Full wwPDB EM Validation Report ⓘ

Aug 9, 2021 – 12:08 pm BST

PDB ID	:	7OVQ
EMDB ID	:	EMD-13087
Title	:	Immature HIV-1 matrix structure
Authors	:	Qu, K.; Ke, Z.L.; Zila, V.; Anders-Oesswein, M.; Glass, B.; Muecksch, F.; Mueller, R.; Schultz, C.; Mueller, B.; Kraeusslich, H.G.; Briggs, J.A.G.
Deposited on	:	2021-06-15
Resolution	:	7.20 Å(reported)
Based on initial model	:	2H3Q

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

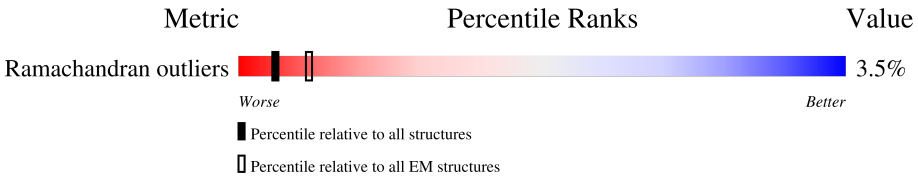
EMDB validation analysis	:	0.0.0.dev97
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.1

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 7.20 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023

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	115	10% 97% .
1	B	115	10% 97% .
1	C	115	10% 97% .
1	D	115	10% 97% .
1	E	115	13% 97% .
1	F	115	14% 97% .
1	I	115	17% 97% .
1	K	115	22% 97% .
1	M	115	17% 97% .
1	O	115	18% 97% .
1	P	115	14% 97% .

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Mol	Chain	Length	Quality of chain
1	Q	115	10% 97%
1	R	115	13% 97%
1	S	115	17% 97%
1	X	115	23% 97%
1	Y	115	17% 97%
1	Z	115	17% 97%
1	b	115	13% 97%
1	c	115	14% 97%
1	d	115	10% 97%
1	f	115	17% 97%
1	h	115	22% 97%
1	l	115	20% 97%
1	m	115	17% 97%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11400 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 Gag polyprotein.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	115	Total 460	C 230	N 115	O 115	0	0
1	B	115	Total 460	C 230	N 115	O 115	0	0
1	C	115	Total 460	C 230	N 115	O 115	0	0
1	D	115	Total 460	C 230	N 115	O 115	0	0
1	P	115	Total 460	C 230	N 115	O 115	0	0
1	b	115	Total 460	C 230	N 115	O 115	0	0
1	E	115	Total 460	C 230	N 115	O 115	0	0
1	Q	115	Total 460	C 230	N 115	O 115	0	0
1	c	115	Total 460	C 230	N 115	O 115	0	0
1	F	115	Total 460	C 230	N 115	O 115	0	0
1	R	115	Total 460	C 230	N 115	O 115	0	0
1	d	115	Total 460	C 230	N 115	O 115	0	0
1	S	115	Total 460	C 230	N 115	O 115	0	0
1	f	115	Total 460	C 230	N 115	O 115	0	0
1	I	115	Total 460	C 230	N 115	O 115	0	0
1	h	115	Total 460	C 230	N 115	O 115	0	0
1	K	115	Total 460	C 230	N 115	O 115	0	0

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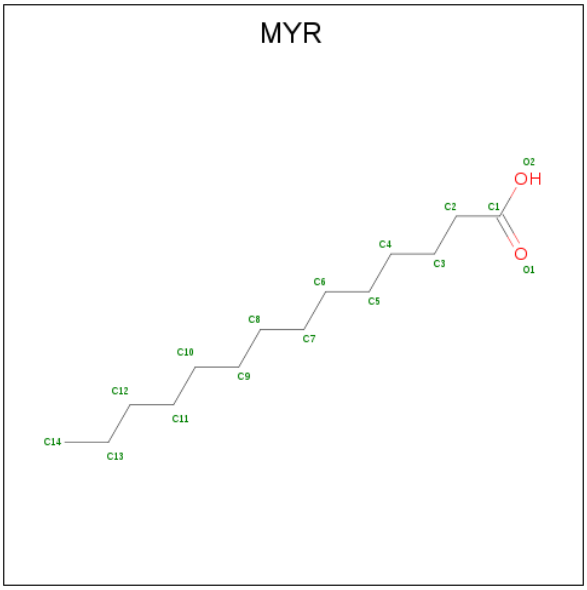
Mol	Chain	Residues	Atoms				AltConf	Trace
1	X	115	Total 460	C 230	N 115	O 115	0	0
1	M	115	Total 460	C 230	N 115	O 115	0	0
1	Y	115	Total 460	C 230	N 115	O 115	0	0
1	Z	115	Total 460	C 230	N 115	O 115	0	0
1	l	115	Total 460	C 230	N 115	O 115	0	0
1	O	115	Total 460	C 230	N 115	O 115	0	0
1	m	115	Total 460	C 230	N 115	O 115	0	0

- Molecule 2 is MYRISTIC ACID (three-letter code: MYR) (formula: $C_{14}H_{28}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
2	A	1	Total 15	C 14	O 1	0
2	B	1	Total 15	C 14	O 1	0
2	C	1	Total 15	C 14	O 1	0
2	D	1	Total 15	C 14	O 1	0

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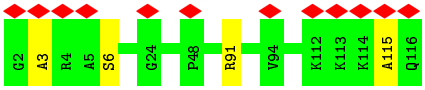
Mol	Chain	Residues	Atoms			AltConf
2	P	1	Total	C	O	0
			15	14	1	
2	b	1	Total	C	O	0
			15	14	1	
2	E	1	Total	C	O	0
			15	14	1	
2	Q	1	Total	C	O	0
			15	14	1	
2	c	1	Total	C	O	0
			15	14	1	
2	F	1	Total	C	O	0
			15	14	1	
2	R	1	Total	C	O	0
			15	14	1	
2	d	1	Total	C	O	0
			15	14	1	
2	S	1	Total	C	O	0
			15	14	1	
2	f	1	Total	C	O	0
			15	14	1	
2	I	1	Total	C	O	0
			15	14	1	
2	h	1	Total	C	O	0
			15	14	1	
2	K	1	Total	C	O	0
			15	14	1	
2	X	1	Total	C	O	0
			15	14	1	
2	M	1	Total	C	O	0
			15	14	1	
2	Y	1	Total	C	O	0
			15	14	1	
2	Z	1	Total	C	O	0
			15	14	1	
2	l	1	Total	C	O	0
			15	14	1	
2	O	1	Total	C	O	0
			15	14	1	
2	m	1	Total	C	O	0
			15	14	1	

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.

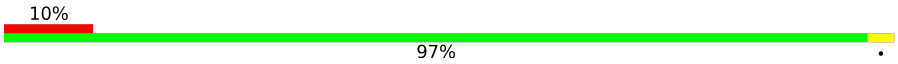
- Molecule 1: Gag polyprotein

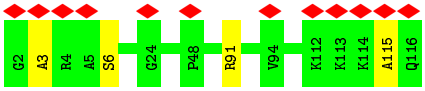
Chain A:



- Molecule 1: Gag polyprotein

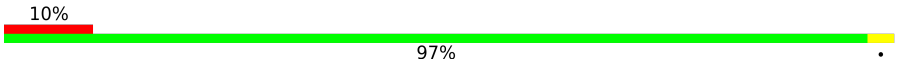
Chain B:

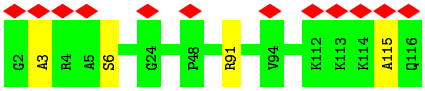




- Molecule 1: Gag polyprotein

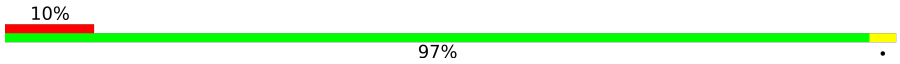
Chain C:

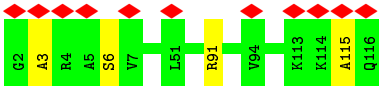




- Molecule 1: Gag polyprotein

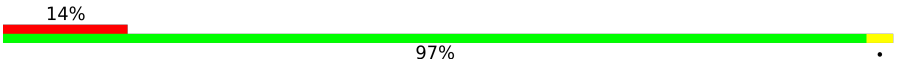
Chain D:

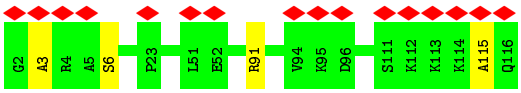




- Molecule 1: Gag polyprotein

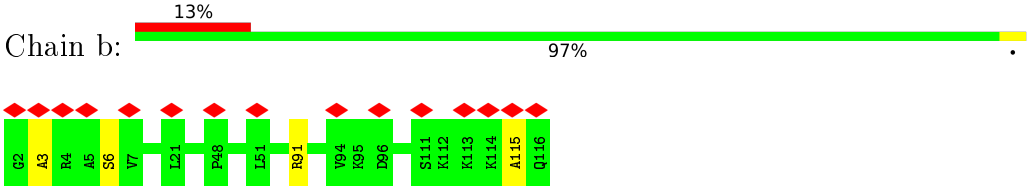
Chain P:





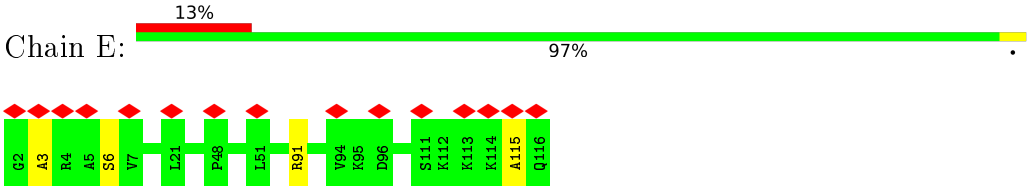
- Molecule 1: Gag polyprotein

Chain b:



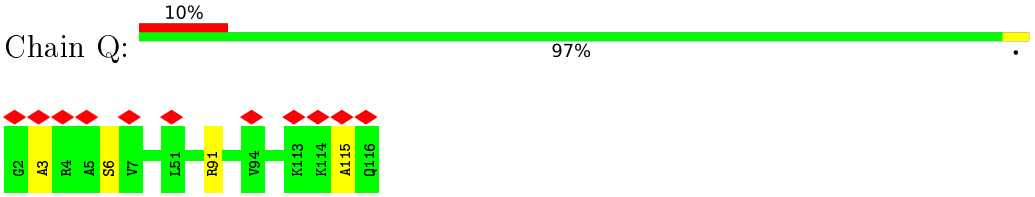
- Molecule 1: Gag polyprotein

Chain E:



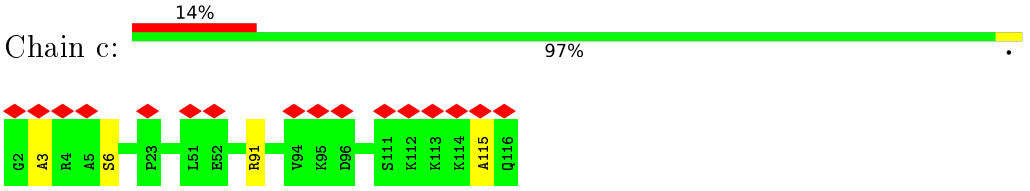
- Molecule 1: Gag polyprotein

Chain Q:



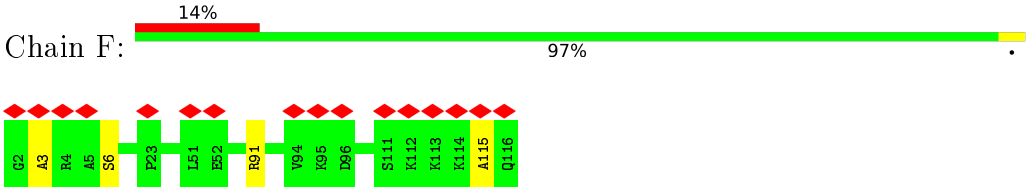
- Molecule 1: Gag polyprotein

Chain c:



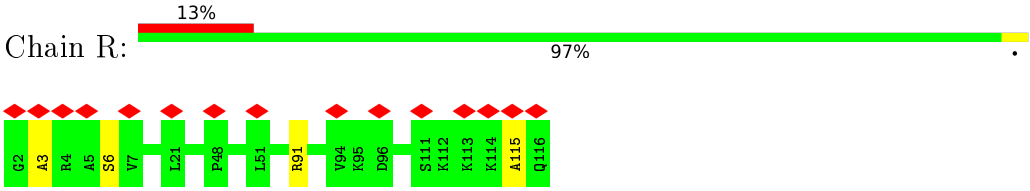
- Molecule 1: Gag polyprotein

Chain F:



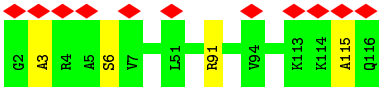
- Molecule 1: Gag polyprotein

Chain R:



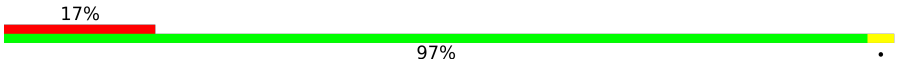
- Molecule 1: Gag polyprotein

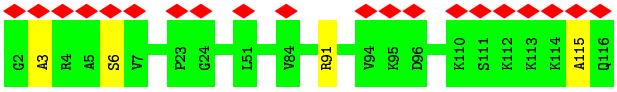
Chain d:



- Molecule 1: Gag polyprotein

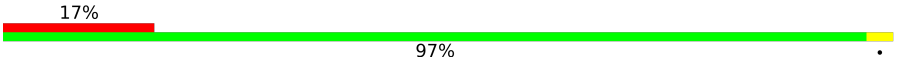
Chain S:

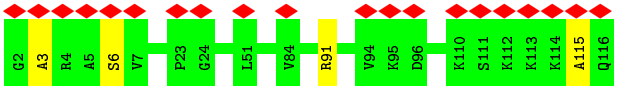




- Molecule 1: Gag polyprotein

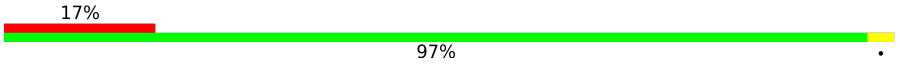
Chain f:

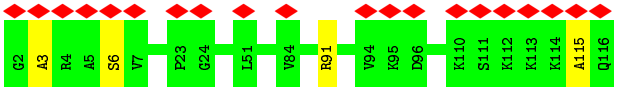




- Molecule 1: Gag polyprotein

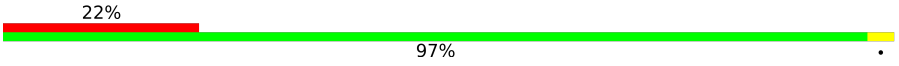
Chain I:

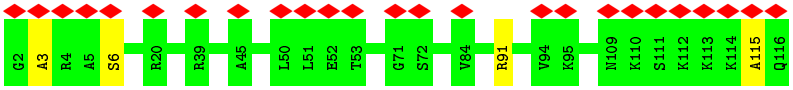




- Molecule 1: Gag polyprotein

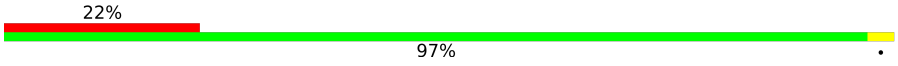
Chain h:

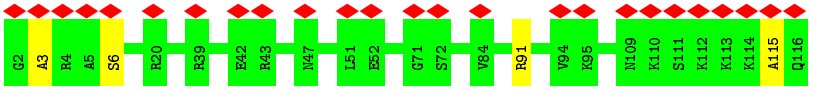




- Molecule 1: Gag polyprotein

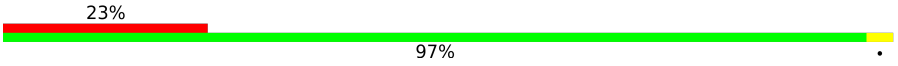
Chain K:

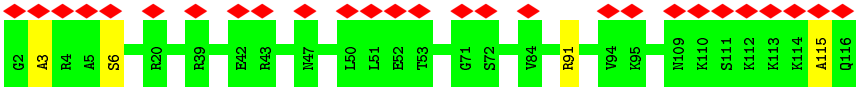




- Molecule 1: Gag polyprotein

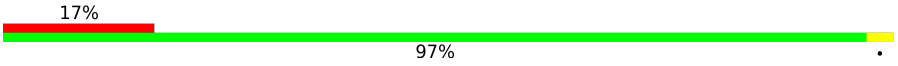
Chain X:

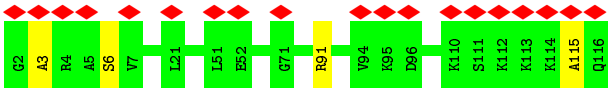




- Molecule 1: Gag polyprotein

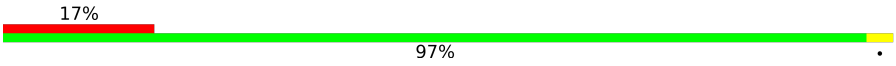
Chain M:

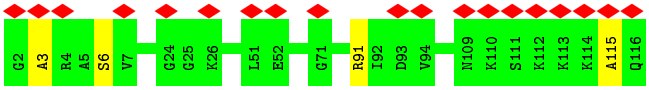




- Molecule 1: Gag polyprotein

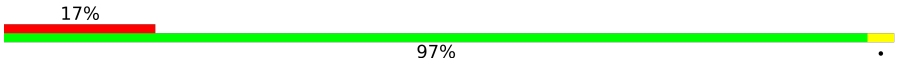
Chain Y:

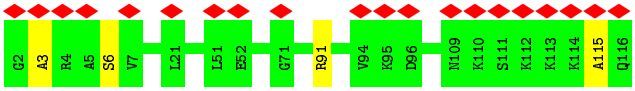




- Molecule 1: Gag polyprotein

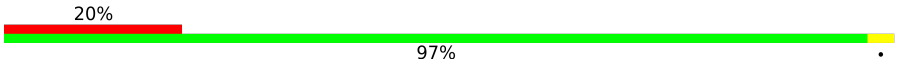
Chain Z:

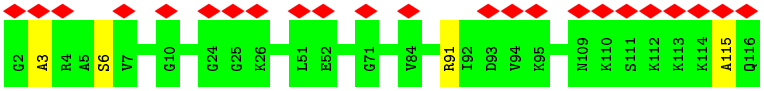




- Molecule 1: Gag polyprotein

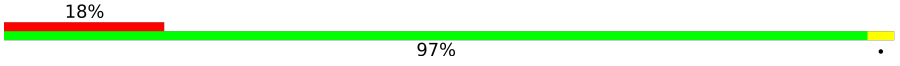
Chain l:

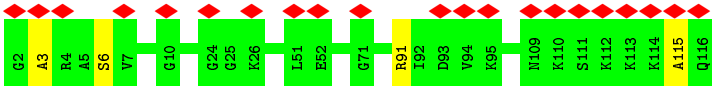




- Molecule 1: Gag polyprotein

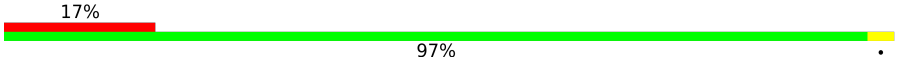
Chain O:

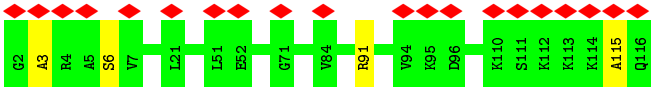




- Molecule 1: Gag polyprotein

Chain m:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of subtomograms used	22417	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 ($e^-/Å^2$)	3	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	15.476	Depositor
Minimum map value	-12.045	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	2.0	Depositor
Map size (Å)	259.2, 259.2, 259.2	wwPDB
Map dimensions	192, 192, 192	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.35, 1.35, 1.35	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.17	0/459	0.30	0/572
1	B	0.17	0/459	0.30	0/572
1	C	0.18	0/459	0.30	0/572
1	D	0.17	0/459	0.30	0/572
1	E	0.17	0/459	0.30	0/572
1	F	0.17	0/459	0.30	0/572
1	I	0.17	0/459	0.30	0/572
1	K	0.17	0/459	0.30	0/572
1	M	0.17	0/459	0.30	0/572
1	O	0.17	0/459	0.30	0/572
1	P	0.17	0/459	0.30	0/572
1	Q	0.17	0/459	0.30	0/572
1	R	0.17	0/459	0.30	0/572
1	S	0.17	0/459	0.30	0/572
1	X	0.17	0/459	0.30	0/572
1	Y	0.17	0/459	0.30	0/572
1	Z	0.18	0/459	0.30	0/572
1	b	0.17	0/459	0.30	0/572
1	c	0.17	0/459	0.30	0/572
1	d	0.17	0/459	0.30	0/572
1	f	0.17	0/459	0.30	0/572
1	h	0.17	0/459	0.30	0/572
1	l	0.17	0/459	0.30	0/572
1	m	0.17	0/459	0.30	0/572
All	All	0.17	0/11016	0.30	0/13728

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

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	113/115 (98%)	103 (91%)	6 (5%)	4 (4%)	3	25
1	B	113/115 (98%)	103 (91%)	6 (5%)	4 (4%)	3	25
1	C	113/115 (98%)	103 (91%)	6 (5%)	4 (4%)	3	25
1	D	113/115 (98%)	103 (91%)	6 (5%)	4 (4%)	3	25
1	E	113/115 (98%)	103 (91%)	6 (5%)	4 (4%)	3	25
1	F	113/115 (98%)	103 (91%)	6 (5%)	4 (4%)	3	25
1	I	113/115 (98%)	103 (91%)	6 (5%)	4 (4%)	3	25
1	K	113/115 (98%)	103 (91%)	6 (5%)	4 (4%)	3	25
1	M	113/115 (98%)	103 (91%)	6 (5%)	4 (4%)	3	25
1	O	113/115 (98%)	103 (91%)	6 (5%)	4 (4%)	3	25
1	P	113/115 (98%)	103 (91%)	6 (5%)	4 (4%)	3	25
1	Q	113/115 (98%)	103 (91%)	6 (5%)	4 (4%)	3	25
1	R	113/115 (98%)	103 (91%)	6 (5%)	4 (4%)	3	25
1	S	113/115 (98%)	103 (91%)	6 (5%)	4 (4%)	3	25
1	X	113/115 (98%)	103 (91%)	6 (5%)	4 (4%)	3	25
1	Y	113/115 (98%)	103 (91%)	6 (5%)	4 (4%)	3	25
1	Z	113/115 (98%)	103 (91%)	6 (5%)	4 (4%)	3	25
1	b	113/115 (98%)	103 (91%)	6 (5%)	4 (4%)	3	25
1	c	113/115 (98%)	103 (91%)	6 (5%)	4 (4%)	3	25
1	d	113/115 (98%)	103 (91%)	6 (5%)	4 (4%)	3	25
1	f	113/115 (98%)	103 (91%)	6 (5%)	4 (4%)	3	25

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	h	113/115 (98%)	103 (91%)	6 (5%)	4 (4%)	3 25
1	l	113/115 (98%)	103 (91%)	6 (5%)	4 (4%)	3 25
1	m	113/115 (98%)	103 (91%)	6 (5%)	4 (4%)	3 25
All	All	2712/2760 (98%)	2472 (91%)	144 (5%)	96 (4%)	6 25

All (96) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	91	ARG
1	B	6	SER
1	B	91	ARG
1	C	91	ARG
1	D	91	ARG
1	P	91	ARG
1	b	91	ARG
1	E	6	SER
1	E	91	ARG
1	Q	91	ARG
1	c	91	ARG
1	F	91	ARG
1	R	91	ARG
1	d	91	ARG
1	S	91	ARG
1	f	91	ARG
1	I	91	ARG
1	h	91	ARG
1	K	91	ARG
1	X	6	SER
1	X	91	ARG
1	M	91	ARG
1	Y	6	SER
1	Y	91	ARG
1	Z	91	ARG
1	l	91	ARG
1	O	91	ARG
1	m	91	ARG
1	A	6	SER
1	A	115	ALA
1	B	115	ALA
1	C	6	SER
1	C	115	ALA

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Mol	Chain	Res	Type
1	D	6	SER
1	D	115	ALA
1	P	6	SER
1	P	115	ALA
1	b	6	SER
1	b	115	ALA
1	E	115	ALA
1	Q	6	SER
1	Q	115	ALA
1	c	6	SER
1	c	115	ALA
1	F	6	SER
1	F	115	ALA
1	R	6	SER
1	R	115	ALA
1	d	6	SER
1	d	115	ALA
1	S	6	SER
1	S	115	ALA
1	f	6	SER
1	f	115	ALA
1	I	6	SER
1	I	115	ALA
1	h	6	SER
1	h	115	ALA
1	K	6	SER
1	K	115	ALA
1	X	115	ALA
1	M	6	SER
1	M	115	ALA
1	Y	115	ALA
1	Z	6	SER
1	Z	115	ALA
1	l	6	SER
1	l	115	ALA
1	O	6	SER
1	O	115	ALA
1	m	6	SER
1	m	115	ALA
1	A	3	ALA
1	B	3	ALA
1	C	3	ALA

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Mol	Chain	Res	Type
1	D	3	ALA
1	P	3	ALA
1	b	3	ALA
1	E	3	ALA
1	Q	3	ALA
1	c	3	ALA
1	F	3	ALA
1	R	3	ALA
1	d	3	ALA
1	S	3	ALA
1	f	3	ALA
1	I	3	ALA
1	h	3	ALA
1	K	3	ALA
1	X	3	ALA
1	M	3	ALA
1	Y	3	ALA
1	Z	3	ALA
1	l	3	ALA
1	O	3	ALA
1	m	3	ALA

5.3.2 Protein sidechains (i)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

24 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	MYR	B	201	1	14,14,15	0.56	0	13,13,15	0.50	0
2	MYR	b	201	1	14,14,15	0.56	0	13,13,15	0.49	0
2	MYR	M	201	1	14,14,15	0.56	0	13,13,15	0.49	0
2	MYR	S	201	1	14,14,15	0.57	0	13,13,15	0.50	0
2	MYR	F	201	1	14,14,15	0.57	0	13,13,15	0.50	0
2	MYR	A	201	1	14,14,15	0.56	0	13,13,15	0.49	0
2	MYR	Z	201	1	14,14,15	0.57	0	13,13,15	0.50	0
2	MYR	h	201	1	14,14,15	0.56	0	13,13,15	0.49	0
2	MYR	Q	201	1	14,14,15	0.56	0	13,13,15	0.50	0
2	MYR	l	201	1	14,14,15	0.56	0	13,13,15	0.49	0
2	MYR	X	201	1	14,14,15	0.56	0	13,13,15	0.50	0
2	MYR	f	201	1	14,14,15	0.56	0	13,13,15	0.49	0
2	MYR	I	201	1	14,14,15	0.56	0	13,13,15	0.49	0
2	MYR	E	201	1	14,14,15	0.56	0	13,13,15	0.49	0
2	MYR	Y	201	1	14,14,15	0.56	0	13,13,15	0.49	0
2	MYR	d	201	1	14,14,15	0.56	0	13,13,15	0.49	0
2	MYR	O	201	1	14,14,15	0.56	0	13,13,15	0.49	0
2	MYR	m	201	1	14,14,15	0.56	0	13,13,15	0.50	0
2	MYR	P	201	1	14,14,15	0.57	0	13,13,15	0.50	0
2	MYR	K	201	1	14,14,15	0.56	0	13,13,15	0.49	0
2	MYR	C	201	1	14,14,15	0.56	0	13,13,15	0.49	0
2	MYR	c	201	1	14,14,15	0.56	0	13,13,15	0.49	0
2	MYR	R	201	1	14,14,15	0.56	0	13,13,15	0.50	0
2	MYR	D	201	1	14,14,15	0.56	0	13,13,15	0.49	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MYR	B	201	1	-	7/11/12/13	-
2	MYR	b	201	1	-	7/11/12/13	-
2	MYR	M	201	1	-	7/11/12/13	-
2	MYR	S	201	1	-	7/11/12/13	-
2	MYR	F	201	1	-	7/11/12/13	-
2	MYR	A	201	1	-	7/11/12/13	-
2	MYR	Z	201	1	-	7/11/12/13	-
2	MYR	h	201	1	-	7/11/12/13	-
2	MYR	Q	201	1	-	7/11/12/13	-
2	MYR	l	201	1	-	7/11/12/13	-
2	MYR	X	201	1	-	7/11/12/13	-
2	MYR	f	201	1	-	7/11/12/13	-
2	MYR	I	201	1	-	7/11/12/13	-
2	MYR	E	201	1	-	7/11/12/13	-
2	MYR	Y	201	1	-	7/11/12/13	-
2	MYR	d	201	1	-	7/11/12/13	-
2	MYR	O	201	1	-	7/11/12/13	-
2	MYR	m	201	1	-	7/11/12/13	-
2	MYR	P	201	1	-	7/11/12/13	-
2	MYR	K	201	1	-	7/11/12/13	-
2	MYR	C	201	1	-	7/11/12/13	-
2	MYR	c	201	1	-	7/11/12/13	-
2	MYR	R	201	1	-	7/11/12/13	-
2	MYR	D	201	1	-	7/11/12/13	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (168) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	201	MYR	C9-C10-C11-C12
2	B	201	MYR	C9-C10-C11-C12
2	Q	201	MYR	C9-C10-C11-C12
2	C	201	MYR	C9-C10-C11-C12
2	D	201	MYR	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
2	P	201	MYR	C9-C10-C11-C12
2	b	201	MYR	C9-C10-C11-C12
2	E	201	MYR	C9-C10-C11-C12
2	c	201	MYR	C9-C10-C11-C12
2	F	201	MYR	C9-C10-C11-C12
2	R	201	MYR	C9-C10-C11-C12
2	d	201	MYR	C9-C10-C11-C12
2	S	201	MYR	C9-C10-C11-C12
2	f	201	MYR	C9-C10-C11-C12
2	I	201	MYR	C9-C10-C11-C12
2	h	201	MYR	C9-C10-C11-C12
2	K	201	MYR	C9-C10-C11-C12
2	X	201	MYR	C9-C10-C11-C12
2	M	201	MYR	C9-C10-C11-C12
2	Y	201	MYR	C9-C10-C11-C12
2	Z	201	MYR	C9-C10-C11-C12
2	l	201	MYR	C9-C10-C11-C12
2	O	201	MYR	C9-C10-C11-C12
2	m	201	MYR	C9-C10-C11-C12
2	Q	201	MYR	C7-C8-C9-C10
2	R	201	MYR	C7-C8-C9-C10
2	S	201	MYR	C7-C8-C9-C10
2	Z	201	MYR	C7-C8-C9-C10
2	A	201	MYR	C7-C8-C9-C10
2	B	201	MYR	C7-C8-C9-C10
2	C	201	MYR	C7-C8-C9-C10
2	D	201	MYR	C7-C8-C9-C10
2	P	201	MYR	C7-C8-C9-C10
2	b	201	MYR	C7-C8-C9-C10
2	E	201	MYR	C7-C8-C9-C10
2	c	201	MYR	C7-C8-C9-C10
2	F	201	MYR	C7-C8-C9-C10
2	d	201	MYR	C7-C8-C9-C10
2	f	201	MYR	C7-C8-C9-C10
2	I	201	MYR	C7-C8-C9-C10
2	h	201	MYR	C7-C8-C9-C10
2	K	201	MYR	C7-C8-C9-C10
2	X	201	MYR	C7-C8-C9-C10
2	M	201	MYR	C7-C8-C9-C10
2	Y	201	MYR	C7-C8-C9-C10
2	l	201	MYR	C7-C8-C9-C10
2	O	201	MYR	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
2	m	201	MYR	C7-C8-C9-C10
2	B	201	MYR	C10-C11-C12-C13
2	D	201	MYR	C10-C11-C12-C13
2	P	201	MYR	C10-C11-C12-C13
2	Q	201	MYR	C10-C11-C12-C13
2	R	201	MYR	C10-C11-C12-C13
2	M	201	MYR	C10-C11-C12-C13
2	A	201	MYR	C10-C11-C12-C13
2	C	201	MYR	C10-C11-C12-C13
2	b	201	MYR	C10-C11-C12-C13
2	E	201	MYR	C10-C11-C12-C13
2	c	201	MYR	C10-C11-C12-C13
2	F	201	MYR	C10-C11-C12-C13
2	d	201	MYR	C10-C11-C12-C13
2	S	201	MYR	C10-C11-C12-C13
2	f	201	MYR	C10-C11-C12-C13
2	I	201	MYR	C10-C11-C12-C13
2	h	201	MYR	C10-C11-C12-C13
2	K	201	MYR	C10-C11-C12-C13
2	X	201	MYR	C10-C11-C12-C13
2	Y	201	MYR	C10-C11-C12-C13
2	Z	201	MYR	C10-C11-C12-C13
2	l	201	MYR	C10-C11-C12-C13
2	O	201	MYR	C10-C11-C12-C13
2	m	201	MYR	C10-C11-C12-C13
2	D	201	MYR	C2-C3-C4-C5
2	Q	201	MYR	C2-C3-C4-C5
2	h	201	MYR	C2-C3-C4-C5
2	M	201	MYR	C2-C3-C4-C5
2	Z	201	MYR	C2-C3-C4-C5
2	l	201	MYR	C2-C3-C4-C5
2	m	201	MYR	C2-C3-C4-C5
2	A	201	MYR	C2-C3-C4-C5
2	B	201	MYR	C2-C3-C4-C5
2	C	201	MYR	C2-C3-C4-C5
2	P	201	MYR	C2-C3-C4-C5
2	b	201	MYR	C2-C3-C4-C5
2	E	201	MYR	C2-C3-C4-C5
2	c	201	MYR	C2-C3-C4-C5
2	F	201	MYR	C2-C3-C4-C5
2	R	201	MYR	C2-C3-C4-C5
2	d	201	MYR	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
2	S	201	MYR	C2-C3-C4-C5
2	f	201	MYR	C2-C3-C4-C5
2	I	201	MYR	C2-C3-C4-C5
2	K	201	MYR	C2-C3-C4-C5
2	X	201	MYR	C2-C3-C4-C5
2	Y	201	MYR	C2-C3-C4-C5
2	O	201	MYR	C2-C3-C4-C5
2	A	201	MYR	C11-C12-C13-C14
2	D	201	MYR	C11-C12-C13-C14
2	F	201	MYR	C11-C12-C13-C14
2	R	201	MYR	C11-C12-C13-C14
2	K	201	MYR	C11-C12-C13-C14
2	M	201	MYR	C11-C12-C13-C14
2	Z	201	MYR	C11-C12-C13-C14
2	O	201	MYR	C11-C12-C13-C14
2	B	201	MYR	C11-C12-C13-C14
2	C	201	MYR	C11-C12-C13-C14
2	P	201	MYR	C11-C12-C13-C14
2	E	201	MYR	C11-C12-C13-C14
2	Q	201	MYR	C11-C12-C13-C14
2	S	201	MYR	C11-C12-C13-C14
2	f	201	MYR	C11-C12-C13-C14
2	I	201	MYR	C11-C12-C13-C14
2	X	201	MYR	C11-C12-C13-C14
2	Y	201	MYR	C11-C12-C13-C14
2	l	201	MYR	C11-C12-C13-C14
2	m	201	MYR	C11-C12-C13-C14
2	b	201	MYR	C11-C12-C13-C14
2	c	201	MYR	C11-C12-C13-C14
2	d	201	MYR	C11-C12-C13-C14
2	h	201	MYR	C11-C12-C13-C14
2	A	201	MYR	C1-C2-C3-C4
2	B	201	MYR	C1-C2-C3-C4
2	C	201	MYR	C1-C2-C3-C4
2	D	201	MYR	C1-C2-C3-C4
2	P	201	MYR	C1-C2-C3-C4
2	b	201	MYR	C1-C2-C3-C4
2	E	201	MYR	C1-C2-C3-C4
2	Q	201	MYR	C1-C2-C3-C4
2	c	201	MYR	C1-C2-C3-C4
2	F	201	MYR	C1-C2-C3-C4
2	R	201	MYR	C1-C2-C3-C4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	d	201	MYR	C1-C2-C3-C4
2	S	201	MYR	C1-C2-C3-C4
2	f	201	MYR	C1-C2-C3-C4
2	I	201	MYR	C1-C2-C3-C4
2	h	201	MYR	C1-C2-C3-C4
2	K	201	MYR	C1-C2-C3-C4
2	X	201	MYR	C1-C2-C3-C4
2	M	201	MYR	C1-C2-C3-C4
2	Y	201	MYR	C1-C2-C3-C4
2	Z	201	MYR	C1-C2-C3-C4
2	l	201	MYR	C1-C2-C3-C4
2	O	201	MYR	C1-C2-C3-C4
2	m	201	MYR	C1-C2-C3-C4
2	A	201	MYR	C5-C6-C7-C8
2	f	201	MYR	C5-C6-C7-C8
2	h	201	MYR	C5-C6-C7-C8
2	X	201	MYR	C5-C6-C7-C8
2	Y	201	MYR	C5-C6-C7-C8
2	Z	201	MYR	C5-C6-C7-C8
2	C	201	MYR	C5-C6-C7-C8
2	Q	201	MYR	C5-C6-C7-C8
2	d	201	MYR	C5-C6-C7-C8
2	l	201	MYR	C5-C6-C7-C8
2	m	201	MYR	C5-C6-C7-C8
2	B	201	MYR	C5-C6-C7-C8
2	D	201	MYR	C5-C6-C7-C8
2	P	201	MYR	C5-C6-C7-C8
2	b	201	MYR	C5-C6-C7-C8
2	E	201	MYR	C5-C6-C7-C8
2	c	201	MYR	C5-C6-C7-C8
2	F	201	MYR	C5-C6-C7-C8
2	R	201	MYR	C5-C6-C7-C8
2	S	201	MYR	C5-C6-C7-C8
2	I	201	MYR	C5-C6-C7-C8
2	K	201	MYR	C5-C6-C7-C8
2	M	201	MYR	C5-C6-C7-C8
2	O	201	MYR	C5-C6-C7-C8

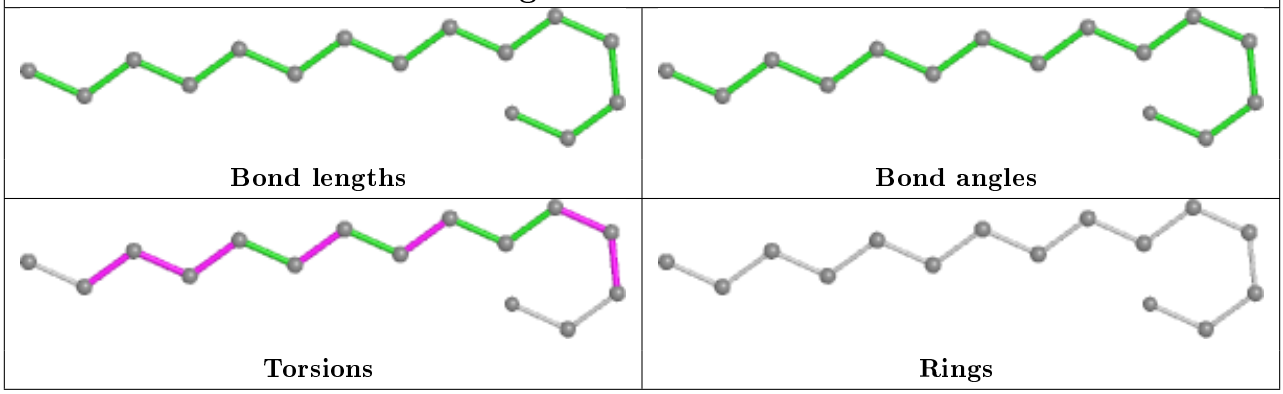
There are no ring outliers.

No monomer is involved in short contacts.

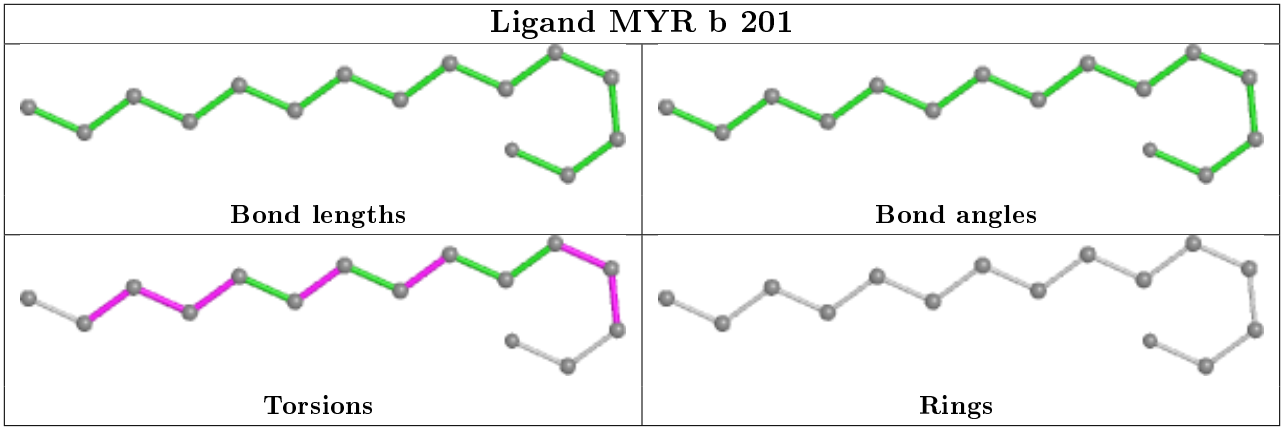
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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.

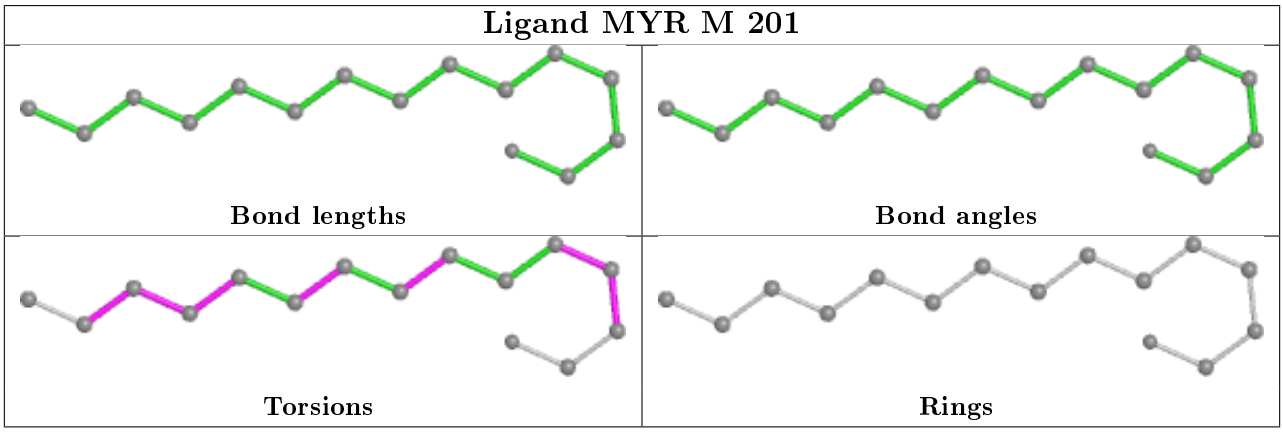
Ligand MYR B 201



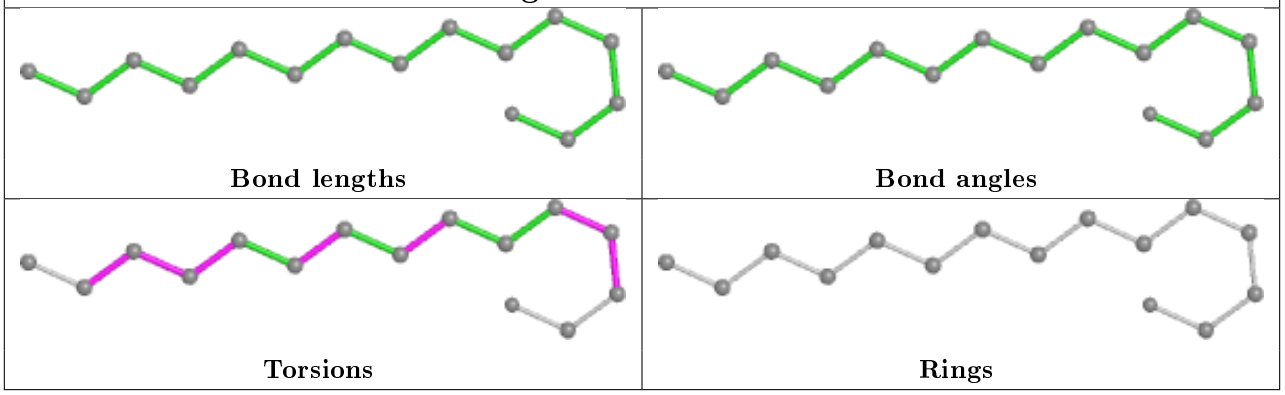
Ligand MYR b 201



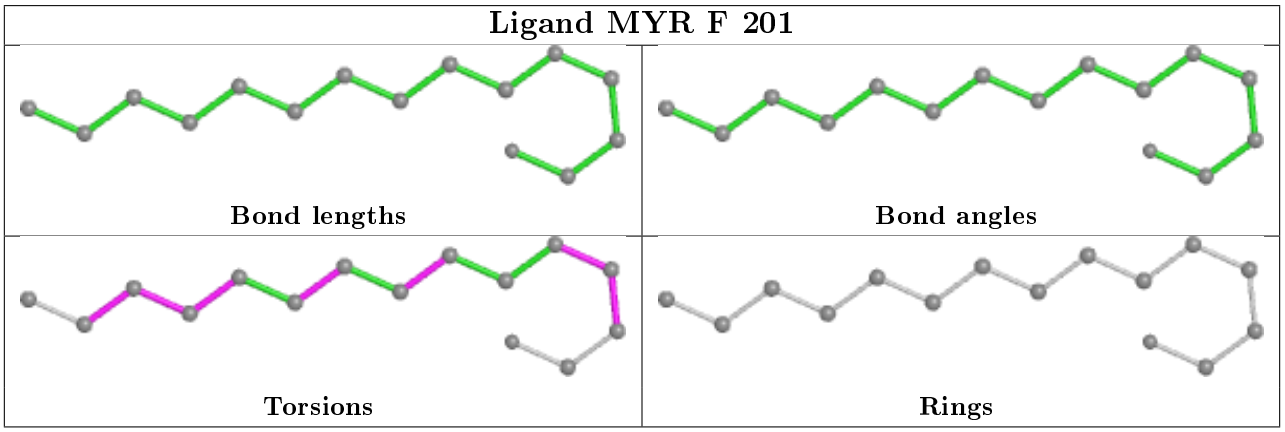
Ligand MYR M 201



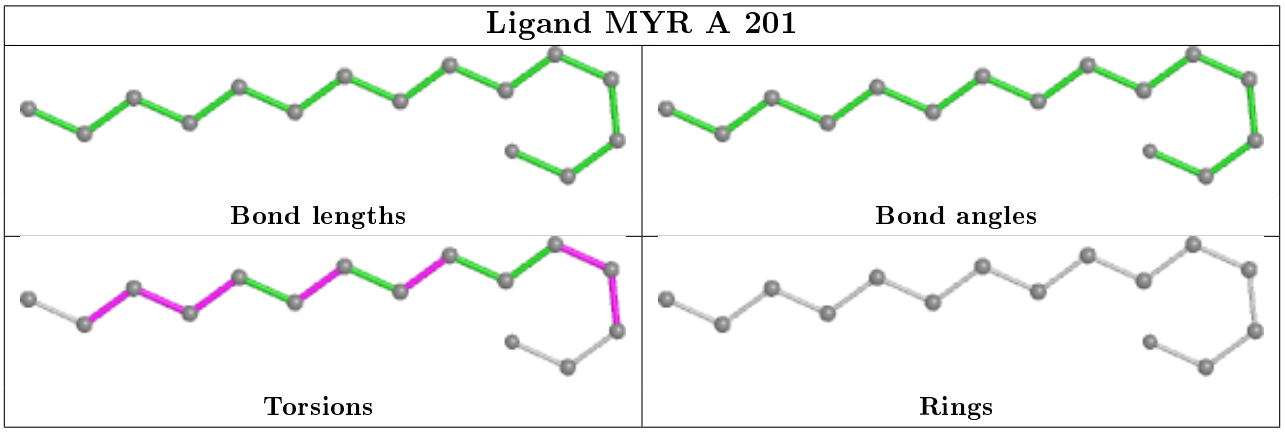
Ligand MYR S 201



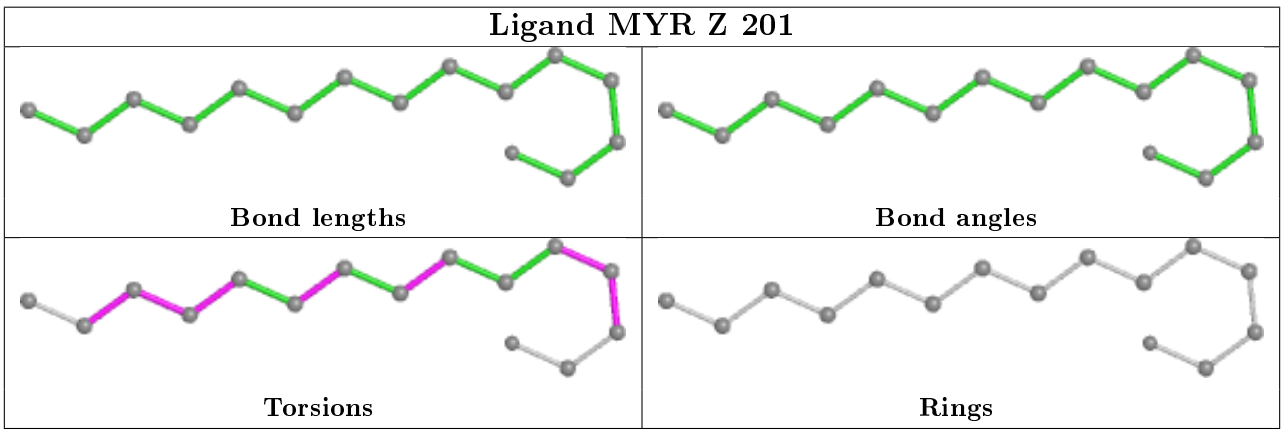
Ligand MYR F 201



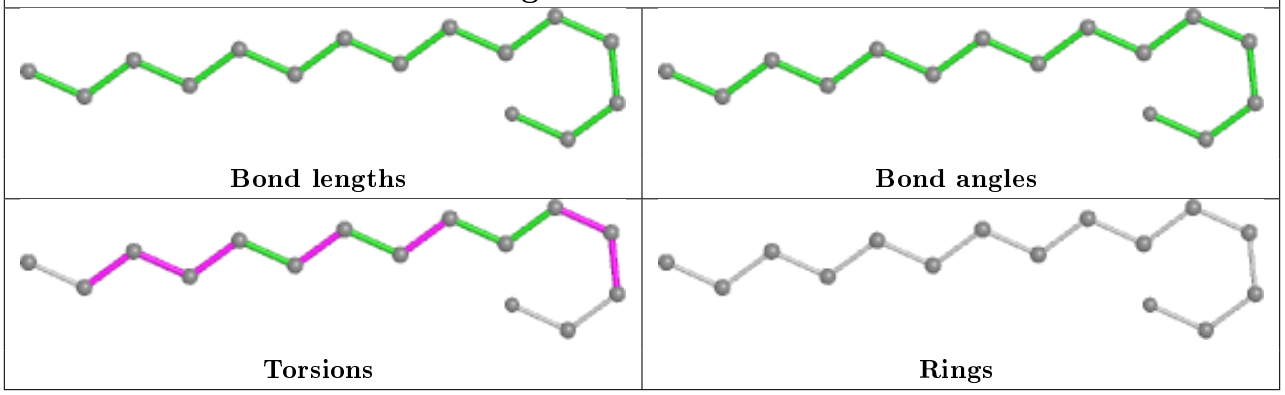
Ligand MYR A 201



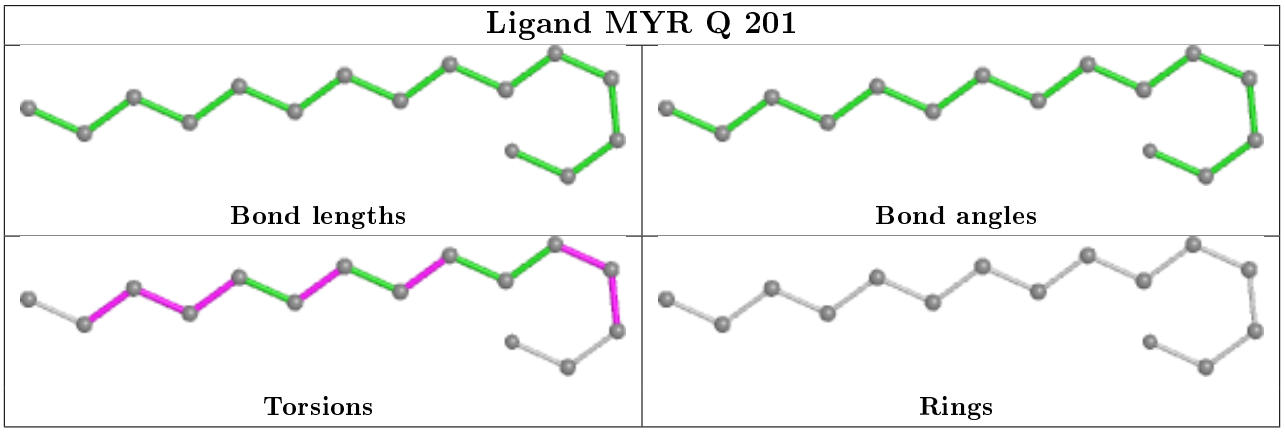
Ligand MYR Z 201



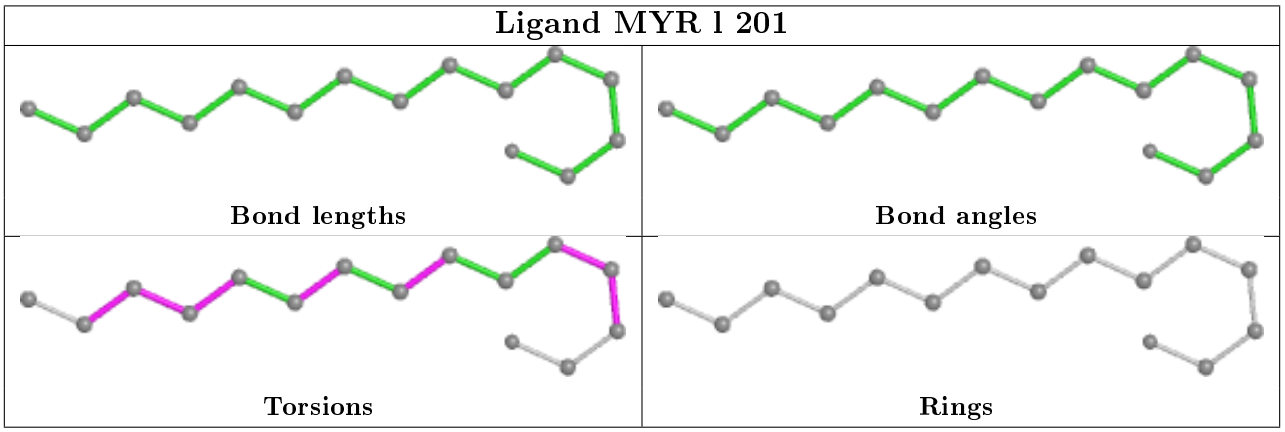
Ligand MYR h 201



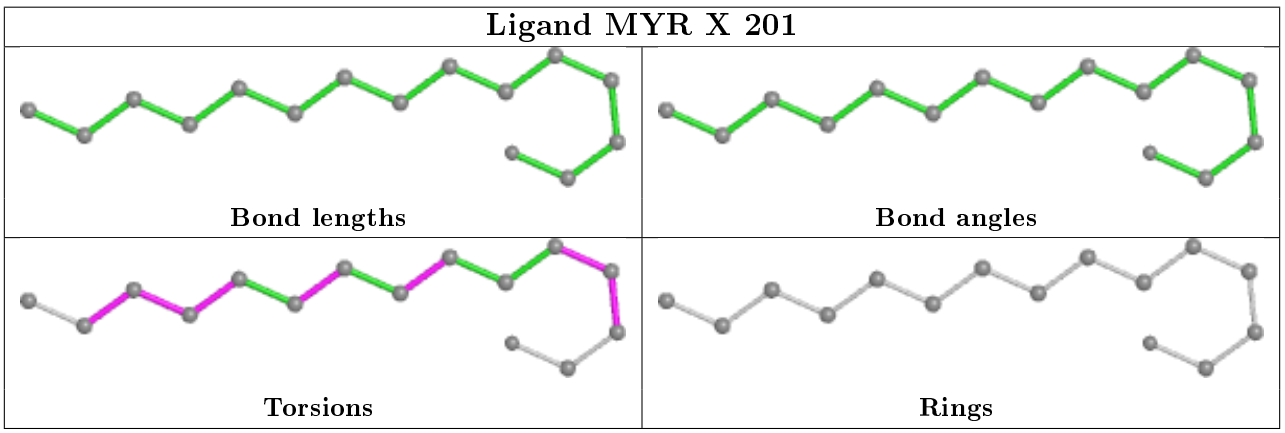
Ligand MYR Q 201



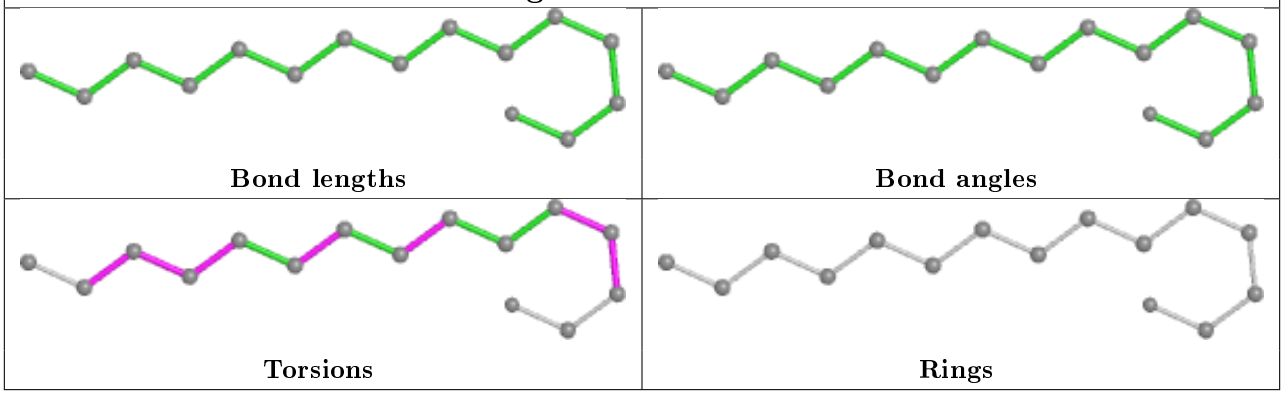
Ligand MYR l 201



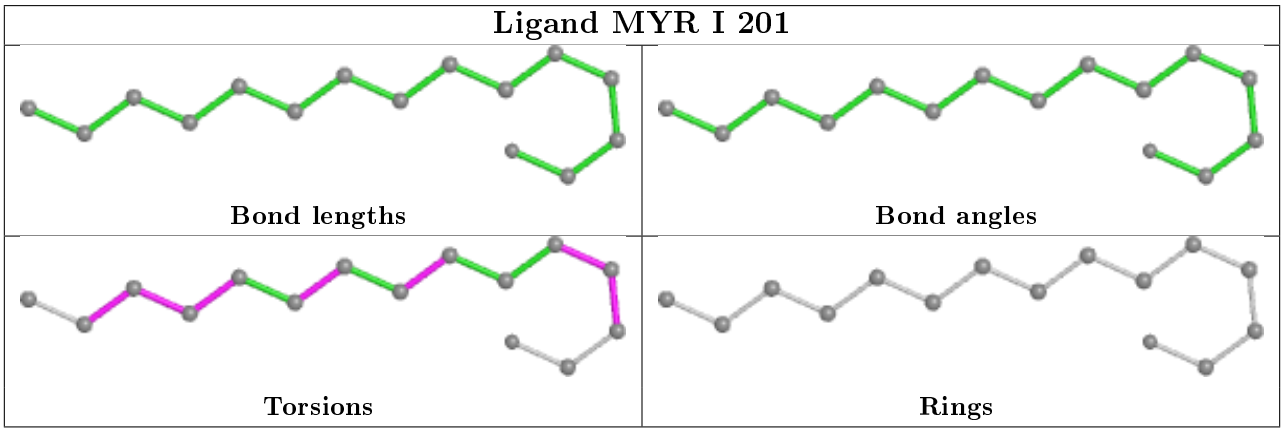
Ligand MYR X 201



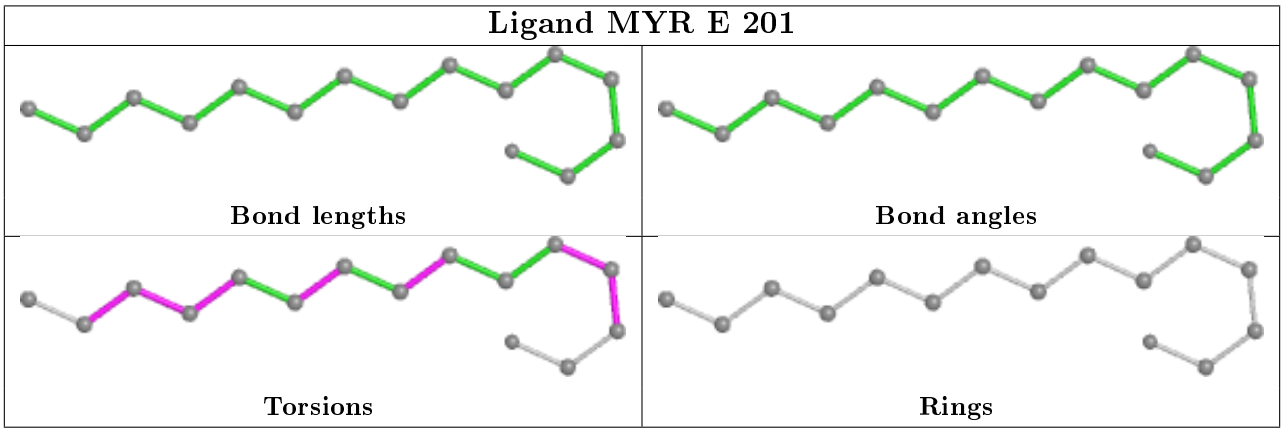
Ligand MYR f 201



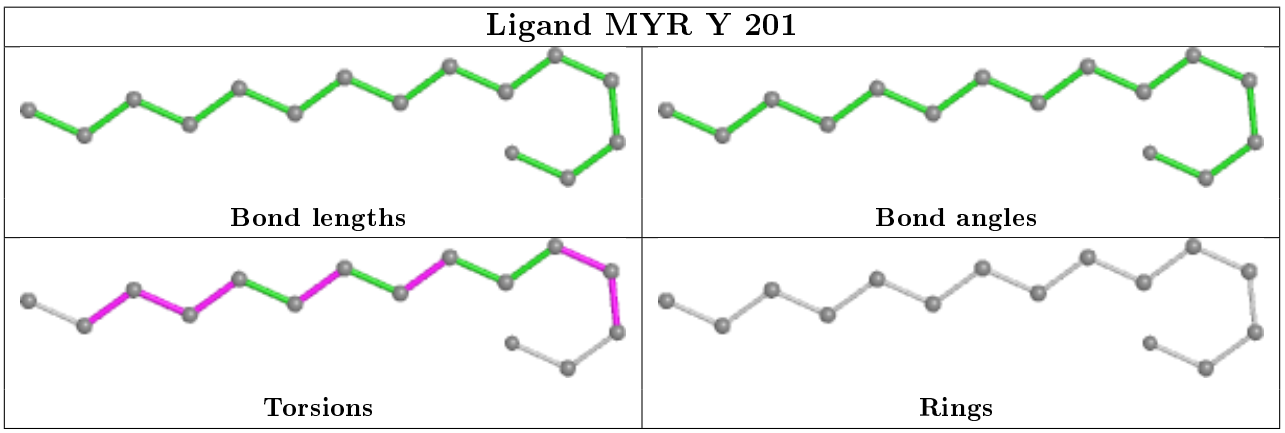
Ligand MYR I 201



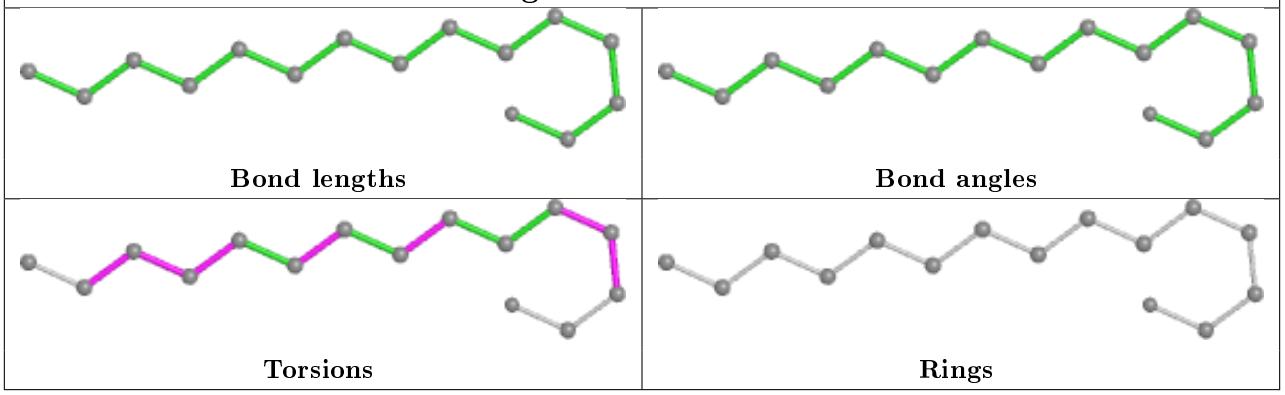
Ligand MYR E 201



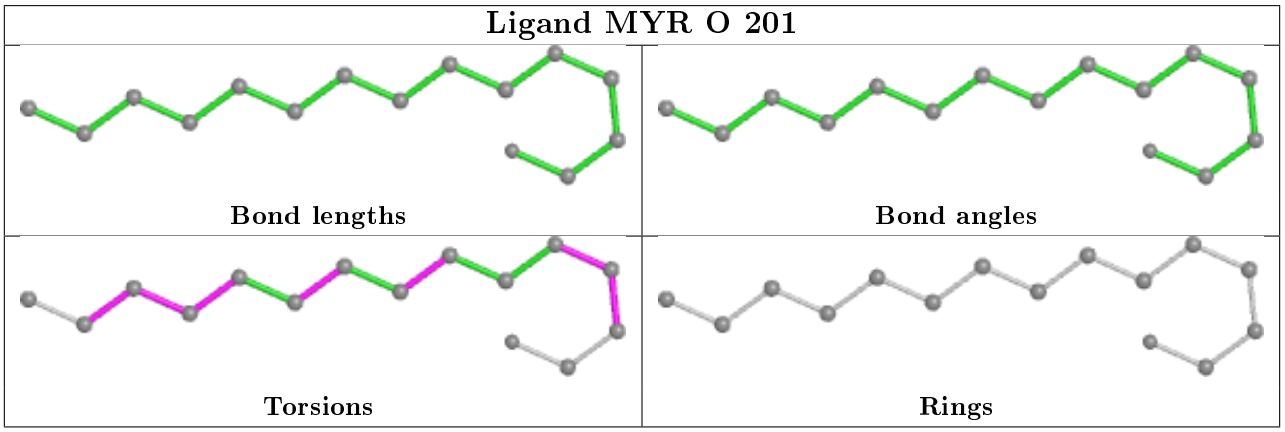
Ligand MYR Y 201



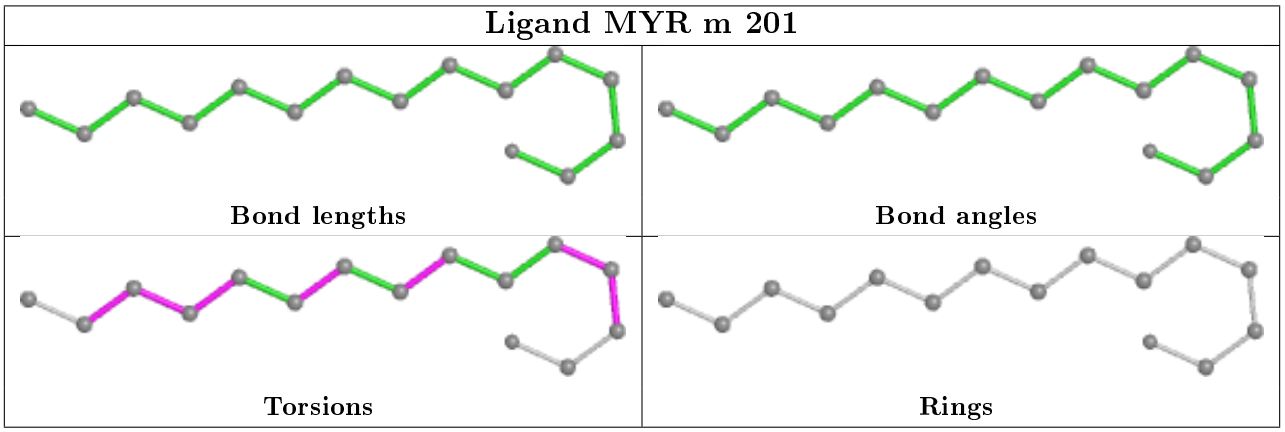
Ligand MYR d 201



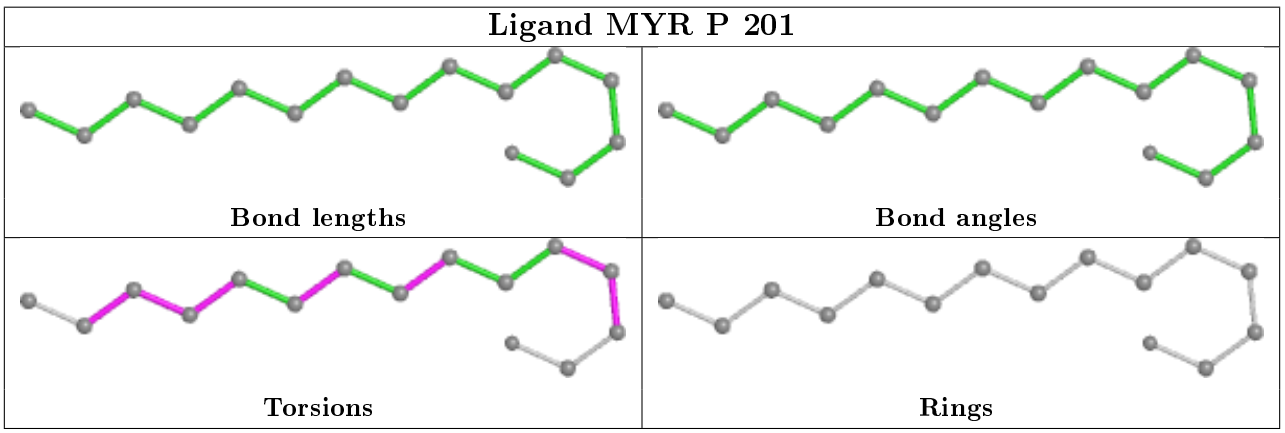
Ligand MYR O 201



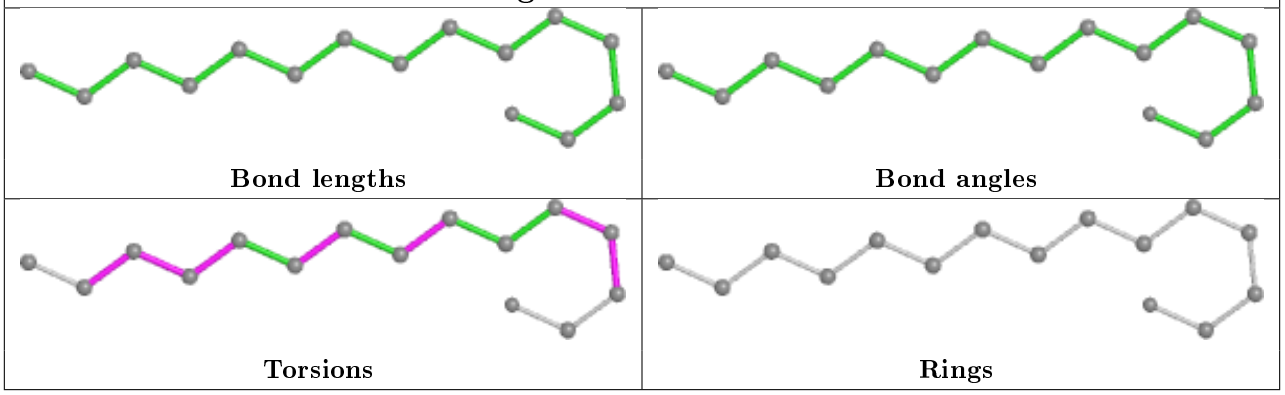
Ligand MYR m 201



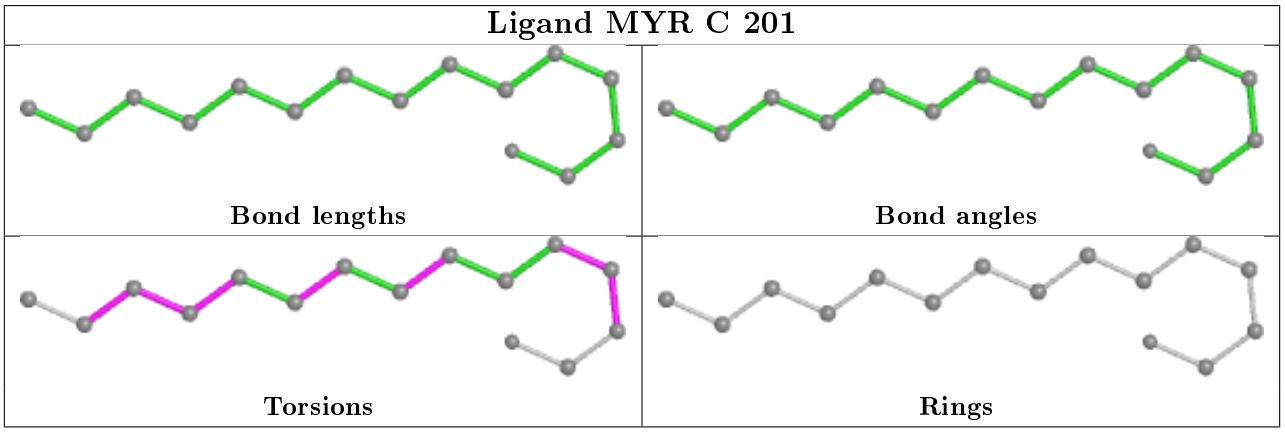
Ligand MYR P 201



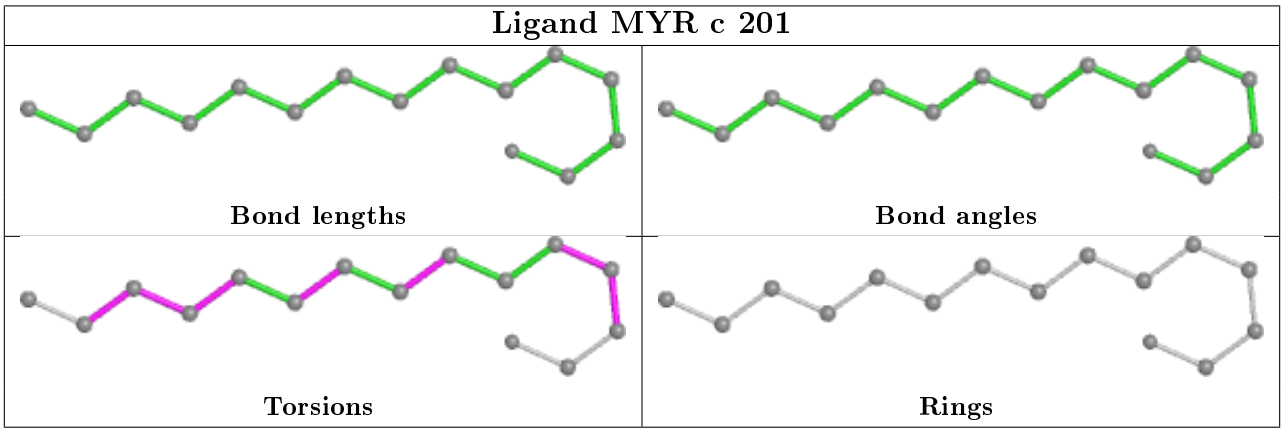
Ligand MYR K 201



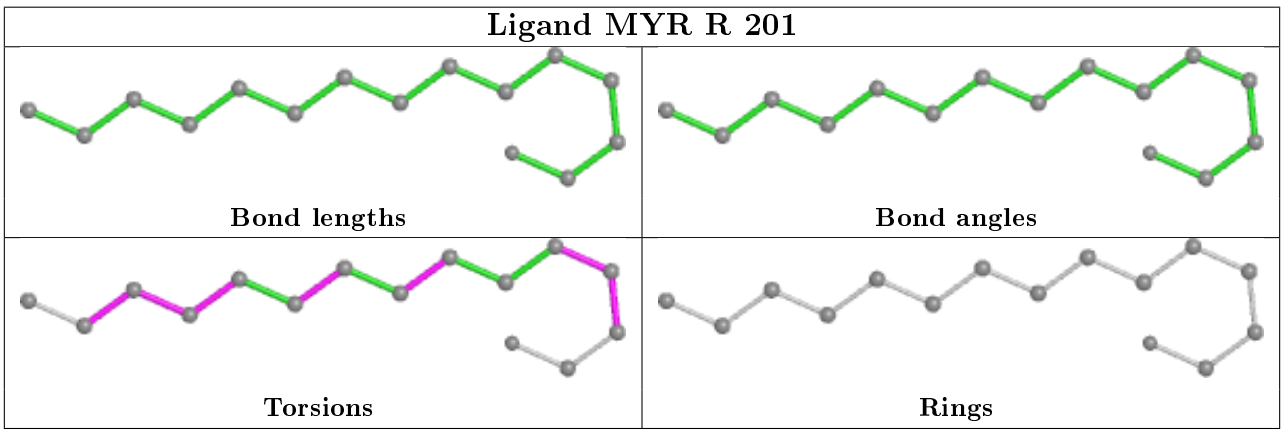
Ligand MYR C 201

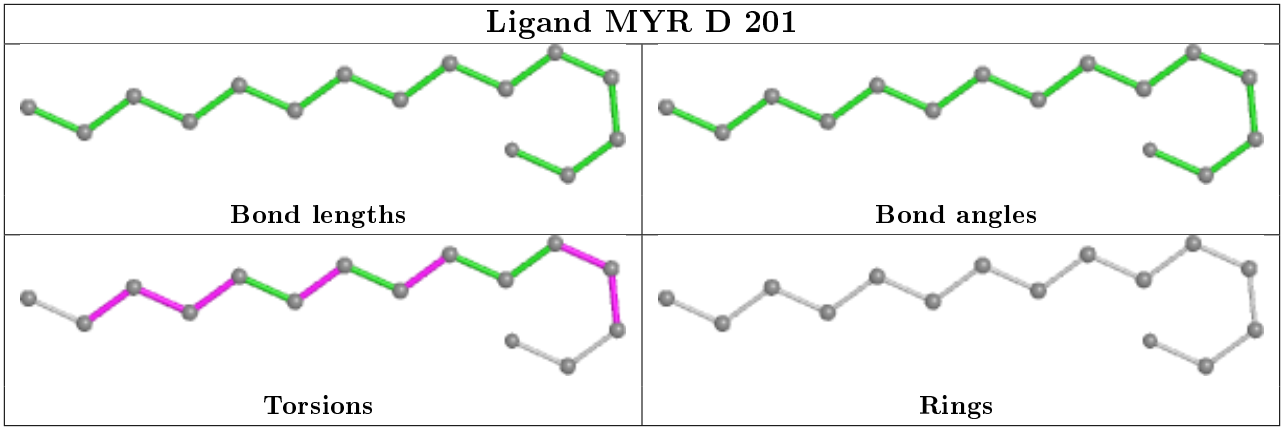


Ligand MYR c 201



Ligand MYR R 201





5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

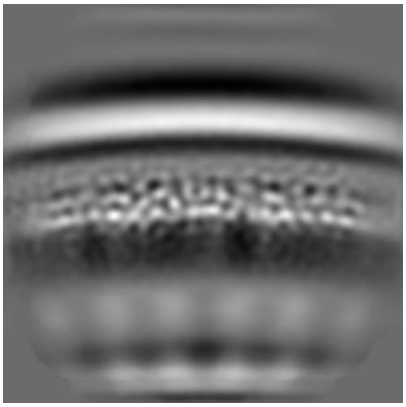
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-13087. These allow visual inspection of the internal detail of the map and identification of artifacts.

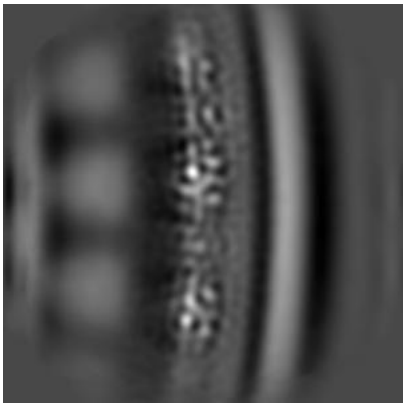
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

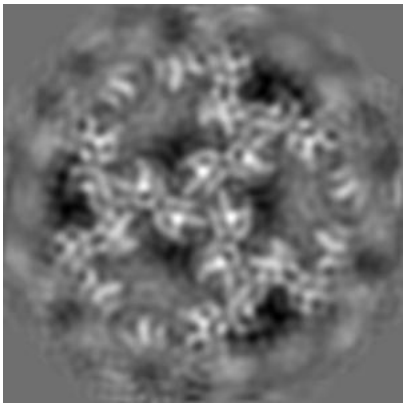
6.1.1 Primary map



X



Y

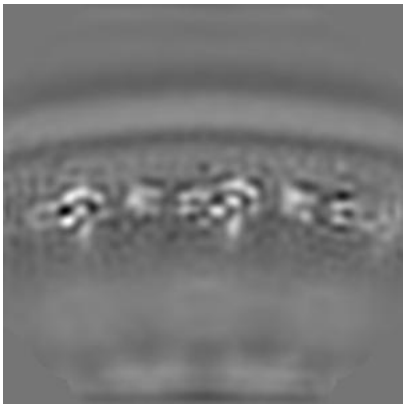


Z

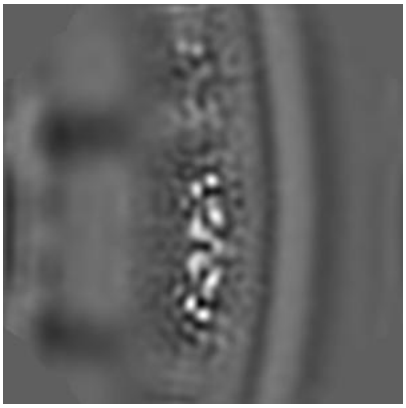
The images above show the map projected in three orthogonal directions.

6.2 Central slices

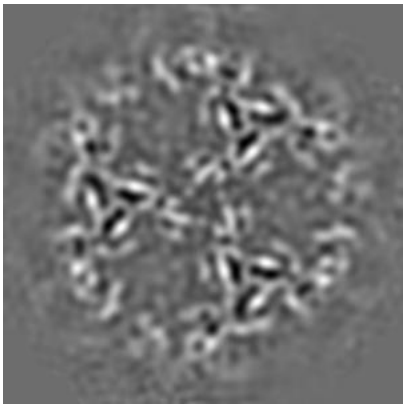
6.2.1 Primary map



X Index: 96



Y Index: 96

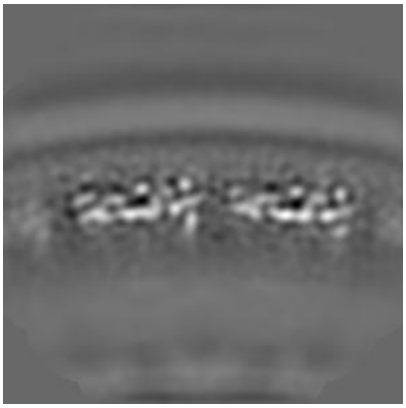


Z Index: 96

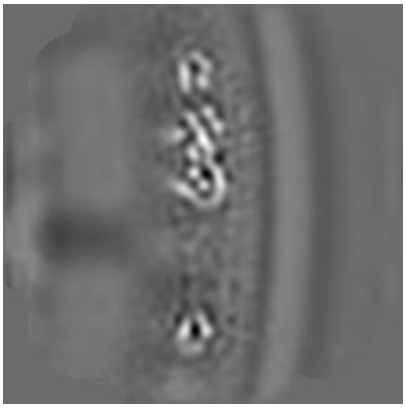
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

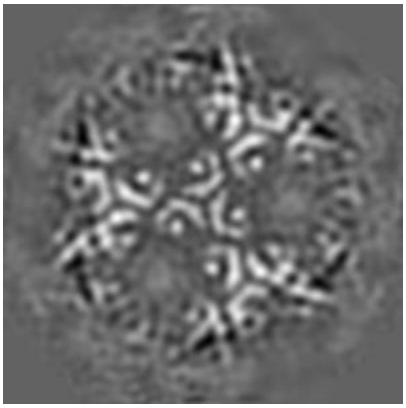
6.3.1 Primary map



X Index: 110



Y Index: 67

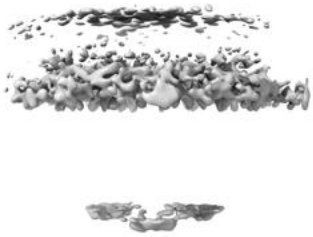


Z Index: 91

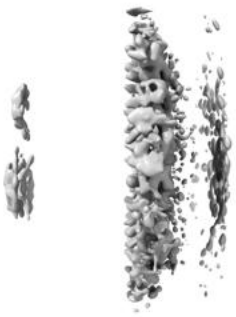
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

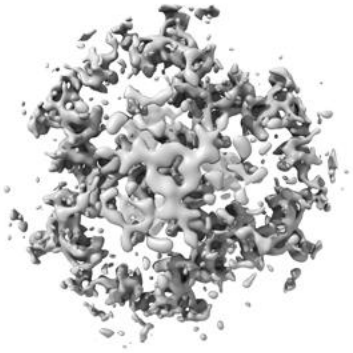
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 2.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

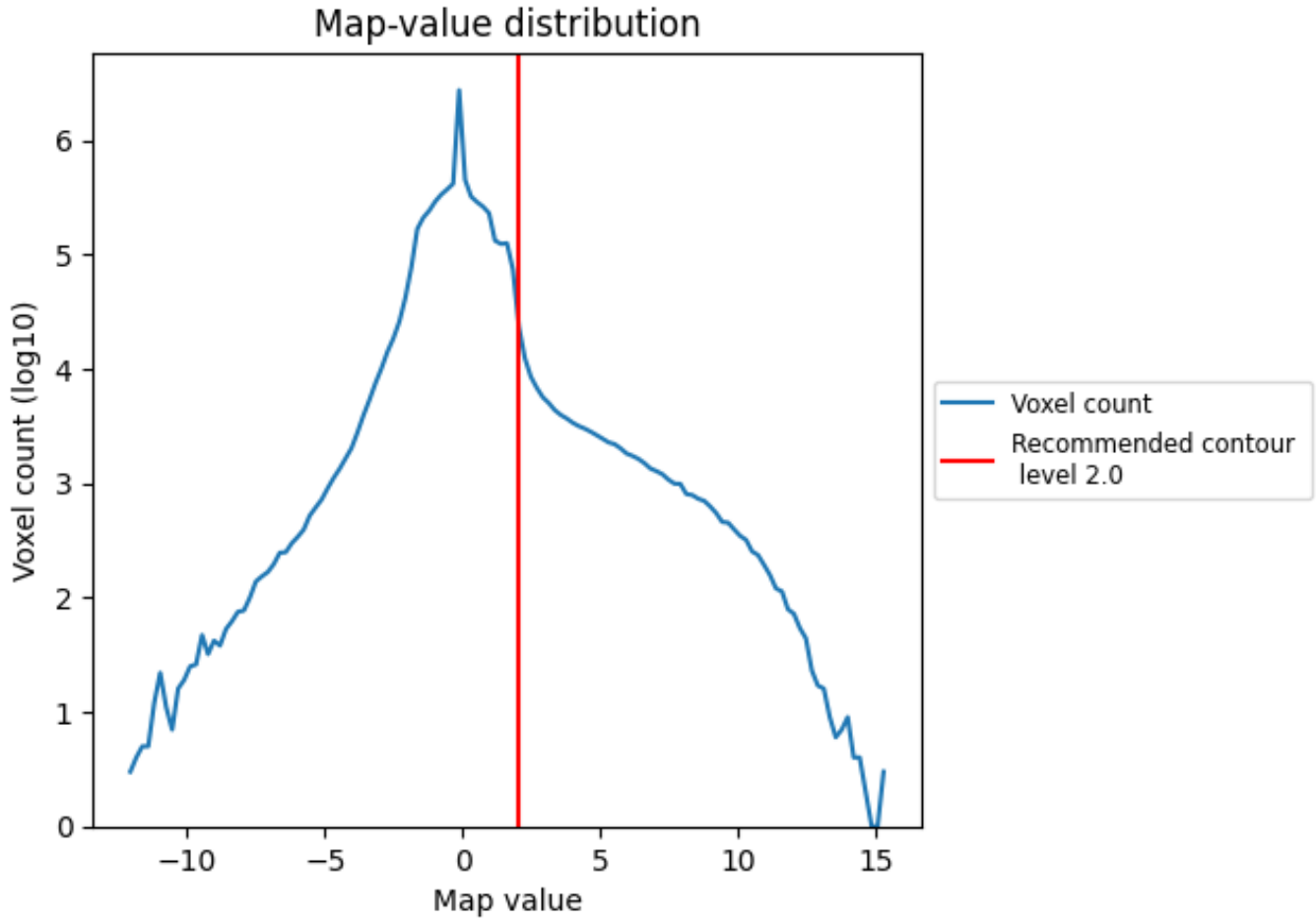
6.5 Mask visualisation (i)

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

7 Map analysis

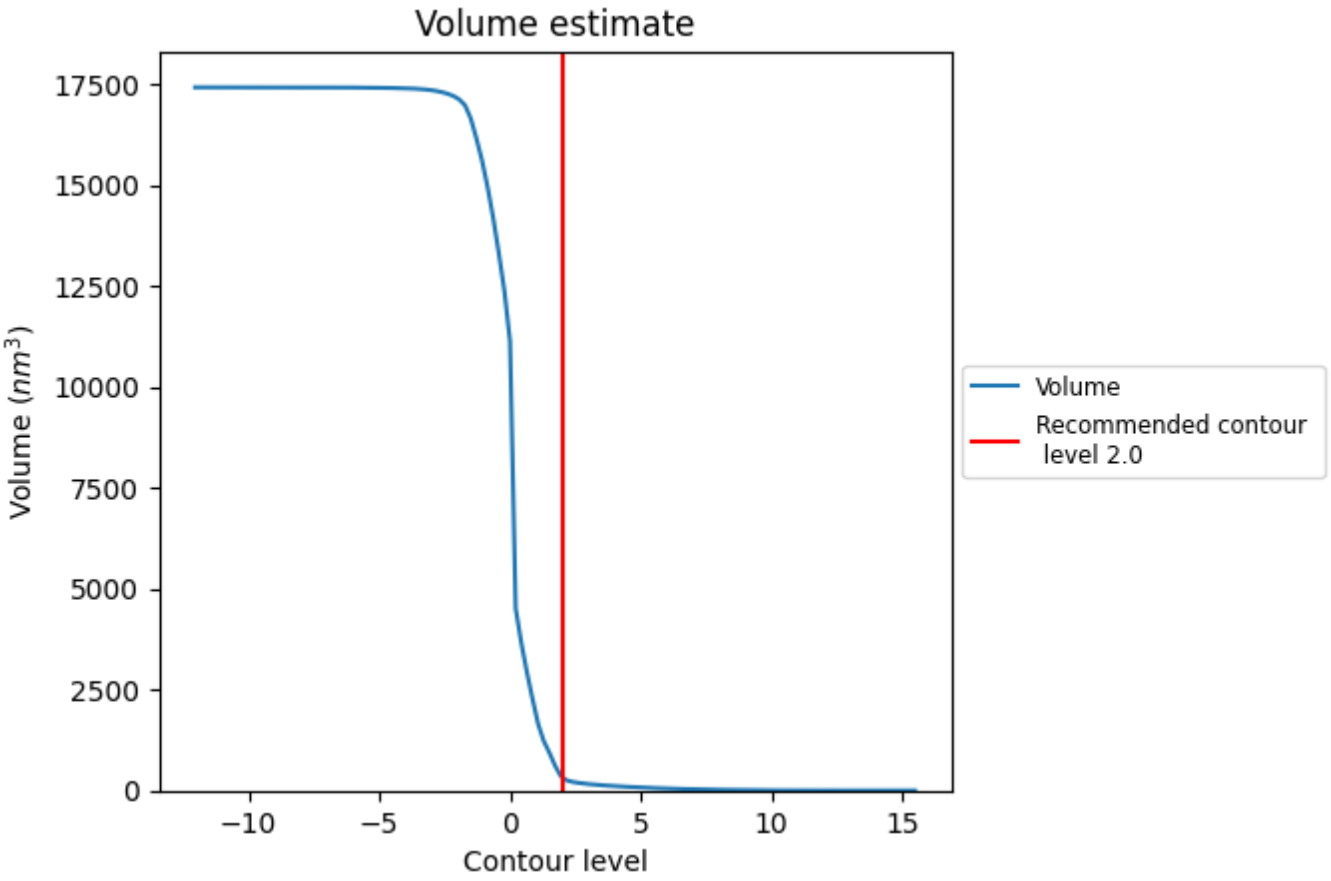
This section contains the results of statistical analysis of the map.

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.

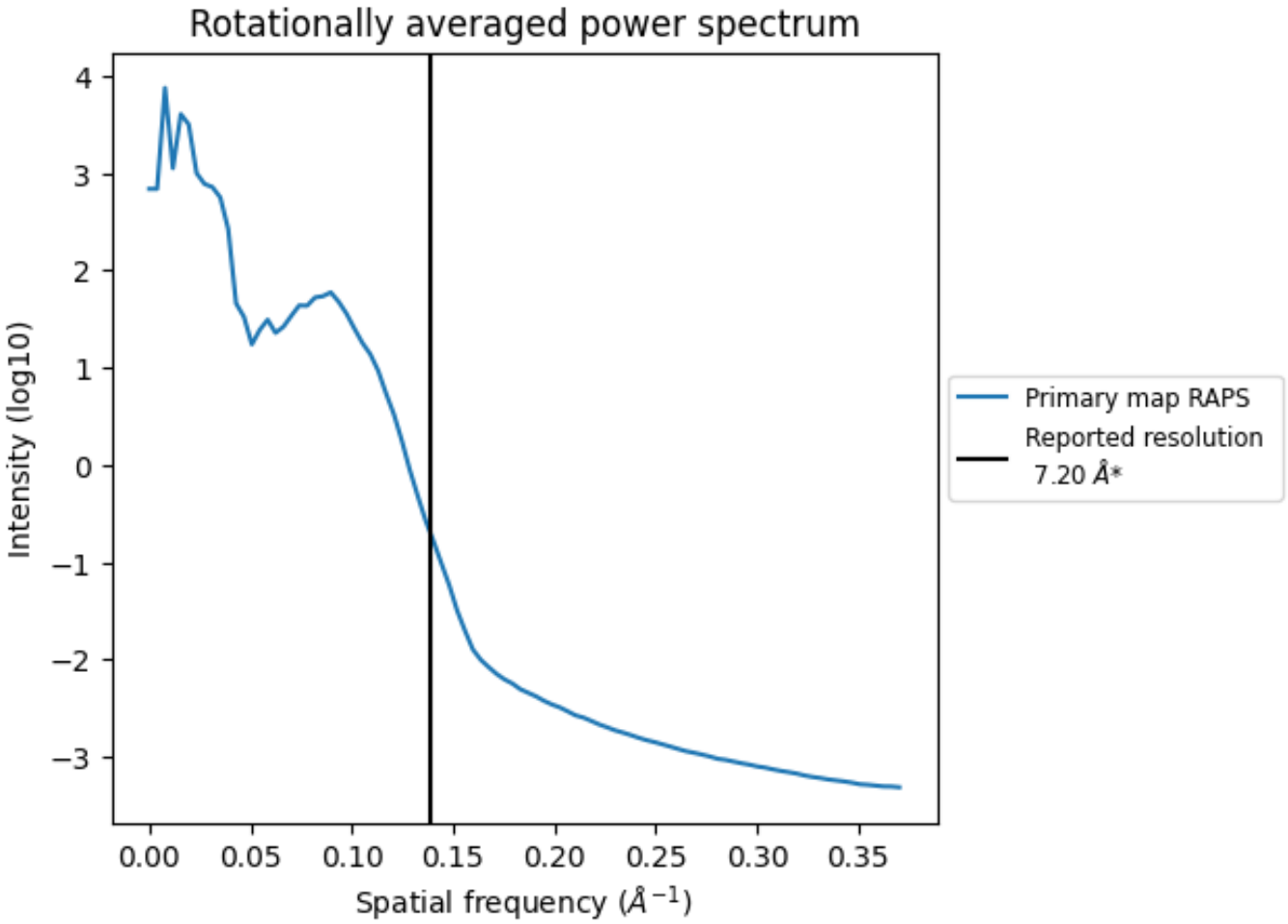
7.2 Volume estimate



The volume at the recommended contour level is 328 nm^3; this corresponds to an approximate mass of 296 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 0.139 Å^{-1}

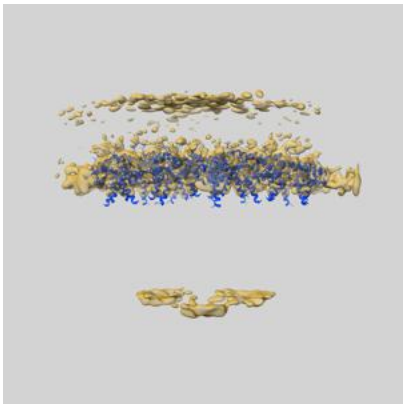
8 Fourier-Shell correlation

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

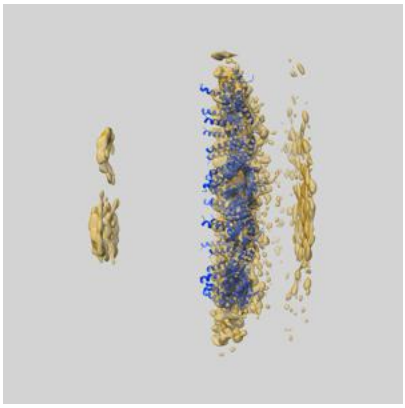
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-13087 and PDB model 7OVQ. Per-residue inclusion information can be found in section 3 on page 7.

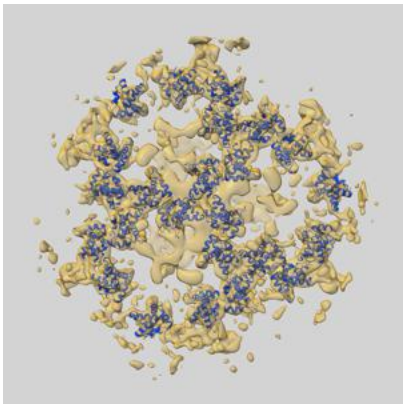
9.1 Map-model overlay



X



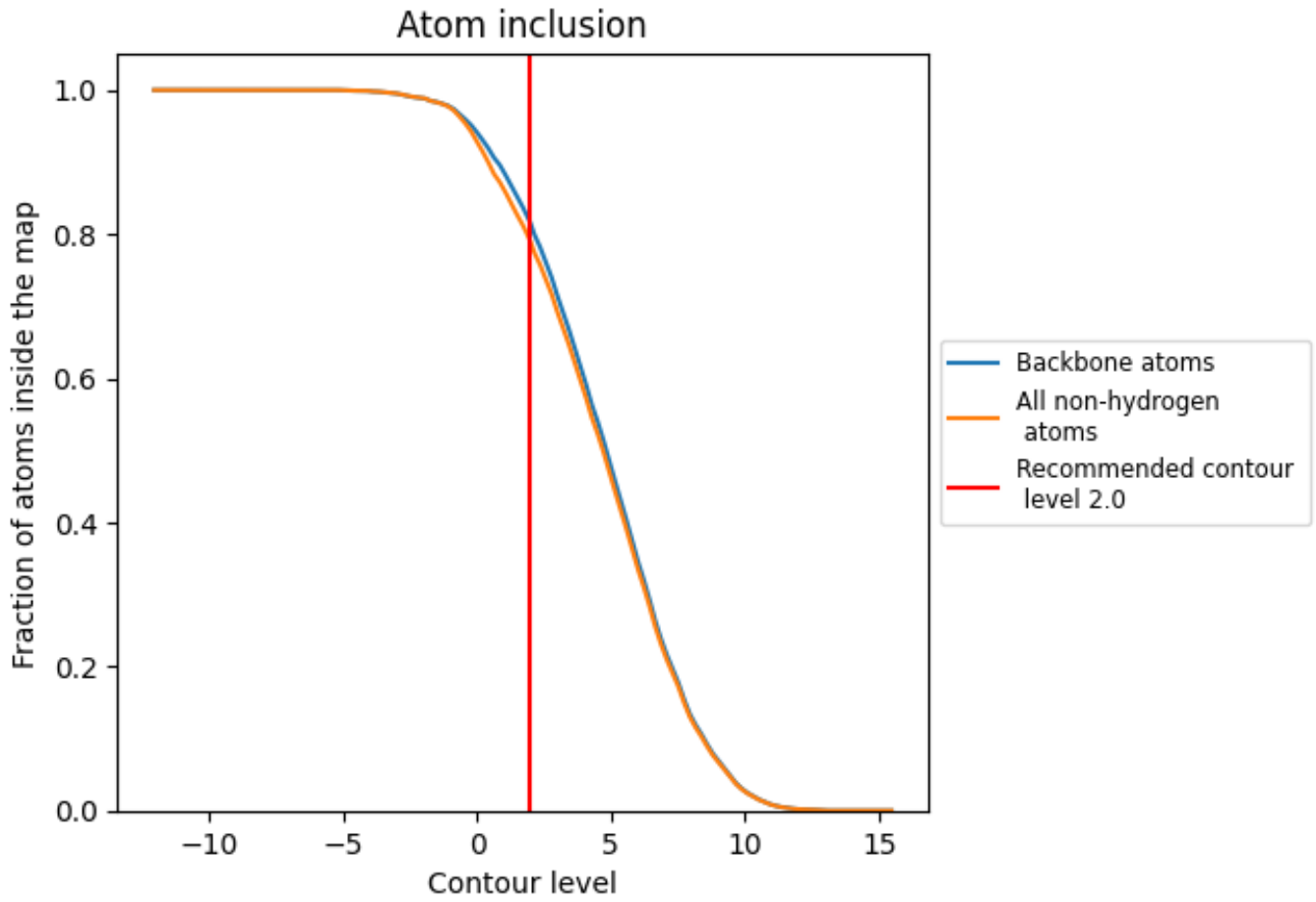
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 2.0 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 Atom inclusion (i)



At the recommended contour level, 82% of all backbone atoms, 79% of all non-hydrogen atoms, are inside the map.