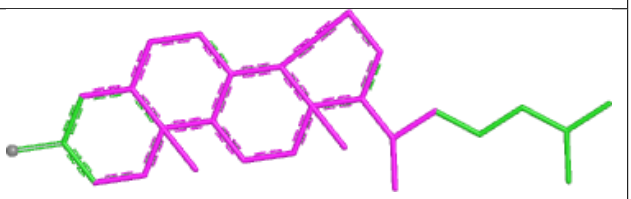
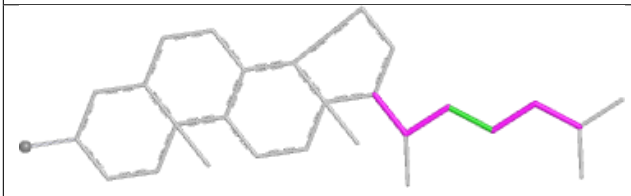
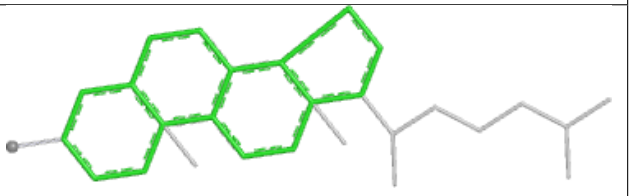
Ligand PCW C 1110



Ligand SPD A 1111



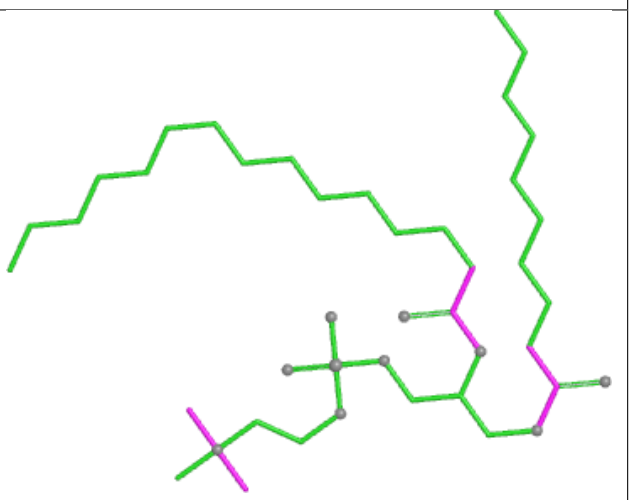
Ligand PCW D 1105	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLR A 1105	
	
Bond lengths	Bond angles
	
Torsions	Rings

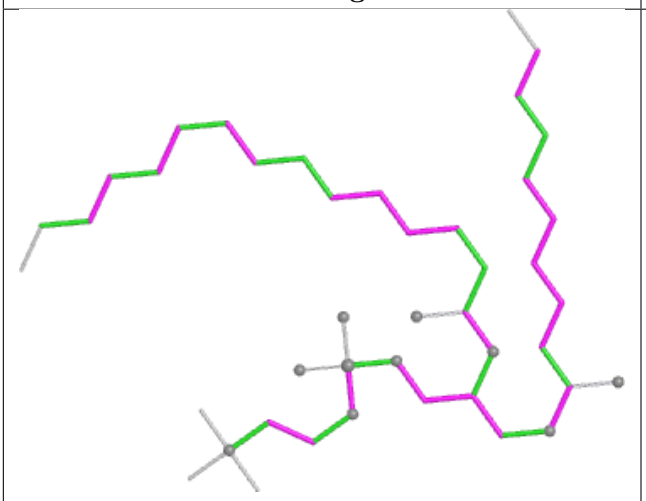
Ligand PCW F 201	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PCW E 202

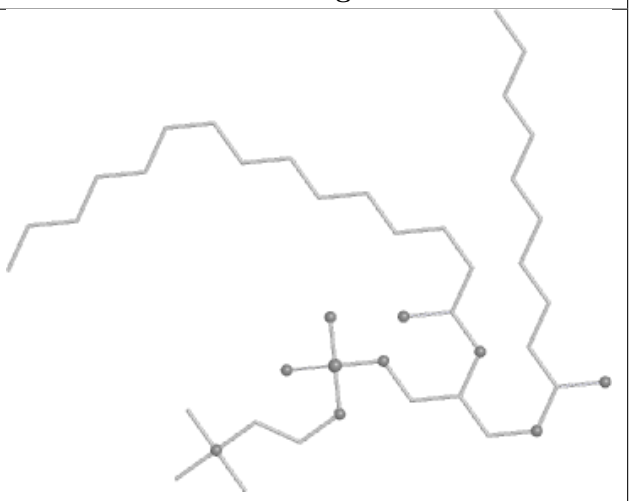
Bond lengths



Bond angles

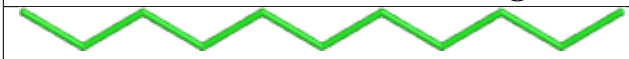


Torsions

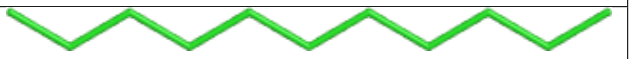


Rings

Ligand PCW C 1108



Bond lengths

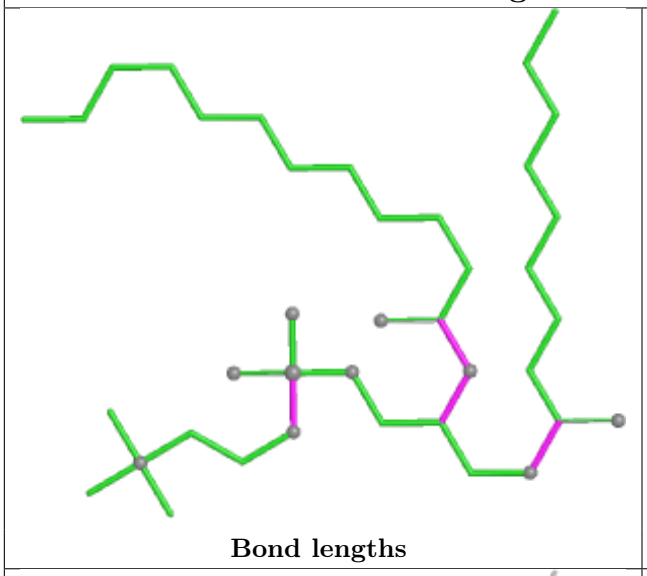


Bond angles

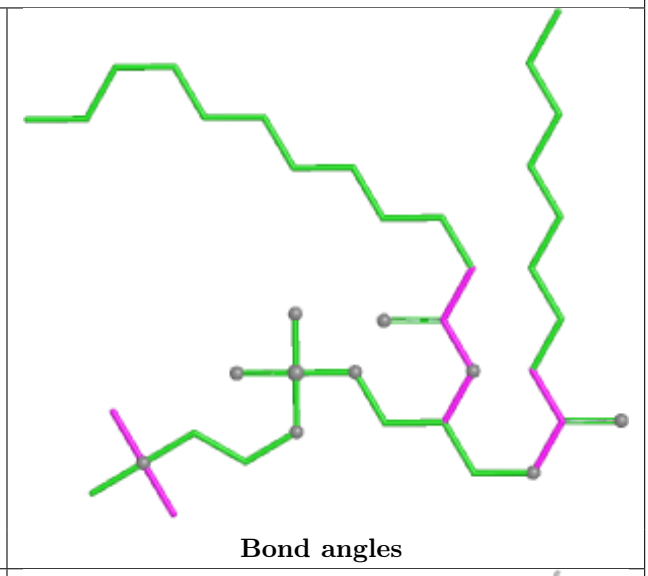
Torsions

Rings

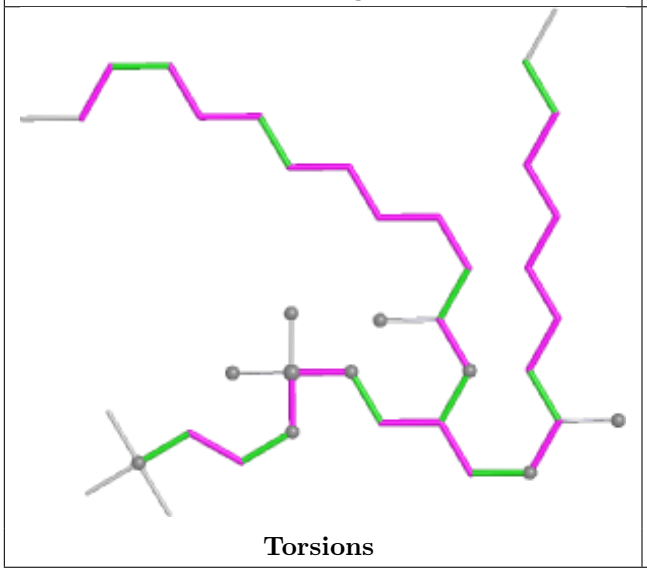
Ligand PCW A 1109



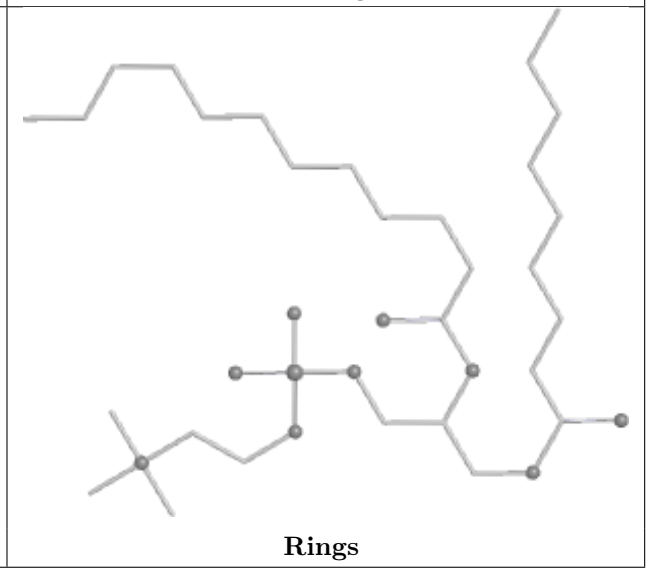
Bond lengths



Bond angles

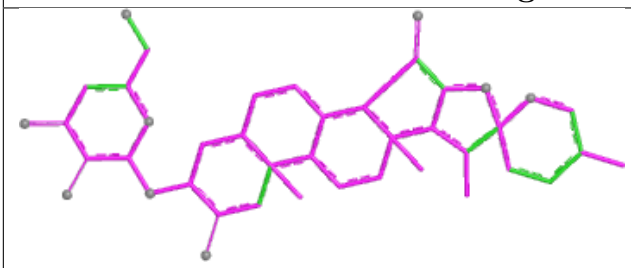


Torsions

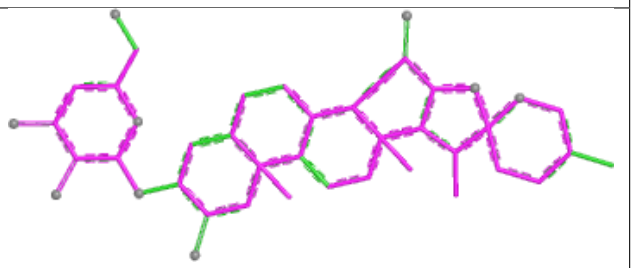


Rings

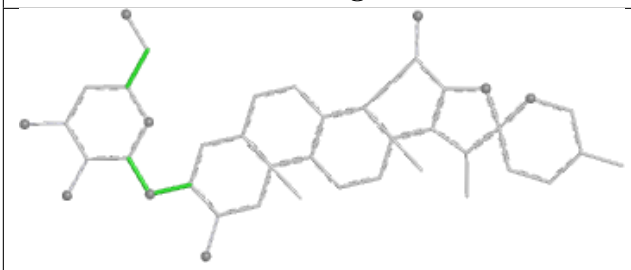
Ligand AJP C 1106



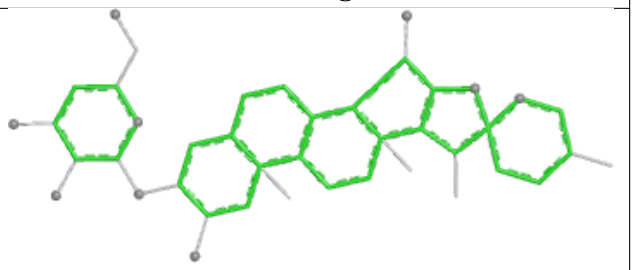
Bond lengths



Bond angles

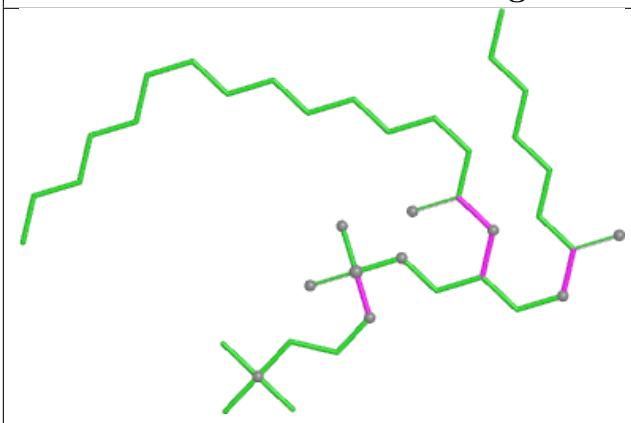


Torsions

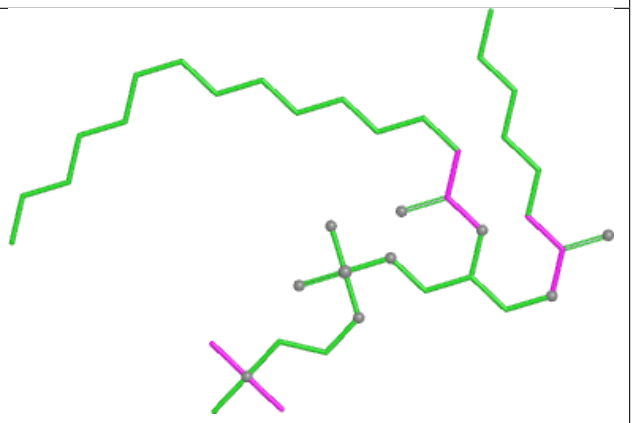


Rings

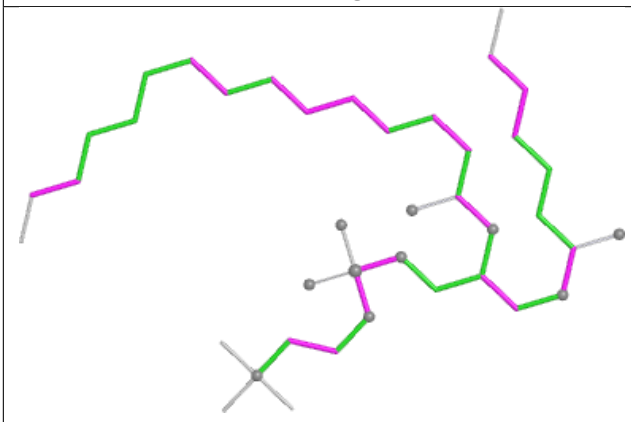
Ligand PCW A 1102



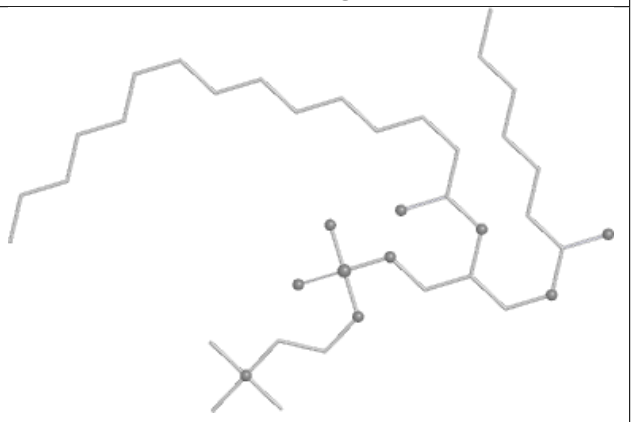
Bond lengths



Bond angles

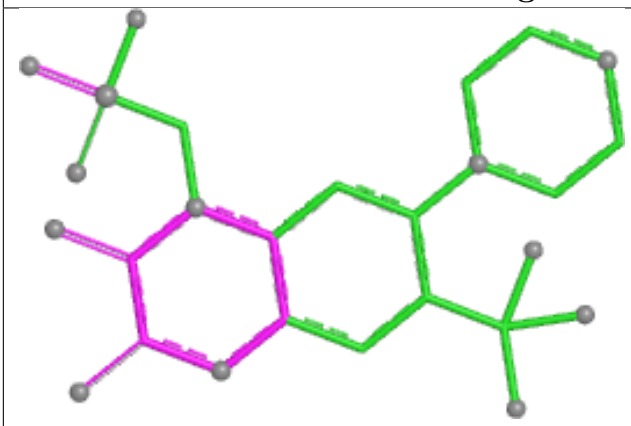


Torsions

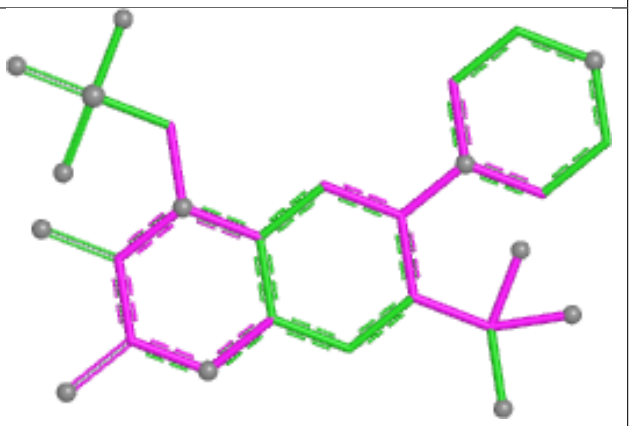


Rings

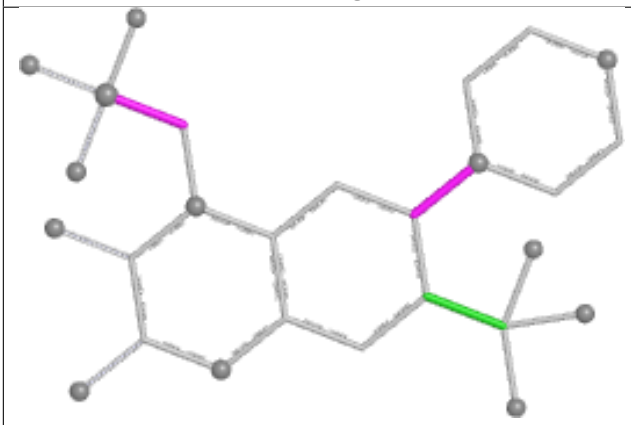
Ligand ZK1 D 1101



Bond lengths



Bond angles



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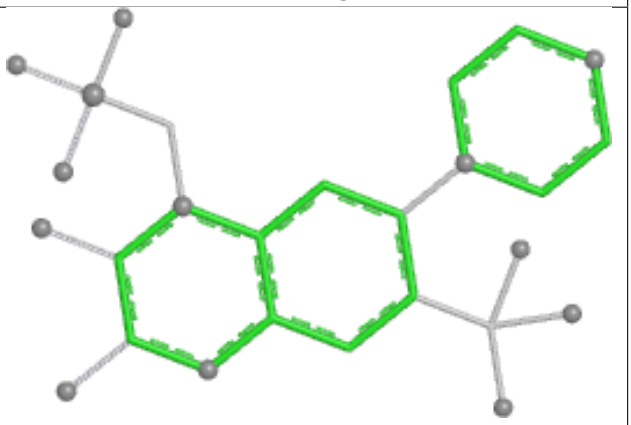
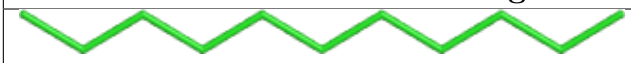


Rings

Ligand PCW A 1104



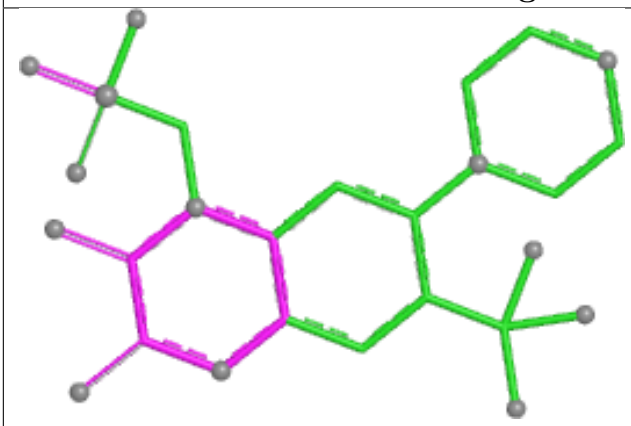
Bond lengths

Bond angles

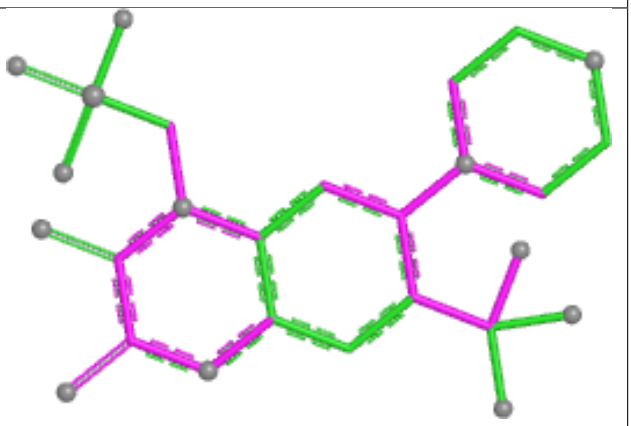
Torsions

Rings

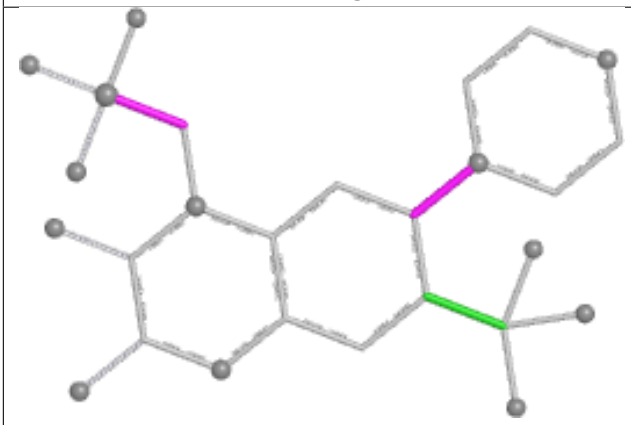
Ligand ZK1 B 1101



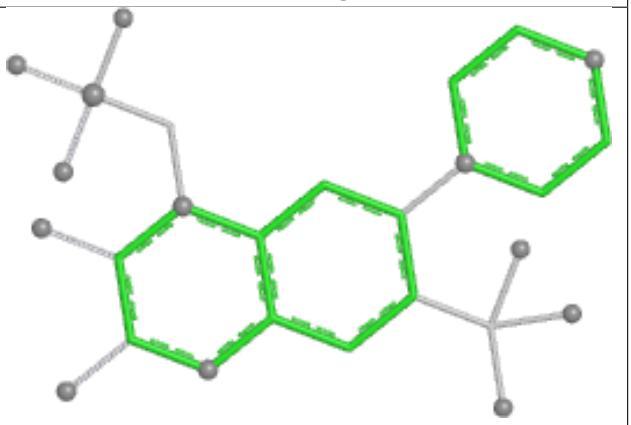
Bond lengths



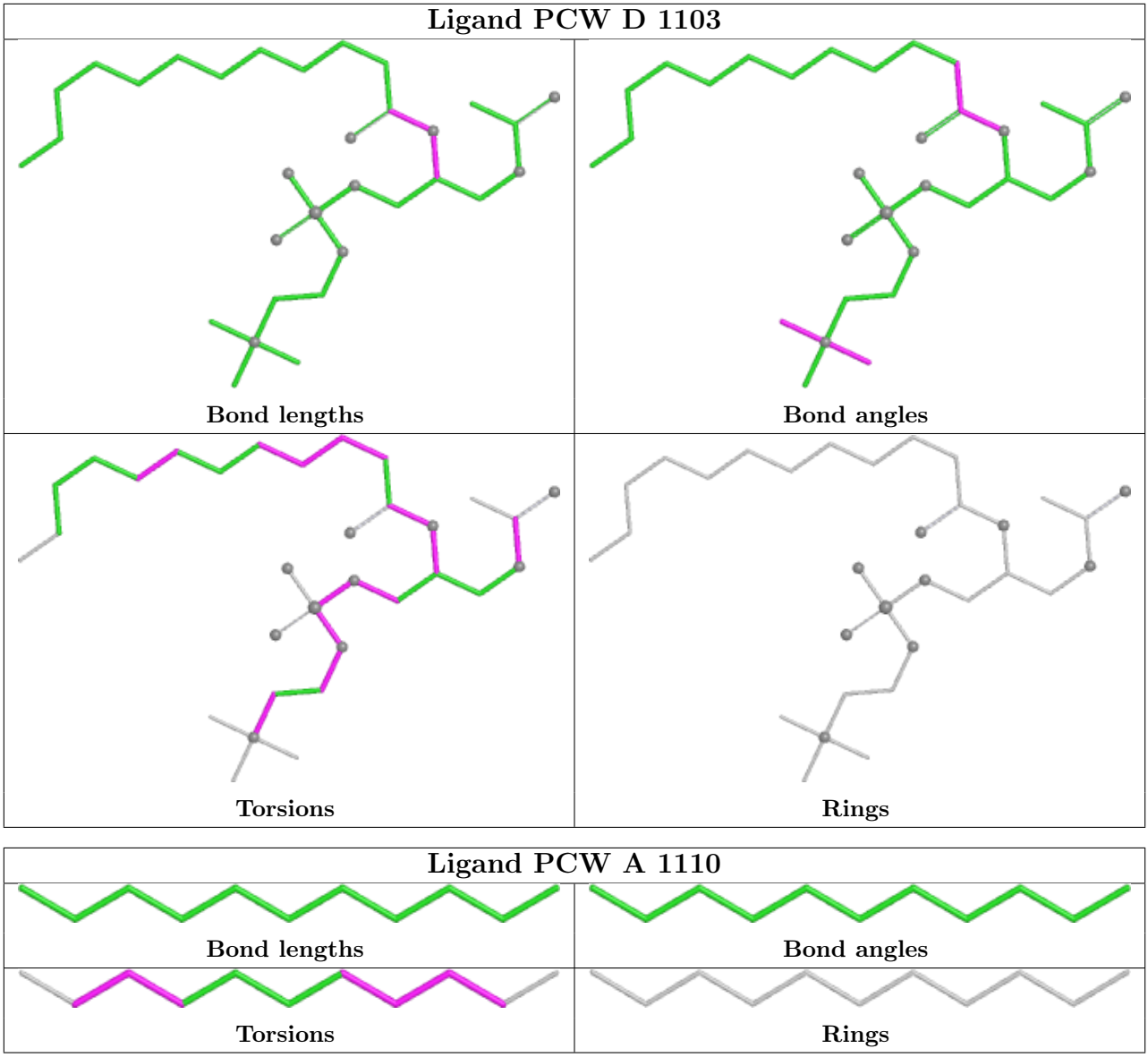
Bond angles



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.

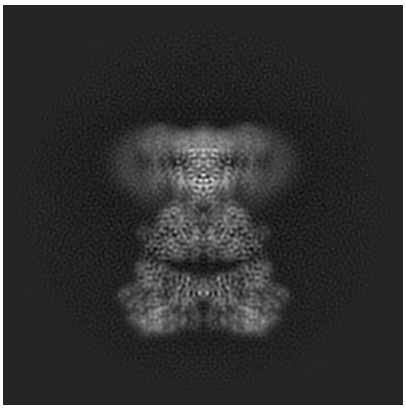
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-40741. These allow visual inspection of the internal detail of the map and identification of artifacts.

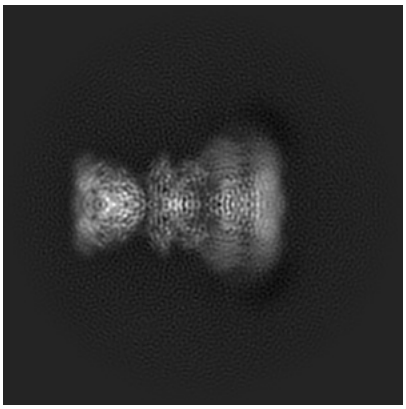
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

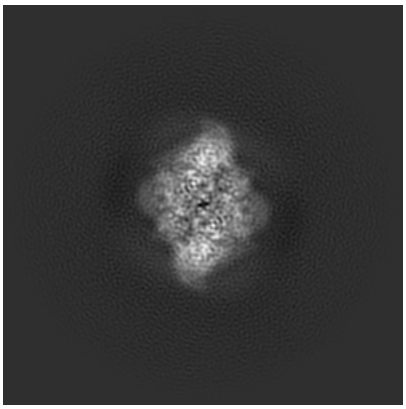
6.1.1 Primary map



X

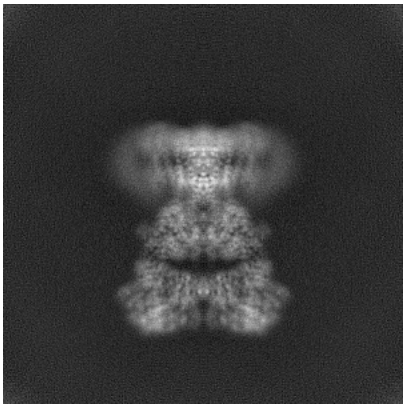


Y

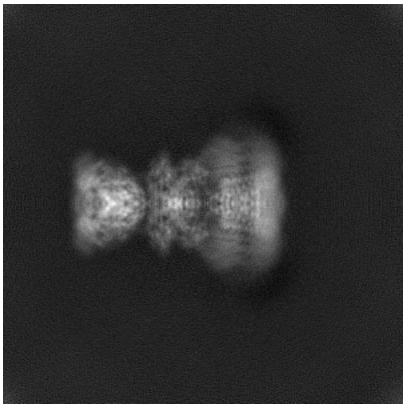


Z

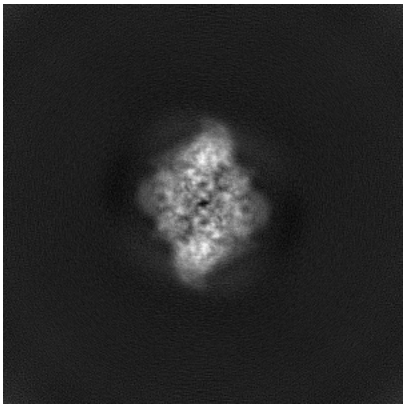
6.1.2 Raw map



X



Y

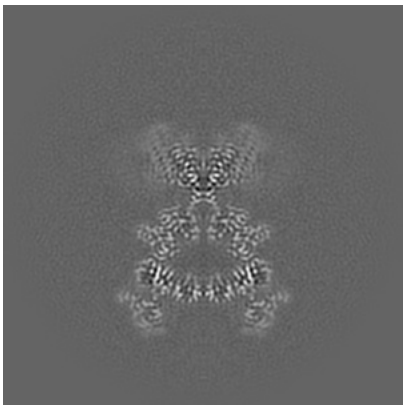


Z

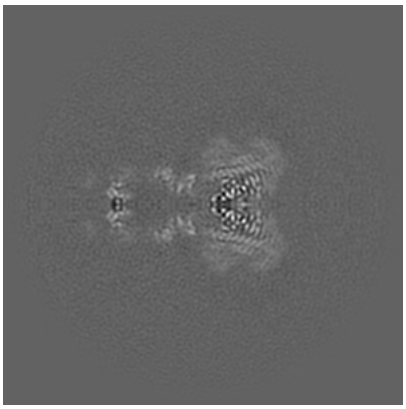
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

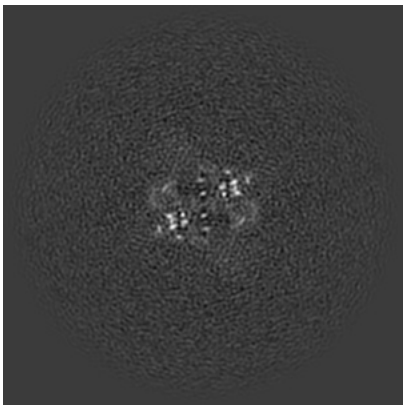
6.2.1 Primary map



X Index: 208

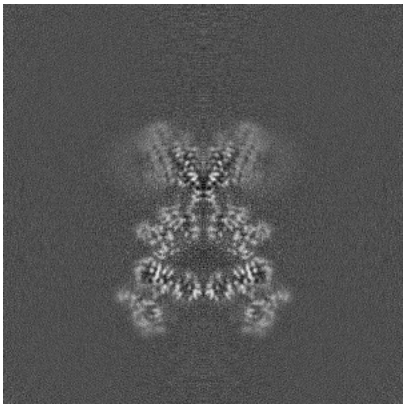


Y Index: 208

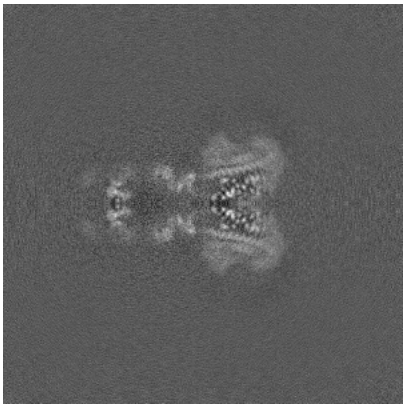


Z Index: 208

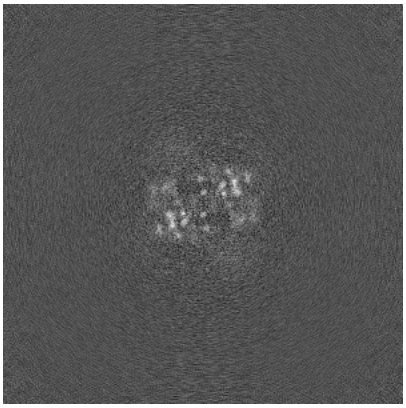
6.2.2 Raw map



X Index: 208



Y Index: 208

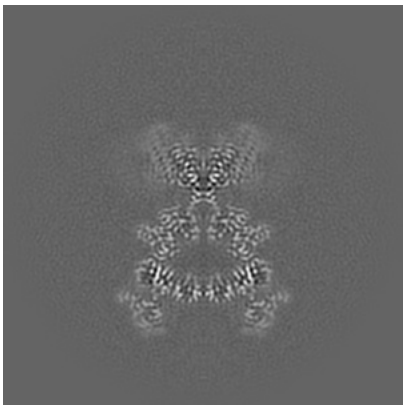


Z Index: 208

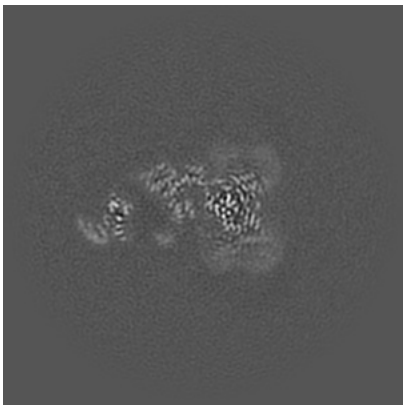
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

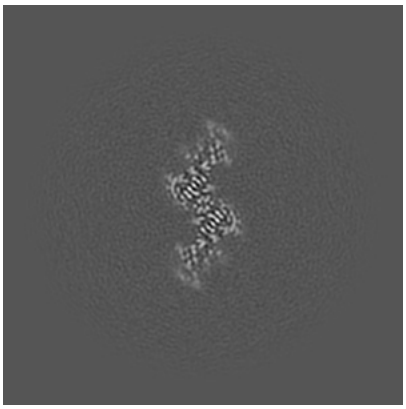
6.3.1 Primary map



X Index: 208

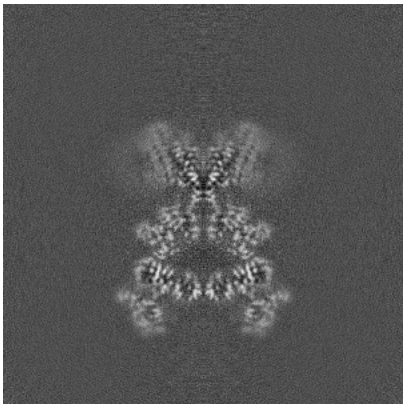


Y Index: 217

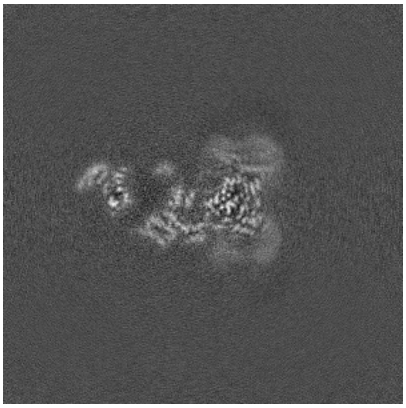


Z Index: 121

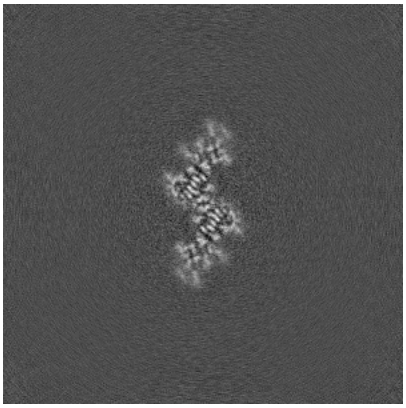
6.3.2 Raw map



X Index: 208



Y Index: 199

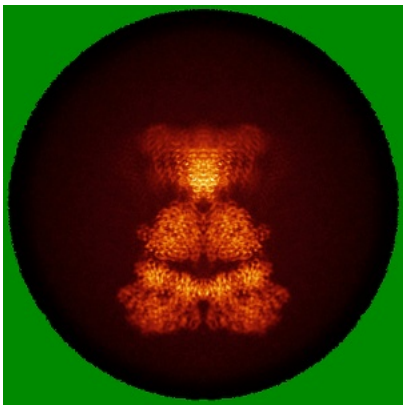


Z Index: 122

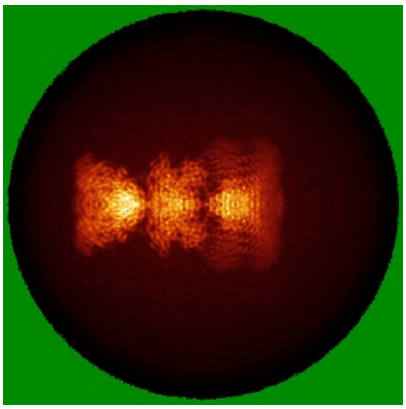
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

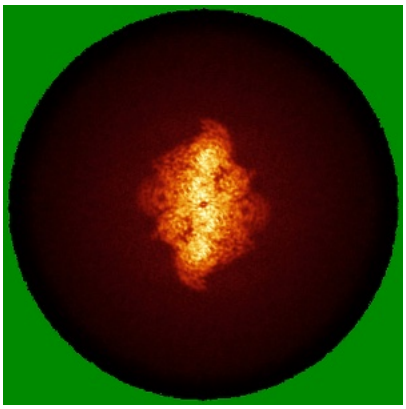
6.4.1 Primary map



X

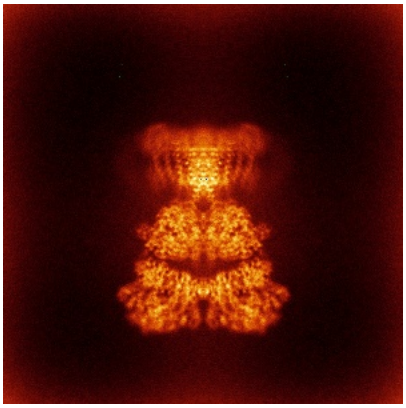


Y

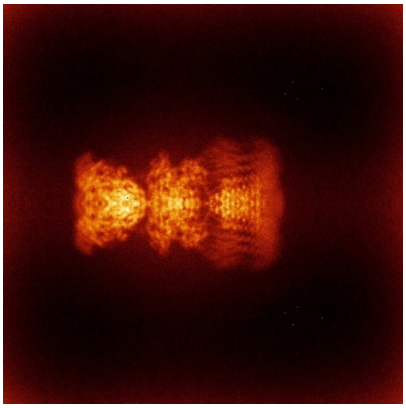


Z

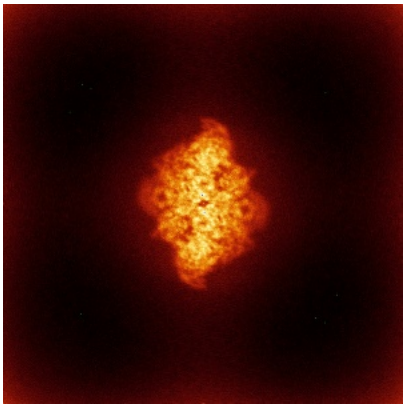
6.4.2 Raw map



X



Y

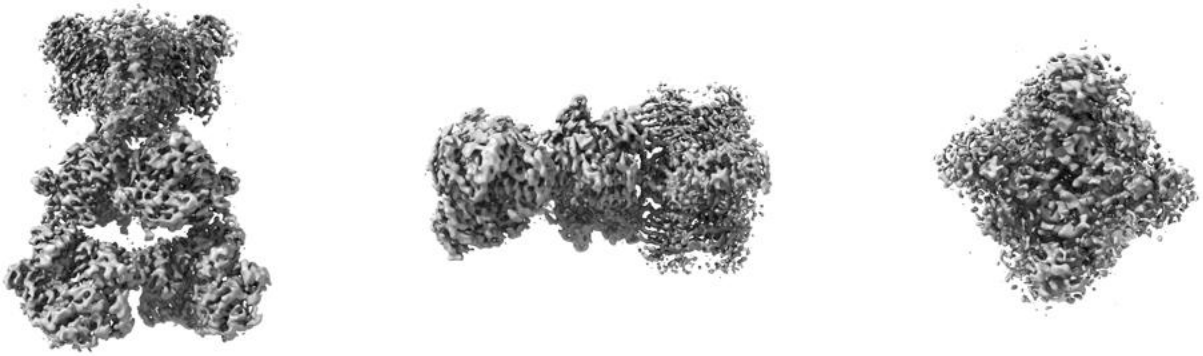


Z

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

6.5 Orthogonal surface views (i)

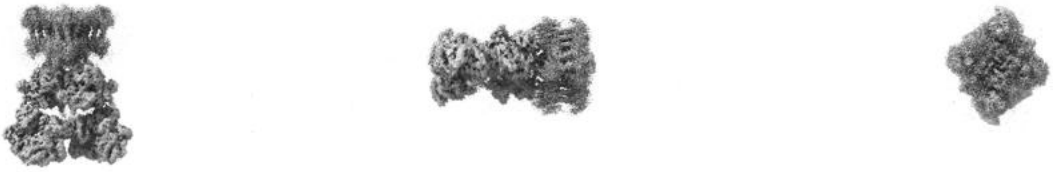
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.13. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

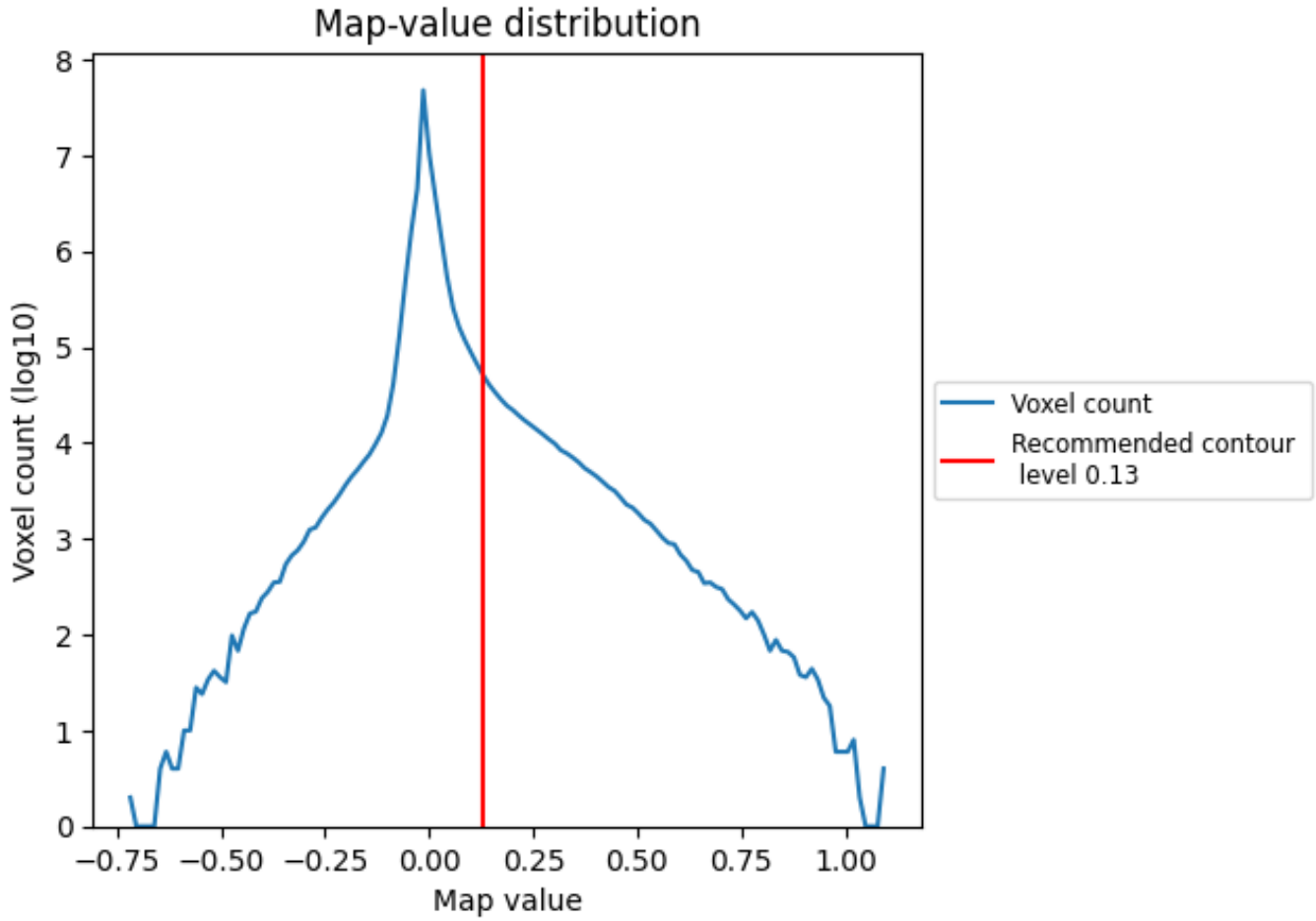
6.6 Mask visualisation (i)

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

7 Map analysis

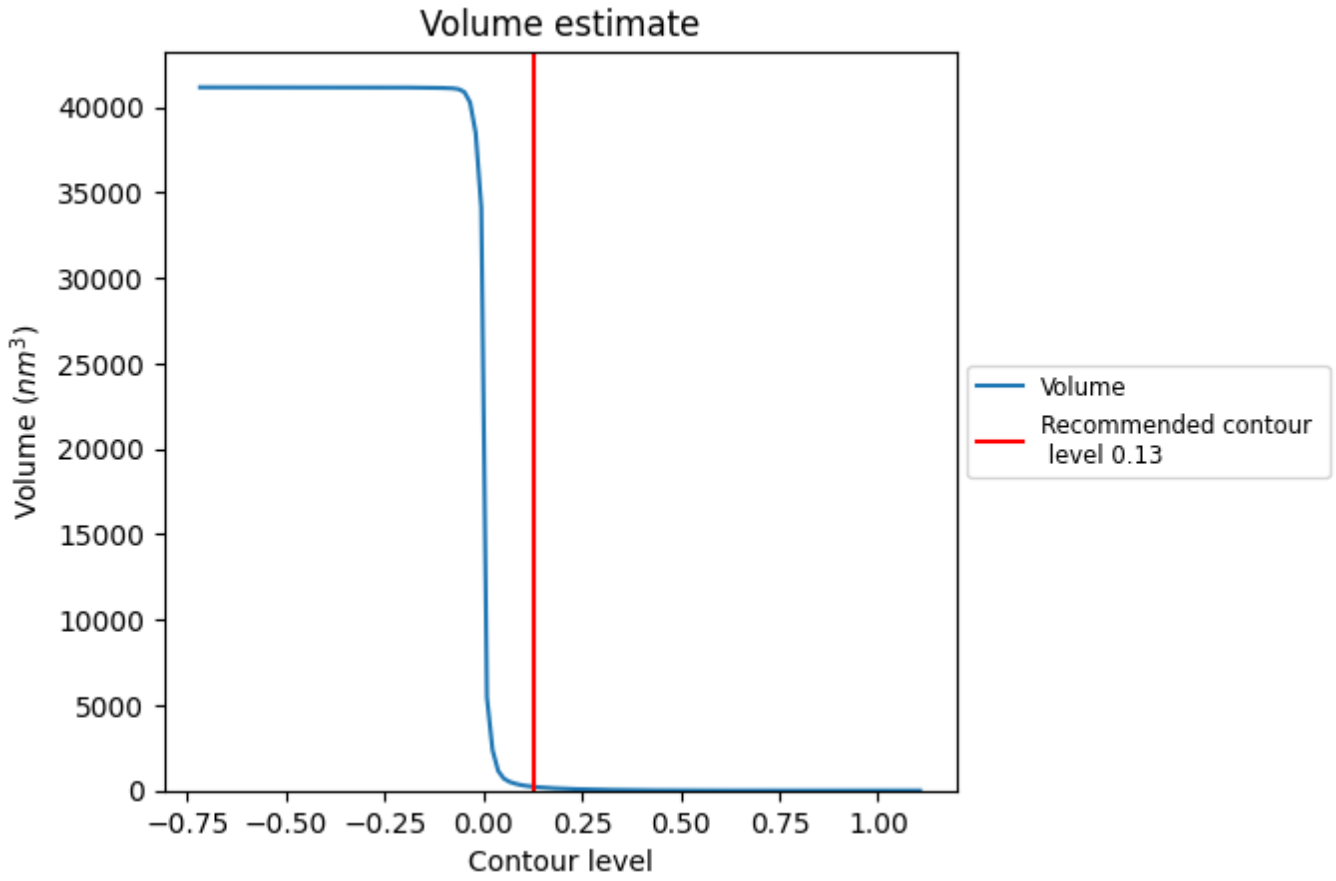
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

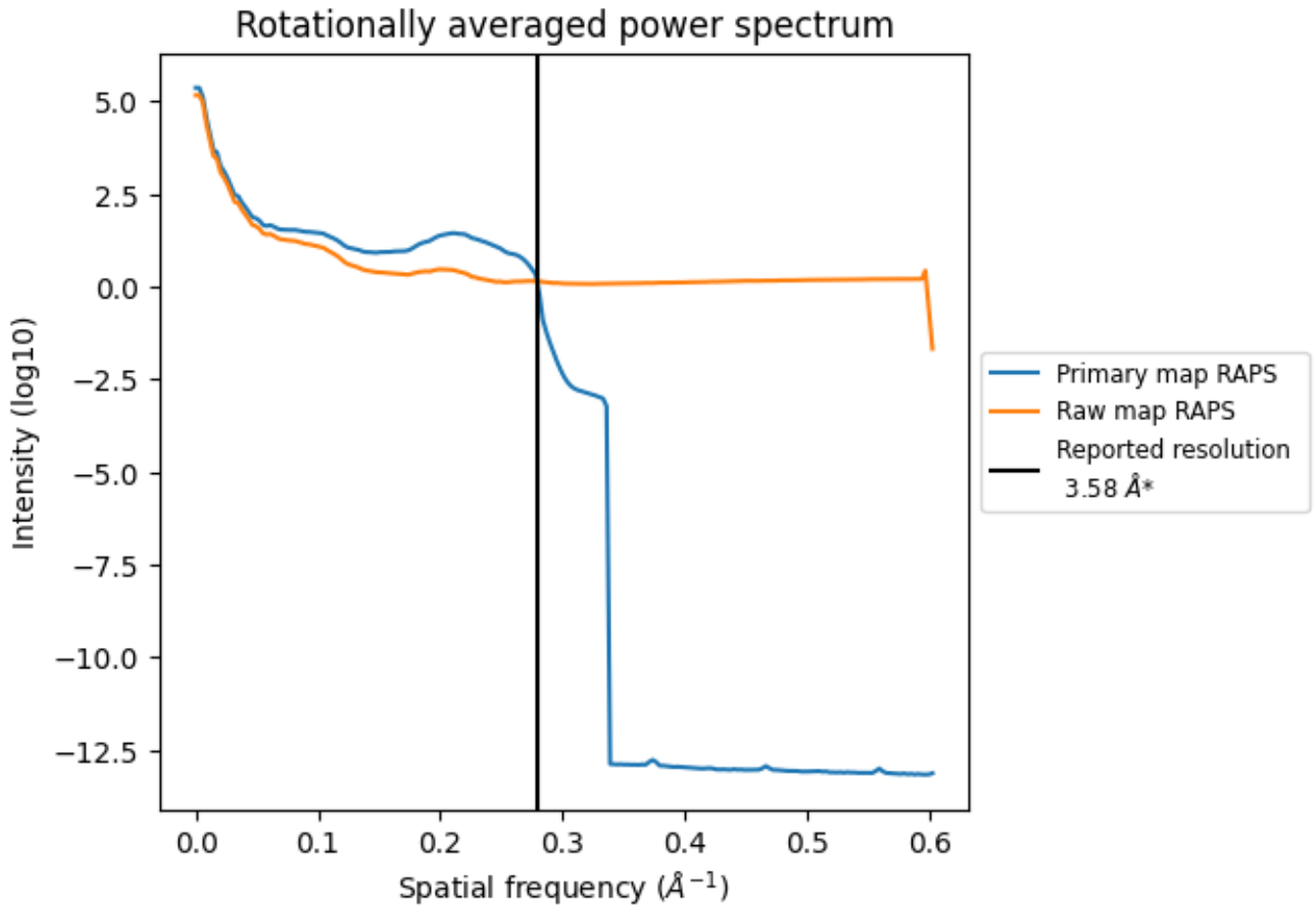
7.2 Volume estimate (i)



The volume at the recommended contour level is 216 nm^3; this corresponds to an approximate mass of 195 kDa.

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

7.3 Rotationally averaged power spectrum (i)

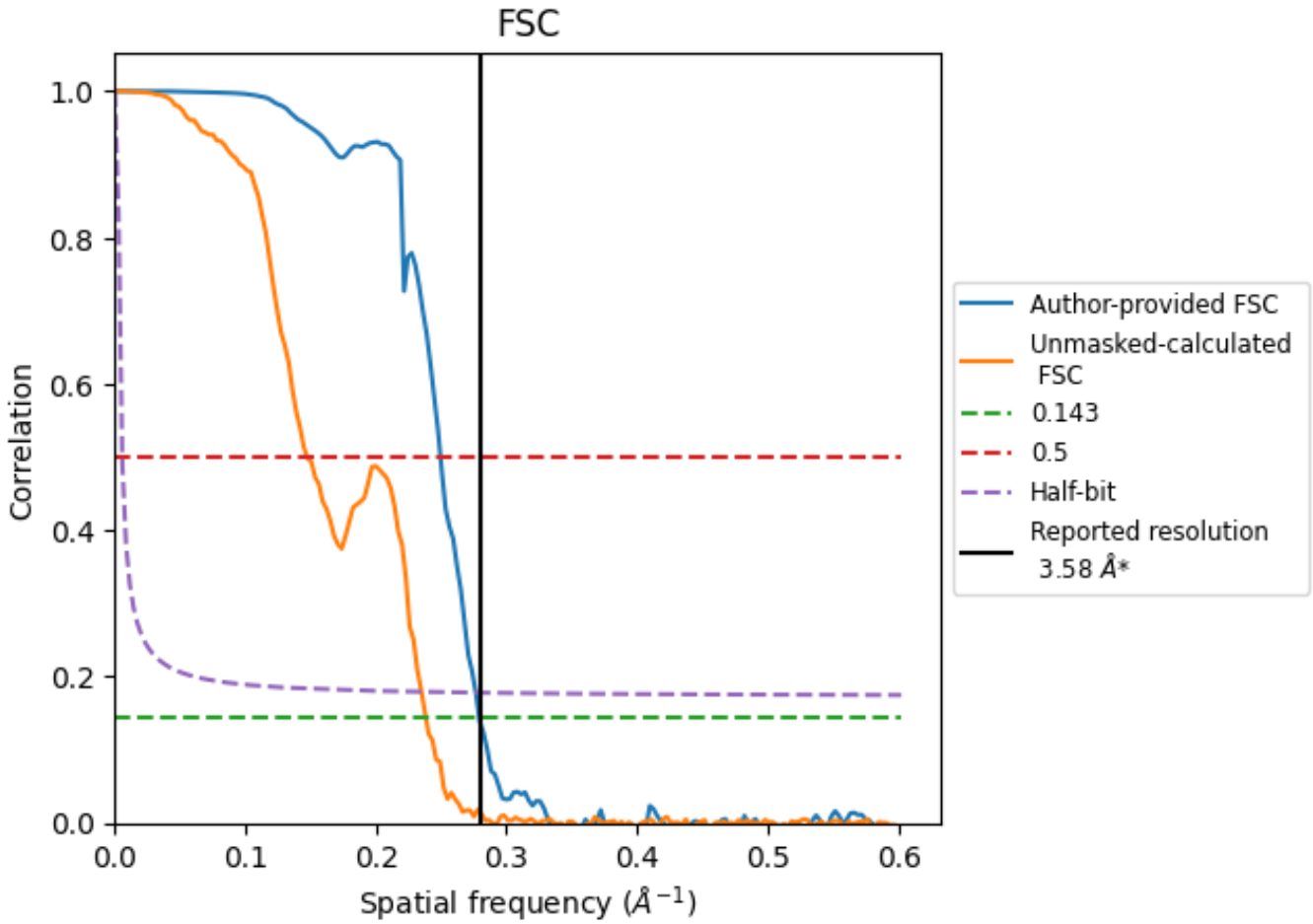


*Reported resolution corresponds to spatial frequency of 0.279 $Å^{-1}$

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.279 Å^{-1}

8.2 Resolution estimates (i)

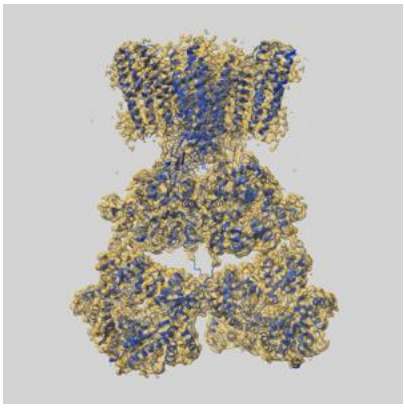
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.58	-	-
Author-provided FSC curve	3.58	4.01	3.62
Unmasked-calculated*	4.20	6.79	4.26

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.20 differs from the reported value 3.58 by more than 10 %

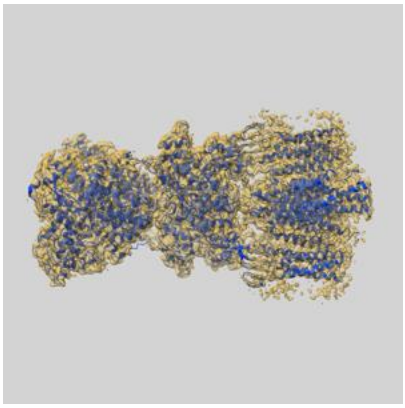
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-40741 and PDB model 8SS2. Per-residue inclusion information can be found in section 3 on page 11.

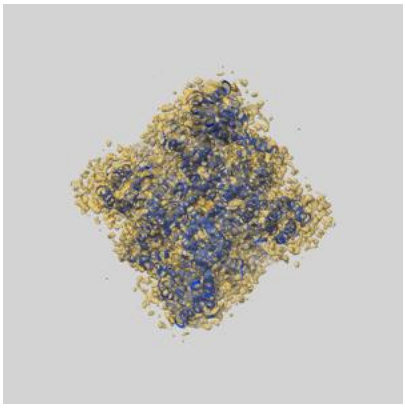
9.1 Map-model overlay



X



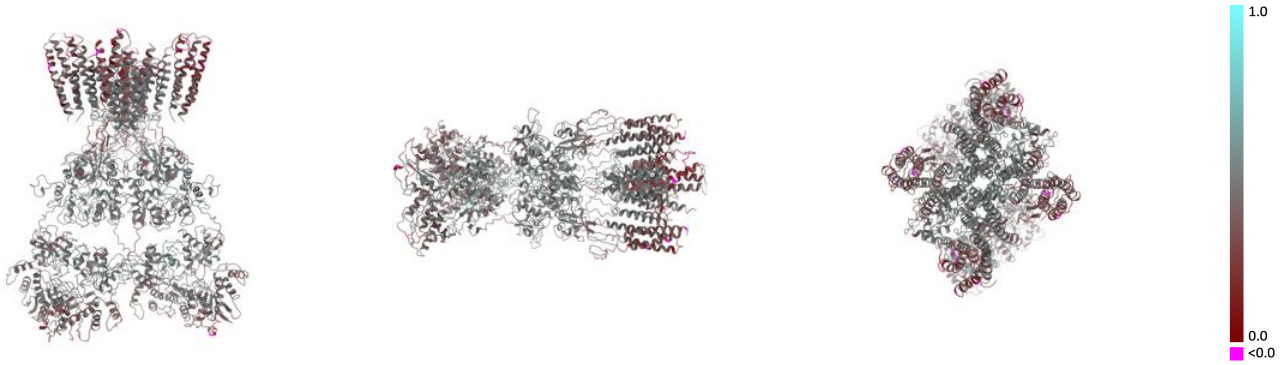
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.13 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.

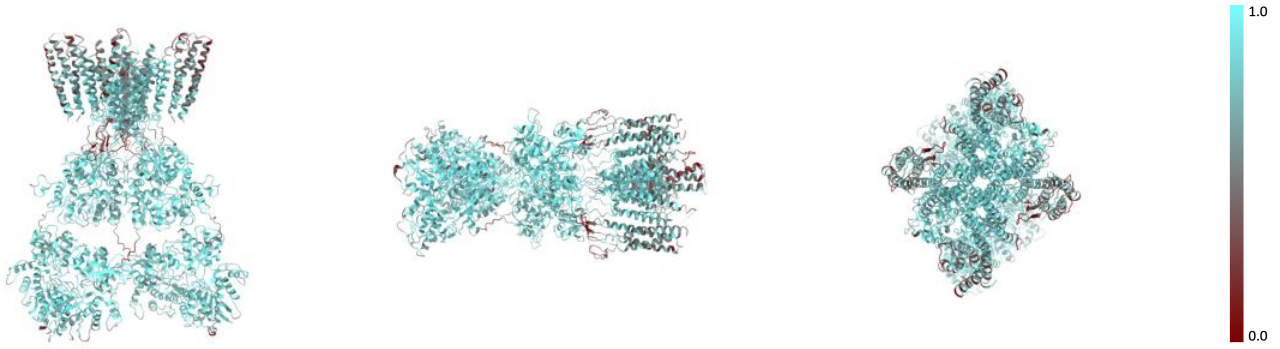
9.2 Q-score mapped to coordinate model



X Y Z

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

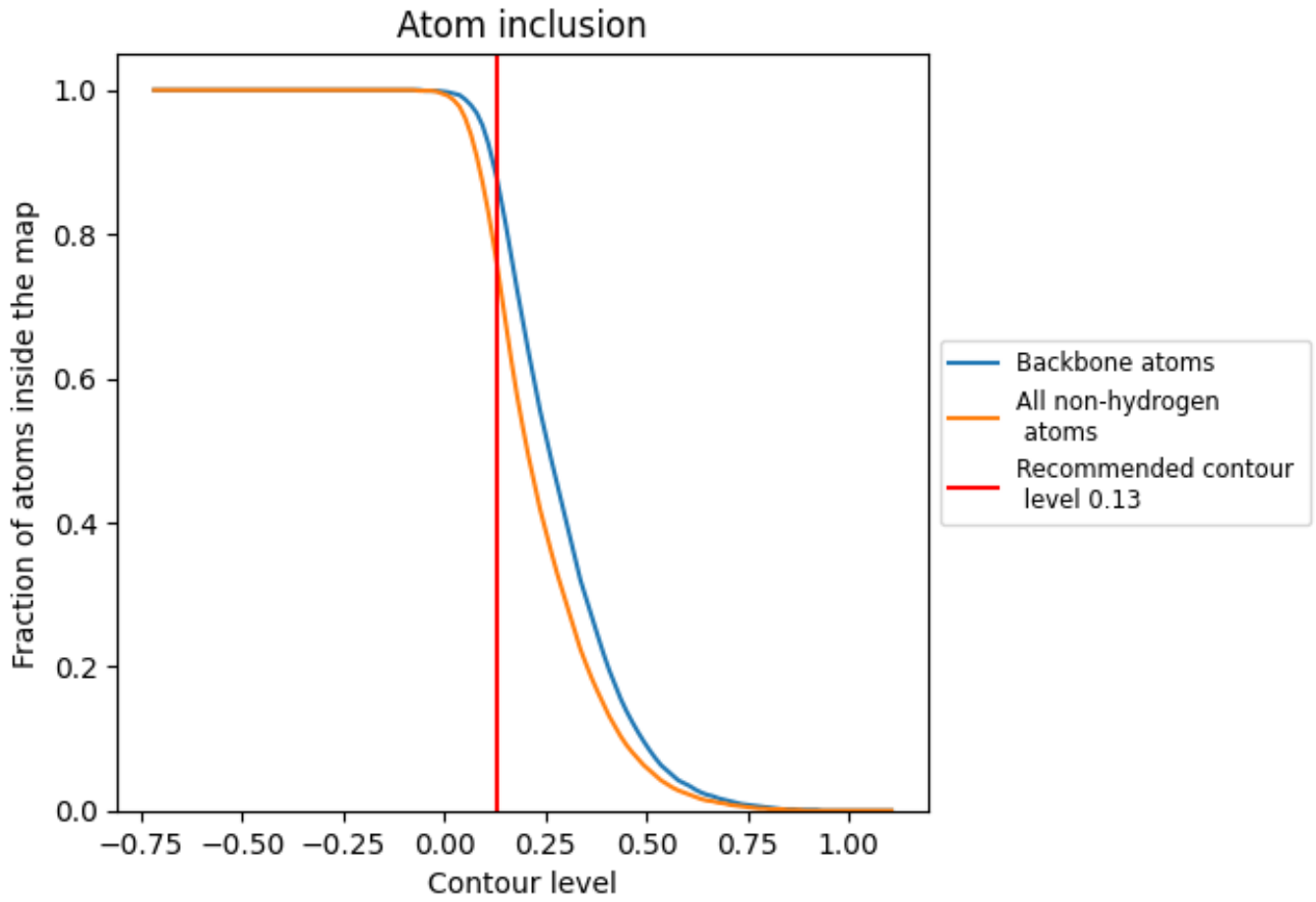
9.3 Atom inclusion mapped to coordinate model



X Y Z

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 (0.13).

9.4 Atom inclusion (i)



At the recommended contour level, 88% of all backbone atoms, 76% 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 (0.13) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7600	0.4380
A	0.7560	0.4420
B	0.8040	0.4580
C	0.7530	0.4380
D	0.8050	0.4550
E	0.5710	0.3300
F	0.5710	0.3270