Full wwPDB EM Validation Report

Mar 28, 2026 – 01:57 PM UTC

PDB ID	:	8U53 / pdb_00008u53
EMDB ID	:	EMD-41911
Title	:	Mechanically activated ion channel OSCA3.1 in nanodiscs
Authors	:	Jojoa-Cruz, S.; Lee, W.H.; Ward, A.B.
Deposited on	:	2023-09-12
Resolution	:	2.60 Å(reported)
Based on initial model	:	.

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

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

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

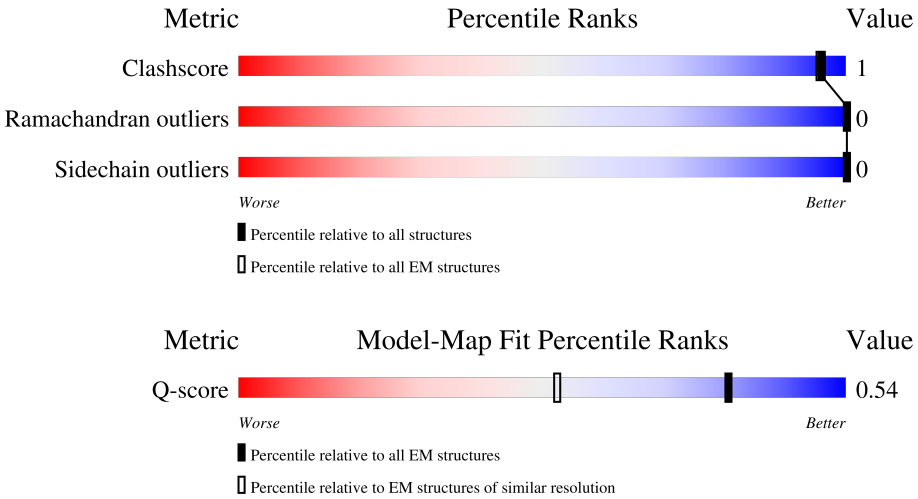
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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 2.60 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	8728 (2.10 - 3.10)

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	734	7% 73% 5% 22%
1	B	734	7% 73% 5% 22%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 9562 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 CSC1-like protein ERD4.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	574	Total	C	N	O	S	0	0
			4517	3013	719	768	17		
1	B	574	Total	C	N	O	S	0	0
			4517	3013	719	768	17		

There are 94 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	234	UNK	SER	conflict	UNP Q9C8G5
A	235	UNK	LYS	conflict	UNP Q9C8G5
A	236	UNK	VAL	conflict	UNP Q9C8G5
A	237	UNK	ASN	conflict	UNP Q9C8G5
A	238	UNK	LYS	conflict	UNP Q9C8G5
A	239	UNK	ILE	conflict	UNP Q9C8G5
A	240	UNK	TRP	conflict	UNP Q9C8G5
A	241	UNK	GLU	conflict	UNP Q9C8G5
A	242	UNK	LYS	conflict	UNP Q9C8G5
A	243	UNK	LEU	conflict	UNP Q9C8G5
A	244	UNK	GLU	conflict	UNP Q9C8G5
A	245	UNK	GLY	conflict	UNP Q9C8G5
A	246	UNK	TYR	conflict	UNP Q9C8G5
A	280	UNK	SER	conflict	UNP Q9C8G5
A	281	UNK	ILE	conflict	UNP Q9C8G5
A	282	UNK	GLU	conflict	UNP Q9C8G5
A	283	UNK	TYR	conflict	UNP Q9C8G5
A	284	UNK	TYR	conflict	UNP Q9C8G5
A	285	UNK	THR	conflict	UNP Q9C8G5
A	286	UNK	GLU	conflict	UNP Q9C8G5
A	287	UNK	LEU	conflict	UNP Q9C8G5
A	288	UNK	ILE	conflict	UNP Q9C8G5
A	289	UNK	ASN	conflict	UNP Q9C8G5
A	290	UNK	GLU	conflict	UNP Q9C8G5
A	291	UNK	SER	conflict	UNP Q9C8G5
A	292	UNK	VAL	conflict	UNP Q9C8G5

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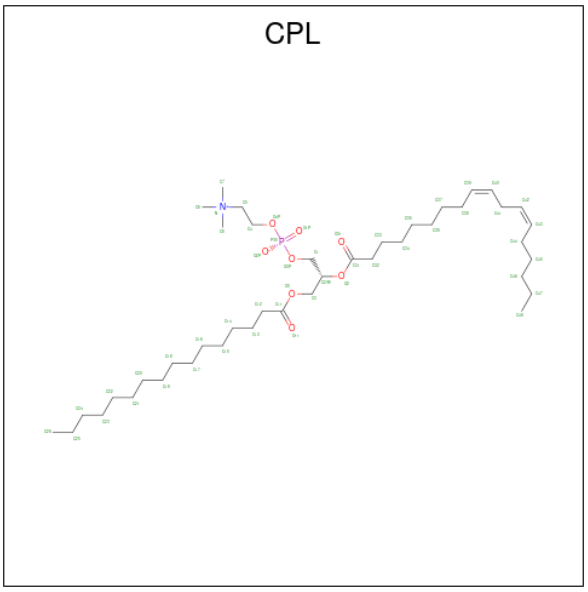
Chain	Residue	Modelled	Actual	Comment	Reference
A	293	UNK	ALA	conflict	UNP Q9C8G5
A	294	UNK	LYS	conflict	UNP Q9C8G5
A	295	UNK	LEU	conflict	UNP Q9C8G5
A	296	UNK	GLU	conflict	UNP Q9C8G5
A	297	UNK	THR	conflict	UNP Q9C8G5
A	298	UNK	GLU	conflict	UNP Q9C8G5
A	299	UNK	GLN	conflict	UNP Q9C8G5
A	300	UNK	LYS	conflict	UNP Q9C8G5
A	301	UNK	ALA	conflict	UNP Q9C8G5
A	302	UNK	VAL	conflict	UNP Q9C8G5
A	303	UNK	LEU	conflict	UNP Q9C8G5
A	725	GLY	-	expression tag	UNP Q9C8G5
A	726	THR	-	expression tag	UNP Q9C8G5
A	727	GLY	-	expression tag	UNP Q9C8G5
A	728	THR	-	expression tag	UNP Q9C8G5
A	729	LEU	-	expression tag	UNP Q9C8G5
A	730	GLU	-	expression tag	UNP Q9C8G5
A	731	VAL	-	expression tag	UNP Q9C8G5
A	732	LEU	-	expression tag	UNP Q9C8G5
A	733	PHE	-	expression tag	UNP Q9C8G5
A	734	GLN	-	expression tag	UNP Q9C8G5
B	234	UNK	SER	conflict	UNP Q9C8G5
B	235	UNK	LYS	conflict	UNP Q9C8G5
B	236	UNK	VAL	conflict	UNP Q9C8G5
B	237	UNK	ASN	conflict	UNP Q9C8G5
B	238	UNK	LYS	conflict	UNP Q9C8G5
B	239	UNK	ILE	conflict	UNP Q9C8G5
B	240	UNK	TRP	conflict	UNP Q9C8G5
B	241	UNK	GLU	conflict	UNP Q9C8G5
B	242	UNK	LYS	conflict	UNP Q9C8G5
B	243	UNK	LEU	conflict	UNP Q9C8G5
B	244	UNK	GLU	conflict	UNP Q9C8G5
B	245	UNK	GLY	conflict	UNP Q9C8G5
B	246	UNK	TYR	conflict	UNP Q9C8G5
B	280	UNK	SER	conflict	UNP Q9C8G5
B	281	UNK	ILE	conflict	UNP Q9C8G5
B	282	UNK	GLU	conflict	UNP Q9C8G5
B	283	UNK	TYR	conflict	UNP Q9C8G5
B	284	UNK	TYR	conflict	UNP Q9C8G5
B	285	UNK	THR	conflict	UNP Q9C8G5
B	286	UNK	GLU	conflict	UNP Q9C8G5
B	287	UNK	LEU	conflict	UNP Q9C8G5

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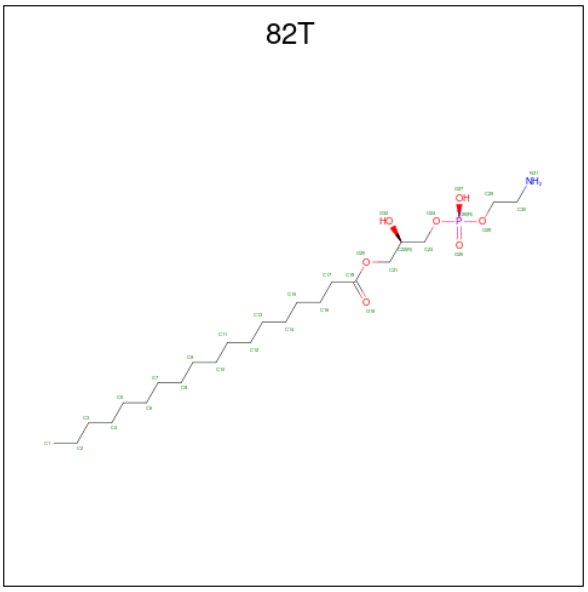
Chain	Residue	Modelled	Actual	Comment	Reference
B	288	UNK	ILE	conflict	UNP Q9C8G5
B	289	UNK	ASN	conflict	UNP Q9C8G5
B	290	UNK	GLU	conflict	UNP Q9C8G5
B	291	UNK	SER	conflict	UNP Q9C8G5
B	292	UNK	VAL	conflict	UNP Q9C8G5
B	293	UNK	ALA	conflict	UNP Q9C8G5
B	294	UNK	LYS	conflict	UNP Q9C8G5
B	295	UNK	LEU	conflict	UNP Q9C8G5
B	296	UNK	GLU	conflict	UNP Q9C8G5
B	297	UNK	THR	conflict	UNP Q9C8G5
B	298	UNK	GLU	conflict	UNP Q9C8G5
B	299	UNK	GLN	conflict	UNP Q9C8G5
B	300	UNK	LYS	conflict	UNP Q9C8G5
B	301	UNK	ALA	conflict	UNP Q9C8G5
B	302	UNK	VAL	conflict	UNP Q9C8G5
B	303	UNK	LEU	conflict	UNP Q9C8G5
B	725	GLY	-	expression tag	UNP Q9C8G5
B	726	THR	-	expression tag	UNP Q9C8G5
B	727	GLY	-	expression tag	UNP Q9C8G5
B	728	THR	-	expression tag	UNP Q9C8G5
B	729	LEU	-	expression tag	UNP Q9C8G5
B	730	GLU	-	expression tag	UNP Q9C8G5
B	731	VAL	-	expression tag	UNP Q9C8G5
B	732	LEU	-	expression tag	UNP Q9C8G5
B	733	PHE	-	expression tag	UNP Q9C8G5
B	734	GLN	-	expression tag	UNP Q9C8G5

- Molecule 2 is 1-PALMITOYL-2-LINOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: CPL) (formula: $C_{42}H_{80}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	B	1	Total	C	N	O	P	0
			52	42	1	8	1	

- Molecule 3 is [(2R)-3-[2-azanylethoxy(oxidanyl)phosphoryl]oxy-2-oxidanyl-propyl] octadecanoate (CCD ID: 82T) (formula: $C_{23}H_{48}NO_7P$).



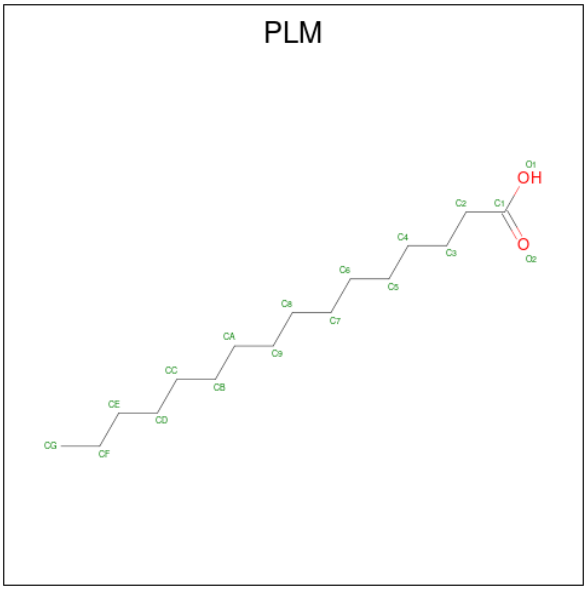
Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			32	23	1	7	1	

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Mol	Chain	Residues	Atoms					AltConf
3	B	1	Total	C	N	O	P	0
			32	23	1	7	1	

- Molecule 4 is PALMITIC ACID (CCD ID: PLM) (formula: $C_{16}H_{32}O_2$).



Mol	Chain	Residues	Atoms			AltConf
4	A	1	Total	C	O	0
			18	16	2	
4	A	1	Total	C	O	0
			18	16	2	
4	A	1	Total	C	O	0
			18	16	2	
4	A	1	Total	C	O	0
			18	16	2	
4	A	1	Total	C	O	0
			18	16	2	
4	A	1	Total	C	O	0
			18	16	2	
4	A	1	Total	C	O	0
			18	16	2	
4	A	1	Total	C	O	0
			18	16	2	
4	A	1	Total	C	O	0
			18	16	2	
4	A	1	Total	C	O	0
			18	16	2	

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Mol	Chain	Residues	Atoms			AltConf
4	B	1	Total	C	O	0
			18	16	2	
4	B	1	Total	C	O	0
			18	16	2	
4	B	1	Total	C	O	0
			18	16	2	
4	B	1	Total	C	O	0
			18	16	2	
4	B	1	Total	C	O	0
			18	16	2	
4	B	1	Total	C	O	0
			18	16	2	
4	B	1	Total	C	O	0
			18	16	2	
4	B	1	Total	C	O	0
			18	16	2	
4	B	1	Total	C	O	0
			18	16	2	
4	B	1	Total	C	O	0
			18	16	2	

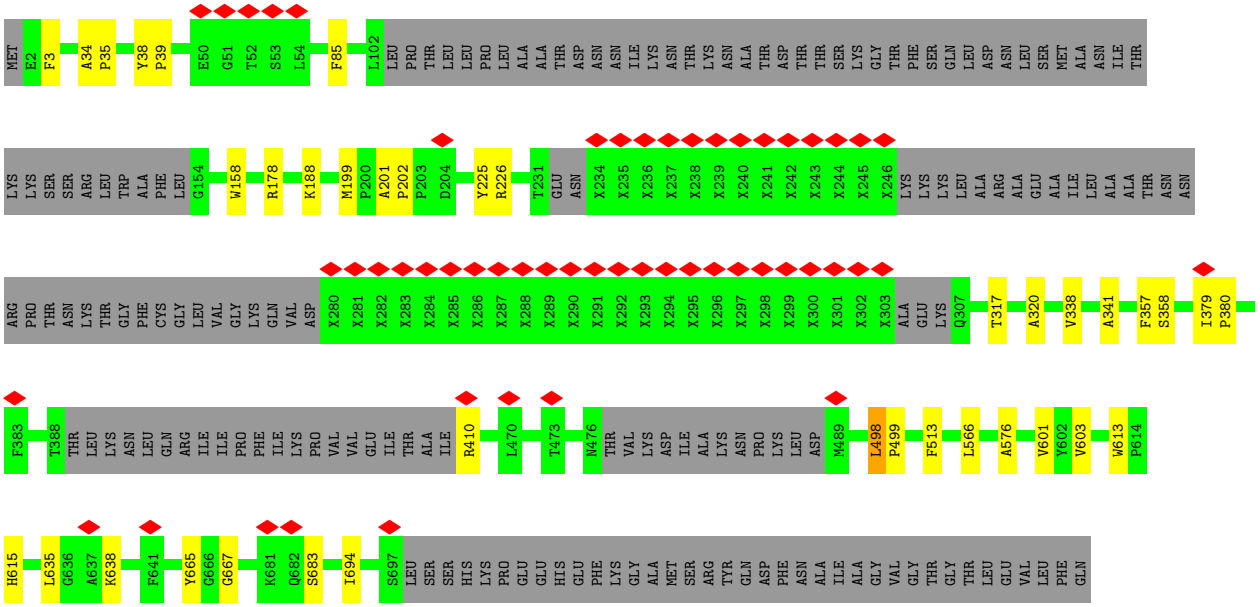
3 Residue-property plots (i)

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: CSC1-like protein ERD4

Chain A:

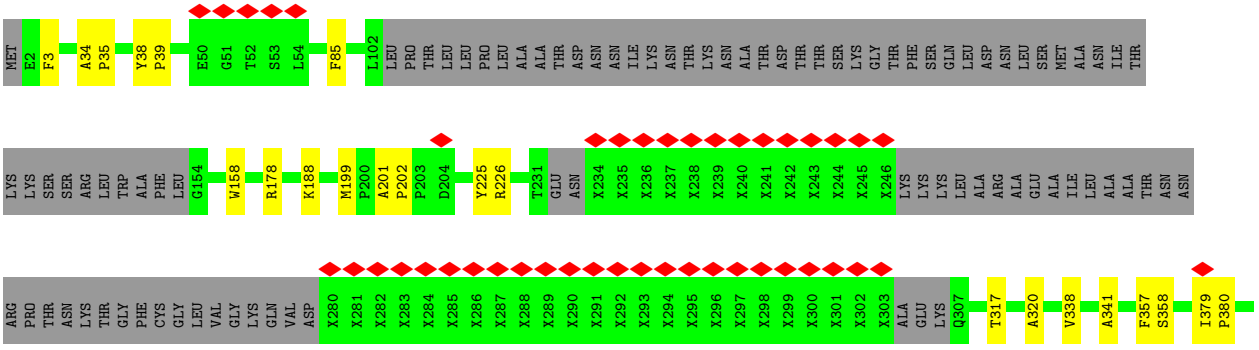


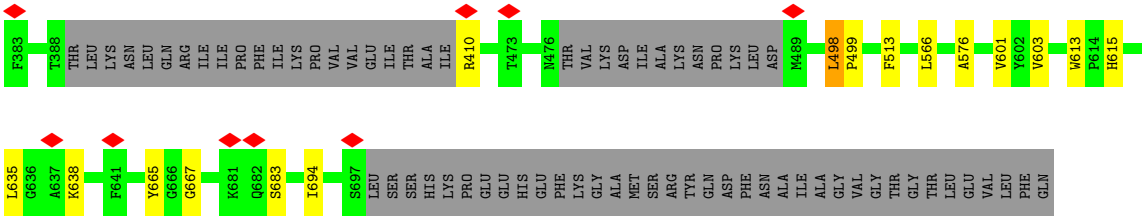


• Molecule 1: CSC1-like protein ERD4

Chain B:






F383
T388
THR LEU LYS ASN LEU GLN ARG ILE ILE PRO PHE ILE LYS PRO VAL VAL GLU ILE THR ALA ILE
R410
T473
M476
THR VAL LYS ASP ILE ALA LYS ASN PRO LYS LEU ASP
M489
L498
P499
F513
L566
A576
V601
Y602
V603
W613
P614
H615
L635
G636
A637
K638
F641
Y665
G666
G667
K681
Q682
S683
I694
S697
LEU SER SER HIS LYS PRO GLU GLU HIS GLU PHE LYS GLY ALA MET SER ARG TYR GLN ASP PHE ASN ALA ILE ALA GLY VAL GLY THR GLY THR LEU GLU VAL LEU PHE GLN

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	197944	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 ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.166	Depositor
Minimum map value	-0.004	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	206.0, 206.0, 206.0	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.03, 1.03, 1.03	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: PLM, 82T, CPL

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	1.23	4/4457 (0.1%)	1.21	35/6061 (0.6%)
1	B	1.23	4/4457 (0.1%)	1.21	35/6061 (0.6%)
All	All	1.23	8/8914 (0.1%)	1.21	70/12122 (0.6%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	566	LEU	CB-CG	-6.63	1.40	1.53
1	A	566	LEU	CB-CG	-6.59	1.40	1.53
1	A	410	ARG	NE-CZ	5.62	1.39	1.33
1	B	410	ARG	NE-CZ	5.61	1.39	1.33
1	A	158	TRP	NE1-CE2	-5.57	1.31	1.37
1	B	158	TRP	NE1-CE2	-5.53	1.31	1.37
1	B	613	TRP	NE1-CE2	-5.14	1.31	1.37
1	A	613	TRP	NE1-CE2	-5.10	1.31	1.37

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	601	VAL	N-CA-C	9.15	118.85	111.62
1	A	601	VAL	N-CA-C	9.12	118.82	111.62
1	A	576	ALA	CA-C-N	9.04	128.78	119.56
1	A	576	ALA	C-N-CA	9.04	128.78	119.56
1	B	576	ALA	CA-C-N	9.02	128.76	119.56
1	B	576	ALA	C-N-CA	9.02	128.76	119.56
1	A	513	PHE	CA-CB-CG	8.61	122.41	113.80
1	B	513	PHE	CA-CB-CG	8.59	122.39	113.80
1	B	357	PHE	CA-CB-CG	-8.20	105.60	113.80
1	A	357	PHE	CA-CB-CG	-8.19	105.61	113.80
1	A	665	TYR	N-CA-C	6.68	118.22	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	665	TYR	N-CA-C	6.66	118.20	111.07
1	B	202	PRO	CA-C-N	6.46	126.43	120.03
1	B	202	PRO	C-N-CA	6.46	126.43	120.03
1	A	202	PRO	CA-C-N	6.45	126.42	120.03
1	A	202	PRO	C-N-CA	6.45	126.42	120.03
1	B	683	SER	CA-C-N	6.32	126.29	119.78
1	B	683	SER	C-N-CA	6.32	126.29	119.78
1	A	683	SER	CA-C-N	6.29	126.26	119.78
1	A	683	SER	C-N-CA	6.29	126.26	119.78
1	A	615	HIS	N-CA-C	-6.23	104.41	111.14
1	B	615	HIS	N-CA-C	-6.23	104.42	111.14
1	B	341	ALA	CA-C-N	6.09	126.00	119.85
1	B	341	ALA	C-N-CA	6.09	126.00	119.85
1	A	341	ALA	CA-C-N	6.06	125.97	119.85
1	A	341	ALA	C-N-CA	6.06	125.97	119.85
1	B	199	MET	CA-C-N	6.02	125.99	120.03
1	B	199	MET	C-N-CA	6.02	125.99	120.03
1	A	199	MET	CA-C-N	5.99	125.95	120.03
1	A	199	MET	C-N-CA	5.99	125.95	120.03
1	B	201	ALA	CA-C-N	5.95	126.50	120.38
1	B	201	ALA	C-N-CA	5.95	126.50	120.38
1	A	201	ALA	CA-C-N	5.93	126.48	120.38
1	A	201	ALA	C-N-CA	5.93	126.48	120.38
1	B	338	VAL	N-CA-C	5.91	116.64	108.12
1	A	338	VAL	N-CA-C	5.91	116.63	108.12
1	A	410	ARG	CA-C-N	5.83	128.10	120.28
1	A	410	ARG	C-N-CA	5.83	128.10	120.28
1	B	410	ARG	CA-C-N	5.82	128.08	120.28
1	B	410	ARG	C-N-CA	5.82	128.08	120.28
1	B	603	VAL	CA-C-N	5.78	125.71	119.76
1	B	603	VAL	C-N-CA	5.78	125.71	119.76
1	A	603	VAL	CA-C-N	5.76	125.69	119.76
1	A	603	VAL	C-N-CA	5.76	125.69	119.76
1	B	498	LEU	CA-C-N	5.60	125.27	119.56
1	B	498	LEU	C-N-CA	5.60	125.27	119.56
1	A	498	LEU	CA-C-N	5.56	125.23	119.56
1	A	498	LEU	C-N-CA	5.56	125.23	119.56
1	B	638	LYS	CA-C-N	5.46	130.12	122.36
1	B	638	LYS	C-N-CA	5.46	130.12	122.36
1	A	638	LYS	CA-C-N	5.45	130.10	122.36
1	A	638	LYS	C-N-CA	5.45	130.10	122.36
1	A	188	LYS	CA-C-N	5.32	125.64	119.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	188	LYS	C-N-CA	5.32	125.64	119.47
1	B	188	LYS	CA-C-N	5.29	125.60	119.47
1	B	188	LYS	C-N-CA	5.29	125.60	119.47
1	B	694	ILE	CA-C-N	5.24	125.44	120.31
1	B	694	ILE	C-N-CA	5.24	125.44	120.31
1	A	694	ILE	CA-C-N	5.22	125.43	120.31
1	A	694	ILE	C-N-CA	5.22	125.43	120.31
1	A	566	LEU	CB-CA-C	-5.21	101.99	110.85
1	B	566	LEU	CB-CA-C	-5.20	102.01	110.85
1	B	635	LEU	N-CA-C	-5.11	105.71	111.28
1	A	635	LEU	N-CA-C	-5.10	105.72	111.28
1	A	3	PHE	N-CA-C	5.08	116.51	111.07
1	A	358	SER	N-CA-C	-5.08	105.93	111.82
1	B	358	SER	N-CA-C	-5.06	105.95	111.82
1	B	85	PHE	CA-CB-CG	-5.05	108.75	113.80
1	B	3	PHE	N-CA-C	5.05	116.47	111.07
1	A	85	PHE	CA-CB-CG	-5.04	108.77	113.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4517	0	4459	7	0
1	B	4517	0	4459	7	0
2	A	52	0	80	0	0
2	B	52	0	80	0	0
3	A	32	0	0	0	0
3	B	32	0	0	0	0
4	A	180	0	310	1	0
4	B	180	0	310	2	0
All	All	9562	0	9698	17	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 1.

All (17) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:498:LEU:HB3	1:B:499:PRO:HD3	1.96	0.47
1:A:498:LEU:HB3	1:A:499:PRO:HD3	1.96	0.47
1:A:225:TYR:CD2	1:A:226:ARG:HG2	2.50	0.47
1:B:317:THR:HG23	1:B:320:ALA:H	1.80	0.46
1:A:317:THR:HG23	1:A:320:ALA:H	1.81	0.46
1:B:225:TYR:CD2	1:B:226:ARG:HG2	2.50	0.46
4:A:809:PLM:HB1	4:A:809:PLM:HE1	1.23	0.45
1:B:38:TYR:N	1:B:39:PRO:CD	2.81	0.44
1:B:178:ARG:NH1	1:B:667:GLY:O	2.50	0.44
1:A:178:ARG:NH1	1:A:667:GLY:O	2.50	0.44
4:B:810:PLM:H51	4:B:810:PLM:H81	1.87	0.43
1:B:379:ILE:HB	1:B:380:PRO:HD3	2.00	0.43
1:A:379:ILE:HB	1:A:380:PRO:HD3	2.00	0.43
1:A:38:TYR:N	1:A:39:PRO:CD	2.81	0.43
1:A:34:ALA:N	1:A:35:PRO:CD	2.83	0.42
1:B:34:ALA:N	1:B:35:PRO:CD	2.83	0.41
4:B:810:PLM:HB1	4:B:810:PLM:HE1	1.23	0.41

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	527/734 (72%)	521 (99%)	6 (1%)	0	100	100
1	B	527/734 (72%)	521 (99%)	6 (1%)	0	100	100
All	All	1054/1468 (72%)	1042 (99%)	12 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	465/601 (77%)	465 (100%)	0	100	100
1	B	465/601 (77%)	465 (100%)	0	100	100
All	All	930/1202 (77%)	930 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	206	GLN
1	A	307	GLN
1	A	597	GLN
1	B	206	GLN
1	B	307	GLN
1	B	597	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	$\#\|Z\| > 2$
4	PLM	B	811	-	17,17,17	0.88	1 (5%)	17,17,17	0.59	0
4	PLM	A	810	-	17,17,17	0.88	1 (5%)	17,17,17	0.59	0
2	CPL	B	802	-	51,51,51	2.04	13 (25%)	57,59,59	0.94	2 (3%)
4	PLM	B	810	-	17,17,17	0.48	0	17,17,17	1.19	1 (5%)
4	PLM	B	801	-	17,17,17	0.77	0	17,17,17	0.83	0
4	PLM	A	807	-	17,17,17	0.90	1 (5%)	17,17,17	0.56	0
4	PLM	B	807	-	17,17,17	0.90	1 (5%)	17,17,17	0.66	0
4	PLM	A	806	-	17,17,17	0.90	1 (5%)	17,17,17	0.66	0
4	PLM	B	808	-	17,17,17	0.90	1 (5%)	17,17,17	0.56	0
3	82T	B	803	-	31,31,31	1.84	8 (25%)	33,35,35	1.27	4 (12%)
4	PLM	B	804	-	17,17,17	0.85	1 (5%)	17,17,17	0.72	0
4	PLM	B	812	-	17,17,17	0.92	1 (5%)	17,17,17	0.65	0
4	PLM	A	805	-	17,17,17	0.84	1 (5%)	17,17,17	0.62	0
4	PLM	B	805	-	17,17,17	0.85	1 (5%)	17,17,17	0.49	0
2	CPL	A	801	-	51,51,51	2.04	13 (25%)	57,59,59	0.94	2 (3%)
4	PLM	A	804	-	17,17,17	0.85	1 (5%)	17,17,17	0.49	0
3	82T	A	802	-	31,31,31	1.84	8 (25%)	33,35,35	1.27	4 (12%)
4	PLM	B	806	-	17,17,17	0.85	1 (5%)	17,17,17	0.63	0
4	PLM	A	808	-	17,17,17	0.89	1 (5%)	17,17,17	0.66	0
4	PLM	A	812	-	17,17,17	0.77	0	17,17,17	0.83	0
4	PLM	B	809	-	17,17,17	0.89	1 (5%)	17,17,17	0.66	0
4	PLM	A	809	-	17,17,17	0.48	0	17,17,17	1.19	1 (5%)
4	PLM	A	803	-	17,17,17	0.85	1 (5%)	17,17,17	0.72	1 (5%)
4	PLM	A	811	-	17,17,17	0.93	1 (5%)	17,17,17	0.65	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
4	PLM	B	811	-	-	8/15/15/15	-
4	PLM	A	810	-	-	8/15/15/15	-
2	CPL	B	802	-	-	19/55/55/55	-
4	PLM	B	810	-	-	11/15/15/15	-
4	PLM	B	801	-	-	2/15/15/15	-
4	PLM	A	807	-	-	7/15/15/15	-
4	PLM	B	807	-	-	6/15/15/15	-
4	PLM	A	806	-	-	6/15/15/15	-
4	PLM	B	808	-	-	7/15/15/15	-
3	82T	B	803	-	-	10/33/33/33	-
4	PLM	B	804	-	-	5/15/15/15	-
4	PLM	B	812	-	-	5/15/15/15	-
4	PLM	A	805	-	-	6/15/15/15	-
4	PLM	B	805	-	-	5/15/15/15	-
2	CPL	A	801	-	-	19/55/55/55	-
4	PLM	A	804	-	-	5/15/15/15	-
3	82T	A	802	-	-	10/33/33/33	-
4	PLM	B	806	-	-	6/15/15/15	-
4	PLM	A	808	-	-	3/15/15/15	-
4	PLM	A	812	-	-	2/15/15/15	-
4	PLM	B	809	-	-	3/15/15/15	-
4	PLM	A	809	-	-	11/15/15/15	-
4	PLM	A	803	-	-	5/15/15/15	-
4	PLM	A	811	-	-	5/15/15/15	-

All (58) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	CPL	P-O4P	5.34	1.80	1.59
2	B	802	CPL	P-O4P	5.34	1.80	1.59
3	B	803	82T	P25-O28	4.75	1.78	1.59
3	A	802	82T	P25-O28	4.74	1.78	1.59
2	B	802	CPL	O2-C31	4.08	1.45	1.34
2	A	801	CPL	O2-C31	4.07	1.45	1.34
2	B	802	CPL	C3-C2	3.85	1.62	1.50
2	A	801	CPL	C3-C2	3.84	1.62	1.50
2	B	802	CPL	O3-C11	3.53	1.43	1.33
2	A	801	CPL	O3-C11	3.51	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	802	82T	C21-C22	3.34	1.62	1.51
3	B	803	82T	C21-C22	3.34	1.62	1.51
2	B	802	CPL	C32-C31	3.27	1.60	1.50
2	A	801	CPL	C32-C31	3.25	1.60	1.50
2	B	802	CPL	P-O3P	3.24	1.72	1.59
2	A	801	CPL	P-O3P	3.23	1.72	1.59
2	A	801	CPL	C1-C2	3.10	1.60	1.50
2	B	802	CPL	C1-C2	3.08	1.60	1.50
2	A	801	CPL	C5-C4	2.97	1.60	1.51
2	B	802	CPL	C5-C4	2.96	1.60	1.51
2	A	801	CPL	C5-N	2.92	1.60	1.51
2	B	802	CPL	C5-N	2.91	1.60	1.51
3	A	802	82T	C23-C22	2.74	1.60	1.51
3	B	803	82T	C23-C22	2.74	1.60	1.51
3	B	803	82T	C9-C10	-2.71	1.38	1.51
3	A	802	82T	C9-C10	-2.70	1.38	1.51
2	A	801	CPL	C33-C32	2.67	1.62	1.52
2	B	802	CPL	C33-C32	2.66	1.61	1.52
3	B	803	82T	O20-C18	2.60	1.40	1.33
3	A	802	82T	O20-C18	2.56	1.40	1.33
3	A	802	82T	P25-O24	2.54	1.69	1.59
3	B	803	82T	P25-O24	2.53	1.69	1.59
3	B	803	82T	C30-C29	2.34	1.59	1.49
3	A	802	82T	C30-C29	2.33	1.59	1.49
2	B	802	CPL	C13-C12	2.28	1.60	1.52
4	B	808	PLM	C2-C1	2.28	1.55	1.50
2	A	801	CPL	C13-C12	2.27	1.60	1.52
4	A	807	PLM	C2-C1	2.27	1.55	1.50
4	A	810	PLM	C2-C1	2.24	1.55	1.50
4	A	808	PLM	C2-C1	2.24	1.55	1.50
4	B	811	PLM	C2-C1	2.22	1.55	1.50
4	B	809	PLM	C2-C1	2.21	1.55	1.50
2	B	802	CPL	C12-C11	2.21	1.57	1.50
2	A	801	CPL	C12-C11	2.21	1.57	1.50
4	B	812	PLM	C2-C1	2.21	1.55	1.50
4	A	804	PLM	C2-C1	2.20	1.55	1.50
4	A	811	PLM	C2-C1	2.19	1.55	1.50
4	B	805	PLM	C2-C1	2.18	1.55	1.50
2	B	802	CPL	C7-N	2.13	1.56	1.50
2	A	801	CPL	C7-N	2.10	1.56	1.50
4	A	803	PLM	C2-C1	2.09	1.55	1.50
4	B	804	PLM	C2-C1	2.08	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	806	PLM	C2-C1	2.07	1.55	1.50
4	A	805	PLM	C2-C1	2.07	1.55	1.50
4	B	807	PLM	C2-C1	2.04	1.55	1.50
3	B	803	82T	C16-C17	2.03	1.59	1.52
4	A	806	PLM	C2-C1	2.03	1.55	1.50
3	A	802	82T	C16-C17	2.02	1.59	1.52

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	802	82T	O20-C18-C17	3.73	123.21	111.83
3	B	803	82T	O20-C18-C17	3.73	123.20	111.83
4	B	810	PLM	C3-C2-C1	-3.00	106.67	114.51
4	A	809	PLM	C3-C2-C1	-3.00	106.69	114.51
3	B	803	82T	O20-C18-O19	-2.84	116.53	123.63
3	A	802	82T	O20-C18-O19	-2.82	116.57	123.63
2	A	801	CPL	O2-C31-C32	2.38	116.64	111.48
2	B	802	CPL	O2-C31-C32	2.38	116.63	111.48
2	A	801	CPL	O3-C3-C2	2.20	114.75	108.40
2	B	802	CPL	O3-C3-C2	2.19	114.72	108.40
3	B	803	82T	C11-C10-C9	2.17	125.32	114.37
3	A	802	82T	C11-C10-C9	2.17	125.32	114.37
3	A	802	82T	C8-C9-C10	2.15	125.24	114.37
3	B	803	82T	C8-C9-C10	2.14	125.21	114.37
4	A	803	PLM	C3-C2-C1	-2.01	109.27	114.51

There are no chirality outliers.

All (174) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	CPL	O4P-C4-C5-N
2	A	801	CPL	C1-O3P-P-O1P
2	A	801	CPL	C4-O4P-P-O1P
2	A	801	CPL	C4-O4P-P-O3P
2	B	802	CPL	O4P-C4-C5-N
2	B	802	CPL	C1-O3P-P-O1P
2	B	802	CPL	C4-O4P-P-O1P
2	B	802	CPL	C4-O4P-P-O3P
3	A	802	82T	C29-O28-P25-O24
3	A	802	82T	C29-O28-P25-O27
3	B	803	82T	C29-O28-P25-O24
3	B	803	82T	C29-O28-P25-O27

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Mol	Chain	Res	Type	Atoms
3	A	802	82T	O19-C18-O20-C21
3	B	803	82T	O19-C18-O20-C21
2	A	801	CPL	C12-C11-O3-C3
2	B	802	CPL	C12-C11-O3-C3
3	A	802	82T	C17-C18-O20-C21
3	B	803	82T	C17-C18-O20-C21
2	A	801	CPL	O11-C11-O3-C3
2	B	802	CPL	O11-C11-O3-C3
4	A	809	PLM	CB-CC-CD-CE
4	B	810	PLM	CB-CC-CD-CE
4	A	806	PLM	C1-C2-C3-C4
4	B	807	PLM	C1-C2-C3-C4
2	A	801	CPL	C44-C45-C46-C47
2	B	802	CPL	C44-C45-C46-C47
4	A	807	PLM	C2-C3-C4-C5
4	B	808	PLM	C2-C3-C4-C5
4	A	810	PLM	C9-CA-CB-CC
4	B	811	PLM	C9-CA-CB-CC
4	A	806	PLM	CA-CB-CC-CD
4	B	807	PLM	CA-CB-CC-CD
4	B	810	PLM	C6-C7-C8-C9
4	A	809	PLM	C6-C7-C8-C9
4	A	804	PLM	C8-C9-CA-CB
4	B	805	PLM	C8-C9-CA-CB
4	B	805	PLM	C7-C8-C9-CA
4	A	804	PLM	C7-C8-C9-CA
4	A	810	PLM	CB-CC-CD-CE
4	B	811	PLM	CB-CC-CD-CE
4	A	808	PLM	C5-C6-C7-C8
4	B	809	PLM	C5-C6-C7-C8
4	A	805	PLM	C8-C9-CA-CB
4	B	806	PLM	C8-C9-CA-CB
3	A	802	82T	C7-C8-C9-C10
3	B	803	82T	C7-C8-C9-C10
4	A	809	PLM	CA-CB-CC-CD
4	B	810	PLM	CA-CB-CC-CD
2	A	801	CPL	C36-C37-C38-C39
2	B	802	CPL	C36-C37-C38-C39
4	B	808	PLM	CB-CC-CD-CE
4	A	807	PLM	CB-CC-CD-CE
4	A	809	PLM	C2-C3-C4-C5
4	B	810	PLM	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
4	A	809	PLM	C8-C9-CA-CB
4	B	810	PLM	C8-C9-CA-CB
2	A	801	CPL	C17-C18-C19-C20
2	B	802	CPL	C17-C18-C19-C20
4	A	810	PLM	C5-C6-C7-C8
4	B	811	PLM	C5-C6-C7-C8
4	A	805	PLM	C1-C2-C3-C4
4	B	806	PLM	C1-C2-C3-C4
3	A	802	82T	C12-C13-C14-C15
3	B	803	82T	C12-C13-C14-C15
4	B	804	PLM	C4-C5-C6-C7
4	A	803	PLM	C4-C5-C6-C7
2	A	801	CPL	O3P-C1-C2-C3
2	B	802	CPL	O3P-C1-C2-C3
4	A	806	PLM	CD-CE-CF-CG
4	B	807	PLM	CD-CE-CF-CG
4	A	805	PLM	CC-CD-CE-CF
4	B	806	PLM	CC-CD-CE-CF
2	A	801	CPL	C13-C14-C15-C16
2	B	802	CPL	C13-C14-C15-C16
3	A	802	82T	C15-C16-C17-C18
3	B	803	82T	C15-C16-C17-C18
4	A	811	PLM	C8-C9-CA-CB
4	B	812	PLM	C8-C9-CA-CB
2	A	801	CPL	O3P-C1-C2-O2
2	B	802	CPL	O3P-C1-C2-O2
2	A	801	CPL	C39-C40-C41-C42
2	A	801	CPL	C40-C41-C42-C43
2	B	802	CPL	C39-C40-C41-C42
2	B	802	CPL	C40-C41-C42-C43
4	B	811	PLM	C4-C5-C6-C7
4	A	810	PLM	C4-C5-C6-C7
4	A	807	PLM	C8-C9-CA-CB
4	B	808	PLM	C8-C9-CA-CB
4	A	809	PLM	C3-C4-C5-C6
4	B	810	PLM	C3-C4-C5-C6
4	A	805	PLM	C6-C7-C8-C9
4	B	806	PLM	C6-C7-C8-C9
4	A	809	PLM	C1-C2-C3-C4
4	B	810	PLM	C1-C2-C3-C4
4	A	809	PLM	C7-C8-C9-CA
4	B	810	PLM	C7-C8-C9-CA

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Mol	Chain	Res	Type	Atoms
4	A	811	PLM	C2-C3-C4-C5
4	B	812	PLM	C2-C3-C4-C5
2	A	801	CPL	C4-O4P-P-O2P
2	B	802	CPL	C4-O4P-P-O2P
2	A	801	CPL	C2-C1-O3P-P
2	B	802	CPL	C2-C1-O3P-P
2	B	802	CPL	C18-C19-C20-C21
2	A	801	CPL	C18-C19-C20-C21
4	B	804	PLM	CC-CD-CE-CF
4	A	803	PLM	CC-CD-CE-CF
4	A	809	PLM	C9-CA-CB-CC
4	B	810	PLM	C9-CA-CB-CC
4	A	809	PLM	O1-C1-C2-C3
4	B	810	PLM	O1-C1-C2-C3
4	A	809	PLM	O2-C1-C2-C3
4	B	810	PLM	O2-C1-C2-C3
2	A	801	CPL	C19-C20-C21-C22
2	B	802	CPL	C19-C20-C21-C22
4	B	812	PLM	CC-CD-CE-CF
4	A	811	PLM	CC-CD-CE-CF
4	A	803	PLM	C7-C8-C9-CA
4	B	804	PLM	C7-C8-C9-CA
4	A	811	PLM	O2-C1-C2-C3
4	B	812	PLM	O2-C1-C2-C3
4	A	808	PLM	O2-C1-C2-C3
4	B	809	PLM	O2-C1-C2-C3
4	A	806	PLM	C3-C4-C5-C6
4	B	807	PLM	C3-C4-C5-C6
4	A	803	PLM	O1-C1-C2-C3
4	A	810	PLM	O1-C1-C2-C3
4	B	804	PLM	O1-C1-C2-C3
4	B	811	PLM	O1-C1-C2-C3
4	A	811	PLM	O1-C1-C2-C3
4	B	812	PLM	O1-C1-C2-C3
4	A	807	PLM	O1-C1-C2-C3
4	B	808	PLM	O1-C1-C2-C3
4	A	810	PLM	O2-C1-C2-C3
4	B	808	PLM	O2-C1-C2-C3
4	B	811	PLM	O2-C1-C2-C3
4	A	805	PLM	O1-C1-C2-C3
4	A	807	PLM	O2-C1-C2-C3
4	B	806	PLM	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
4	B	804	PLM	O2-C1-C2-C3
4	B	809	PLM	O1-C1-C2-C3
4	A	803	PLM	O2-C1-C2-C3
4	A	808	PLM	O1-C1-C2-C3
4	A	810	PLM	C6-C7-C8-C9
4	B	811	PLM	C6-C7-C8-C9
4	A	806	PLM	O1-C1-C2-C3
4	B	807	PLM	O1-C1-C2-C3
4	B	801	PLM	O1-C1-C2-C3
4	A	805	PLM	O2-C1-C2-C3
4	A	812	PLM	O1-C1-C2-C3
4	B	806	PLM	O2-C1-C2-C3
4	A	806	PLM	O2-C1-C2-C3
4	B	807	PLM	O2-C1-C2-C3
4	B	805	PLM	O1-C1-C2-C3
4	A	804	PLM	O1-C1-C2-C3
4	A	812	PLM	O2-C1-C2-C3
4	B	801	PLM	O2-C1-C2-C3
4	B	808	PLM	C7-C8-C9-CA
4	A	807	PLM	C7-C8-C9-CA
3	A	802	82T	C13-C14-C15-C16
3	B	803	82T	C13-C14-C15-C16
3	B	803	82T	C14-C15-C16-C17
3	A	802	82T	C14-C15-C16-C17
4	B	805	PLM	O2-C1-C2-C3
4	A	804	PLM	O2-C1-C2-C3
2	A	801	CPL	C14-C15-C16-C17
2	B	802	CPL	C14-C15-C16-C17
3	A	802	82T	C6-C7-C8-C9
3	B	803	82T	C6-C7-C8-C9
4	A	807	PLM	CC-CD-CE-CF
4	B	808	PLM	CC-CD-CE-CF
4	A	804	PLM	C6-C7-C8-C9
4	B	805	PLM	C6-C7-C8-C9
4	B	811	PLM	CD-CE-CF-CG
4	A	810	PLM	CD-CE-CF-CG

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	810	PLM	2	0

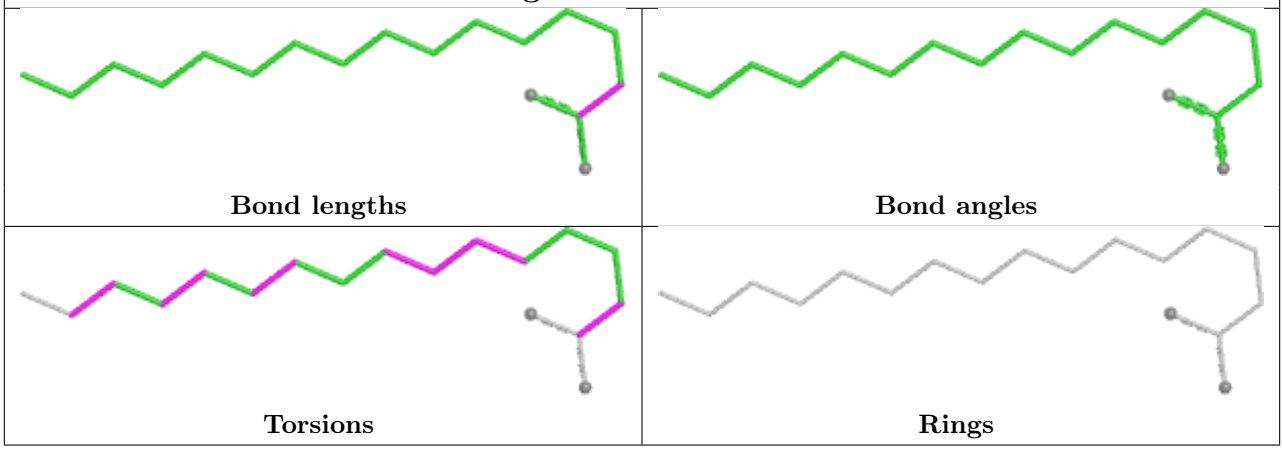
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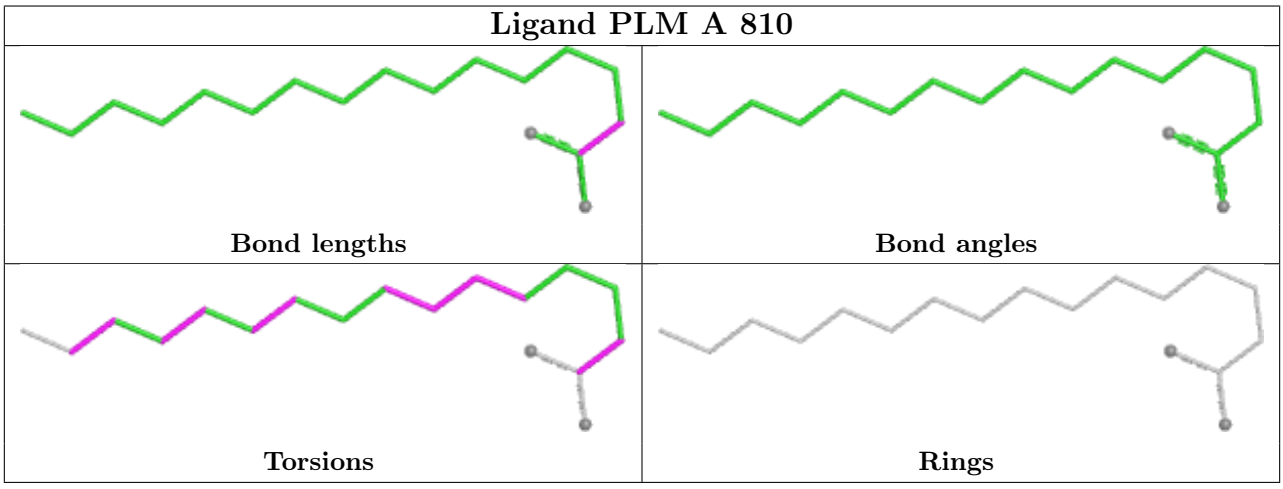
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	809	PLM	1	0

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.

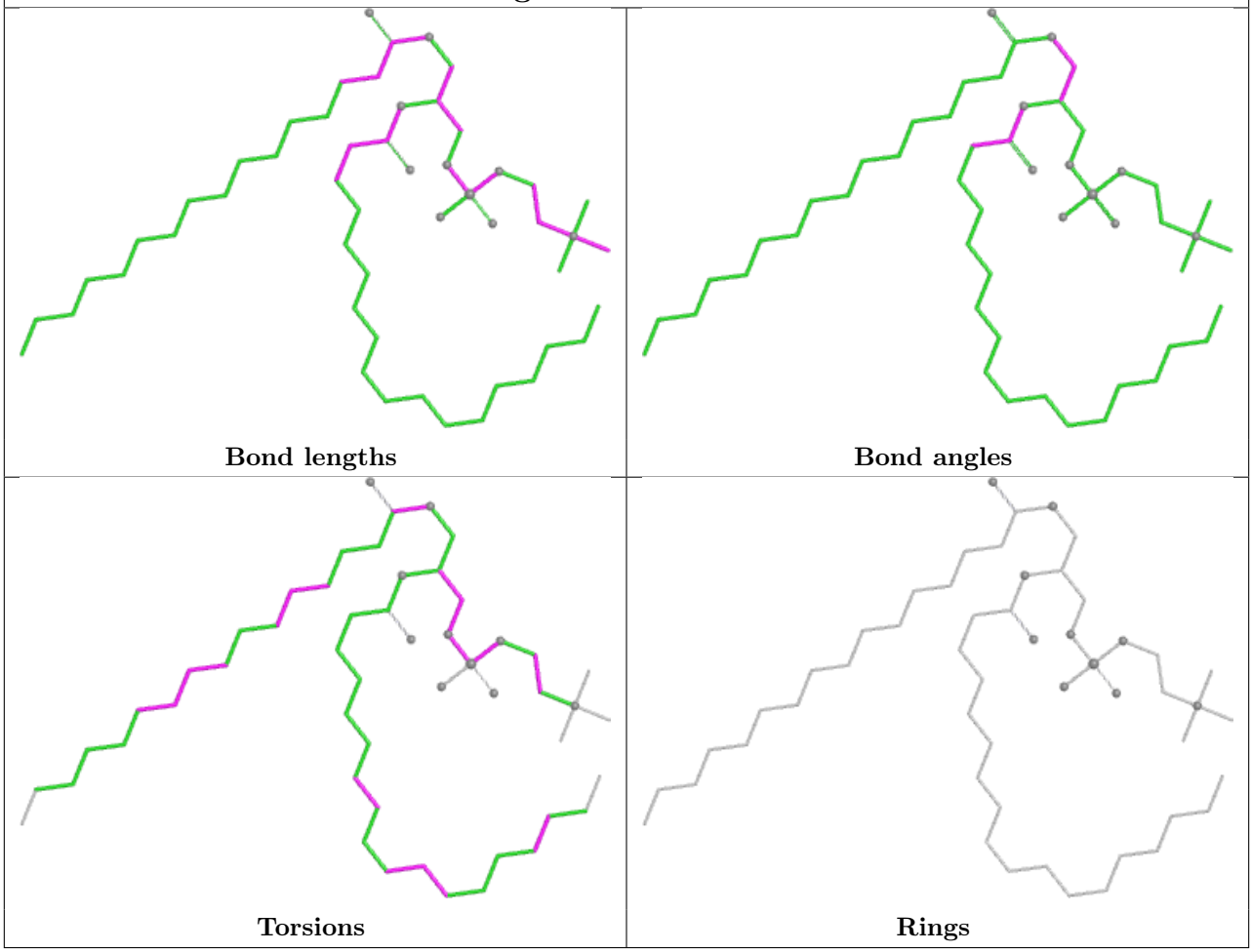
Ligand PLM B 811



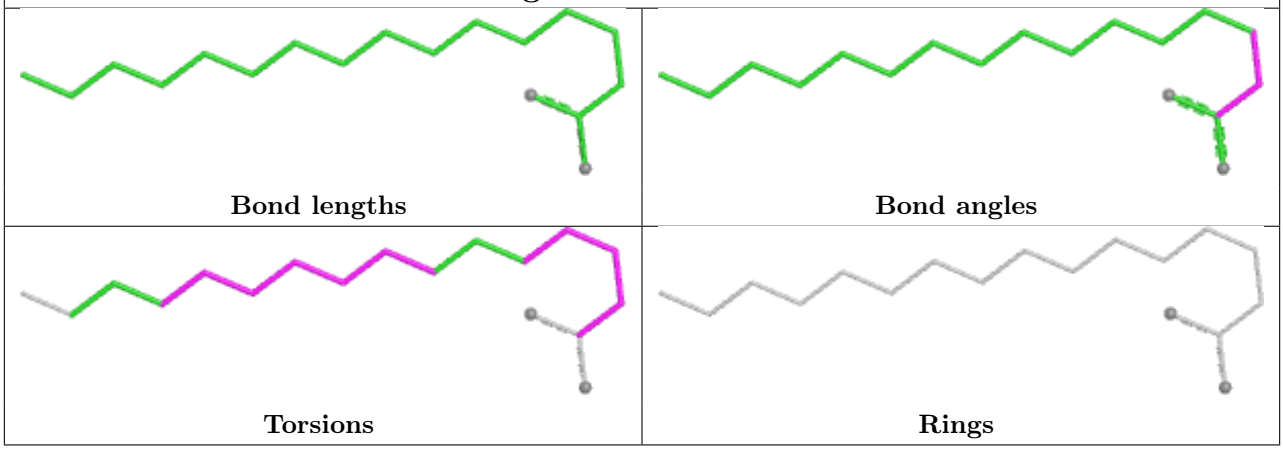
Ligand PLM A 810



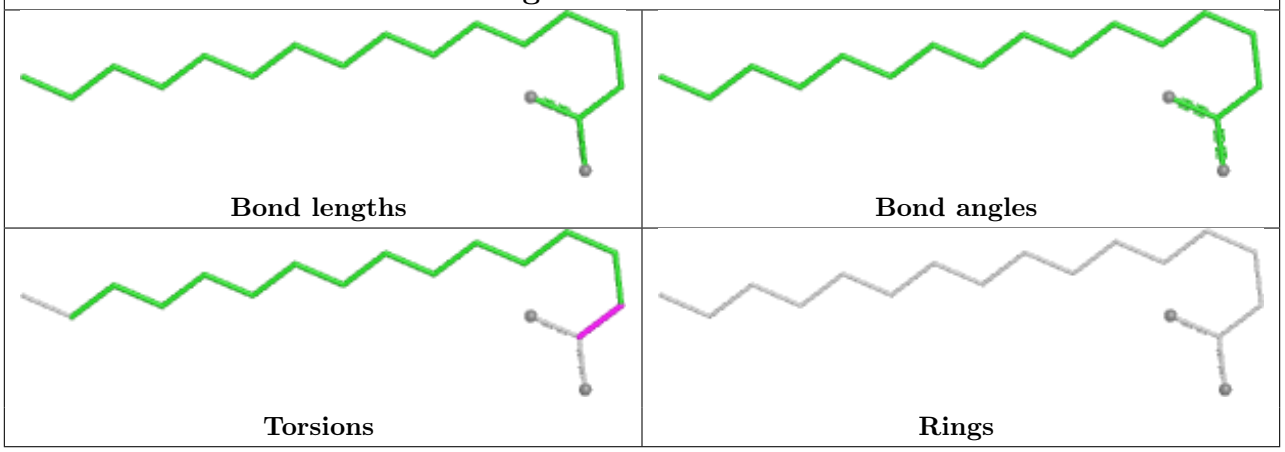
Ligand CPL B 802



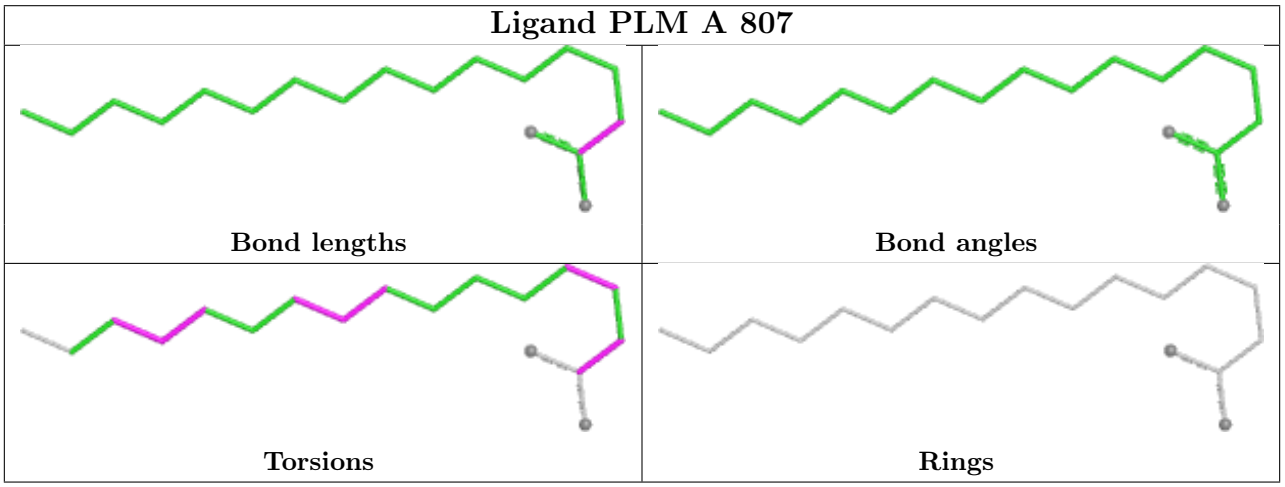
Ligand PLM B 810



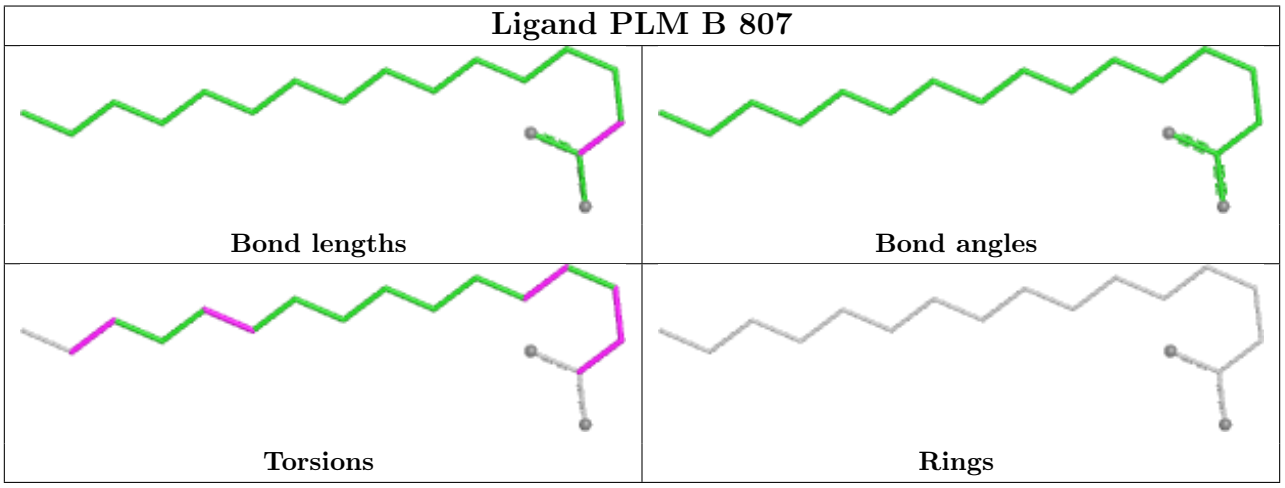
Ligand PLM B 801



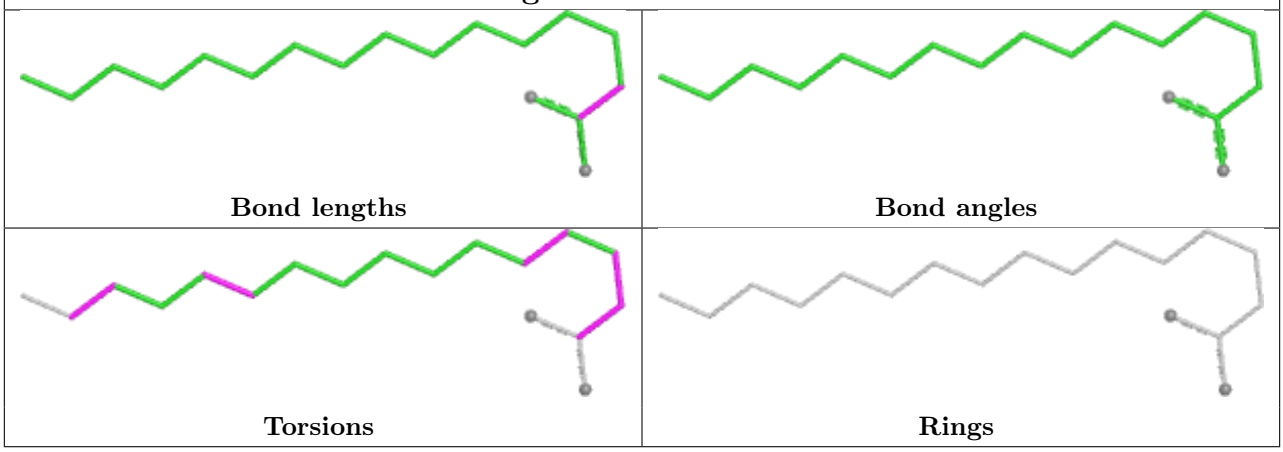
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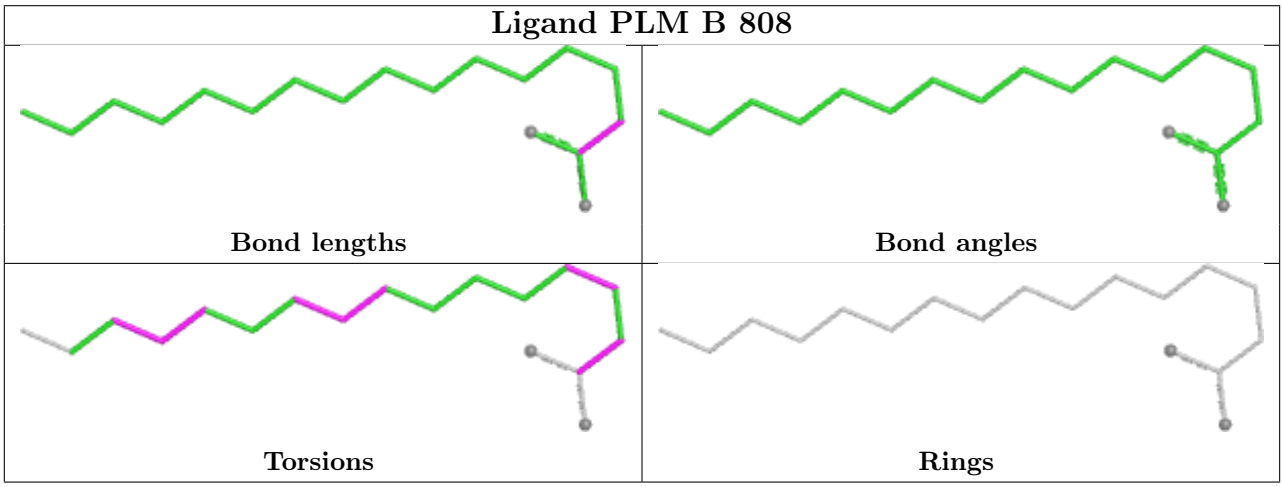
Ligand PLM B 807



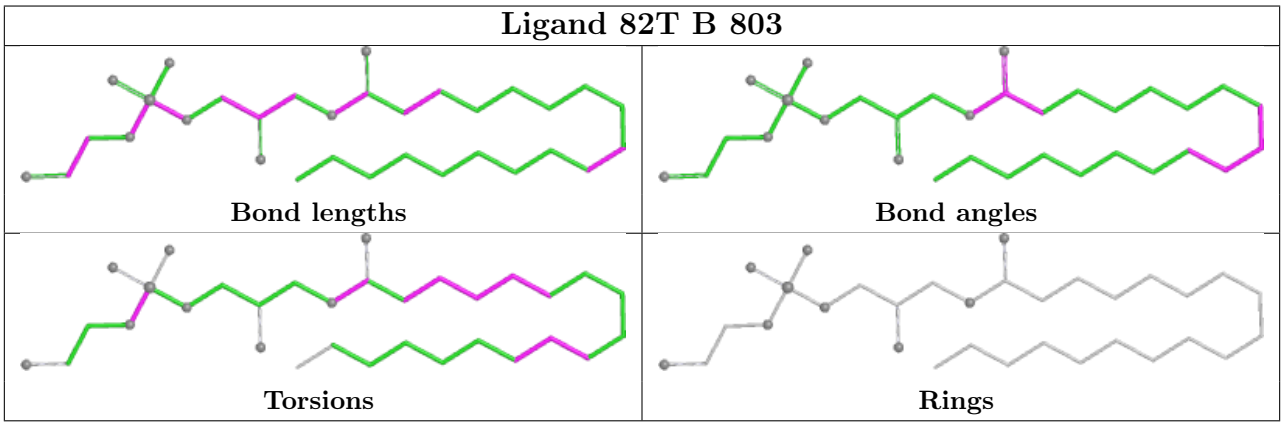
Ligand PLM A 806



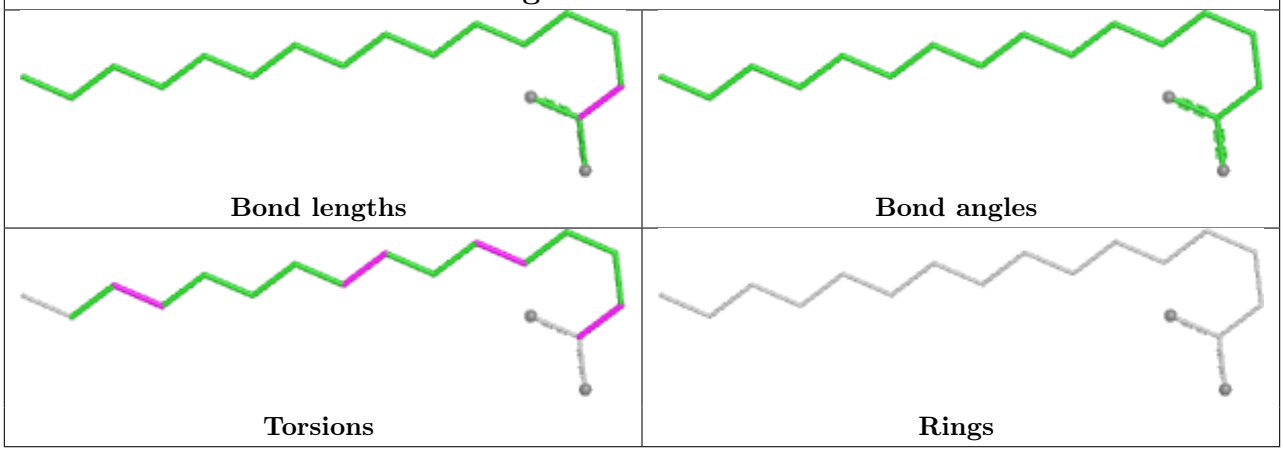
Ligand PLM B 808



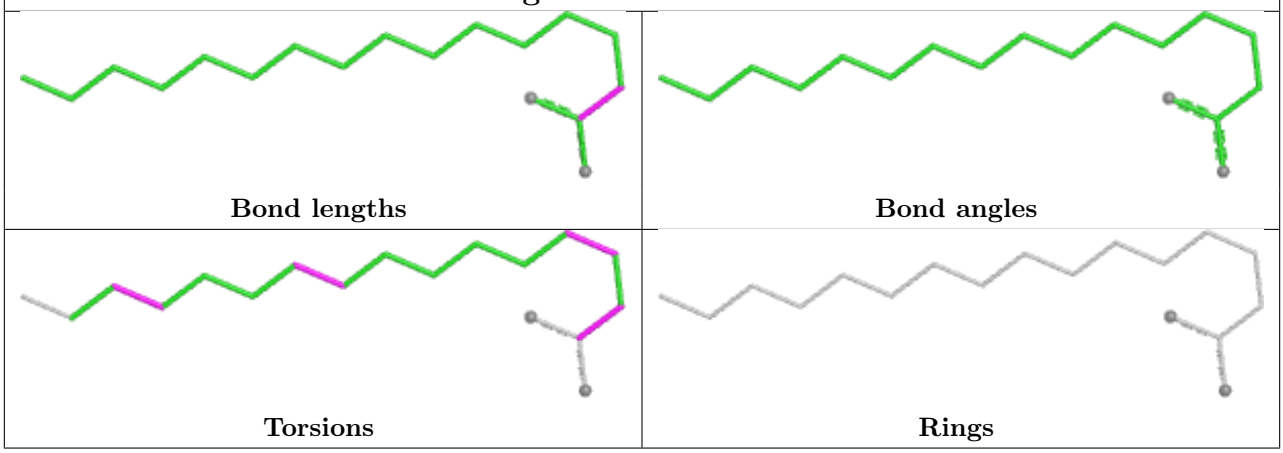
Ligand 82T B 803



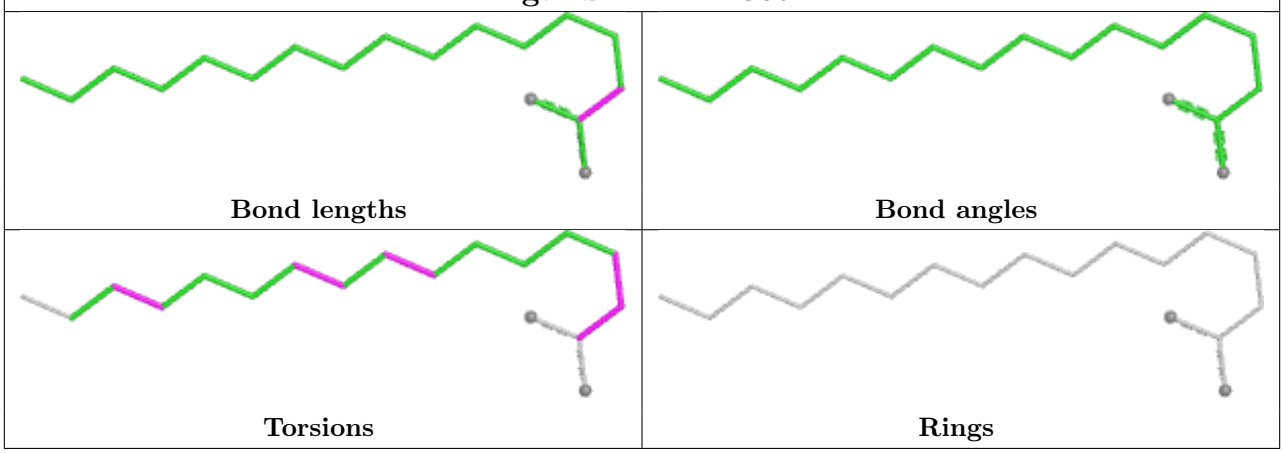
Ligand PLM B 804



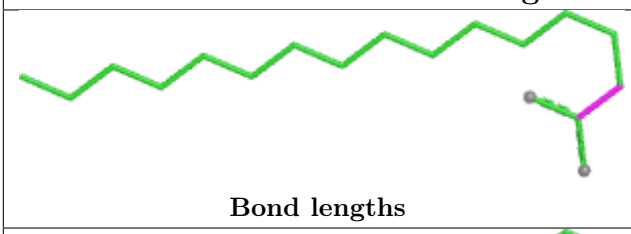
Ligand PLM B 812



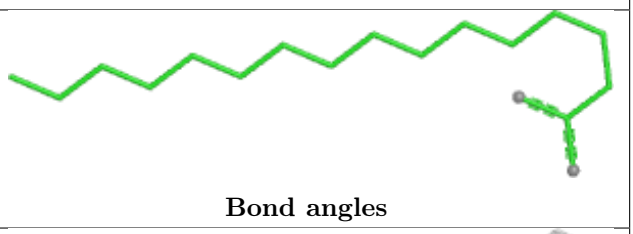
Ligand PLM A 805



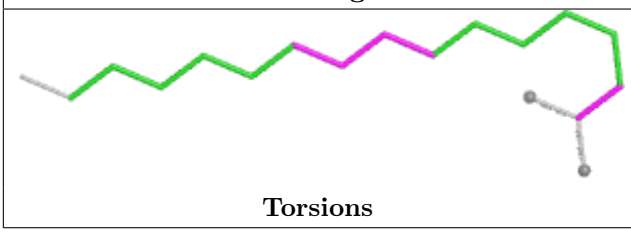
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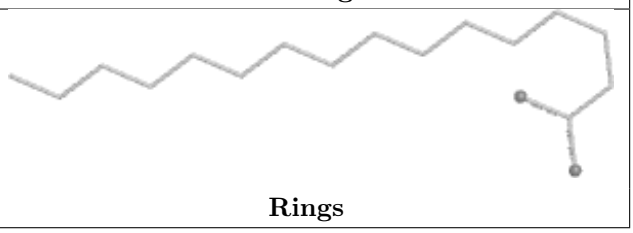
Bond lengths



Bond angles

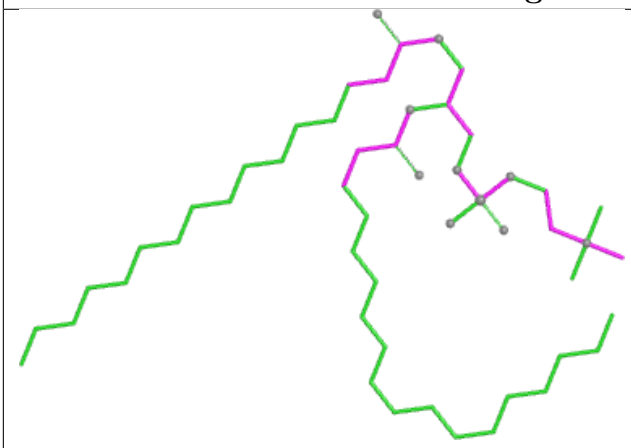


Torsions

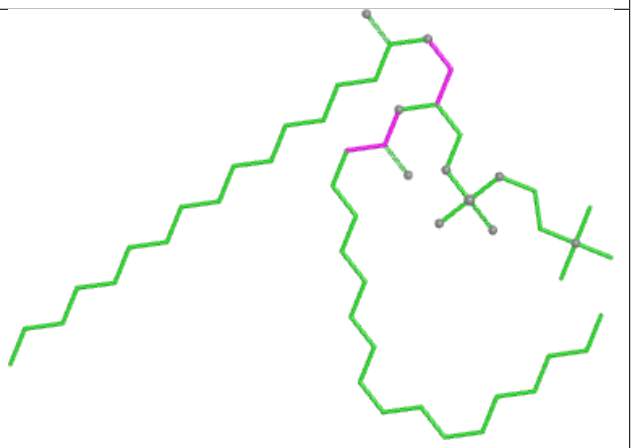


Rings

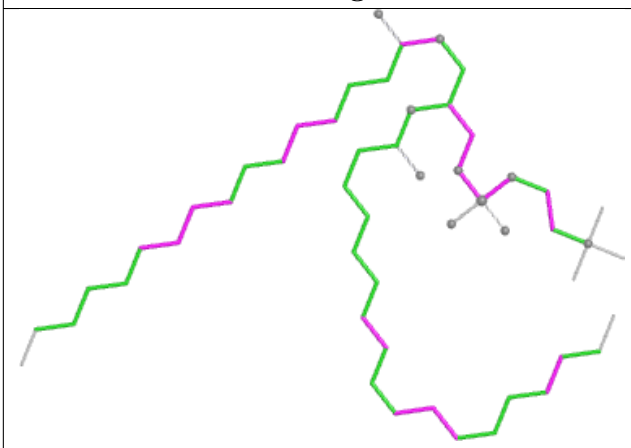
Ligand CPL A 801



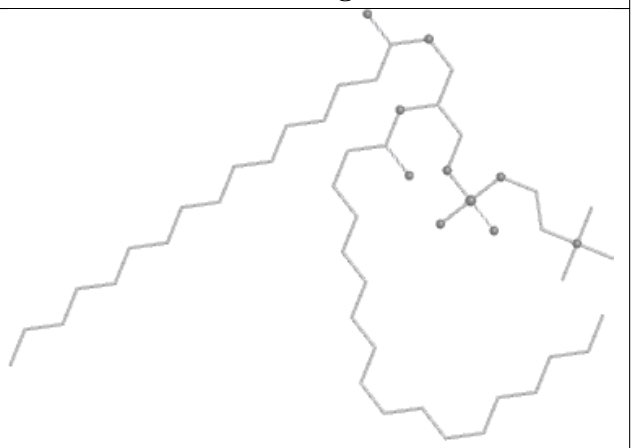
Bond lengths



Bond angles

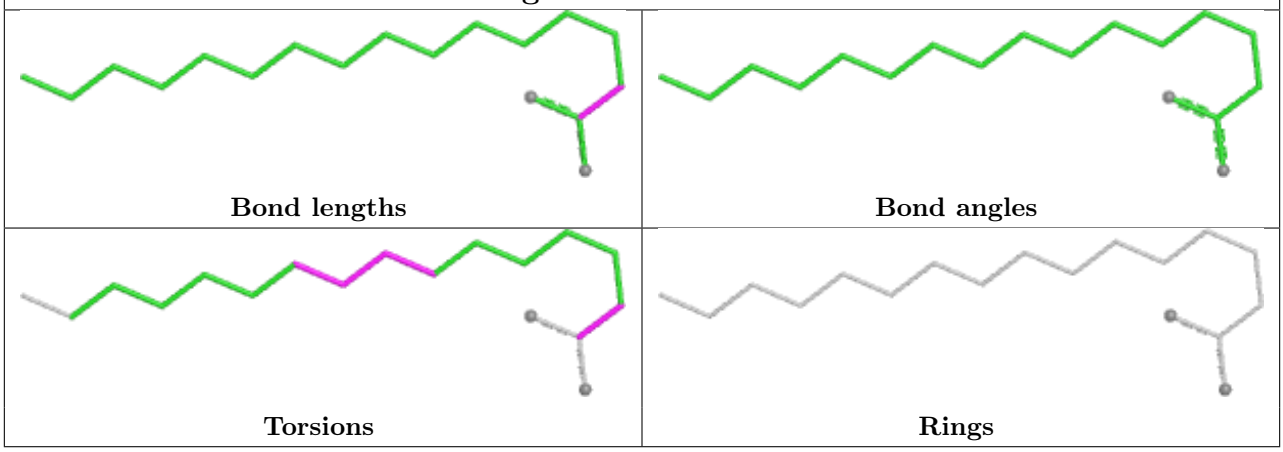


Torsions

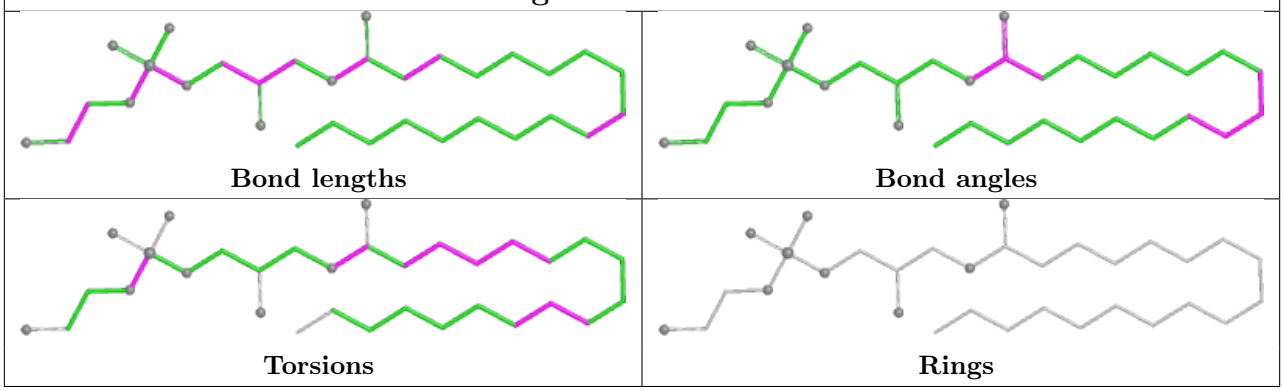


Rings

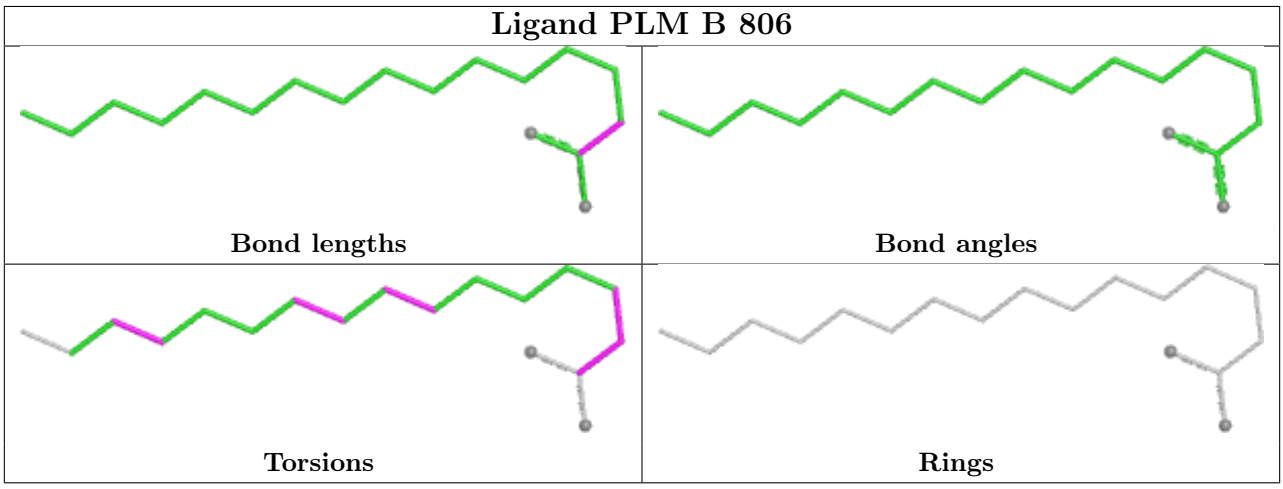
Ligand PLM A 804



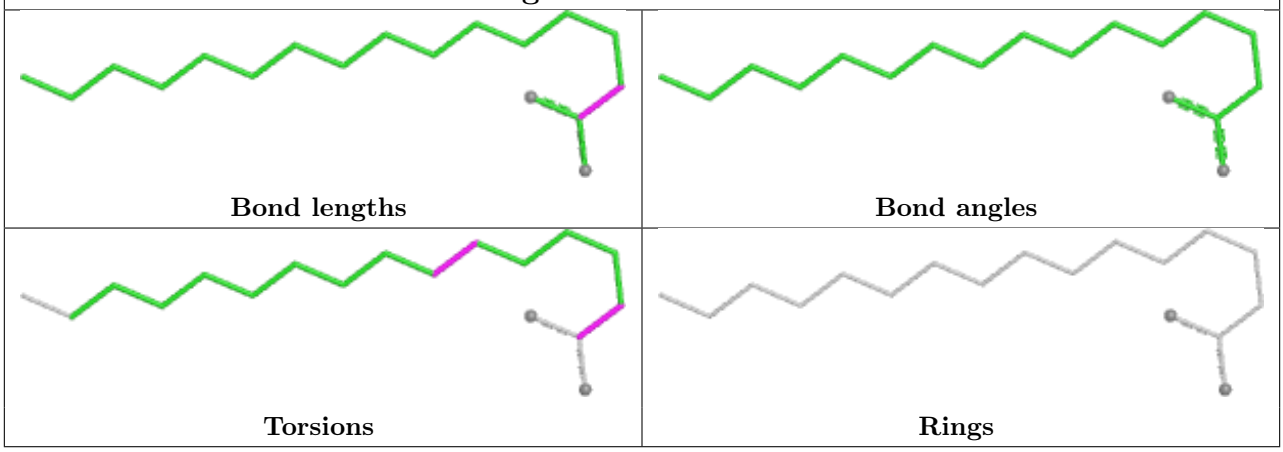
Ligand 82T A 802



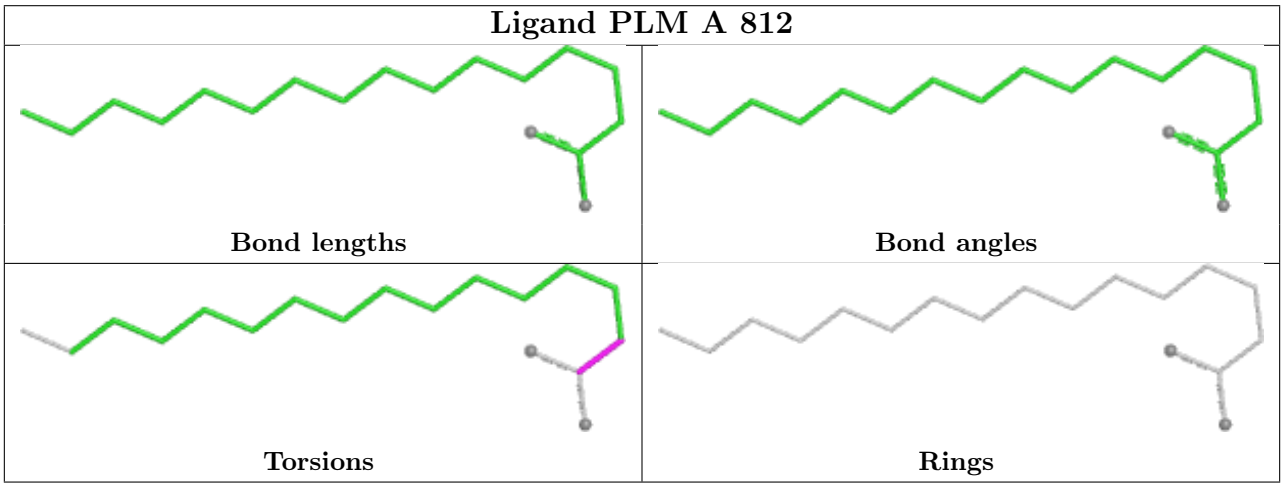
Ligand PLM B 806



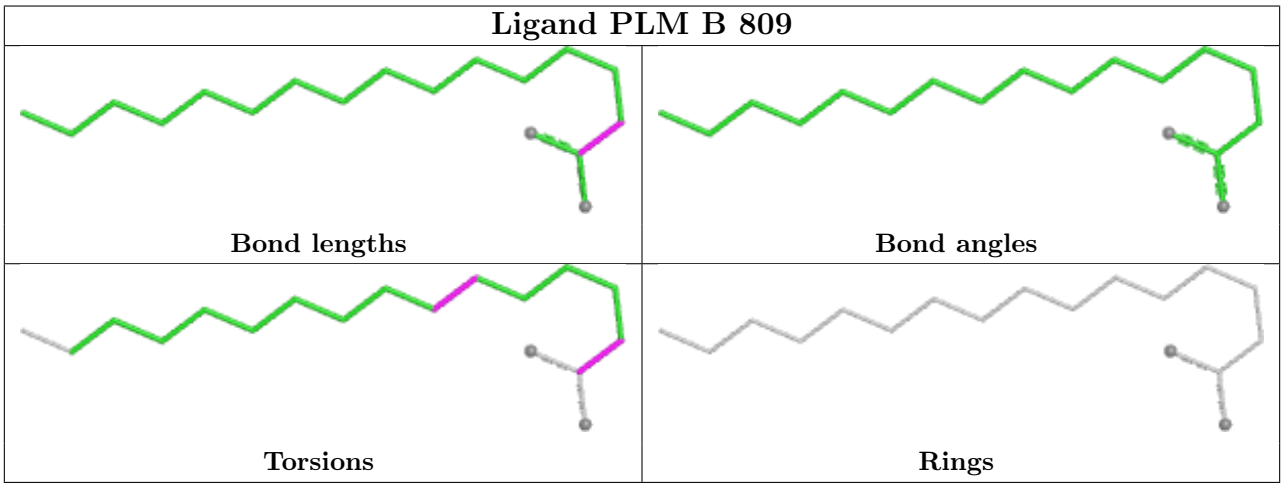
Ligand PLM A 808



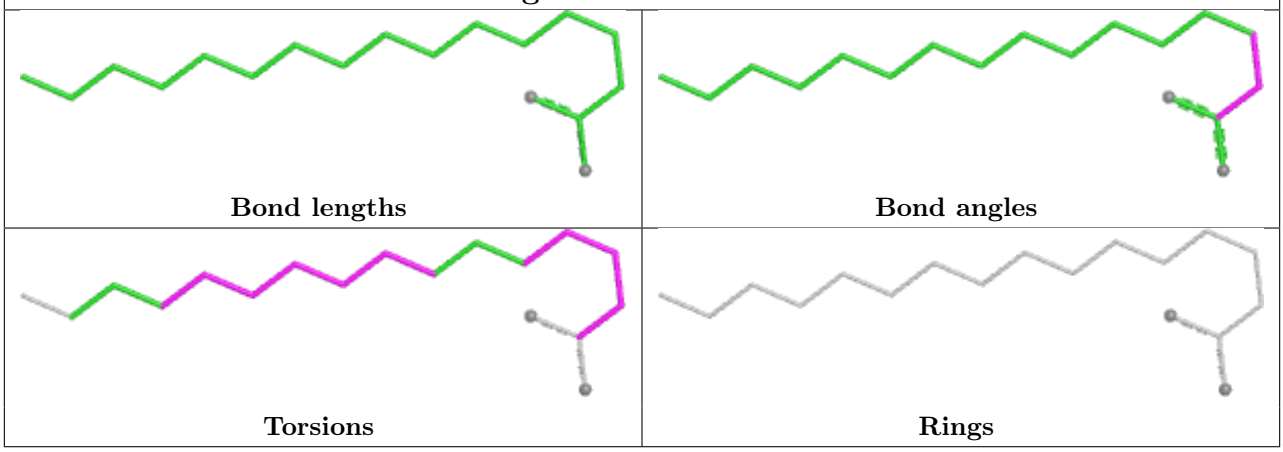
Ligand PLM A 812



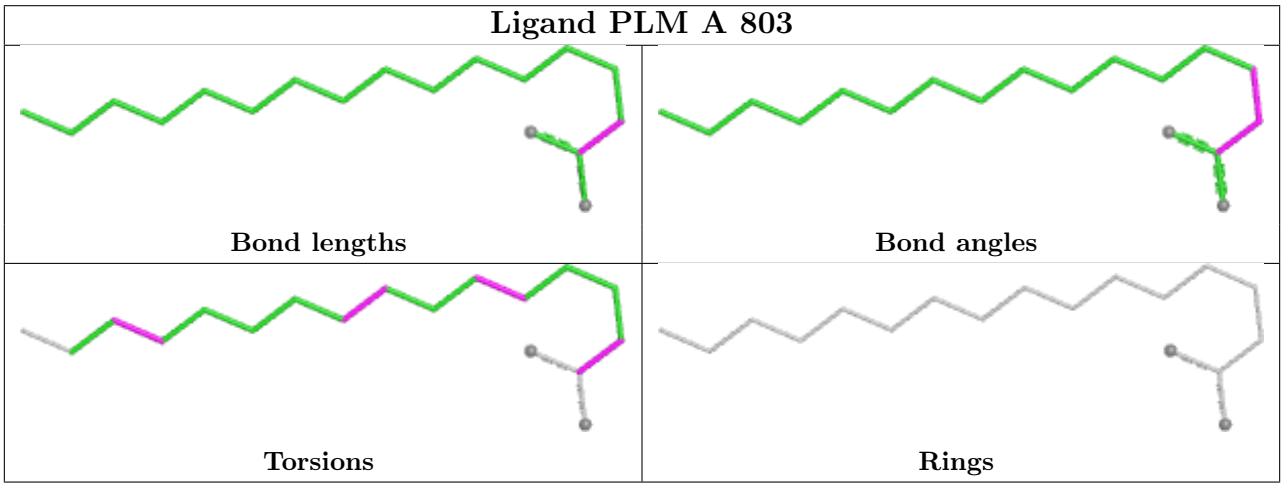
Ligand PLM B 809



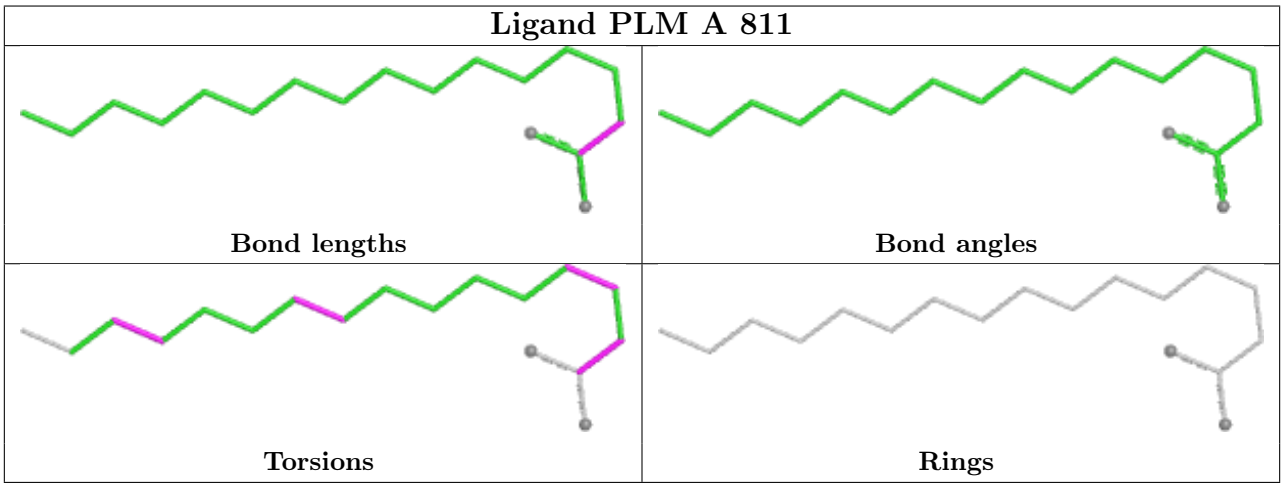
Ligand PLM A 809



Ligand PLM A 803



Ligand PLM A 811



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.

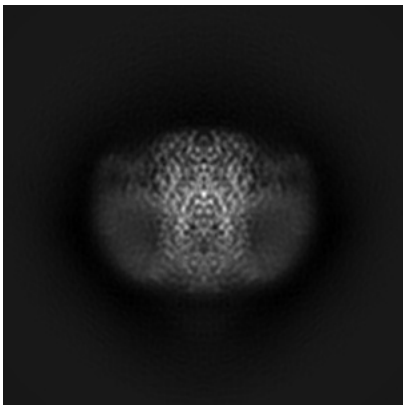
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-41911. These allow visual inspection of the internal detail of the map and identification of artifacts.

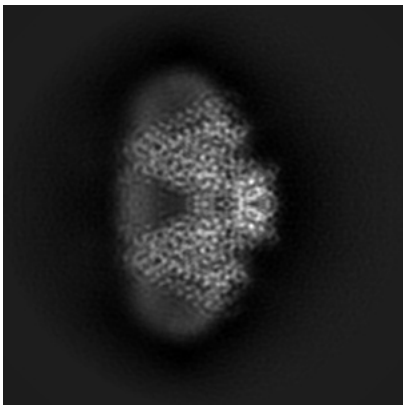
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

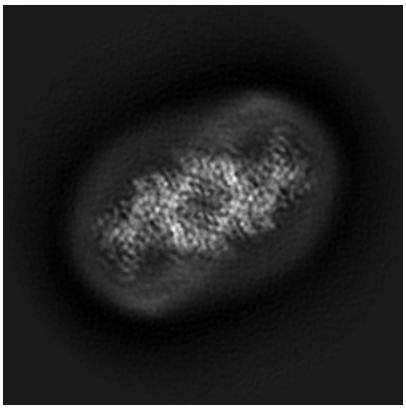
6.1.1 Primary map



X

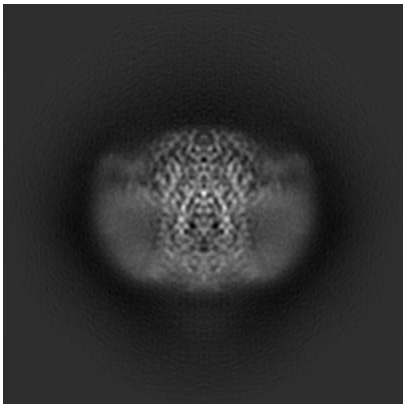


Y

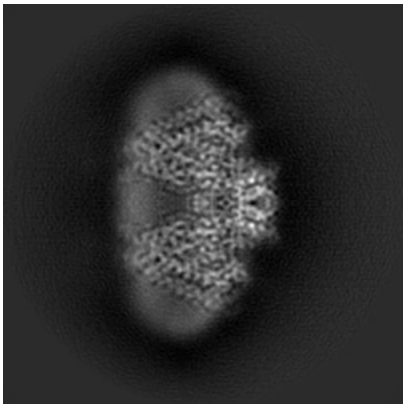


Z

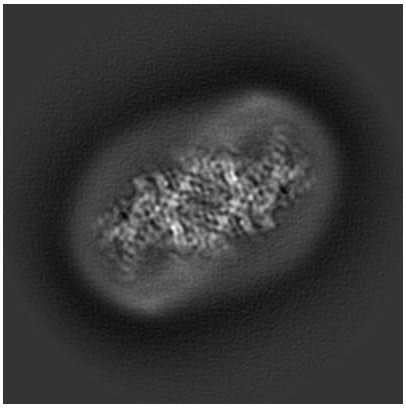
6.1.2 Raw map



X



Y



Z

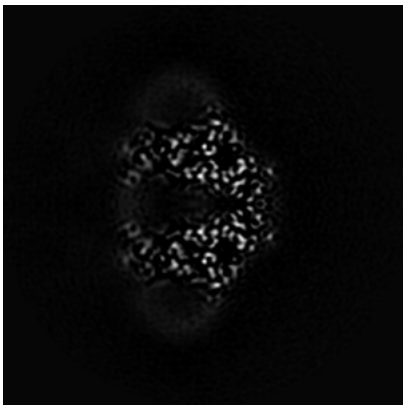
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

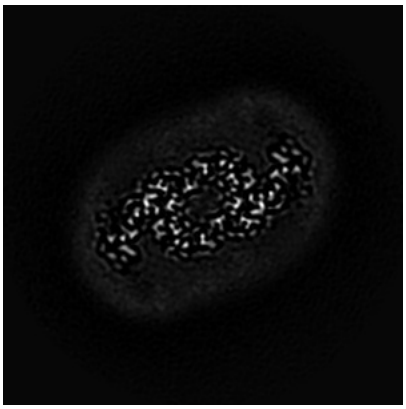
6.2.1 Primary map



X Index: 100

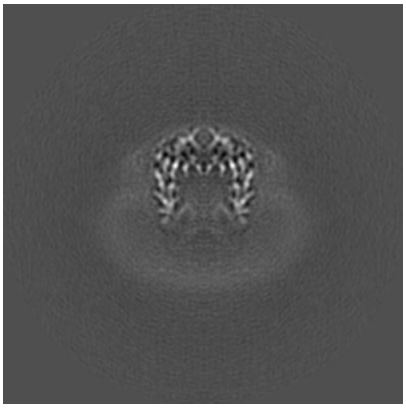


Y Index: 100

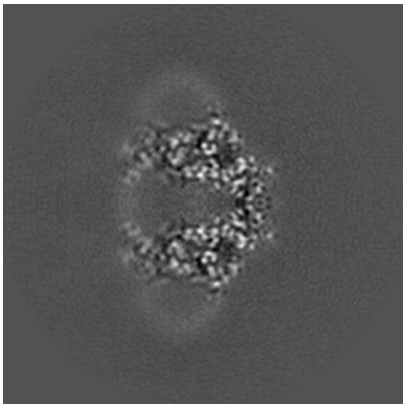


Z Index: 100

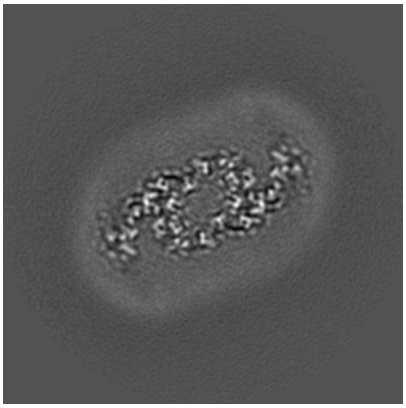
6.2.2 Raw map



X Index: 100



Y Index: 100

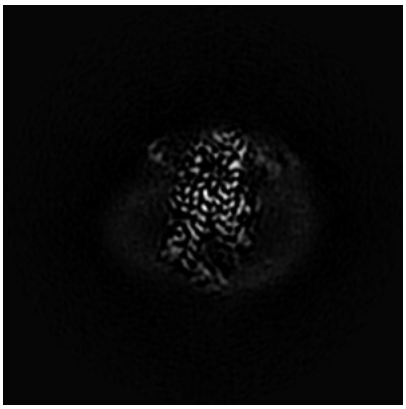


Z Index: 100

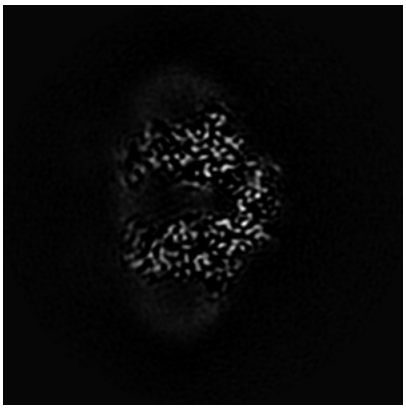
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

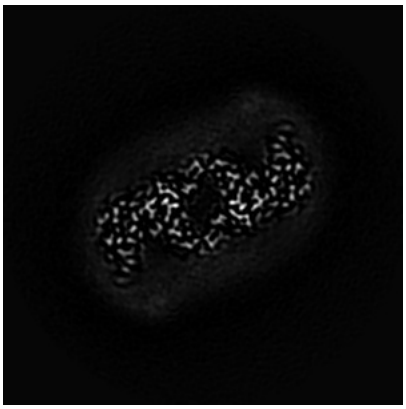
6.3.1 Primary map



X Index: 114

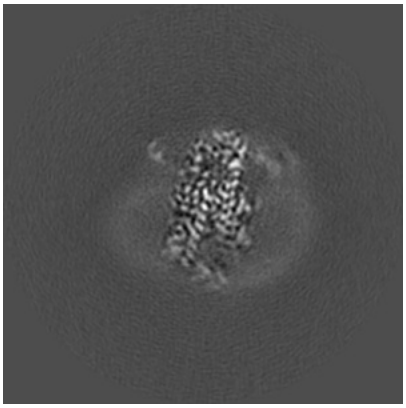


Y Index: 103

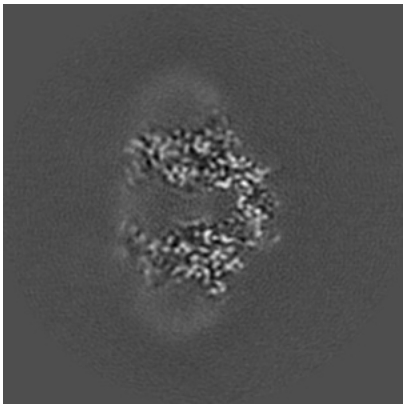


Z Index: 105

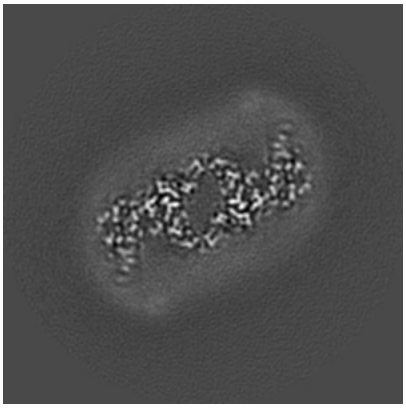
6.3.2 Raw map



X Index: 114



Y Index: 97

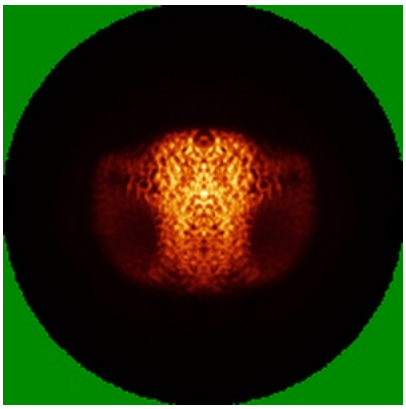


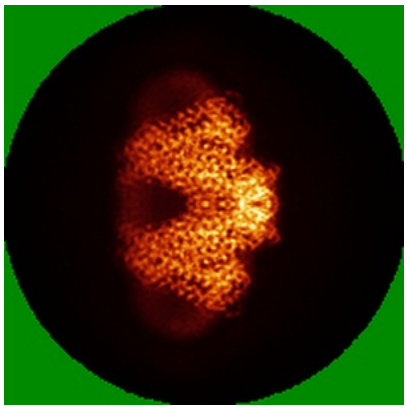
Z Index: 105

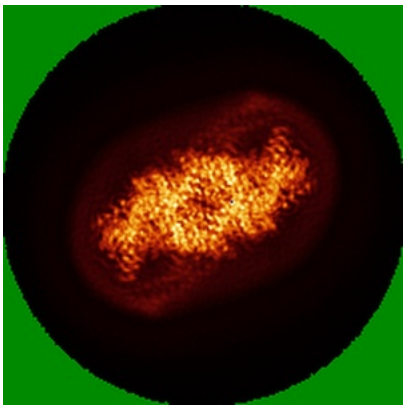
The images above show the largest variance slices of the map in three orthogonal directions.

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

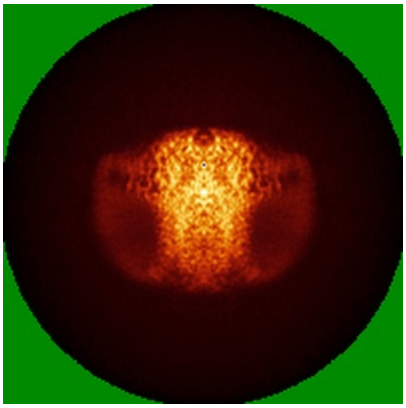
6.4.1 Primary map

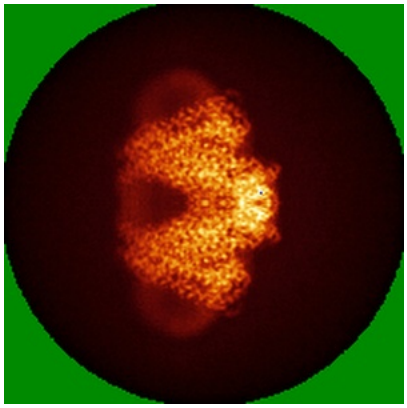

X

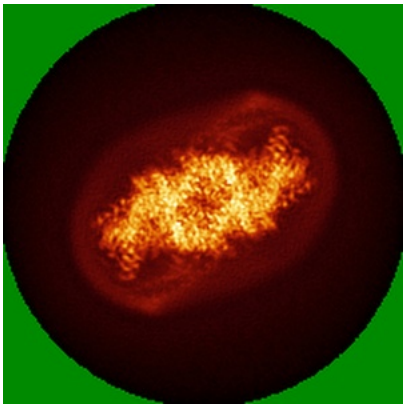

Y


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 0.02. 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.

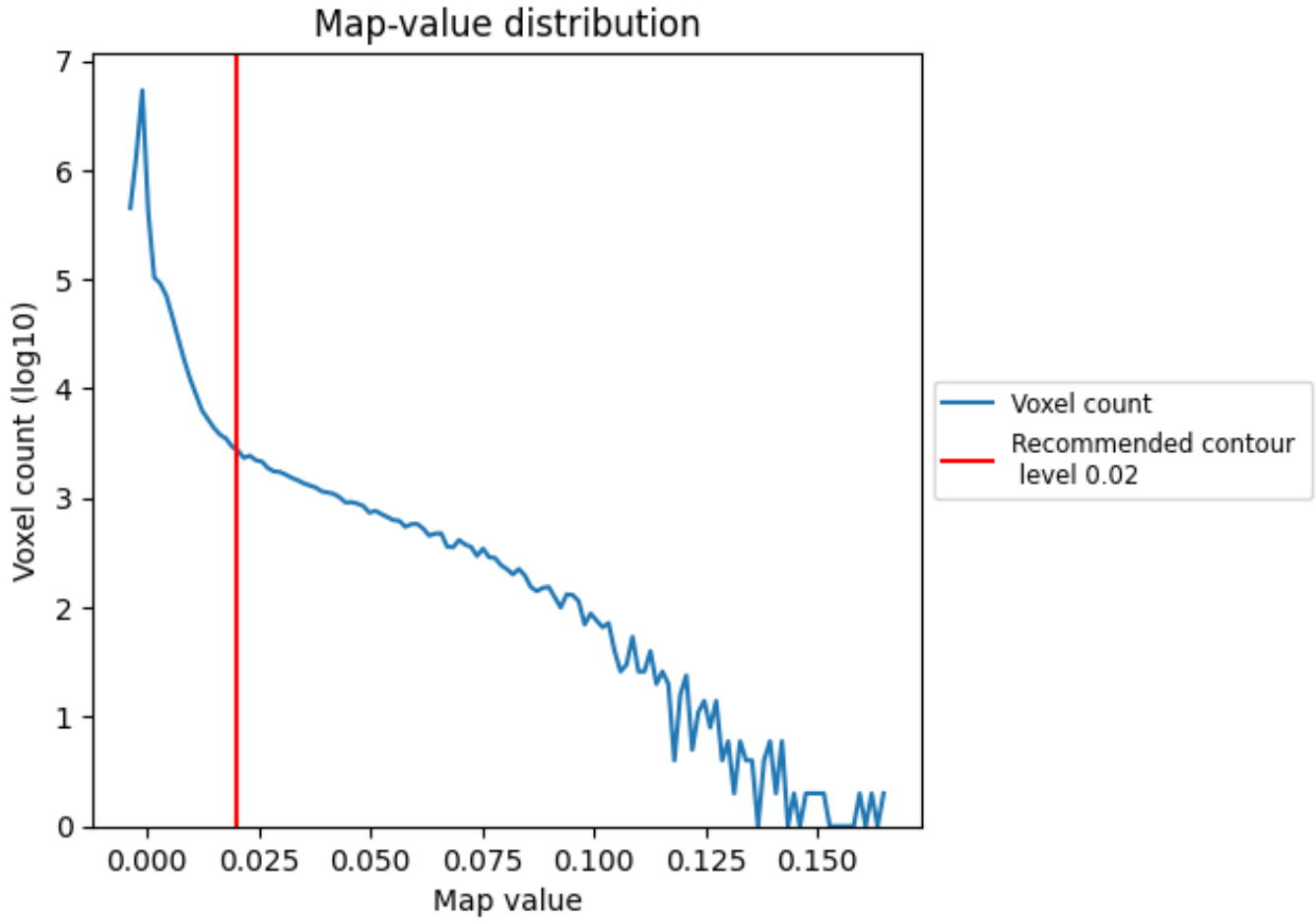
6.6 Mask visualisation (i)

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

7 Map analysis

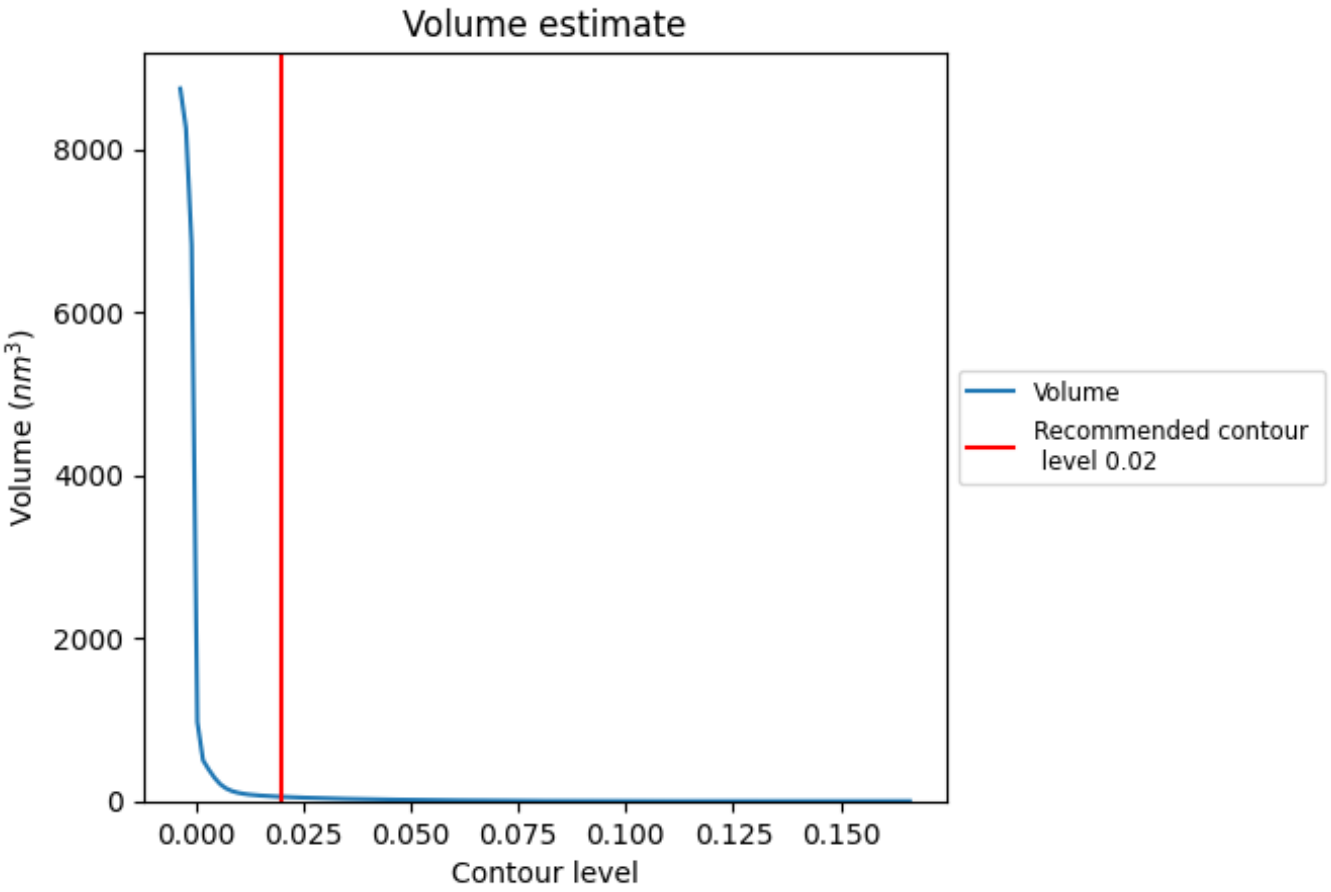
This section contains the results of statistical analysis of the map.

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.

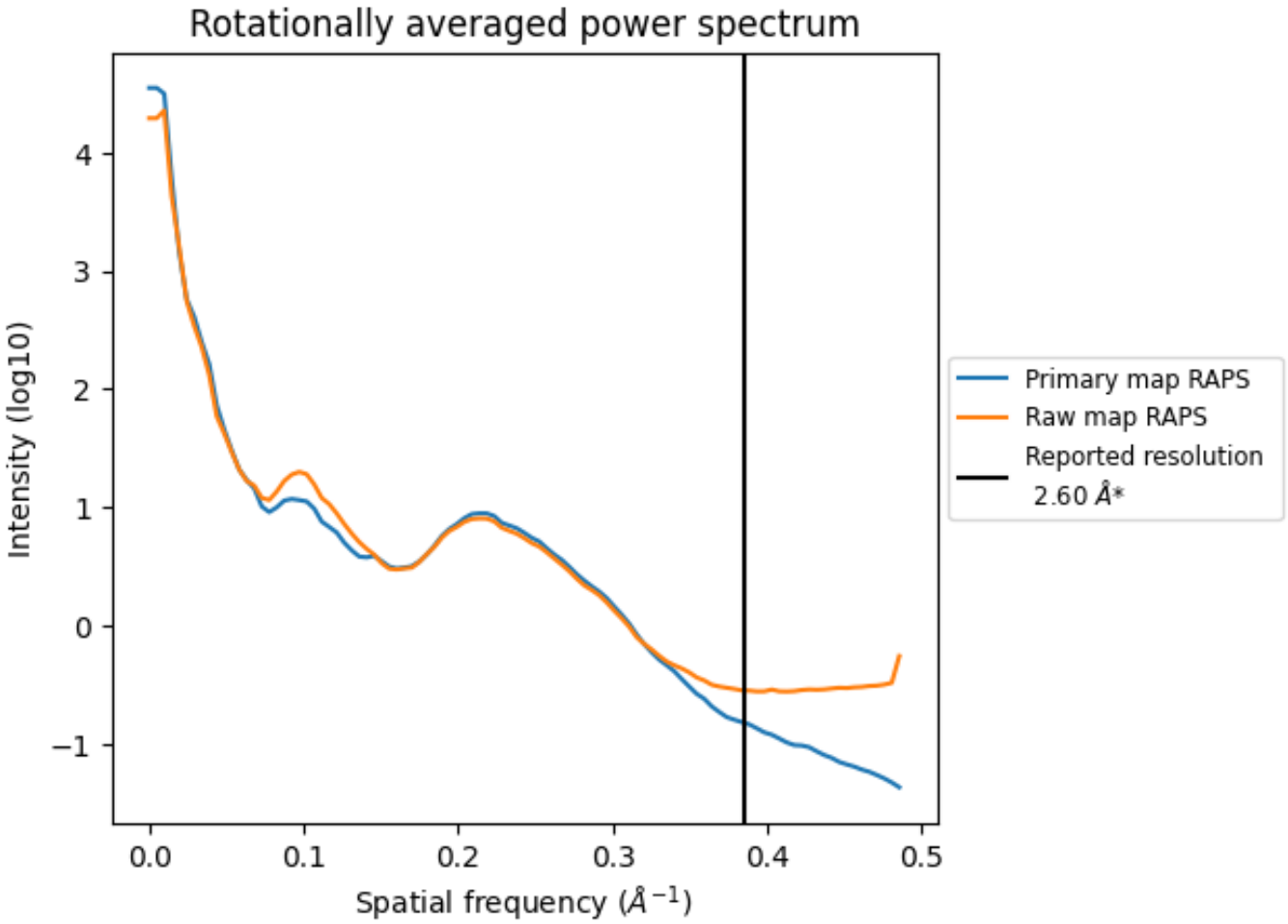
7.2 Volume estimate



The volume at the recommended contour level is 53 nm^3; this corresponds to an approximate mass of 48 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)

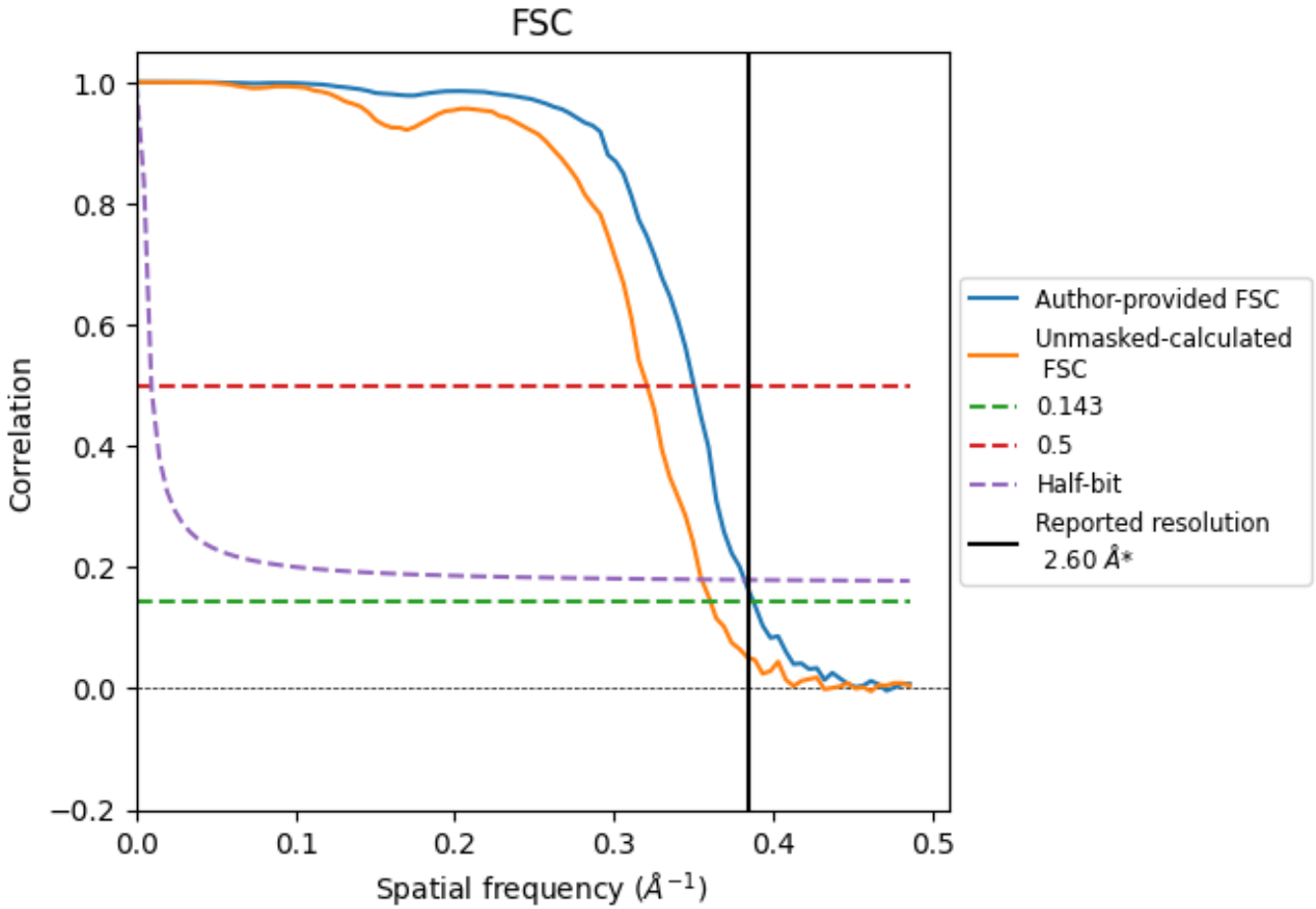


*Reported resolution corresponds to spatial frequency of 0.385 $Å^{-1}$

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 0.385 Å^{-1}

8.2 Resolution estimates (i)

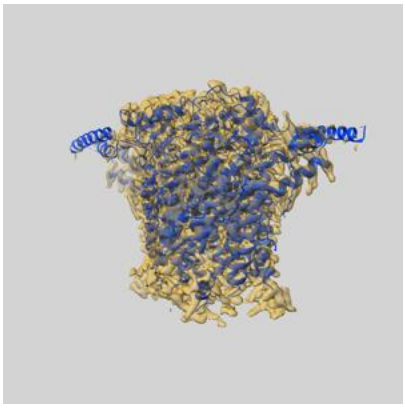
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.60	-	-
Author-provided FSC curve	2.58	2.86	2.62
Unmasked-calculated*	2.77	3.12	2.82

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

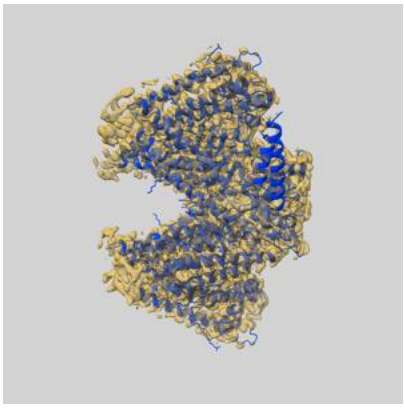
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-41911 and PDB model 8U53. Per-residue inclusion information can be found in section 3 on page 9.

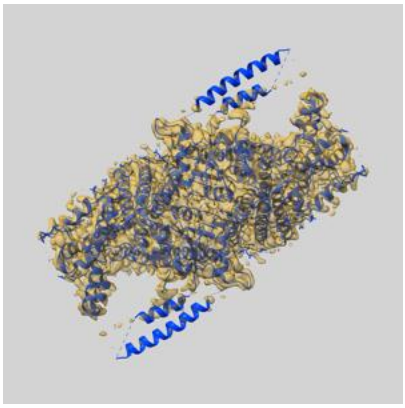
9.1 Map-model overlay



X



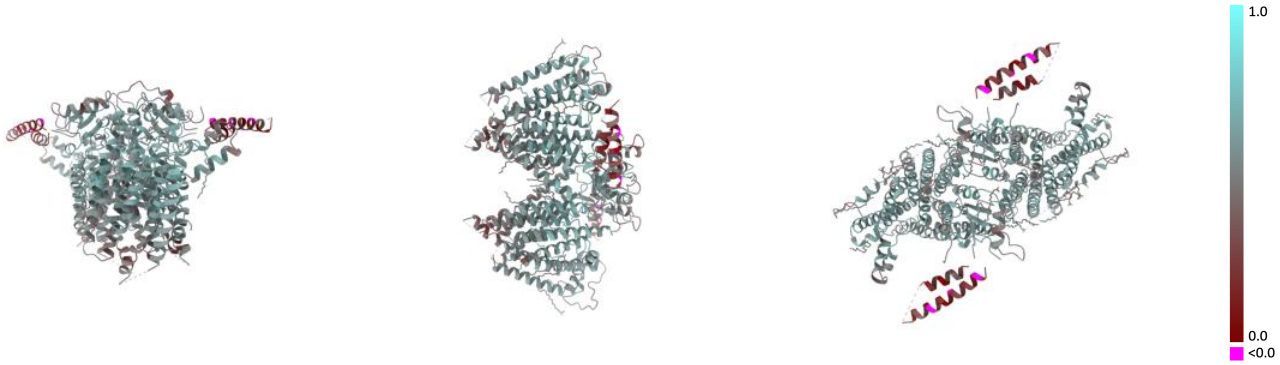
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

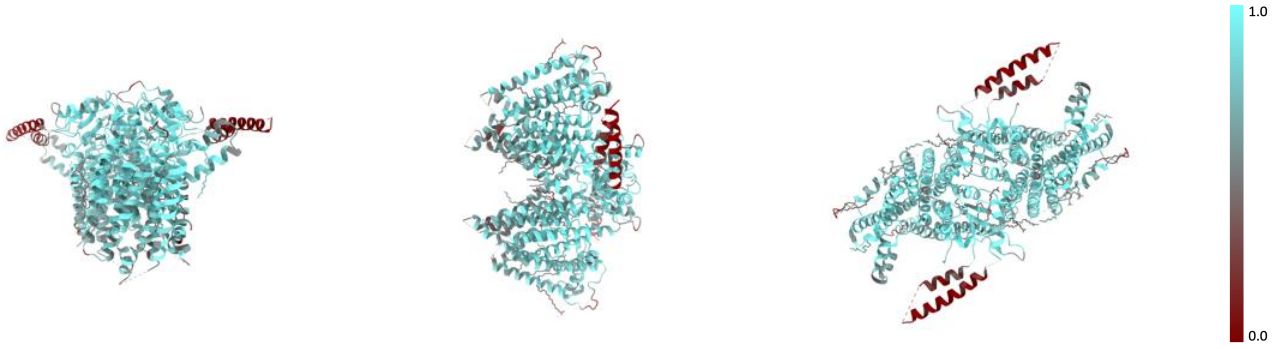
9.2 Q-score mapped to coordinate model (i)



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.

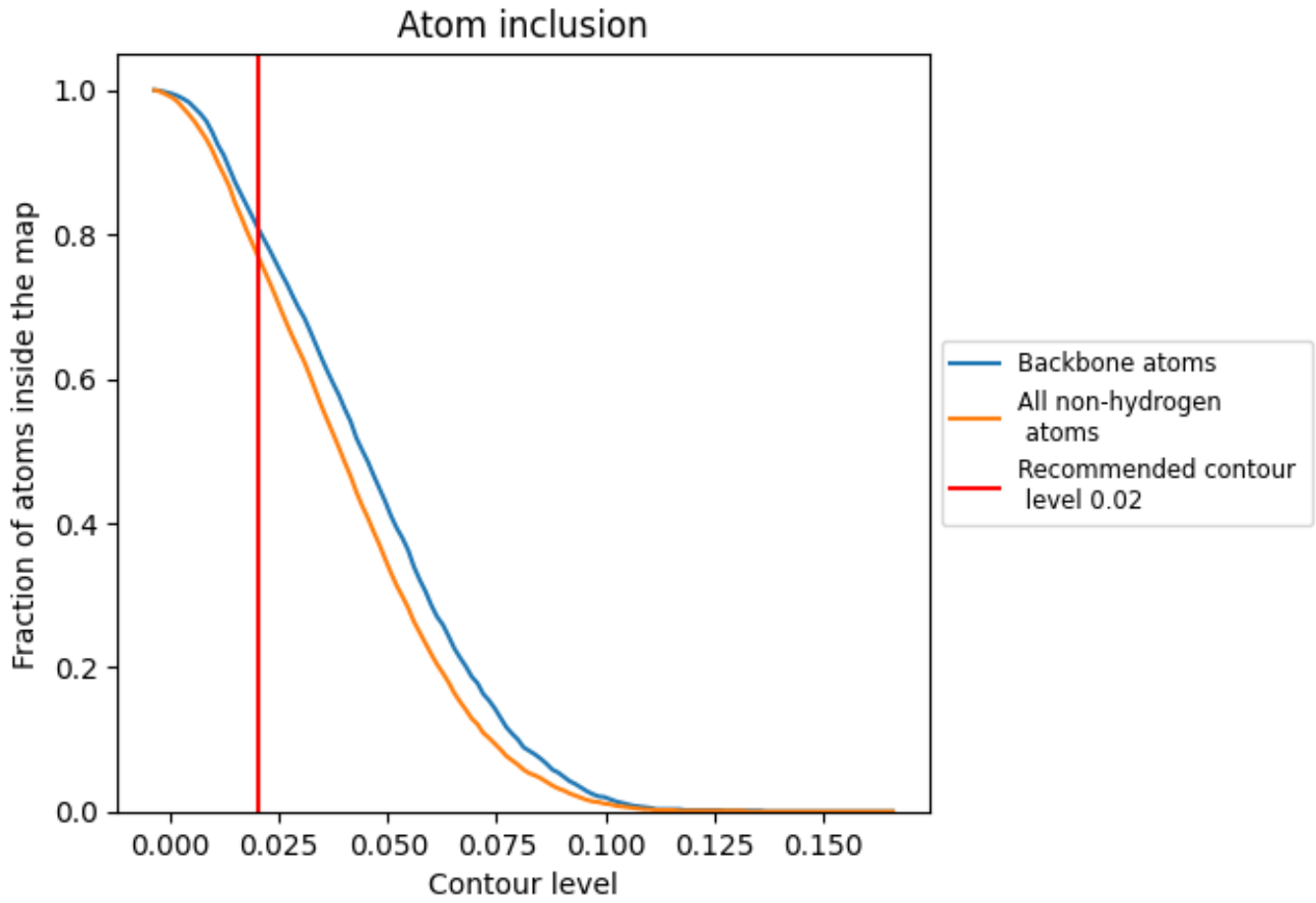
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.02).

9.4 Atom inclusion (i)



At the recommended contour level, 81% of all backbone atoms, 77% 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 (0.02) and Q-score for the entire model and for each chain.



Chain	Atom inclusion	Q-score
All	0.7720	0.5400
A	0.7740	0.5400
B	0.7710	0.5410