Full wwPDB EM Validation Report ⓘ

Dec 17, 2022 – 09:13 am GMT

PDB ID	:	6Z16
EMDB ID	:	EMD-11027
Title	:	Structure of the Mrp antiporter complex
Authors	:	Steiner, J.; Sazanov, L.A.
Deposited on	:	2020-05-12
Resolution	:	2.98 Å(reported)
Based on initial models	:	6CFW, 4HEA

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:

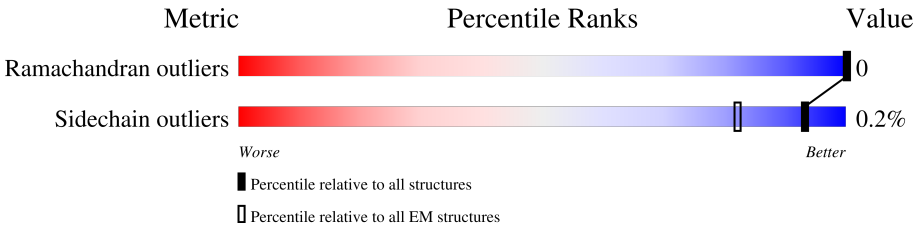
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 2.98 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
Sidechain outliers	154315	3826

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	821	17% 96%
1	a	821	20% 96%
2	B	140	11% 99%
2	b	140	16% 99%
3	C	109	8% 98%
3	c	109	8% 98%
4	D	490	99%
4	d	490	99%
5	E	158	32% 97%

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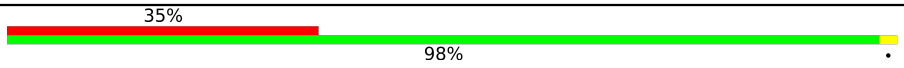
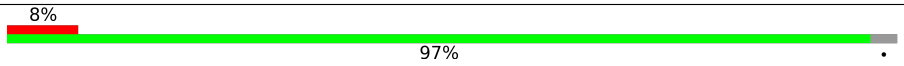
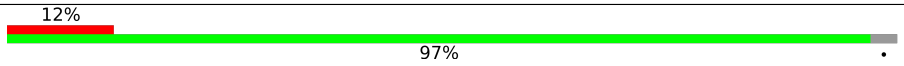
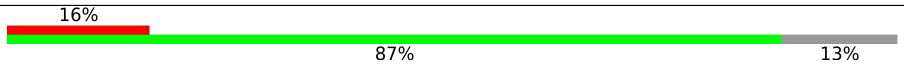
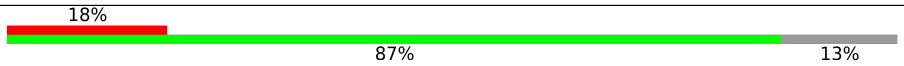
Mol	Chain	Length	Quality of chain
5	e	158	
6	F	91	
6	f	91	
7	G	119	
7	g	119	

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 30250 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 Multisubunit Na+/H+ antiporter, A subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	788	Total	C	N	O	S	0	0
			6221	4180	979	1029	33		
1	a	788	Total	C	N	O	S	0	0
			6221	4180	979	1029	33		

- Molecule 2 is a protein called Multisubunit Na+/H+ antiporter, B subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	138	Total	C	N	O	S	0	0
			1070	716	167	182	5		
2	b	138	Total	C	N	O	S	0	0
			1070	716	167	182	5		

- Molecule 3 is a protein called Multisubunit Na+/H+ antiporter, C subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	107	Total	C	N	O	S	0	0
			802	531	128	137	6		
3	c	107	Total	C	N	O	S	0	0
			802	531	128	137	6		

- Molecule 4 is a protein called Multisubunit Na+/H+ antiporter, D subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	489	Total	C	N	O	S	0	0
			3796	2570	577	635	14		
4	d	489	Total	C	N	O	S	0	0
			3796	2570	577	635	14		

- Molecule 5 is a protein called Multisubunit Na+/H+ antiporter, E subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	158	Total	C	N	O	S	0	0
			1274	860	193	215	6		
5	e	158	Total	C	N	O	S	0	0
			1274	860	193	215	6		

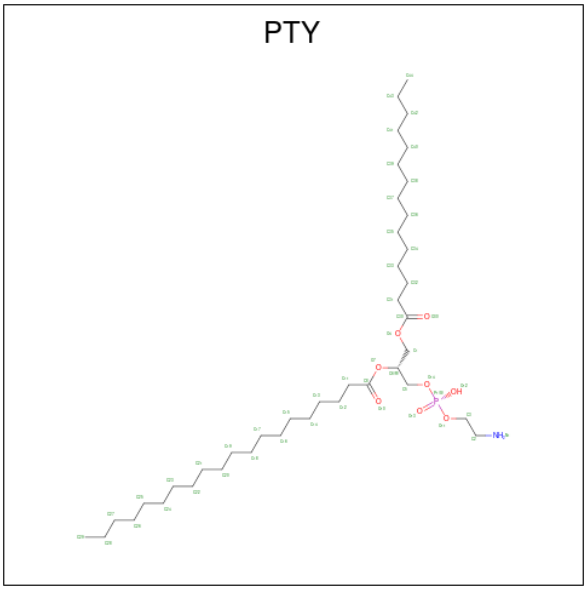
- Molecule 6 is a protein called Multisubunit Na+/H+ antiporter, F subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	88	Total	C	N	O	S	0	0
			648	431	103	110	4		
6	f	88	Total	C	N	O	S	0	0
			648	431	103	110	4		

- Molecule 7 is a protein called Multisubunit Na+/H+ antiporter, G subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	104	Total	C	N	O	S	0	0
			804	527	137	137	3		
7	g	104	Total	C	N	O	S	0	0
			804	527	137	137	3		

- Molecule 8 is PHOSPHATIDYLETHANOLAMINE (three-letter code: PTY) (formula: $C_{40}H_{80}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
8	A	1	Total	C	N	O	P	0
			275	205	7	56	7	

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Mol	Chain	Residues	Atoms	AltConf
8	A	1	Total C N O P 275 205 7 56 7	0
8	A	1	Total C N O P 275 205 7 56 7	0
8	A	1	Total C N O P 275 205 7 56 7	0
8	A	1	Total C N O P 275 205 7 56 7	0
8	A	1	Total C N O P 275 205 7 56 7	0
8	A	1	Total C N O P 275 205 7 56 7	0
8	B	1	Total C N O P 34 24 1 8 1	0
8	D	1	Total C N O P 116 86 3 24 3	0
8	D	1	Total C N O P 116 86 3 24 3	0
8	D	1	Total C N O P 116 86 3 24 3	0
8	E	1	Total C N O P 34 24 1 8 1	0
8	F	1	Total C N O P 83 63 2 16 2	0
8	F	1	Total C N O P 83 63 2 16 2	0
8	a	1	Total C N O P 275 205 7 56 7	0
8	a	1	Total C N O P 275 205 7 56 7	0
8	a	1	Total C N O P 275 205 7 56 7	0
8	a	1	Total C N O P 275 205 7 56 7	0
8	a	1	Total C N O P 275 205 7 56 7	0
8	a	1	Total C N O P 275 205 7 56 7	0
8	a	1	Total C N O P 275 205 7 56 7	0
8	d	1	Total C N O P 116 86 3 24 3	0

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Mol	Chain	Residues	Atoms					AltConf
8	d	1	Total	C	N	O	P	0
			116	86	3	24	3	
8	d	1	Total	C	N	O	P	0
			116	86	3	24	3	
8	f	1	Total	C	N	O	P	0
			83	63	2	16	2	
8	f	1	Total	C	N	O	P	0
			83	63	2	16	2	

- Molecule 9 is POTASSIUM ION (three-letter code: K) (formula: K).

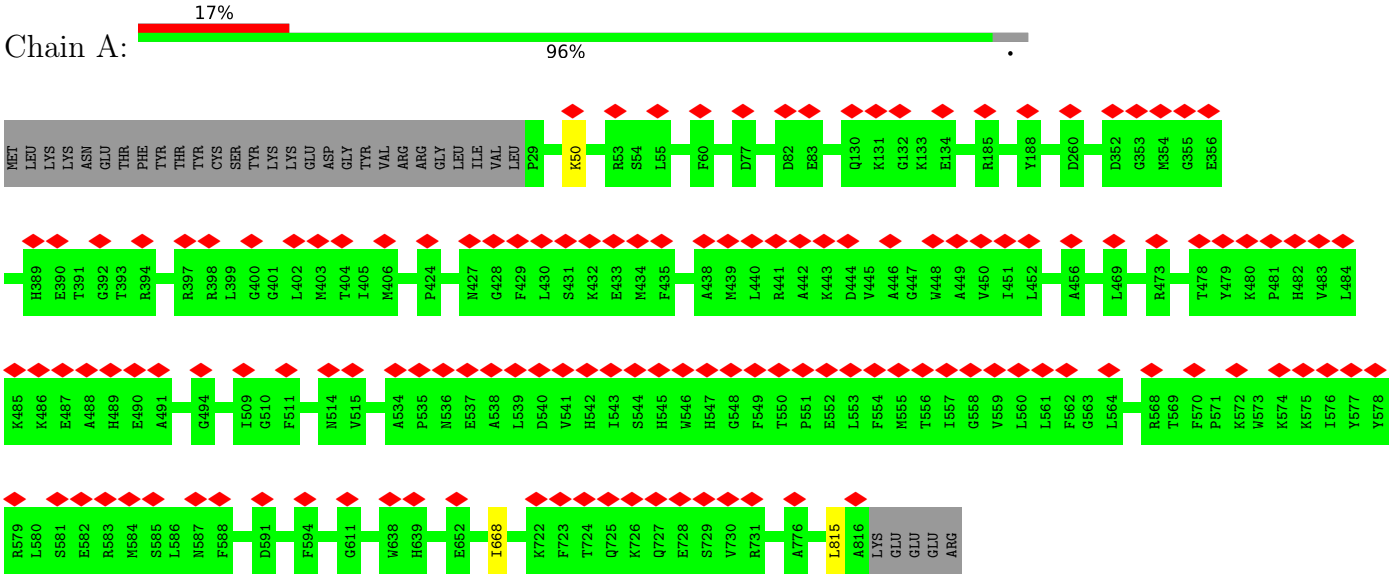
Mol	Chain	Residues	Atoms		AltConf
9	A	1	Total	K	0
			1	1	
9	C	1	Total	K	0
			1	1	
9	a	1	Total	K	0
			1	1	
9	c	1	Total	K	0
			1	1	

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.

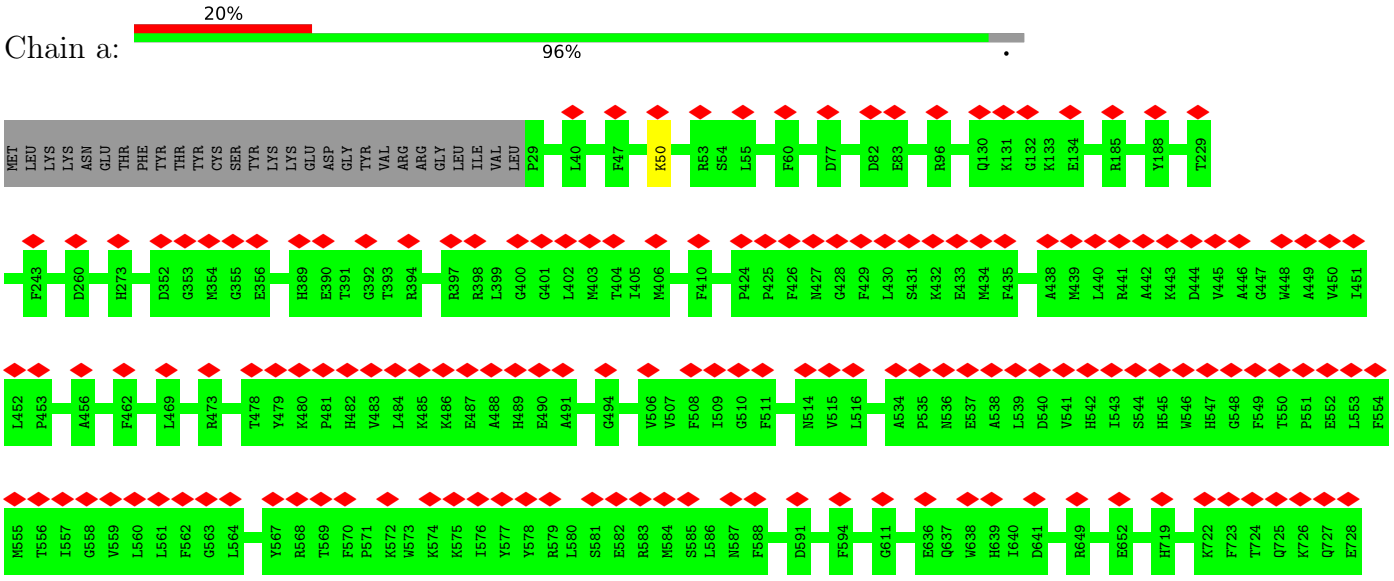
• Molecule 1: Multisubunit Na+/H+ antiporter, A subunit

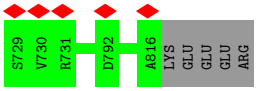
Chain A:



• Molecule 1: Multisubunit Na+/H+ antiporter, A subunit

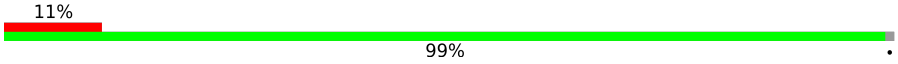
Chain a:

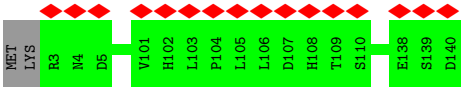




• Molecule 2: Multisubunit Na+/H+ antiporter, B subunit

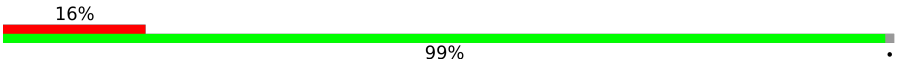
Chain B:

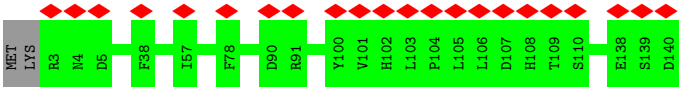




• Molecule 2: Multisubunit Na+/H+ antiporter, B subunit

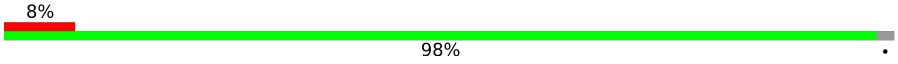
Chain b:

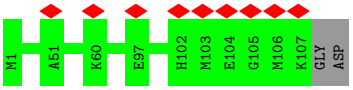




• Molecule 3: Multisubunit Na+/H+ antiporter, C subunit

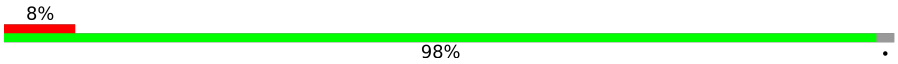
Chain C:

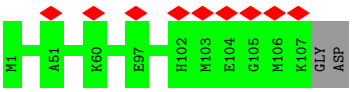




• Molecule 3: Multisubunit Na+/H+ antiporter, C subunit

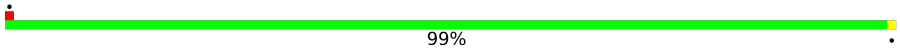
Chain c:

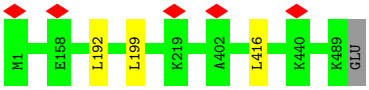




• Molecule 4: Multisubunit Na+/H+ antiporter, D subunit

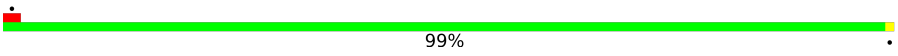
Chain D:

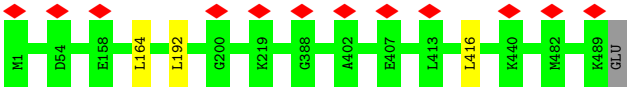




• Molecule 4: Multisubunit Na+/H+ antiporter, D subunit

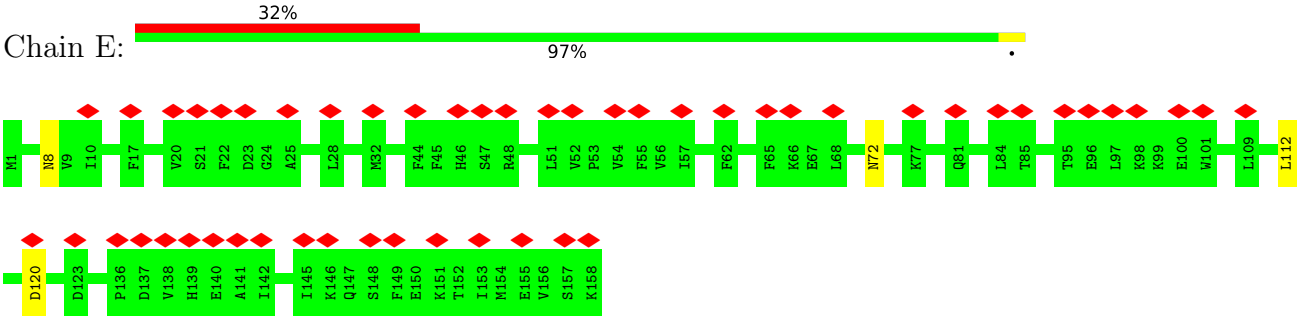
Chain d:





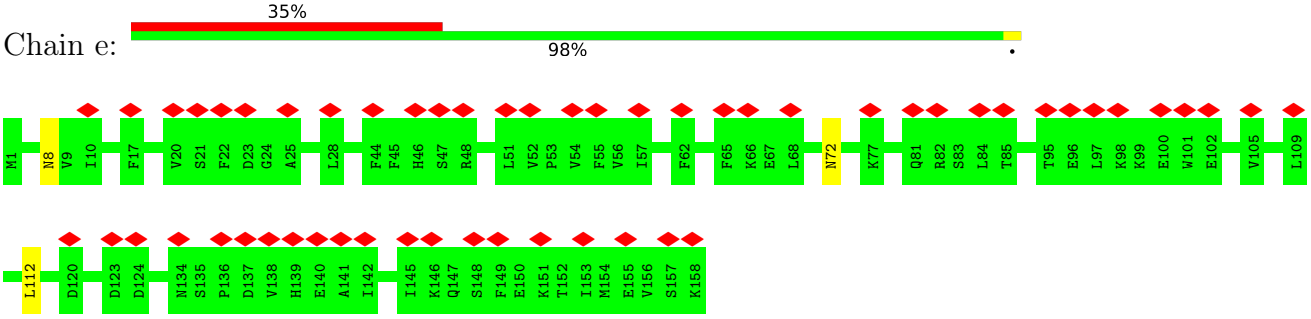
• Molecule 5: Multisubunit Na+/H+ antiporter, E subunit

Chain E:



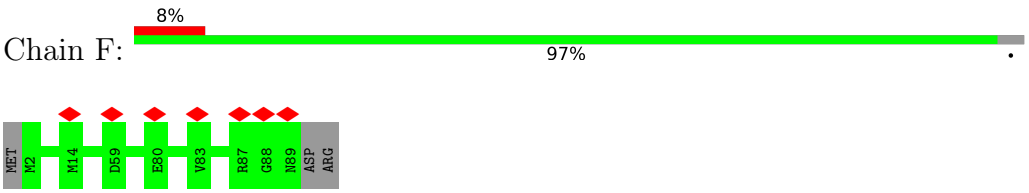
• Molecule 5: Multisubunit Na+/H+ antiporter, E subunit

Chain e:



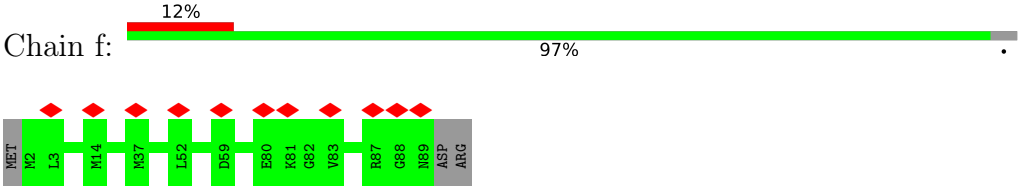
• Molecule 6: Multisubunit Na+/H+ antiporter, F subunit

Chain F:



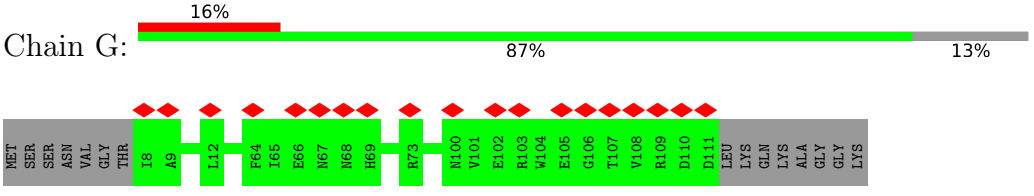
• Molecule 6: Multisubunit Na+/H+ antiporter, F subunit

Chain f:



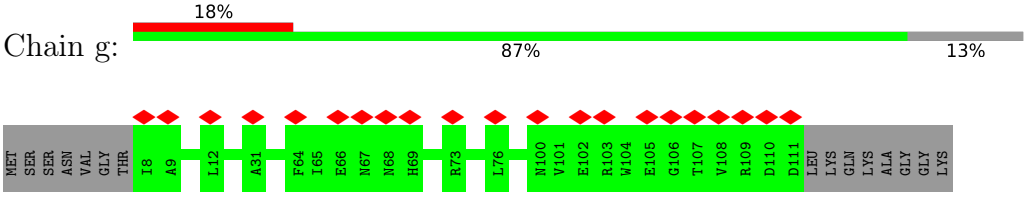
• Molecule 7: Multisubunit Na+/H+ antiporter, G subunit

Chain G:



• Molecule 7: Multisubunit Na+/H+ antiporter, G subunit

Chain g:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	285688	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 ($e^-/Å^2$)	88	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.097	Depositor
Minimum map value	-0.050	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.018	Depositor
Map size (Å)	213.36, 222.59999, 91.56	wwPDB
Map dimensions	109, 265, 254	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.84, 0.84, 0.84	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.38	0/6402	0.59	2/8721 (0.0%)
1	a	0.36	0/6402	0.57	0/8721
2	B	0.36	0/1097	0.66	0/1497
2	b	0.35	0/1097	0.65	0/1497
3	C	0.34	0/816	0.58	0/1105
3	c	0.33	0/816	0.57	0/1105
4	D	0.39	0/3893	0.61	3/5315 (0.1%)
4	d	0.38	0/3893	0.59	3/5315 (0.1%)
5	E	0.34	0/1304	0.59	1/1768 (0.1%)
5	e	0.33	0/1304	0.59	1/1768 (0.1%)
6	F	0.35	0/654	0.58	0/886
6	f	0.34	0/654	0.59	0/886
7	G	0.33	0/820	0.63	0/1117
7	g	0.33	0/820	0.62	0/1117
All	All	0.36	0/29972	0.59	10/40818 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
5	E	0	1

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	d	192	LEU	CA-CB-CG	7.09	131.62	115.30
4	D	192	LEU	CA-CB-CG	6.29	129.78	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	e	112	LEU	CA-CB-CG	6.28	129.74	115.30
5	E	112	LEU	CA-CB-CG	6.19	129.53	115.30
4	D	416	LEU	CB-CG-CD1	-5.73	101.26	111.00
4	D	199	LEU	CA-CB-CG	5.37	127.65	115.30
4	d	164	LEU	CA-CB-CG	5.18	127.22	115.30
4	d	416	LEU	CB-CG-CD1	-5.14	102.27	111.00
1	A	668	ILE	CG1-CB-CG2	-5.05	100.28	111.40
1	A	815	LEU	CA-CB-CG	5.00	126.81	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	E	120	ASP	Peptide

5.2 Too-close contacts (i)

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

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	786/821 (96%)	752 (96%)	34 (4%)	0	100	100
1	a	786/821 (96%)	746 (95%)	40 (5%)	0	100	100
2	B	136/140 (97%)	128 (94%)	8 (6%)	0	100	100
2	b	136/140 (97%)	130 (96%)	6 (4%)	0	100	100
3	C	105/109 (96%)	102 (97%)	3 (3%)	0	100	100
3	c	105/109 (96%)	102 (97%)	3 (3%)	0	100	100
4	D	487/490 (99%)	469 (96%)	18 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	d	487/490 (99%)	470 (96%)	17 (4%)	0	100	100
5	E	156/158 (99%)	148 (95%)	8 (5%)	0	100	100
5	e	156/158 (99%)	148 (95%)	8 (5%)	0	100	100
6	F	86/91 (94%)	82 (95%)	4 (5%)	0	100	100
6	f	86/91 (94%)	83 (96%)	3 (4%)	0	100	100
7	G	102/119 (86%)	95 (93%)	7 (7%)	0	100	100
7	g	102/119 (86%)	95 (93%)	7 (7%)	0	100	100
All	All	3716/3856 (96%)	3550 (96%)	166 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	659/690 (96%)	658 (100%)	1 (0%)	93	98
1	a	659/690 (96%)	658 (100%)	1 (0%)	93	98
2	B	116/118 (98%)	116 (100%)	0	100	100
2	b	116/118 (98%)	116 (100%)	0	100	100
3	C	85/86 (99%)	85 (100%)	0	100	100
3	c	85/86 (99%)	85 (100%)	0	100	100
4	D	409/411 (100%)	409 (100%)	0	100	100
4	d	409/411 (100%)	409 (100%)	0	100	100
5	E	143/143 (100%)	141 (99%)	2 (1%)	67	86
5	e	143/143 (100%)	141 (99%)	2 (1%)	67	86
6	F	69/72 (96%)	69 (100%)	0	100	100
6	f	69/72 (96%)	69 (100%)	0	100	100
7	G	86/97 (89%)	86 (100%)	0	100	100
7	g	86/97 (89%)	86 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3134/3234 (97%)	3128 (100%)	6 (0%)	93 98

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	LYS
5	E	8	ASN
5	E	72	ASN
1	a	50	LYS
5	e	8	ASN
5	e	72	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	158	HIS
1	A	273	HIS
2	B	31	HIS
7	G	90	HIS
1	a	138	ASN
1	a	158	HIS
1	a	273	HIS
2	b	31	HIS
7	g	90	HIS

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)

Of 30 ligands modelled in this entry, 4 are monoatomic - leaving 26 for Mogul analysis.

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	$\#\|Z\| > 2$
8	PTY	d	503	-	42,42,49	0.36	0	45,47,54	0.52	1 (2%)
8	PTY	d	502	-	38,38,49	0.32	0	41,43,54	0.30	0
8	PTY	d	501	-	33,33,49	0.33	0	36,38,54	0.35	0
8	PTY	A	907	-	46,46,49	0.32	0	49,51,54	0.51	1 (2%)
8	PTY	a	907	-	46,46,49	0.32	0	49,51,54	0.51	1 (2%)
8	PTY	f	1801	-	49,49,49	0.29	0	52,54,54	0.45	0
8	PTY	a	906	-	33,33,49	1.08	3 (9%)	36,38,54	0.59	1 (2%)
8	PTY	F	1801	-	49,49,49	0.30	0	52,54,54	0.47	1 (1%)
8	PTY	D	503	-	42,42,49	0.35	0	45,47,54	0.52	1 (2%)
8	PTY	F	1802	-	32,32,49	0.37	0	35,37,54	0.31	0
8	PTY	A	905	-	46,46,49	0.30	0	49,51,54	0.26	0
8	PTY	A	902	-	33,33,49	1.04	3 (9%)	36,38,54	0.31	0
8	PTY	A	901	-	29,29,49	0.36	0	32,34,54	0.30	0
8	PTY	A	903	-	42,42,49	0.33	0	45,47,54	0.28	0
8	PTY	a	905	-	46,46,49	0.30	0	49,51,54	0.25	0
8	PTY	B	201	-	33,33,49	1.08	3 (9%)	36,38,54	0.56	0
8	PTY	a	902	-	33,33,49	1.04	3 (9%)	36,38,54	0.31	0
8	PTY	a	903	-	42,42,49	0.33	0	45,47,54	0.28	0
8	PTY	A	904	-	39,39,49	0.34	0	42,44,54	0.39	0
8	PTY	f	1802	-	32,32,49	0.36	0	35,37,54	0.31	0
8	PTY	E	201	-	33,33,49	1.07	3 (9%)	36,38,54	0.56	0
8	PTY	a	904	-	39,39,49	0.35	0	42,44,54	0.37	0
8	PTY	D	502	-	38,38,49	0.31	0	41,43,54	0.32	0
8	PTY	a	901	-	29,29,49	0.37	0	32,34,54	0.30	0
8	PTY	A	906	-	33,33,49	1.07	3 (9%)	36,38,54	0.59	1 (2%)
8	PTY	D	501	-	33,33,49	0.33	0	36,38,54	0.35	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
8	PTY	d	503	-	-	13/46/46/53	-
8	PTY	d	502	-	-	9/42/42/53	-
8	PTY	d	501	-	-	5/37/37/53	-
8	PTY	A	907	-	-	11/50/50/53	-
8	PTY	a	907	-	-	10/50/50/53	-
8	PTY	f	1801	-	-	15/53/53/53	-
8	PTY	a	906	-	-	10/37/37/53	-
8	PTY	F	1801	-	-	13/53/53/53	-
8	PTY	D	503	-	-	12/46/46/53	-
8	PTY	F	1802	-	-	5/36/36/53	-
8	PTY	A	905	-	-	11/50/50/53	-
8	PTY	A	902	-	-	9/37/37/53	-
8	PTY	A	901	-	-	7/33/33/53	-
8	PTY	A	903	-	-	8/46/46/53	-
8	PTY	a	905	-	-	10/50/50/53	-
8	PTY	B	201	-	-	13/37/37/53	-
8	PTY	a	902	-	-	6/37/37/53	-
8	PTY	a	903	-	-	8/46/46/53	-
8	PTY	A	904	-	-	12/43/43/53	-
8	PTY	f	1802	-	-	5/36/36/53	-
8	PTY	E	201	-	-	16/37/37/53	-
8	PTY	a	904	-	-	12/43/43/53	-
8	PTY	D	502	-	-	10/42/42/53	-
8	PTY	a	901	-	-	5/33/33/53	-
8	PTY	A	906	-	-	10/37/37/53	-
8	PTY	D	501	-	-	10/37/37/53	-

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	201	PTY	P1-O12	-4.08	1.36	1.55
8	A	906	PTY	P1-O12	-4.06	1.36	1.55
8	E	201	PTY	P1-O12	-4.03	1.36	1.55
8	a	906	PTY	P1-O12	-4.03	1.36	1.55
8	A	902	PTY	P1-O12	-3.98	1.36	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	a	902	PTY	P1-O12	-3.93	1.36	1.55
8	B	201	PTY	P1-O14	-3.13	1.46	1.59
8	E	201	PTY	P1-O14	-3.03	1.47	1.59
8	a	906	PTY	P1-O14	-3.03	1.47	1.59
8	E	201	PTY	P1-O13	-2.99	1.40	1.50
8	A	902	PTY	P1-O13	-2.99	1.40	1.50
8	a	902	PTY	P1-O13	-2.98	1.40	1.50
8	a	906	PTY	P1-O13	-2.98	1.40	1.50
8	A	906	PTY	P1-O13	-2.97	1.40	1.50
8	B	201	PTY	P1-O13	-2.97	1.40	1.50
8	A	906	PTY	P1-O14	-2.93	1.47	1.59
8	a	902	PTY	P1-O14	-2.92	1.47	1.59
8	A	902	PTY	P1-O14	-2.83	1.47	1.59

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	F	1801	PTY	O4-C1-C6	2.21	114.86	108.43
8	d	503	PTY	C6-O7-C8	2.09	122.94	117.79
8	A	907	PTY	C6-O7-C8	2.09	122.94	117.79
8	a	907	PTY	C6-O7-C8	2.09	122.93	117.79
8	A	906	PTY	C6-O7-C8	2.08	122.92	117.79
8	a	906	PTY	C6-O7-C8	2.06	122.85	117.79
8	D	503	PTY	C6-O7-C8	2.03	122.80	117.79

There are no chirality outliers.

All (255) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	901	PTY	N1-C2-C3-O11
8	A	902	PTY	N1-C2-C3-O11
8	A	902	PTY	C5-O14-P1-O13
8	A	903	PTY	C5-O14-P1-O12
8	A	903	PTY	C5-O14-P1-O13
8	A	904	PTY	N1-C2-C3-O11
8	A	904	PTY	C3-O11-P1-O12
8	A	904	PTY	C3-O11-P1-O13
8	A	905	PTY	N1-C2-C3-O11
8	A	905	PTY	C3-O11-P1-O12
8	A	905	PTY	C3-O11-P1-O13
8	A	907	PTY	N1-C2-C3-O11
8	A	907	PTY	C3-O11-P1-O12

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Mol	Chain	Res	Type	Atoms
8	A	907	PTY	C3-O11-P1-O13
8	B	201	PTY	N1-C2-C3-O11
8	B	201	PTY	C3-O11-P1-O12
8	B	201	PTY	C3-O11-P1-O13
8	B	201	PTY	C5-O14-P1-O12
8	D	501	PTY	N1-C2-C3-O11
8	D	501	PTY	C3-O11-P1-O13
8	D	501	PTY	C5-O14-P1-O13
8	D	502	PTY	C5-O14-P1-O11
8	D	503	PTY	N1-C2-C3-O11
8	D	503	PTY	C3-O11-P1-O13
8	D	503	PTY	C5-O14-P1-O13
8	E	201	PTY	N1-C2-C3-O11
8	E	201	PTY	C3-O11-P1-O12
8	E	201	PTY	C3-O11-P1-O13
8	E	201	PTY	C5-O14-P1-O12
8	F	1801	PTY	C3-O11-P1-O12
8	F	1801	PTY	C3-O11-P1-O13
8	F	1802	PTY	C3-O11-P1-O14
8	a	901	PTY	N1-C2-C3-O11
8	a	902	PTY	C3-O11-P1-O13
8	a	902	PTY	C5-O14-P1-O13
8	a	903	PTY	C5-O14-P1-O12
8	a	904	PTY	N1-C2-C3-O11
8	a	904	PTY	C3-O11-P1-O12
8	a	904	PTY	C3-O11-P1-O13
8	a	905	PTY	N1-C2-C3-O11
8	a	905	PTY	C3-O11-P1-O12
8	a	905	PTY	C3-O11-P1-O13
8	a	907	PTY	N1-C2-C3-O11
8	a	907	PTY	C3-O11-P1-O12
8	a	907	PTY	C3-O11-P1-O13
8	d	502	PTY	N1-C2-C3-O11
8	d	502	PTY	C3-O11-P1-O13
8	d	502	PTY	C5-O14-P1-O11
8	d	503	PTY	N1-C2-C3-O11
8	d	503	PTY	C3-O11-P1-O13
8	f	1801	PTY	C3-O11-P1-O12
8	f	1801	PTY	C3-O11-P1-O13
8	f	1802	PTY	C3-O11-P1-O12
8	E	201	PTY	C8-C11-C12-C13
8	B	201	PTY	C8-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
8	d	501	PTY	C8-C11-C12-C13
8	A	902	PTY	C5-O14-P1-O11
8	A	904	PTY	C3-O11-P1-O14
8	A	905	PTY	C3-O11-P1-O14
8	A	905	PTY	C5-O14-P1-O11
8	A	906	PTY	C3-O11-P1-O14
8	A	906	PTY	C5-O14-P1-O11
8	A	907	PTY	C3-O11-P1-O14
8	B	201	PTY	C3-O11-P1-O14
8	B	201	PTY	C5-O14-P1-O11
8	D	501	PTY	C5-O14-P1-O11
8	E	201	PTY	C3-O11-P1-O14
8	E	201	PTY	C5-O14-P1-O11
8	F	1801	PTY	C3-O11-P1-O14
8	a	902	PTY	C5-O14-P1-O11
8	a	904	PTY	C3-O11-P1-O14
8	a	905	PTY	C3-O11-P1-O14
8	a	905	PTY	C5-O14-P1-O11
8	a	906	PTY	C3-O11-P1-O14
8	a	906	PTY	C5-O14-P1-O11
8	a	907	PTY	C3-O11-P1-O14
8	a	907	PTY	C5-O14-P1-O11
8	d	502	PTY	C3-O11-P1-O14
8	f	1801	PTY	C3-O11-P1-O14
8	f	1802	PTY	C3-O11-P1-O14
8	D	501	PTY	C8-C11-C12-C13
8	f	1801	PTY	C24-C25-C26-C27
8	D	503	PTY	C11-C12-C13-C14
8	D	503	PTY	C33-C34-C35-C36
8	d	503	PTY	C11-C12-C13-C14
8	d	503	PTY	C33-C34-C35-C36
8	F	1801	PTY	C24-C25-C26-C27
8	f	1801	PTY	C35-C36-C37-C38
8	A	907	PTY	C32-C33-C34-C35
8	A	901	PTY	C12-C13-C14-C15
8	A	905	PTY	C14-C15-C16-C17
8	d	503	PTY	C8-C11-C12-C13
8	D	503	PTY	C8-C11-C12-C13
8	a	905	PTY	C14-C15-C16-C17
8	a	907	PTY	C32-C33-C34-C35
8	A	906	PTY	O4-C1-C6-O7
8	D	503	PTY	C3-O11-P1-O14

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Mol	Chain	Res	Type	Atoms
8	D	503	PTY	C5-O14-P1-O11
8	a	901	PTY	C5-O14-P1-O11
8	a	903	PTY	C5-O14-P1-O11
8	d	503	PTY	C3-O11-P1-O14
8	A	903	PTY	O14-C5-C6-C1
8	F	1801	PTY	O14-C5-C6-C1
8	a	903	PTY	O14-C5-C6-C1
8	a	906	PTY	O14-C5-C6-C1
8	d	503	PTY	O14-C5-C6-C1
8	f	1801	PTY	O14-C5-C6-C1
8	D	503	PTY	C31-C32-C33-C34
8	A	905	PTY	C31-C32-C33-C34
8	B	201	PTY	O4-C1-C6-C5
8	a	903	PTY	C13-C14-C15-C16
8	a	905	PTY	C31-C32-C33-C34
8	B	201	PTY	O14-C5-C6-O7
8	a	906	PTY	O4-C1-C6-O7
8	A	903	PTY	C13-C14-C15-C16
8	A	906	PTY	O14-C5-C6-C1
8	A	901	PTY	C6-C5-O14-P1
8	A	902	PTY	C6-C5-O14-P1
8	a	901	PTY	C6-C5-O14-P1
8	a	904	PTY	C6-C5-O14-P1
8	E	201	PTY	O4-C1-C6-C5
8	A	902	PTY	C3-O11-P1-O14
8	A	903	PTY	C5-O14-P1-O11
8	D	501	PTY	C3-O11-P1-O14
8	D	501	PTY	O4-C1-C6-O7
8	A	904	PTY	C6-C5-O14-P1
8	A	906	PTY	C6-C5-O14-P1
8	F	1801	PTY	C6-C5-O14-P1
8	F	1802	PTY	C6-C5-O14-P1
8	a	902	PTY	C6-C5-O14-P1
8	f	1802	PTY	C6-C5-O14-P1
8	a	905	PTY	C15-C16-C17-C18
8	D	503	PTY	O14-C5-C6-C1
8	f	1801	PTY	C31-C30-O4-C1
8	D	501	PTY	O4-C1-C6-C5
8	f	1801	PTY	O4-C1-C6-C5
8	f	1801	PTY	C6-C5-O14-P1
8	A	903	PTY	O14-C5-C6-O7
8	E	201	PTY	O14-C5-C6-O7

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Mol	Chain	Res	Type	Atoms
8	a	903	PTY	O14-C5-C6-O7
8	a	906	PTY	O14-C5-C6-O7
8	A	905	PTY	C15-C16-C17-C18
8	B	201	PTY	O4-C1-C6-O7
8	f	1801	PTY	O4-C1-C6-O7
8	F	1801	PTY	C19-C20-C21-C22
8	A	901	PTY	C5-O14-P1-O11
8	D	502	PTY	C3-O11-P1-O14
8	a	902	PTY	C3-O11-P1-O14
8	d	503	PTY	C5-O14-P1-O11
8	A	903	PTY	C16-C17-C18-C19
8	A	902	PTY	C3-O11-P1-O12
8	A	902	PTY	C5-O14-P1-O12
8	A	905	PTY	C5-O14-P1-O12
8	A	905	PTY	C5-O14-P1-O13
8	A	906	PTY	C3-O11-P1-O13
8	A	906	PTY	C5-O14-P1-O13
8	D	501	PTY	C5-O14-P1-O12
8	D	502	PTY	C5-O14-P1-O12
8	D	503	PTY	C3-O11-P1-O12
8	F	1802	PTY	C3-O11-P1-O12
8	a	901	PTY	C5-O14-P1-O12
8	a	902	PTY	C5-O14-P1-O12
8	a	903	PTY	C5-O14-P1-O13
8	a	905	PTY	C5-O14-P1-O12
8	a	906	PTY	C3-O11-P1-O13
8	a	906	PTY	C5-O14-P1-O13
8	d	502	PTY	C3-O11-P1-O12
8	d	502	PTY	C5-O14-P1-O12
8	d	503	PTY	C3-O11-P1-O12
8	F	1801	PTY	C31-C30-O4-C1
8	a	903	PTY	C11-C12-C13-C14
8	a	903	PTY	C16-C17-C18-C19
8	f	1802	PTY	C2-C3-O11-P1
8	A	904	PTY	O14-C5-C6-O7
8	A	906	PTY	O14-C5-C6-O7
8	F	1801	PTY	O14-C5-C6-O7
8	a	904	PTY	O14-C5-C6-O7
8	f	1801	PTY	O14-C5-C6-O7
8	a	904	PTY	C19-C20-C21-C22
8	F	1801	PTY	O4-C1-C6-C5
8	E	201	PTY	C6-C5-O14-P1

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Mol	Chain	Res	Type	Atoms
8	f	1801	PTY	C19-C20-C21-C22
8	A	903	PTY	C11-C12-C13-C14
8	D	502	PTY	C17-C18-C19-C20
8	a	904	PTY	C14-C15-C16-C17
8	a	906	PTY	C6-C5-O14-P1
8	A	904	PTY	O4-C1-C6-O7
8	E	201	PTY	O4-C1-C6-O7
8	F	1801	PTY	O4-C1-C6-O7
8	A	904	PTY	C5-O14-P1-O11
8	a	904	PTY	C5-O14-P1-O11
8	d	501	PTY	C3-O11-P1-O14
8	d	503	PTY	C31-C32-C33-C34
8	A	906	PTY	O4-C1-C6-C5
8	B	201	PTY	C6-C5-O14-P1
8	A	904	PTY	C14-C15-C16-C17
8	d	502	PTY	C17-C18-C19-C20
8	f	1801	PTY	O30-C30-O4-C1
8	F	1801	PTY	O30-C30-O4-C1
8	D	502	PTY	N1-C2-C3-O11
8	d	501	PTY	O4-C1-C6-O7
8	A	904	PTY	C19-C20-C21-C22
8	a	906	PTY	O4-C1-C6-C5
8	d	501	PTY	O4-C1-C6-C5
8	B	201	PTY	C1-C6-O7-C8
8	E	201	PTY	C1-C6-O7-C8
8	d	503	PTY	O14-C5-C6-O7
8	A	904	PTY	O14-C5-C6-C1
8	a	904	PTY	O4-C1-C6-O7
8	d	503	PTY	O4-C1-C6-O7
8	A	902	PTY	O4-C1-C6-C5
8	A	902	PTY	C14-C15-C16-C17
8	D	501	PTY	O14-C5-C6-O7
8	E	201	PTY	O14-C5-C6-C1
8	a	904	PTY	O14-C5-C6-C1
8	D	503	PTY	O4-C1-C6-O7
8	A	907	PTY	C5-O14-P1-O11
8	A	907	PTY	C11-C12-C13-C14
8	E	201	PTY	O4-C30-C31-C32
8	a	907	PTY	C15-C16-C17-C18
8	D	502	PTY	O4-C30-C31-C32
8	A	907	PTY	C41-C42-C43-C44
8	D	502	PTY	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
8	a	904	PTY	C17-C18-C19-C20
8	D	502	PTY	C6-C5-O14-P1
8	A	901	PTY	C8-C11-C12-C13
8	f	1802	PTY	C12-C13-C14-C15
8	A	901	PTY	C5-O14-P1-O12
8	D	502	PTY	C3-O11-P1-O12
8	F	1801	PTY	C5-O14-P1-O13
8	a	905	PTY	C5-O14-P1-O13
8	a	907	PTY	C5-O14-P1-O13
8	d	501	PTY	C3-O11-P1-O13
8	d	503	PTY	C5-O14-P1-O13
8	A	905	PTY	O4-C30-C31-C32
8	B	201	PTY	O14-C5-C6-C1
8	A	901	PTY	C2-C3-O11-P1
8	A	906	PTY	C5-C6-O7-C8
8	A	907	PTY	C1-C6-O7-C8
8	E	201	PTY	C2-C3-O11-P1
8	F	1802	PTY	C2-C3-O11-P1
8	a	906	PTY	C5-C6-O7-C8
8	f	1801	PTY	C2-C3-O11-P1
8	A	907	PTY	O4-C30-C31-C32
8	A	907	PTY	C15-C16-C17-C18
8	D	502	PTY	O30-C30-C31-C32
8	a	907	PTY	O4-C30-C31-C32
8	d	502	PTY	O4-C30-C31-C32
8	f	1801	PTY	C21-C22-C23-C24
8	E	201	PTY	O30-C30-C31-C32
8	a	907	PTY	O30-C30-C31-C32
8	F	1802	PTY	C12-C13-C14-C15
8	A	904	PTY	C17-C18-C19-C20
8	a	901	PTY	C8-C11-C12-C13
8	d	502	PTY	O30-C30-C31-C32

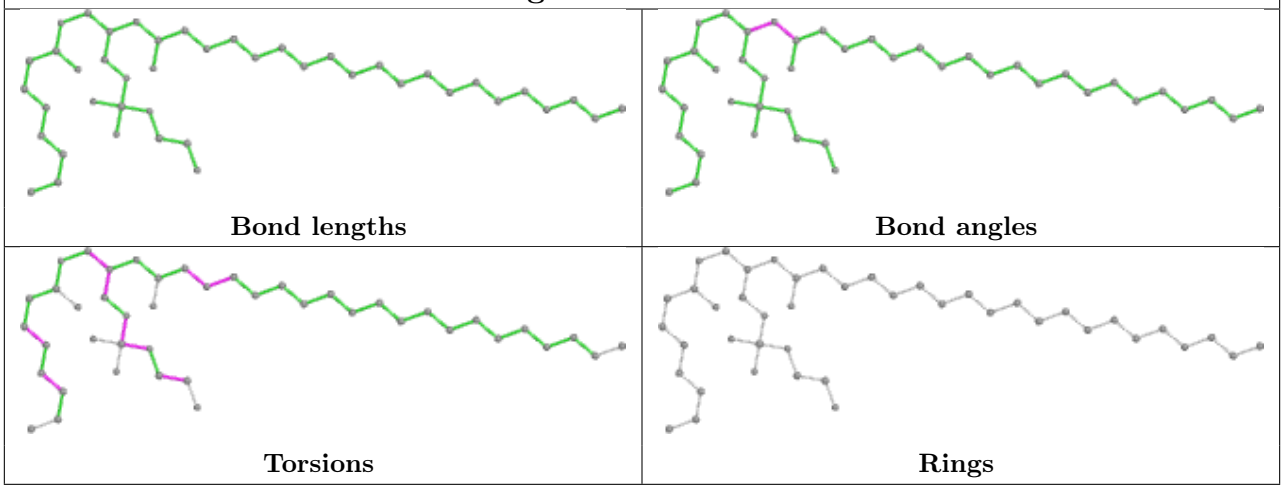
There are no ring outliers.

No monomer is involved in short contacts.

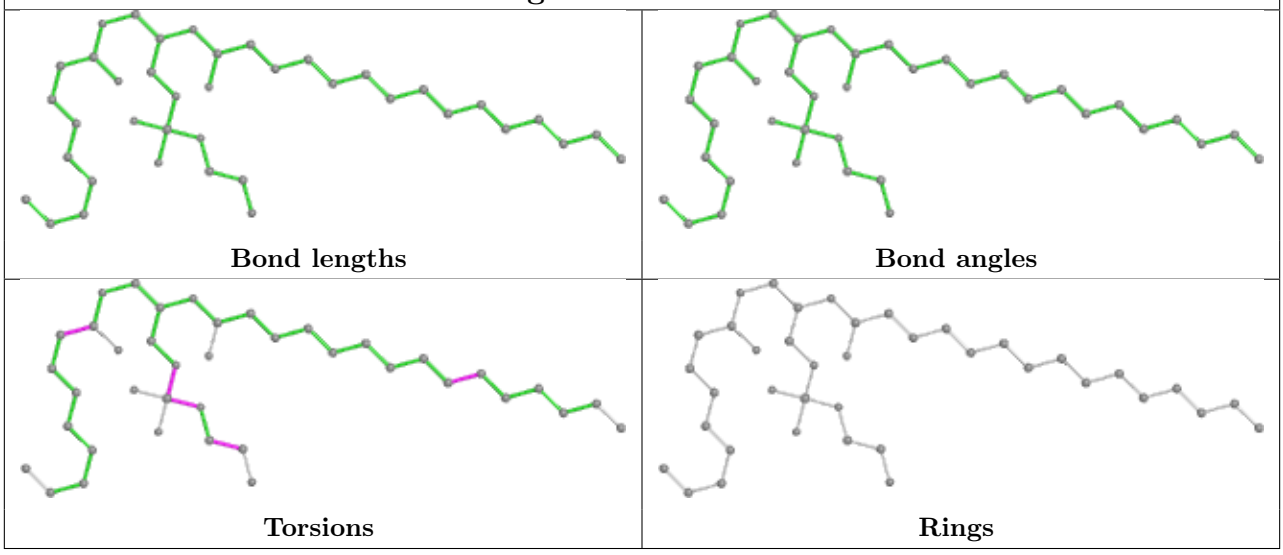
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

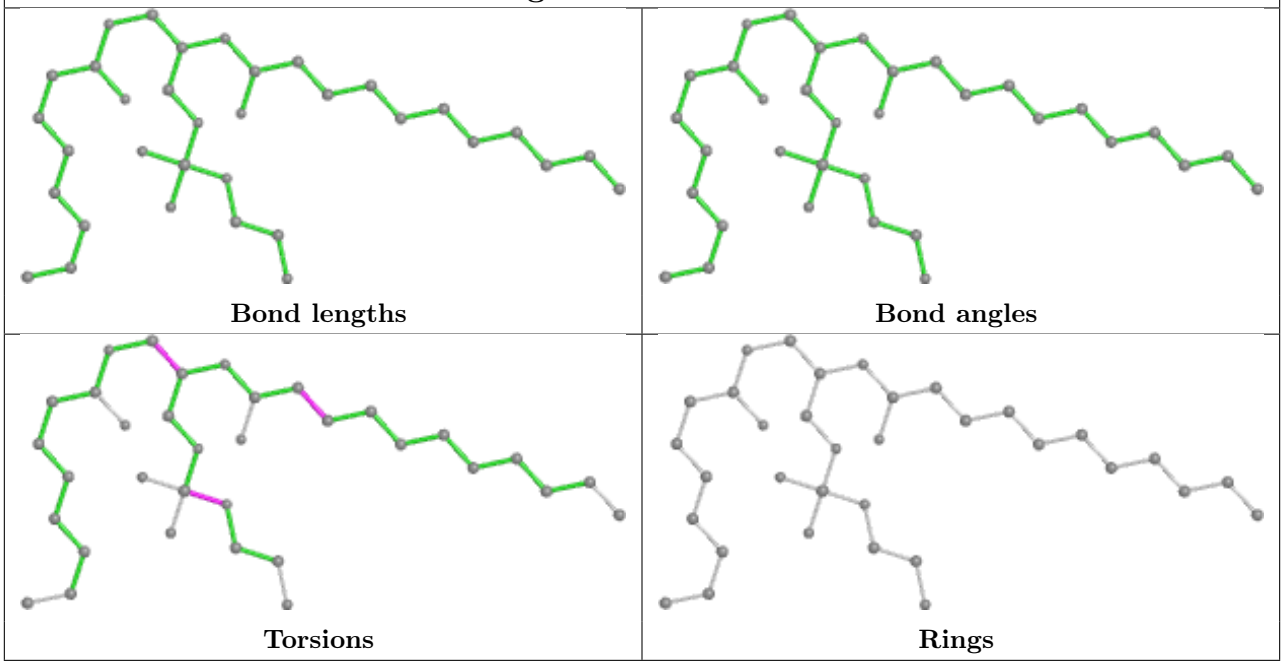
Ligand PTY d 503



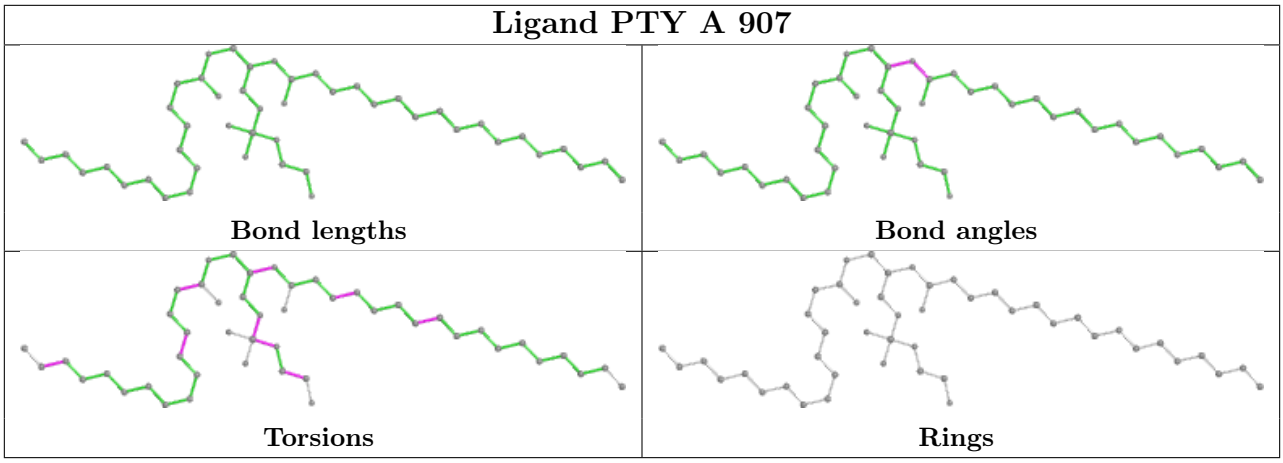
Ligand PTY d 502



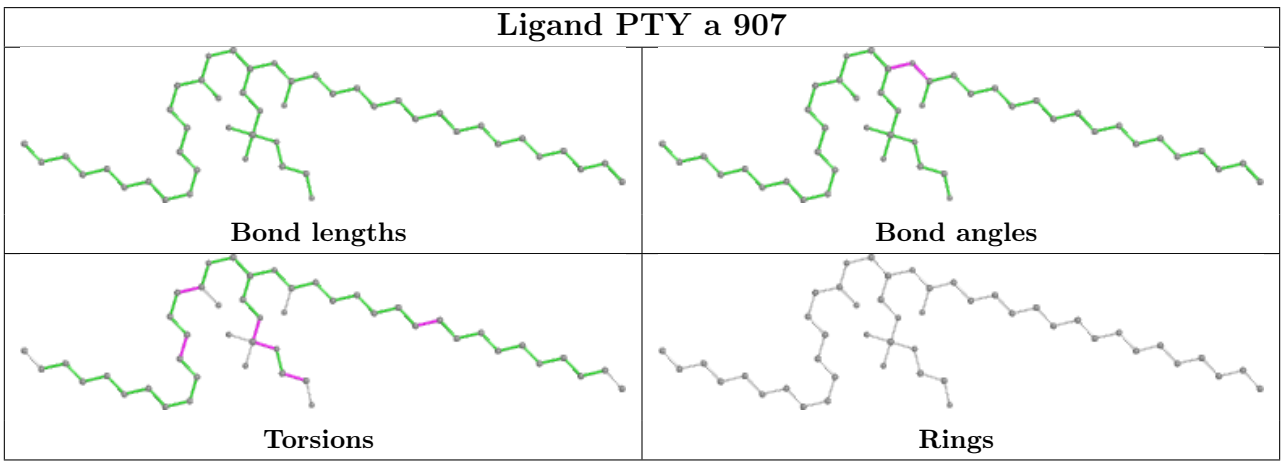
Ligand PTY d 501



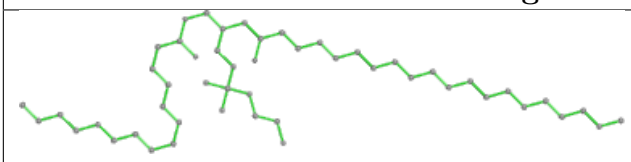
Ligand PTY A 907

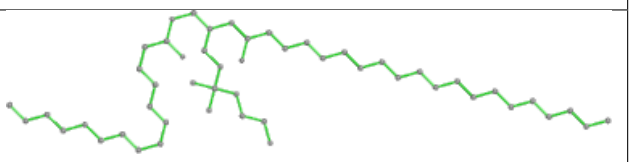


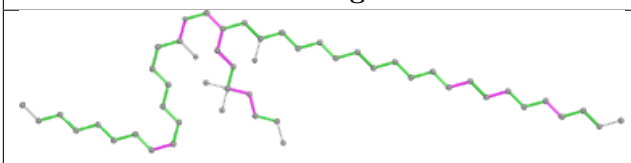
Ligand PTY a 907

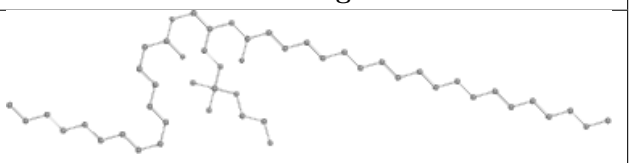


Ligand PTY f 1801

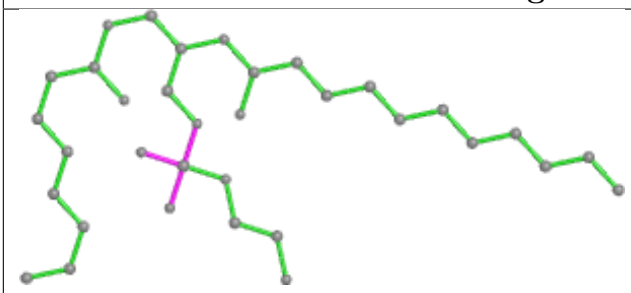

Bond lengths

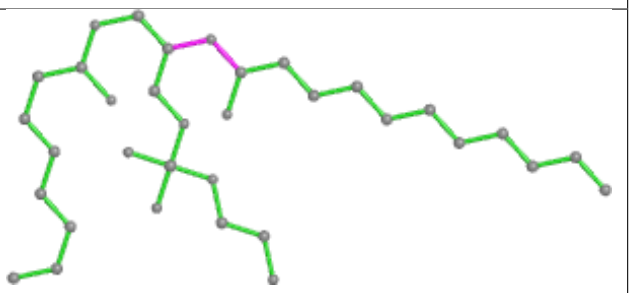

Bond angles

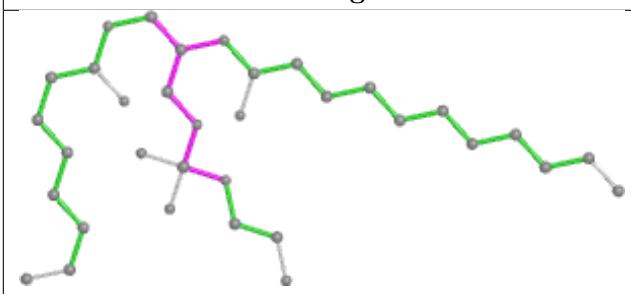

Torsions

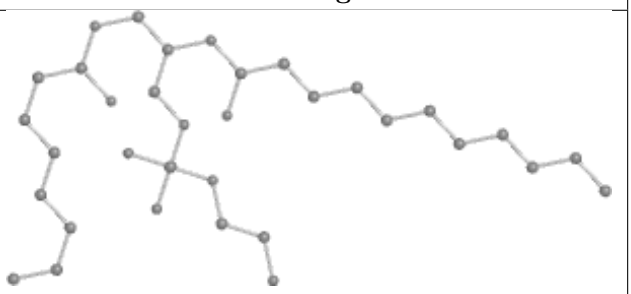

Rings

Ligand PTY a 906

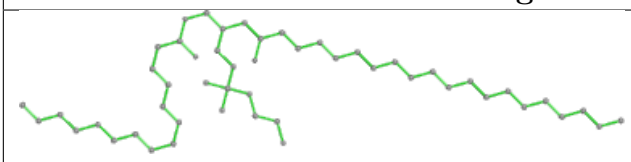

Bond lengths

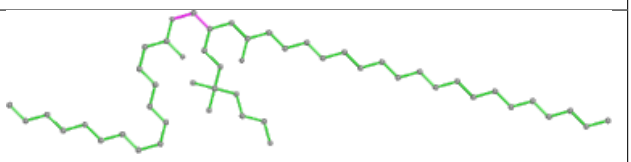

Bond angles

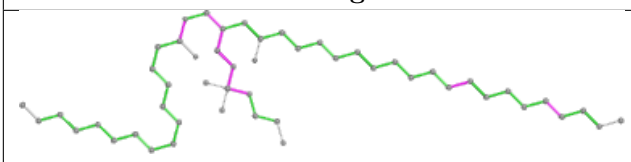

Torsions

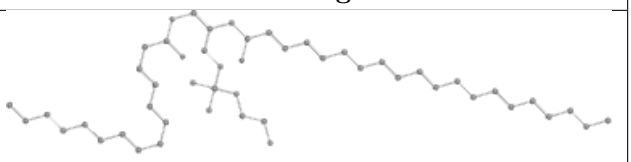

Rings

Ligand PTY F 1801

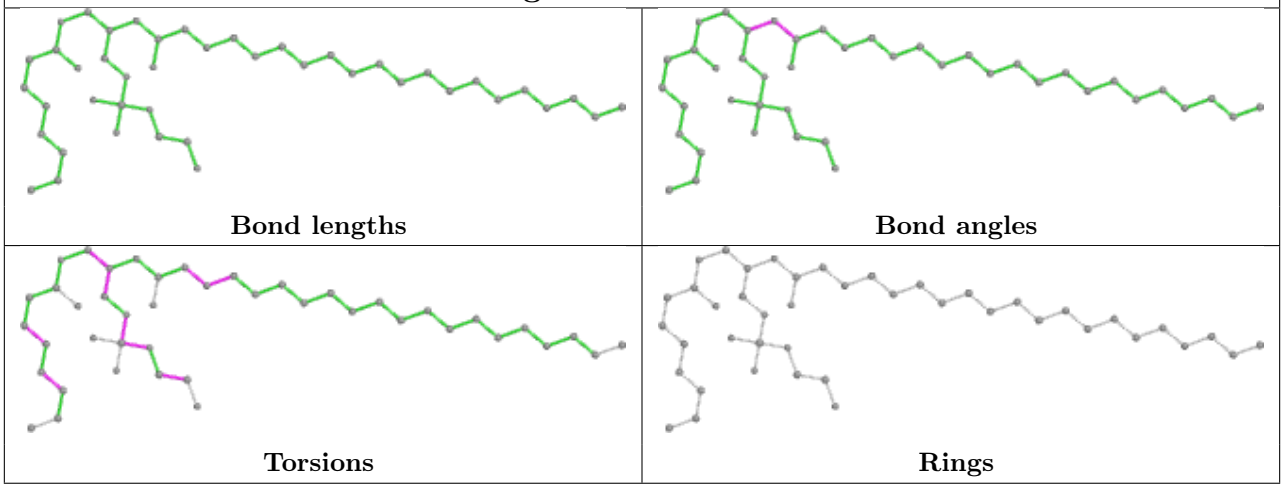

Bond lengths


Bond angles

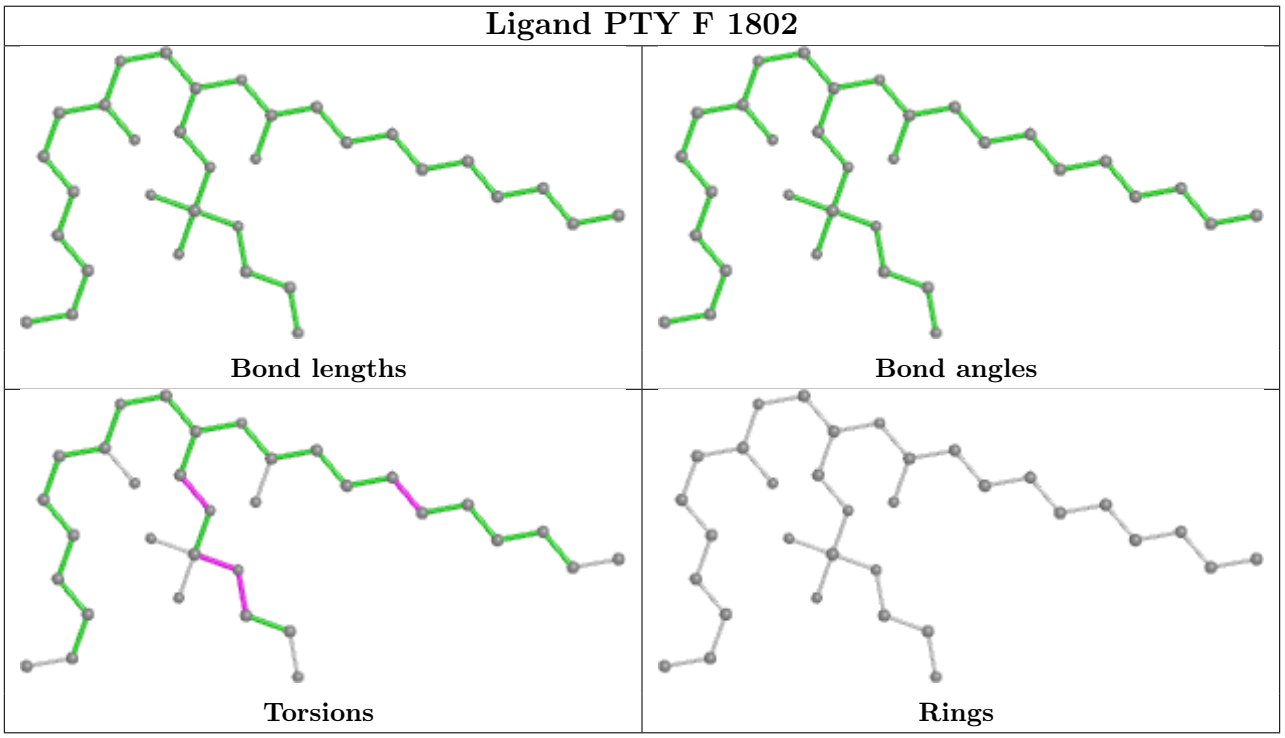

Torsions


Rings

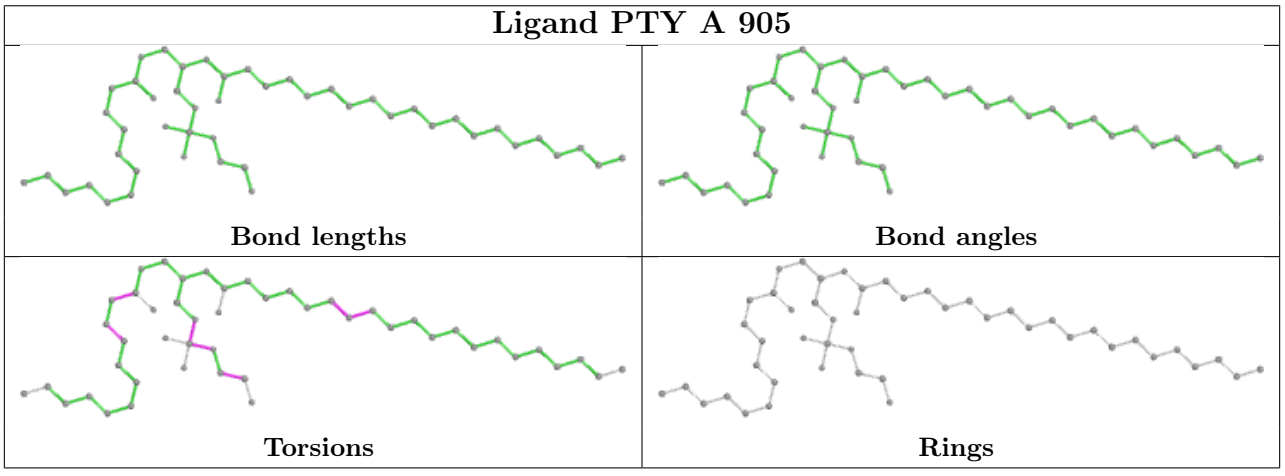
Ligand PTY D 503



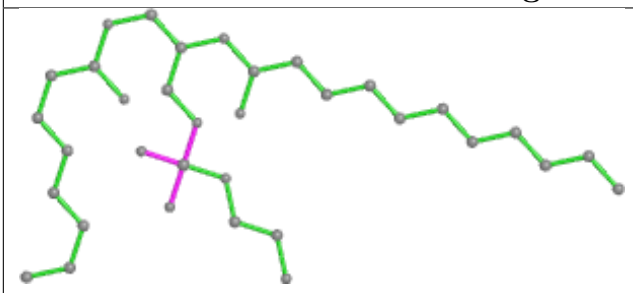
Ligand PTY F 1802



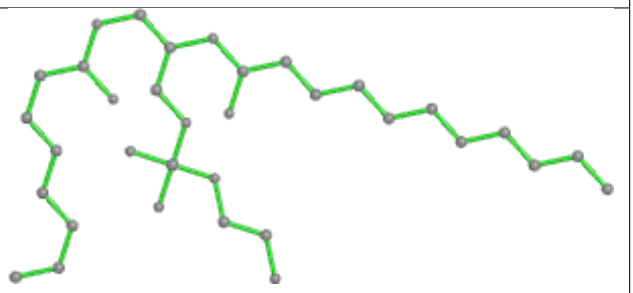
Ligand PTY A 905



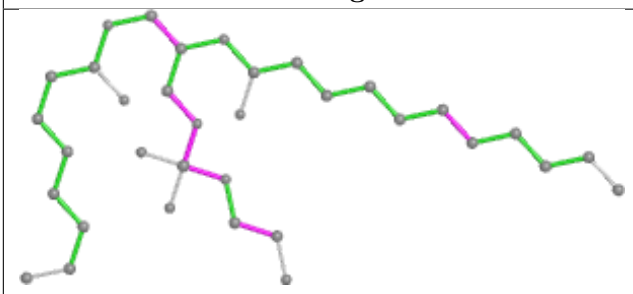
Ligand PTY A 902



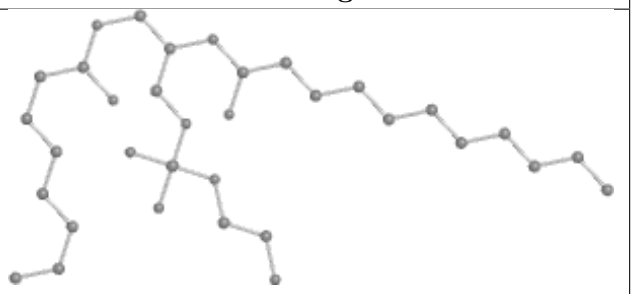
Bond lengths



Bond angles

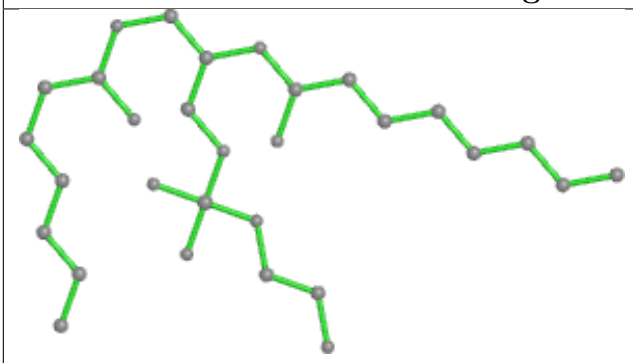


Torsions

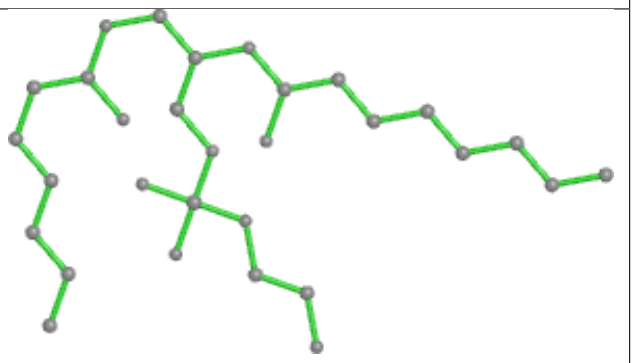


Rings

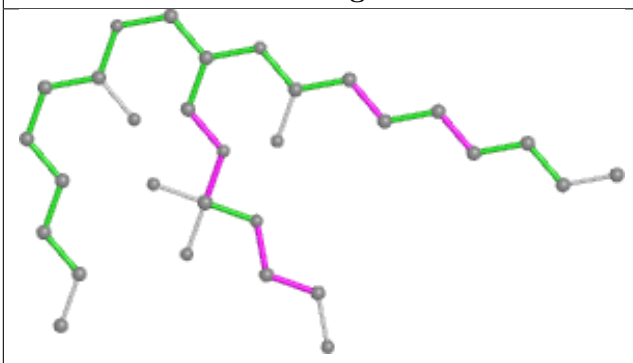
Ligand PTY A 901



Bond lengths



Bond angles



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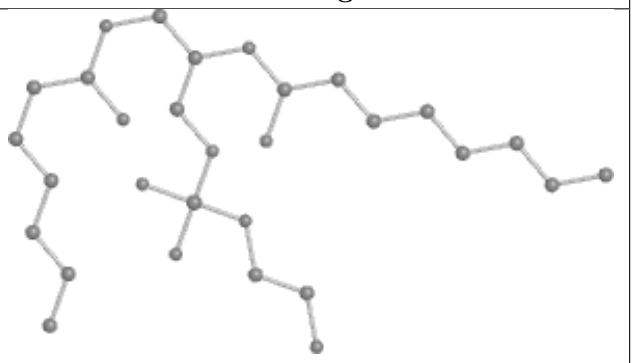
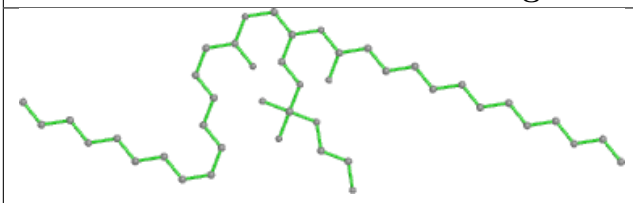
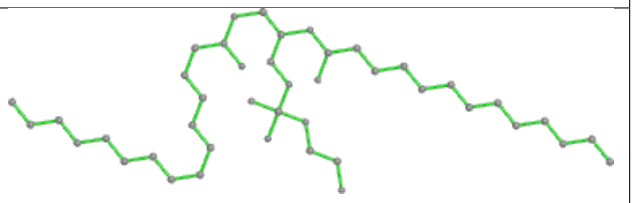


Rings

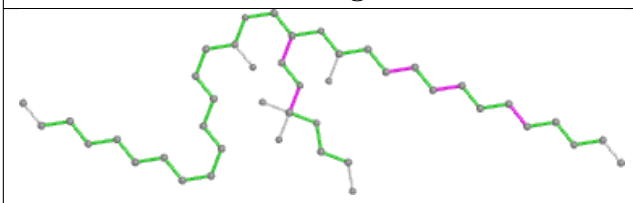
Ligand PTY A 903



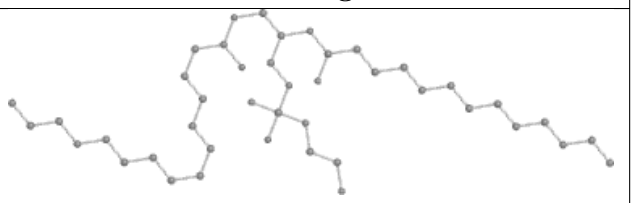
Bond lengths



Bond angles

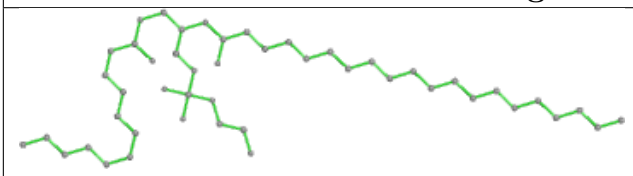


Torsions

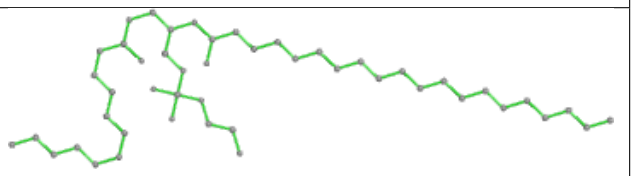


Rings

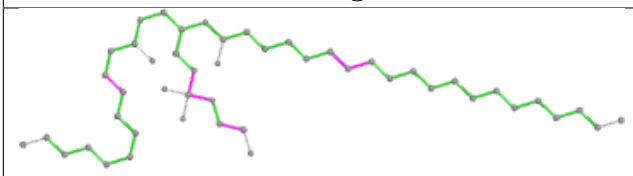
Ligand PTY a 905



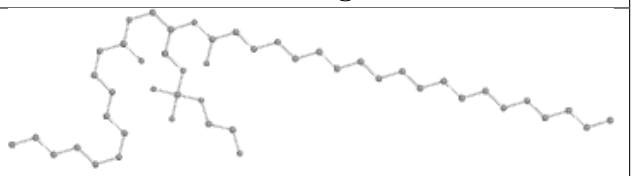
Bond lengths



Bond angles

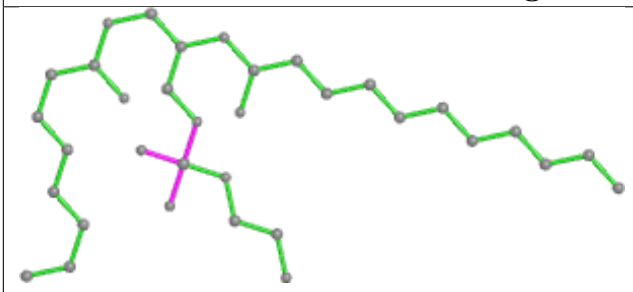


Torsions

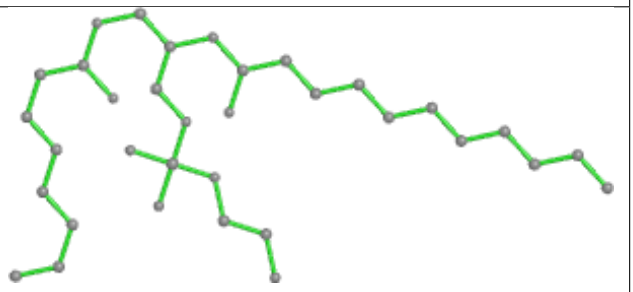


Rings

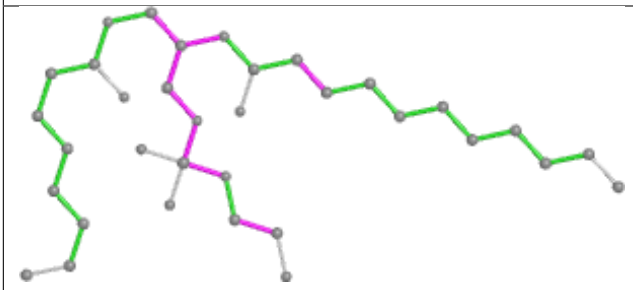
Ligand PTY B 201



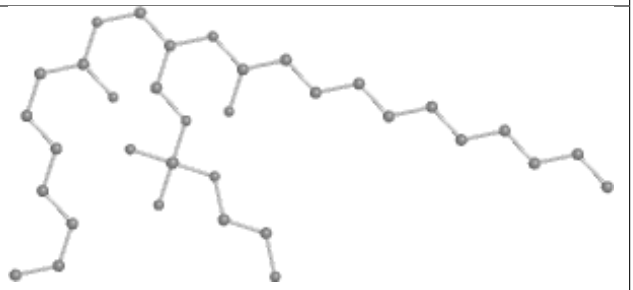
Bond lengths



Bond angles

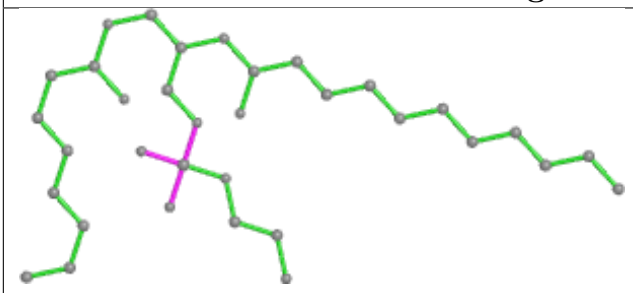


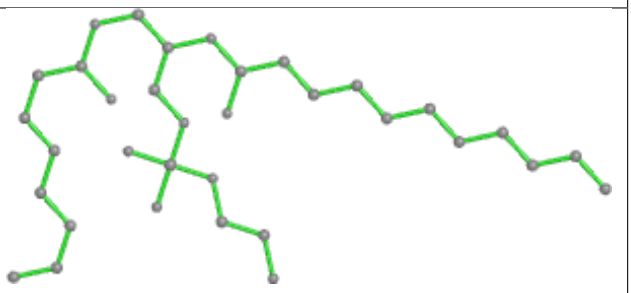
Torsions

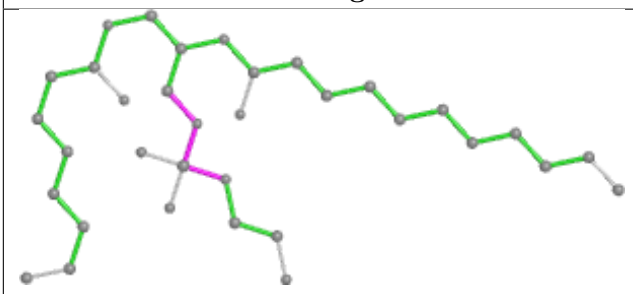


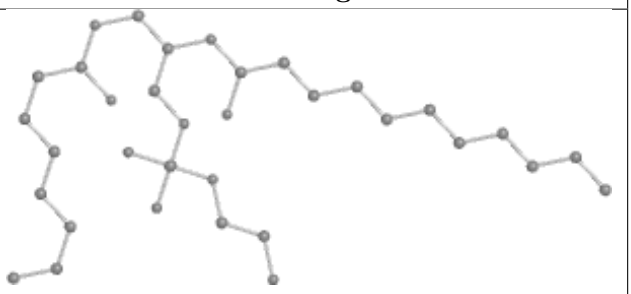
Rings

Ligand PTY a 902

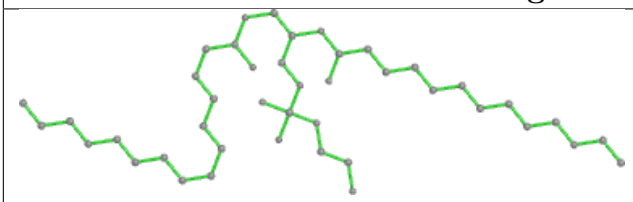

Bond lengths

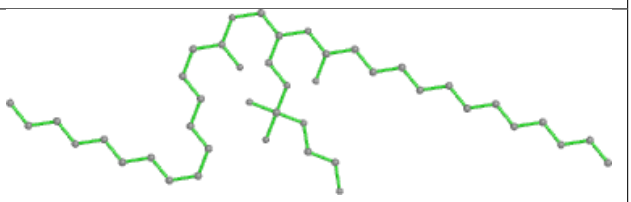

Bond angles

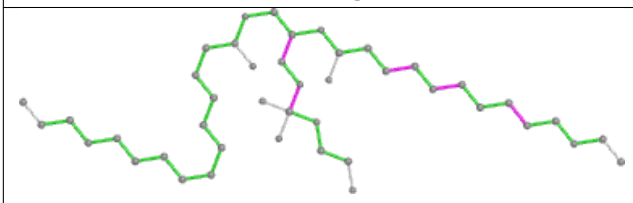

Torsions

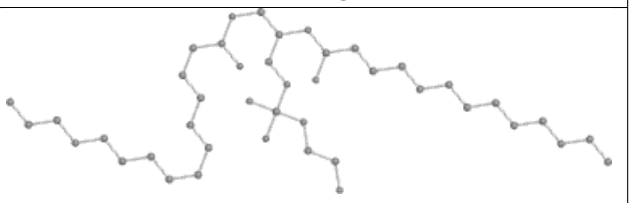

Rings

Ligand PTY a 903

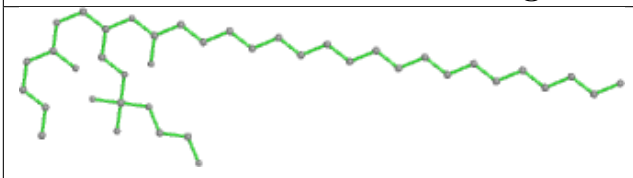

Bond lengths

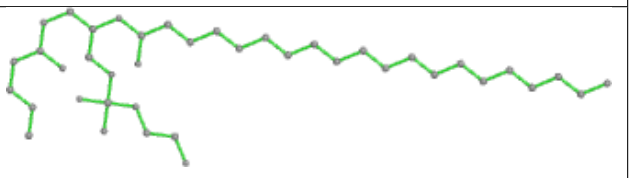

Bond angles

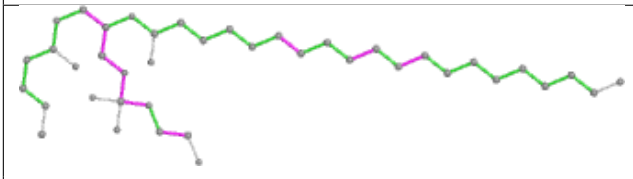

Torsions

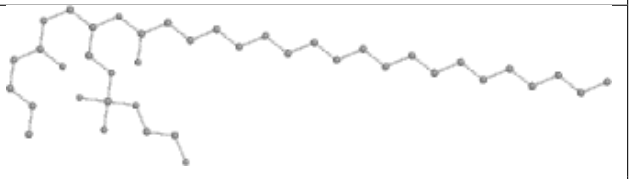

Rings

Ligand PTY A 904

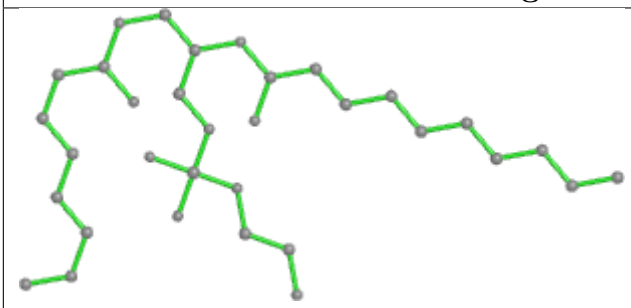

Bond lengths


Bond angles

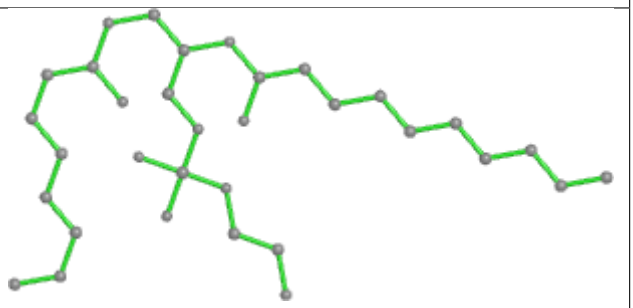

Torsions


Rings

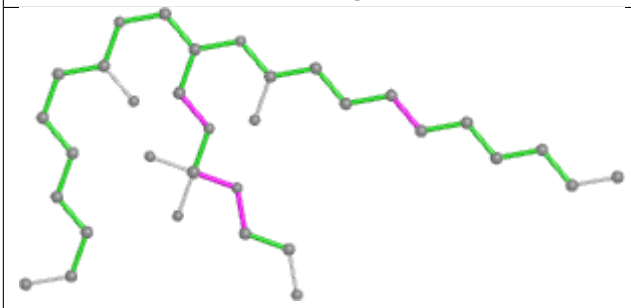
Ligand PTY f 1802



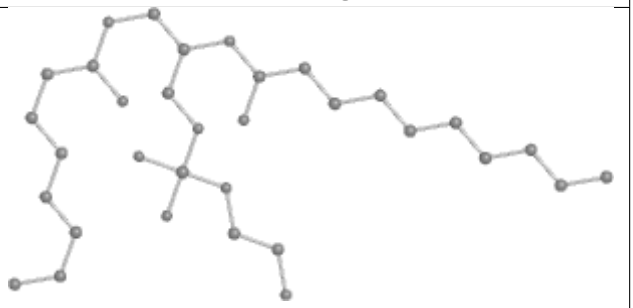
Bond lengths



Bond angles

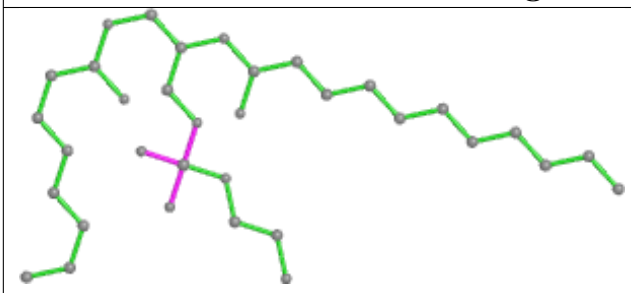


Torsions

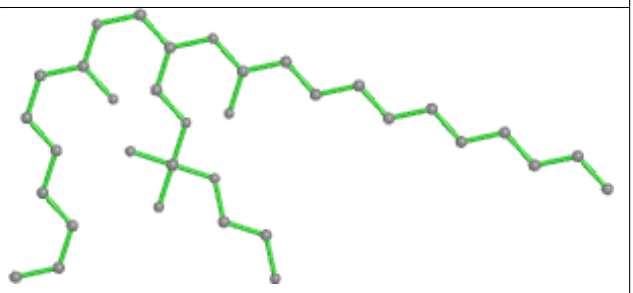


Rings

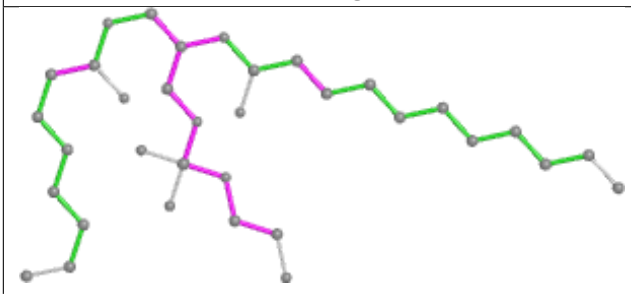
Ligand PTY E 201



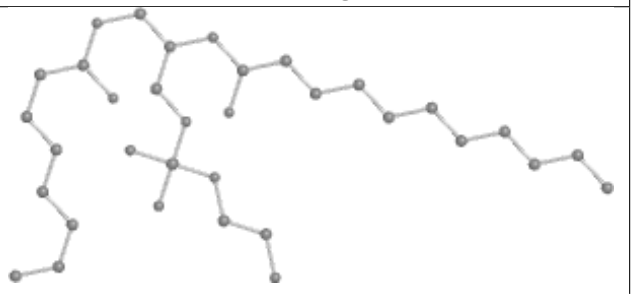
Bond lengths



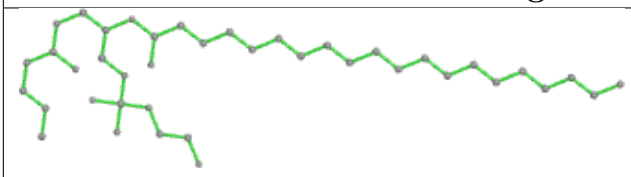
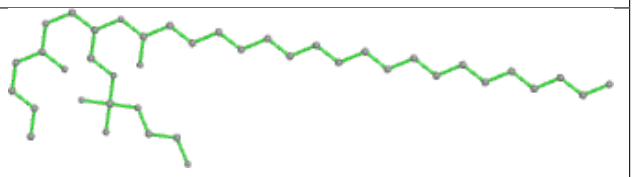
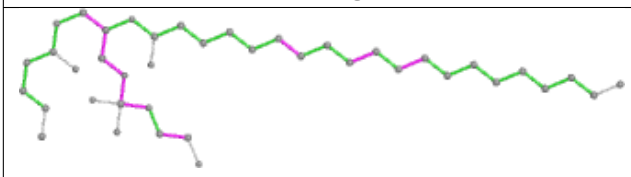
Bond angles

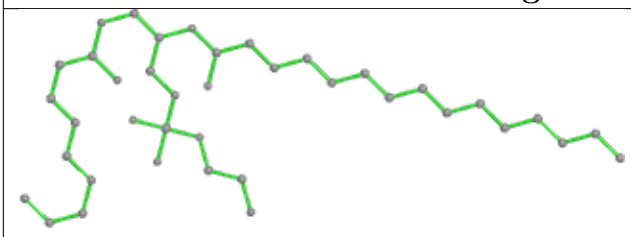
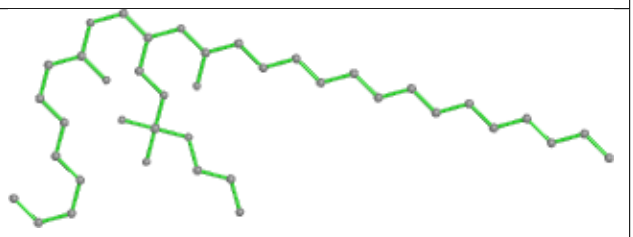
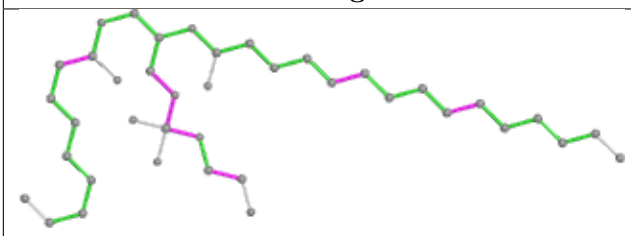


Torsions

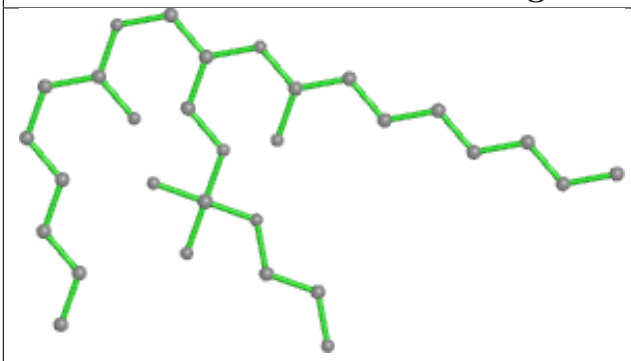


Rings

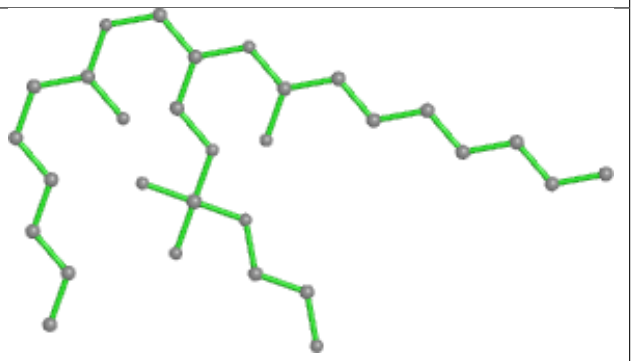
Ligand PTY a 904	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PTY D 502	
 Bond lengths	 Bond angles
 Torsions	 Rings

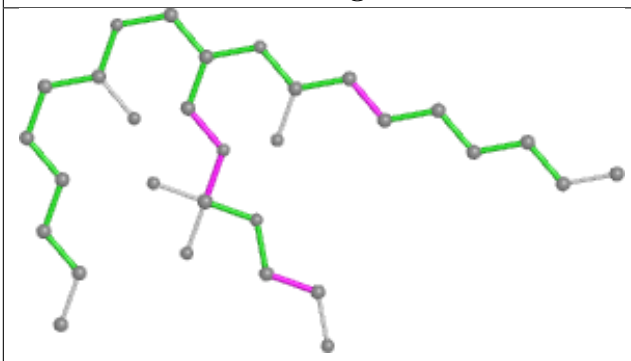
Ligand PTY a 901



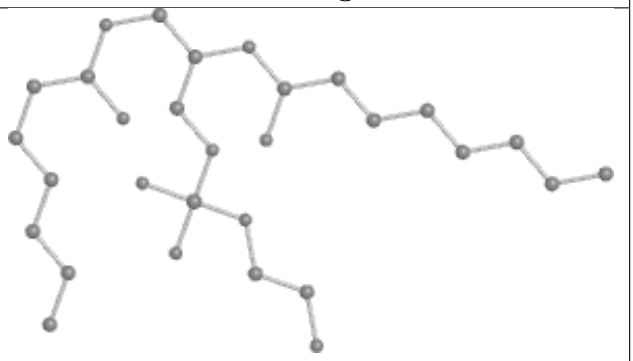
Bond lengths



Bond angles

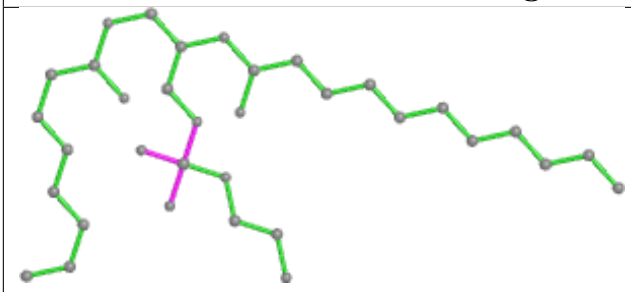


Torsions

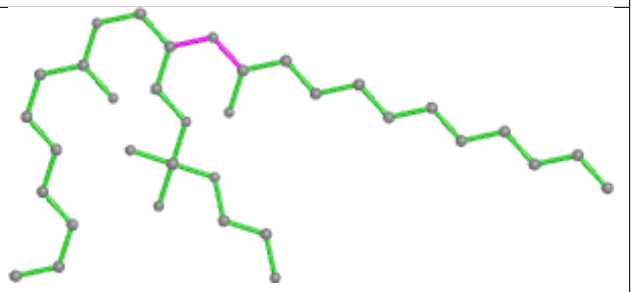


Rings

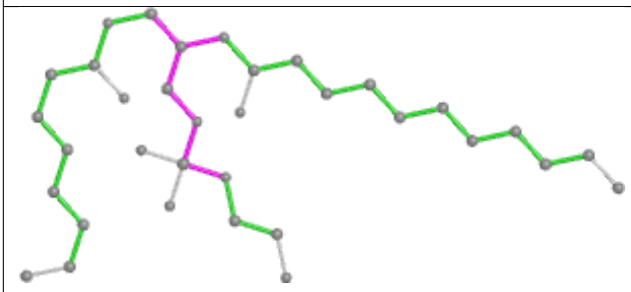
Ligand PTY A 906



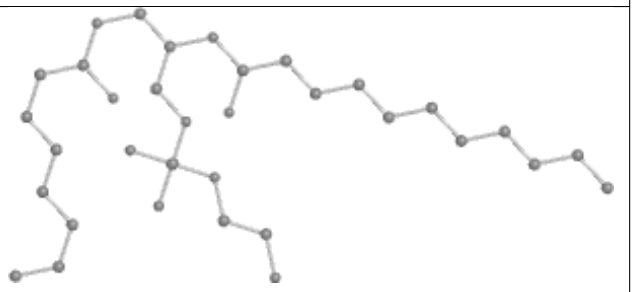
Bond lengths



Bond angles

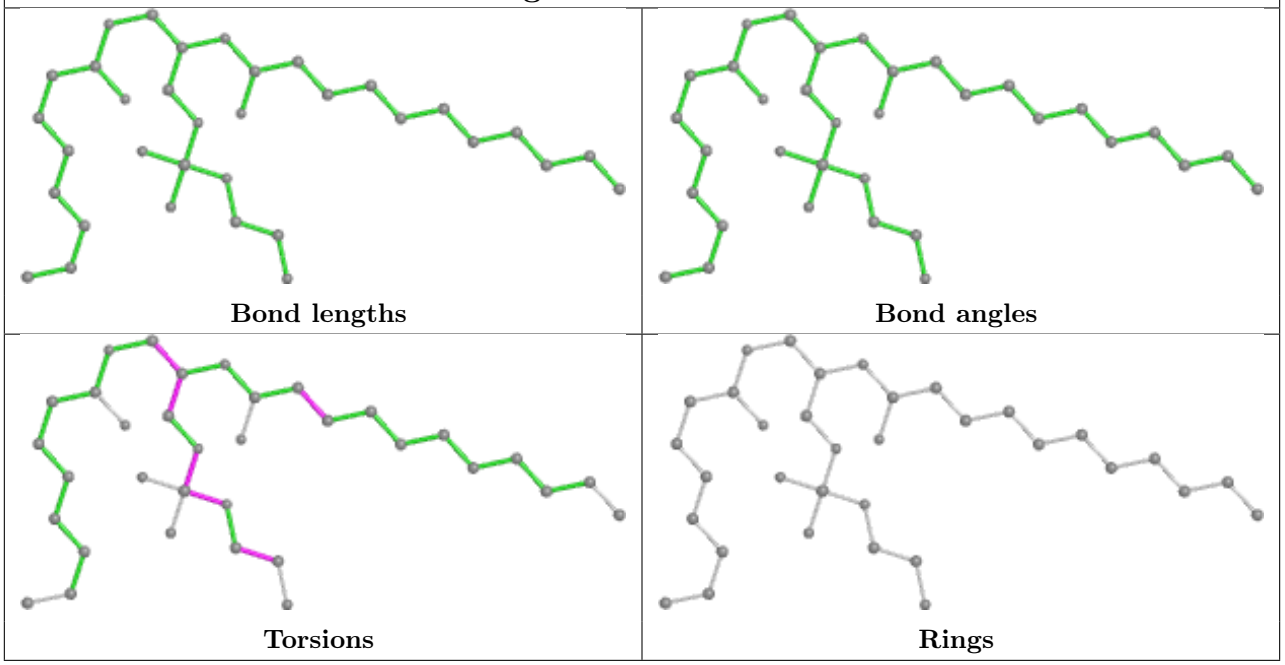


Torsions



Rings

Ligand PTY D 501



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.

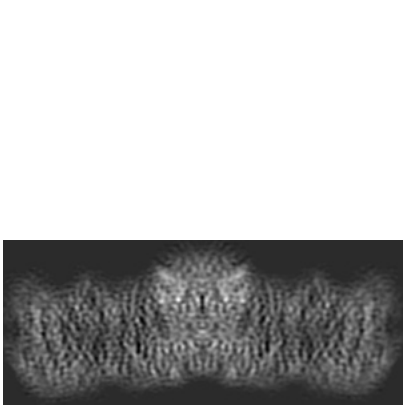
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-11027. 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.

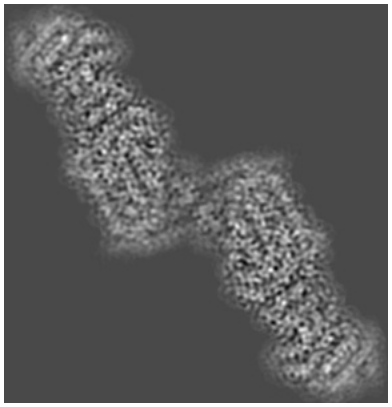
6.1 Orthogonal projections

6.1.1 Primary map



X

Y



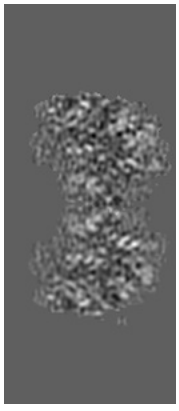
Z

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

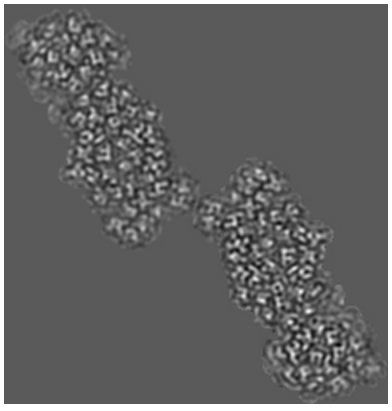
6.2 Central slices

6.2.1 Primary map

X Index: 127



Y Index: 132

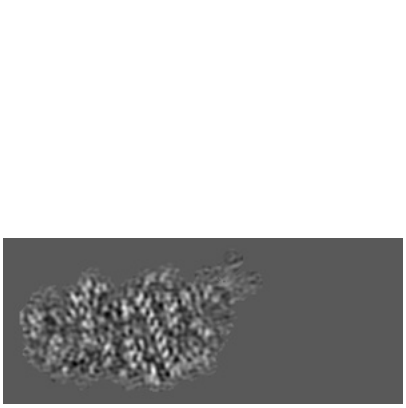


Z Index: 54

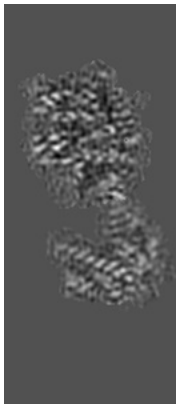
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

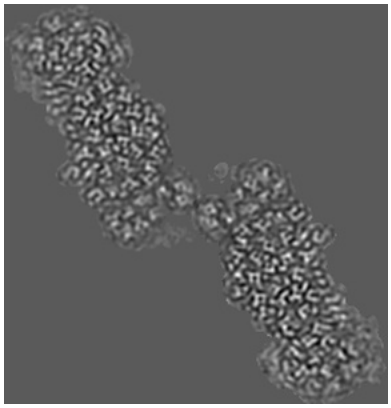
6.3.1 Primary map



X Index: 187



Y Index: 116



Z Index: 58

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

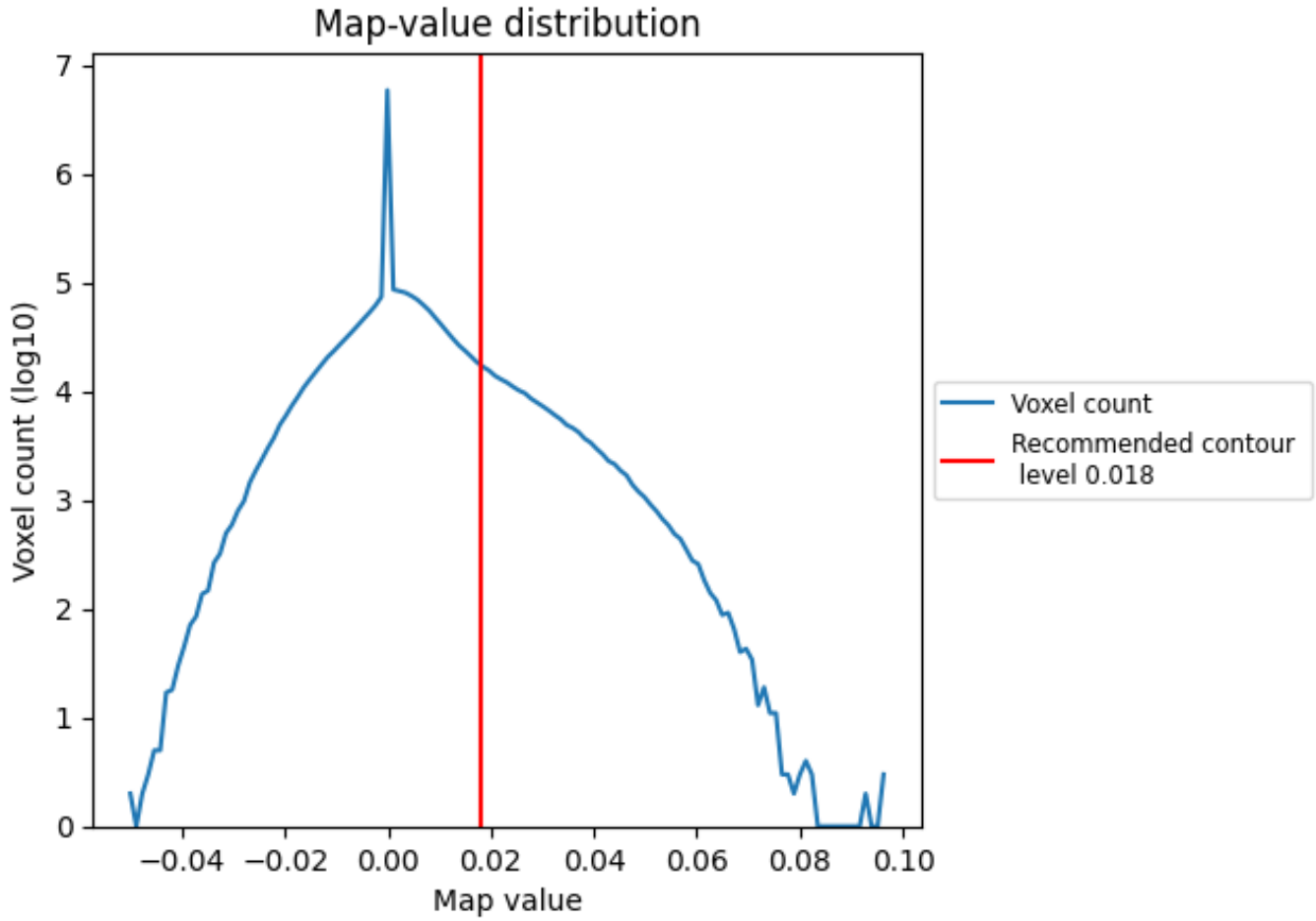
6.5 Mask visualisation (i)

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

7 Map analysis

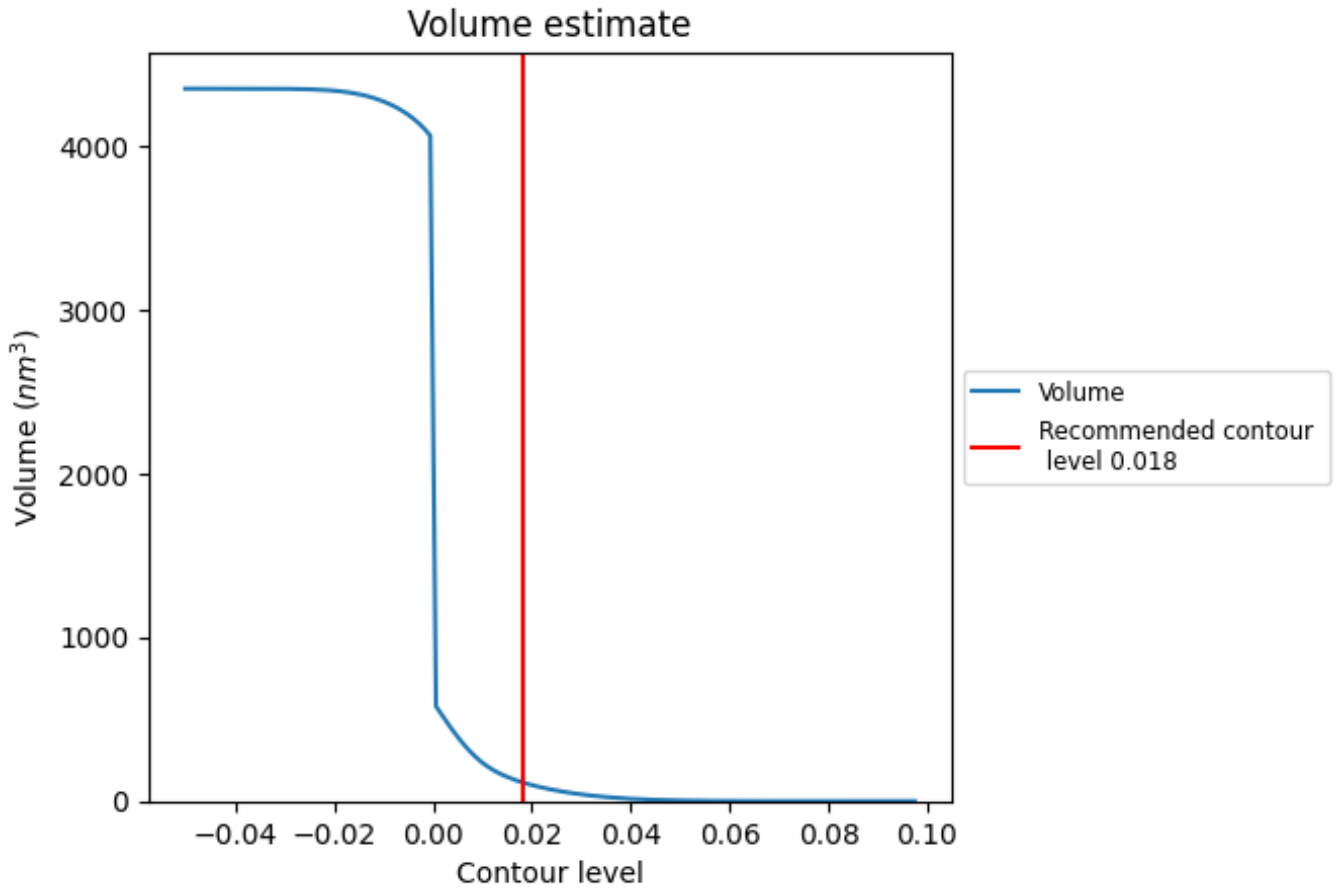
This section contains the results of statistical analysis of the map.

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 (i)



The volume at the recommended contour level is 115 nm^3; this corresponds to an approximate mass of 104 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.

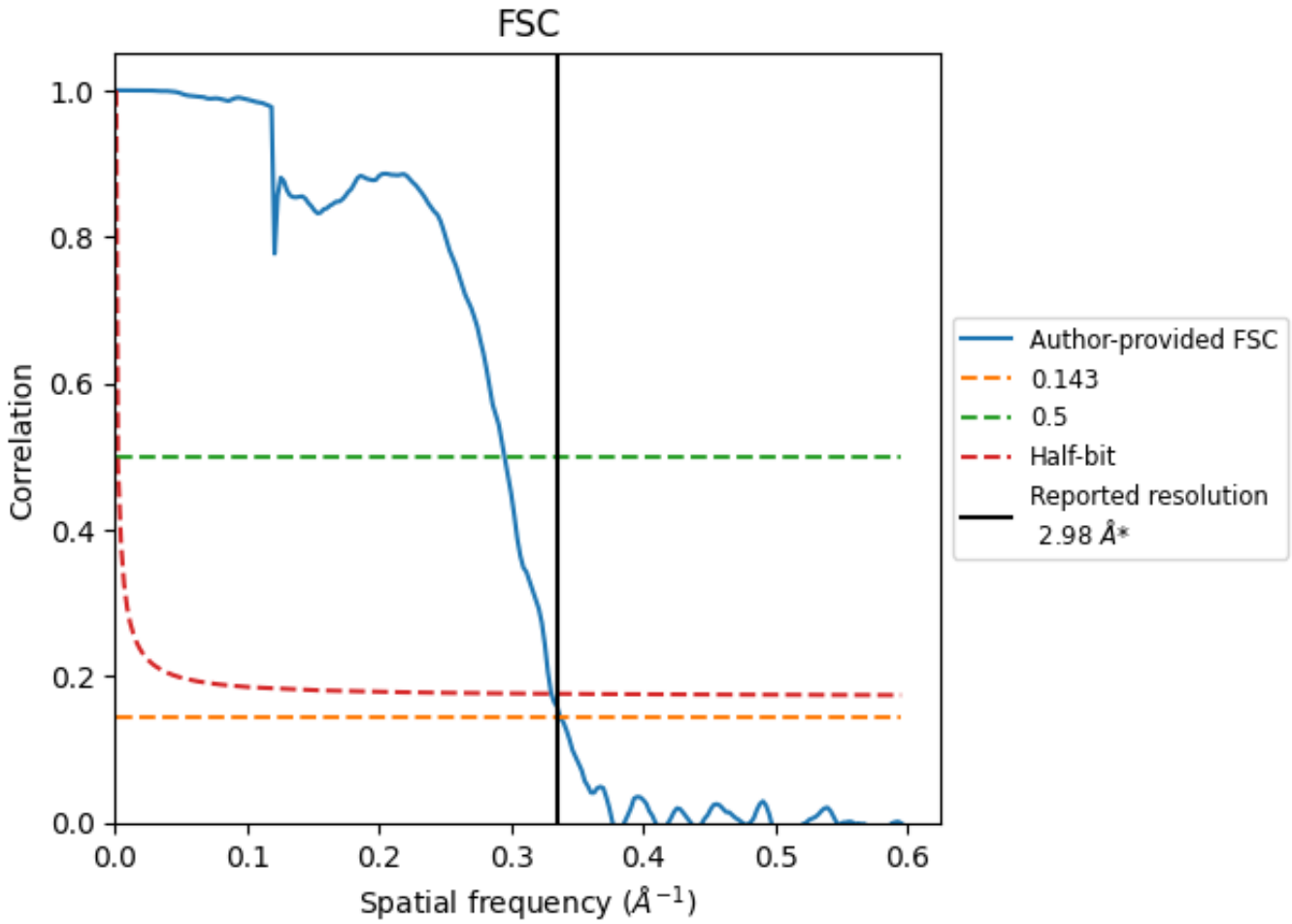
7.3 Rotationally averaged power spectrum (i)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

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 0.336 Å^{-1}

8.2 Resolution estimates (i)

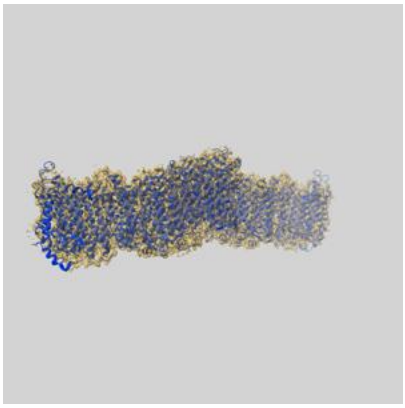
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.98	-	-
Author-provided FSC curve	2.97	3.39	3.03
Unmasked-calculated*	-	-	-

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

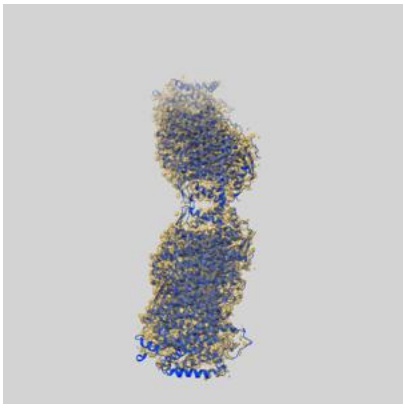
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-11027 and PDB model 6Z16. Per-residue inclusion information can be found in section 3 on page 8.

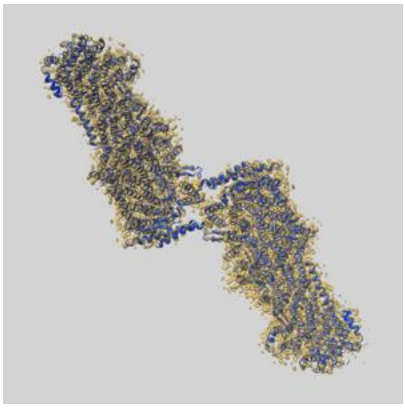
9.1 Map-model overlay



X



Y



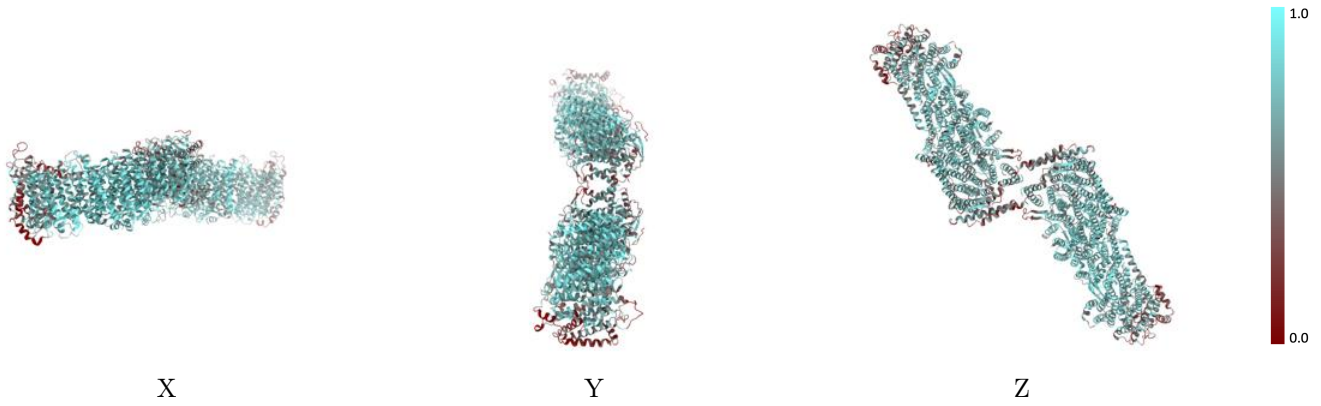
Z

The images above show the 3D surface view of the map at the recommended contour level 0.018 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)

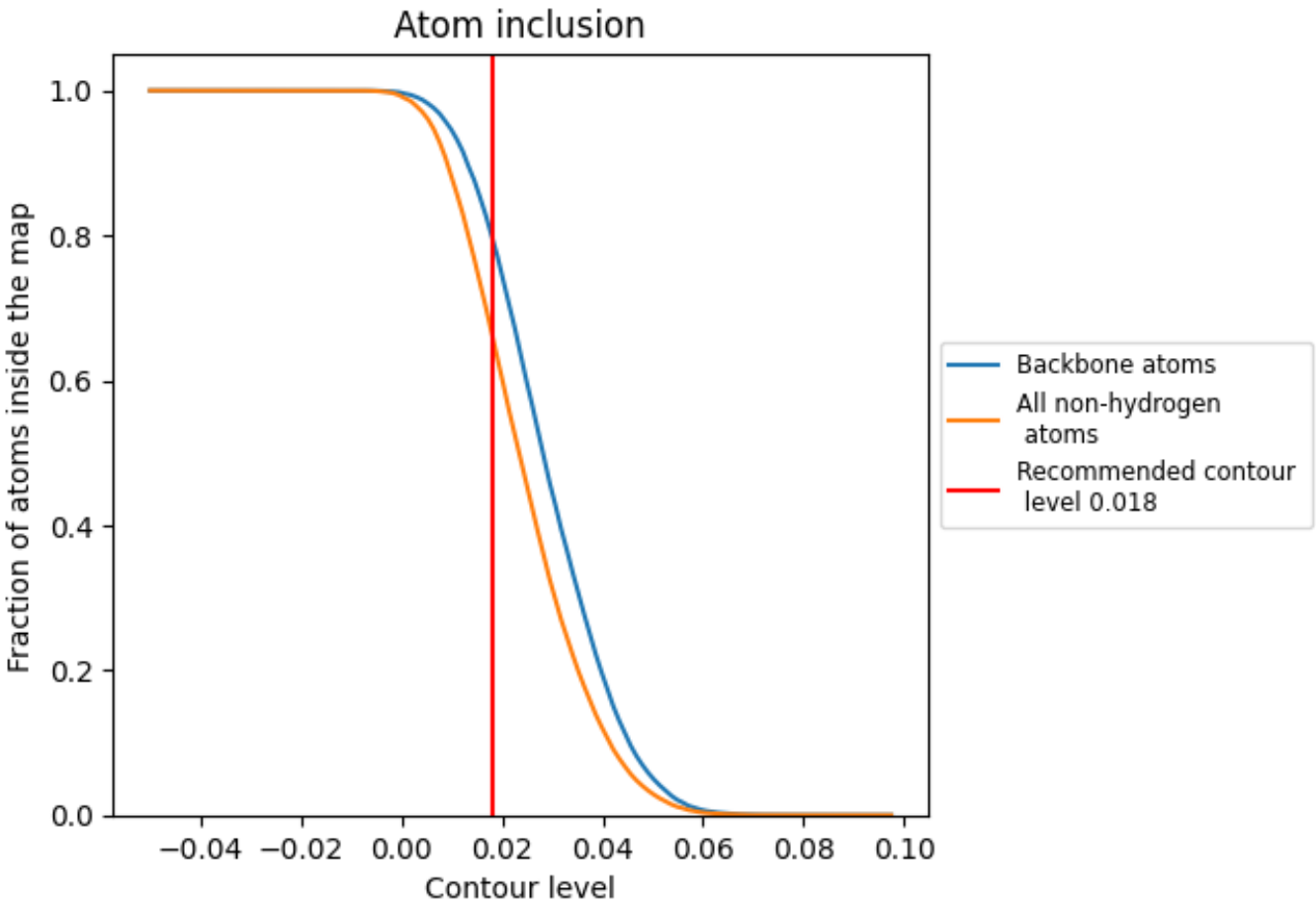
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model (i)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.018).

9.4 Atom inclusion (i)



At the recommended contour level, 80% of all backbone atoms, 66% 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 (0.018) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6629	0.5230
A	0.6502	0.5090
B	0.6575	0.5220
C	0.7554	0.5610
D	0.8211	0.5740
E	0.5027	0.4670
F	0.6312	0.5290
G	0.6104	0.5010
a	0.5944	0.5020
b	0.6284	0.5160
c	0.7163	0.5540
d	0.7776	0.5690
e	0.4972	0.4610
f	0.5856	0.5200
g	0.5736	0.4920