wwPDB X-ray Structure Validation Summary Report (i)

Jun 1, 2022 – 01:38 am BST

PDB ID	:	7PGB
Title	:	NaV_Ae1/Sp1CTD_pore-SAT09 complex
Authors	:	Lolicato, M.; Arrigoni, C.
Deposited on	:	2021-08-13
Resolution	:	3.60 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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

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

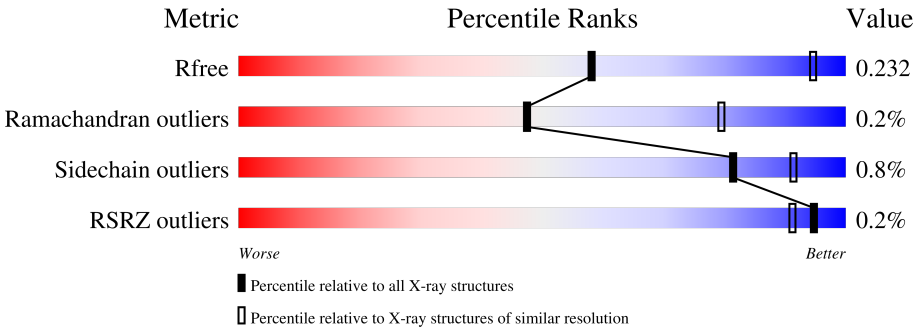
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.28.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.28.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1257 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)
RSRZ outliers	127900	1161 (3.70-3.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	234	92% · 6%
1	H	234	92% · 6%
1	R	234	93% · 6%
1	U	234	% 93% · 6%
1	X	234	93% · 6%
1	a	234	93% · 6%

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Mol	Chain	Length	Quality of chain
1	f	234	92% 6%
1	i	234	92% 6%
1	m	234	% 93% 6%
1	p	234	93% 6%
2	B	215	97%
2	L	215	97%
2	S	215	97%
2	V	215	97%
2	Y	215	97%
2	b	215	97%
2	g	215	97%
2	k	215	97%
2	n	215	97%
2	q	215	97%
3	C	143	77% 21%
3	T	143	% 77% 21%
3	W	143	% 78% 21%
3	Z	143	78% 21%
3	c	143	77% 21%
3	d	143	78% 21%
3	e	143	78% 21%
3	h	143	78% 21%
3	l	143	78% 21%
3	o	143	% 78% 21%

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

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	D12	e	304	-	-	-	X
13	GOL	h	305	-	-	-	X
4	4NB	T	302	-	-	-	X
4	4NB	Z	302	-	-	-	X
4	4NB	h	302	-	-	-	X
6	OCT	U	303	-	-	-	X
6	OCT	X	304	-	-	-	X
6	OCT	a	303	-	-	-	X
6	OCT	c	301	-	-	-	X
6	OCT	l	305	-	-	-	X
6	OCT	o	304	-	-	-	X
8	LNK	Z	304	-	-	-	X
8	LNK	d	303	-	-	-	X
8	LNK	d	304	-	-	-	X

2 Entry composition (i)

There are 14 unique types of molecules in this entry. The entry contains 42734 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 SAT09 fab fragment, heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	219	Total	C	N	O	S	0	0	0
			1640	1041	271	323	5			
1	A	219	Total	C	N	O	S	0	0	0
			1640	1041	271	323	5			
1	R	219	Total	C	N	O	S	0	0	0
			1640	1041	271	323	5			
1	U	219	Total	C	N	O	S	0	0	0
			1640	1041	271	323	5			
1	X	219	Total	C	N	O	S	0	0	0
			1640	1041	271	323	5			
1	a	219	Total	C	N	O	S	0	0	0
			1640	1041	271	323	5			
1	m	219	Total	C	N	O	S	0	0	0
			1640	1041	271	323	5			
1	p	219	Total	C	N	O	S	0	0	0
			1640	1041	271	323	5			
1	f	219	Total	C	N	O	S	0	0	0
			1640	1041	271	323	5			
1	i	219	Total	C	N	O	S	0	0	0
			1640	1041	271	323	5			

- Molecule 2 is a protein called SAT09 fab fragment, light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	211	Total	C	N	O	S	0	0	0
			1612	1006	274	327	5			
2	B	211	Total	C	N	O	S	0	0	0
			1612	1006	274	327	5			
2	S	211	Total	C	N	O	S	0	0	0
			1612	1006	274	327	5			
2	V	211	Total	C	N	O	S	0	0	0
			1612	1006	274	327	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Y	211	Total	C	N	O	S	0	0	0
			1612	1006	274	327	5			
2	b	211	Total	C	N	O	S	0	0	0
			1612	1006	274	327	5			
2	n	211	Total	C	N	O	S	0	0	0
			1612	1006	274	327	5			
2	q	211	Total	C	N	O	S	0	0	0
			1612	1006	274	327	5			
2	g	211	Total	C	N	O	S	0	0	0
			1612	1006	274	327	5			
2	k	211	Total	C	N	O	S	0	0	0
			1612	1006	274	327	5			

- Molecule 3 is a protein called Ion transport protein,Voltage-gated sodium channel.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	c	113	Total	C	N	O	S	0	0	0
			910	612	136	157	5			
3	C	113	Total	C	N	O	S	0	0	0
			906	610	136	155	5			
3	T	113	Total	C	N	O	S	0	0	0
			899	604	135	155	5			
3	W	113	Total	C	N	O	S	0	0	0
			899	604	135	155	5			
3	Z	113	Total	C	N	O	S	0	0	0
			899	604	135	155	5			
3	d	113	Total	C	N	O	S	0	0	0
			899	604	135	155	5			
3	l	113	Total	C	N	O	S	0	0	0
			899	604	135	155	5			
3	o	113	Total	C	N	O	S	0	0	0
			899	604	135	155	5			
3	h	113	Total	C	N	O	S	0	0	0
			899	604	135	155	5			
3	e	113	Total	C	N	O	S	0	0	0
			899	604	135	155	5			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
c	137	GLY	-	expression tag	UNP Q0ABW0
c	138	PRO	-	expression tag	UNP Q0ABW0
c	139	SER	-	expression tag	UNP Q0ABW0

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Chain	Residue	Modelled	Actual	Comment	Reference
c	140	SER	-	expression tag	UNP Q0ABW0
c	141	PRO	-	expression tag	UNP Q0ABW0
c	142	SER	-	expression tag	UNP Q0ABW0
C	137	GLY	-	expression tag	UNP Q0ABW0
C	138	PRO	-	expression tag	UNP Q0ABW0
C	139	SER	-	expression tag	UNP Q0ABW0
C	140	SER	-	expression tag	UNP Q0ABW0
C	141	PRO	-	expression tag	UNP Q0ABW0
C	142	SER	-	expression tag	UNP Q0ABW0
T	137	GLY	-	expression tag	UNP Q0ABW0
T	138	PRO	-	expression tag	UNP Q0ABW0
T	139	SER	-	expression tag	UNP Q0ABW0
T	140	SER	-	expression tag	UNP Q0ABW0
T	141	PRO	-	expression tag	UNP Q0ABW0
T	142	SER	-	expression tag	UNP Q0ABW0
W	137	GLY	-	expression tag	UNP Q0ABW0
W	138	PRO	-	expression tag	UNP Q0ABW0
W	139	SER	-	expression tag	UNP Q0ABW0
W	140	SER	-	expression tag	UNP Q0ABW0
W	141	PRO	-	expression tag	UNP Q0ABW0
W	142	SER	-	expression tag	UNP Q0ABW0
Z	137	GLY	-	expression tag	UNP Q0ABW0
Z	138	PRO	-	expression tag	UNP Q0ABW0
Z	139	SER	-	expression tag	UNP Q0ABW0
Z	140	SER	-	expression tag	UNP Q0ABW0
Z	141	PRO	-	expression tag	UNP Q0ABW0
Z	142	SER	-	expression tag	UNP Q0ABW0
d	137	GLY	-	expression tag	UNP Q0ABW0
d	138	PRO	-	expression tag	UNP Q0ABW0
d	139	SER	-	expression tag	UNP Q0ABW0
d	140	SER	-	expression tag	UNP Q0ABW0
d	141	PRO	-	expression tag	UNP Q0ABW0
d	142	SER	-	expression tag	UNP Q0ABW0
l	137	GLY	-	expression tag	UNP Q0ABW0
l	138	PRO	-	expression tag	UNP Q0ABW0
l	139	SER	-	expression tag	UNP Q0ABW0
l	140	SER	-	expression tag	UNP Q0ABW0
l	141	PRO	-	expression tag	UNP Q0ABW0
l	142	SER	-	expression tag	UNP Q0ABW0
o	137	GLY	-	expression tag	UNP Q0ABW0
o	138	PRO	-	expression tag	UNP Q0ABW0
o	139	SER	-	expression tag	UNP Q0ABW0

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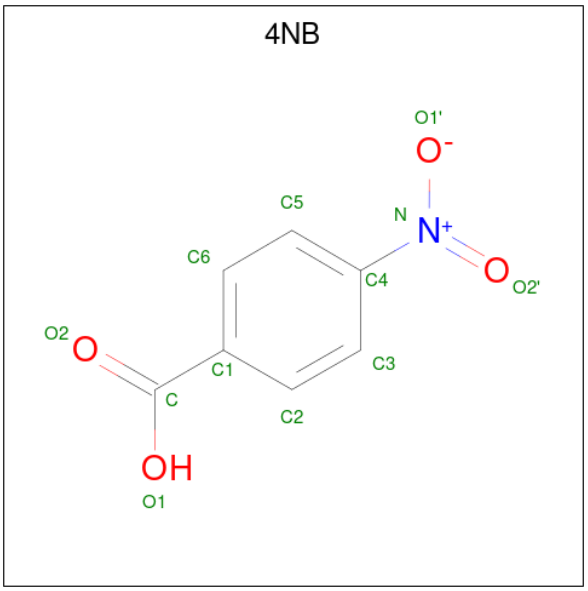
Chain	Residue	Modelled	Actual	Comment	Reference
o	140	SER	-	expression tag	UNP Q0ABW0
o	141	PRO	-	expression tag	UNP Q0ABW0
o	142	SER	-	expression tag	UNP Q0ABW0
h	137	GLY	-	expression tag	UNP Q0ABW0
h	138	PRO	-	expression tag	UNP Q0ABW0
h	139	SER	-	expression tag	UNP Q0ABW0
h	140	SER	-	expression tag	UNP Q0ABW0
h	141	PRO	-	expression tag	UNP Q0ABW0
h	142	SER	-	expression tag	UNP Q0ABW0
e	137	GLY	-	expression tag	UNP Q0ABW0
e	138	PRO	-	expression tag	UNP Q0ABW0
e	139	SER	-	expression tag	UNP Q0ABW0
e	140	SER	-	expression tag	UNP Q0ABW0
e	141	PRO	-	expression tag	UNP Q0ABW0
e	142	SER	-	expression tag	UNP Q0ABW0

- Molecule 4 is 4-NITROBENZOIC ACID (three-letter code: 4NB) (formula: $C_7H_5NO_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	H	1	Total	C	N	O	0	0
			12	7	1	4		
4	H	1	Total	C	N	O	0	0
			12	7	1	4		
4	C	1	Total	C	N	O	0	0
			12	7	1	4		
4	C	1	Total	C	N	O	0	0
			12	7	1	4		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	R	1	Total	C	N	O	0	0
			12	7	1	4		
4	T	1	Total	C	N	O	0	0
			12	7	1	4		
4	T	1	Total	C	N	O	0	0
			12	7	1	4		
4	T	1	Total	C	N	O	0	0
			12	7	1	4		
4	U	1	Total	C	N	O	0	0
			12	7	1	4		
4	W	1	Total	C	N	O	0	0
			12	7	1	4		
4	X	1	Total	C	N	O	0	0
			12	7	1	4		
4	X	1	Total	C	N	O	0	0
			12	7	1	4		
4	Z	1	Total	C	N	O	0	0
			12	7	1	4		
4	Z	1	Total	C	N	O	0	0
			12	7	1	4		
4	Z	1	Total	C	N	O	0	0
			12	7	1	4		
4	d	1	Total	C	N	O	0	0
			12	7	1	4		
4	d	1	Total	C	N	O	0	0
			12	7	1	4		
4	m	1	Total	C	N	O	0	0
			12	7	1	4		
4	l	1	Total	C	N	O	0	0
			12	7	1	4		
4	l	1	Total	C	N	O	0	0
			12	7	1	4		
4	l	1	Total	C	N	O	0	0
			12	7	1	4		
4	l	1	Total	C	N	O	0	0
			12	7	1	4		
4	p	1	Total	C	N	O	0	0
			12	7	1	4		
4	o	1	Total	C	N	O	0	0
			12	7	1	4		
4	o	1	Total	C	N	O	0	0
			12	7	1	4		

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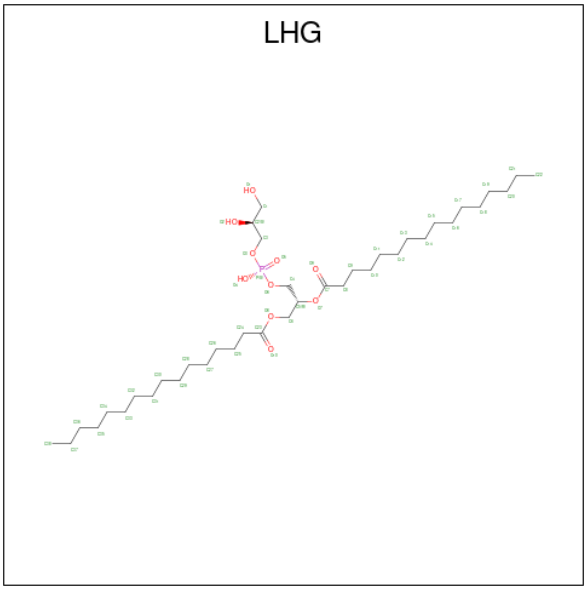
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	f	1	Total C N O 12 7 1 4	0	0
4	i	1	Total C N O 12 7 1 4	0	0
4	h	1	Total C N O 12 7 1 4	0	0
4	h	1	Total C N O 12 7 1 4	0	0
4	e	1	Total C N O 12 7 1 4	0	0
4	e	1	Total C N O 12 7 1 4	0	0
4	e	1	Total C N O 12 7 1 4	0	0

- Molecule 5 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	H	1	Total C O P 49 38 10 1	0	0
5	A	1	Total C O P 49 38 10 1	0	0
5	R	1	Total C O P 49 38 10 1	0	0
5	U	1	Total C O P 49 38 10 1	0	0

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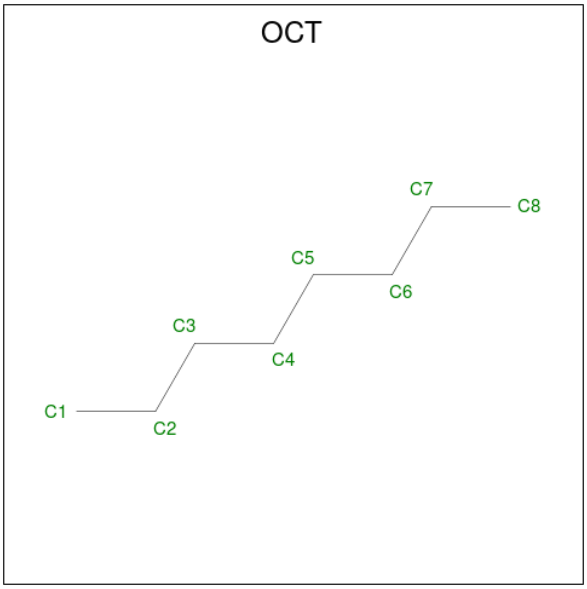
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	X	1	Total C O P 49 38 10 1	0	0
5	a	1	Total C O P 49 38 10 1	0	0
5	m	1	Total C O P 49 38 10 1	0	0
5	p	1	Total C O P 49 38 10 1	0	0
5	f	1	Total C O P 49 38 10 1	0	0
5	i	1	Total C O P 49 38 10 1	0	0

- Molecule 6 is N-OCTANE (three-letter code: OCT) (formula: C_8H_{18}).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	H	1	Total C 8 8	0	0
6	c	1	Total C 8 8	0	0
6	C	1	Total C 8 8	0	0
6	T	1	Total C 8 8	0	0
6	U	1	Total C 8 8	0	0

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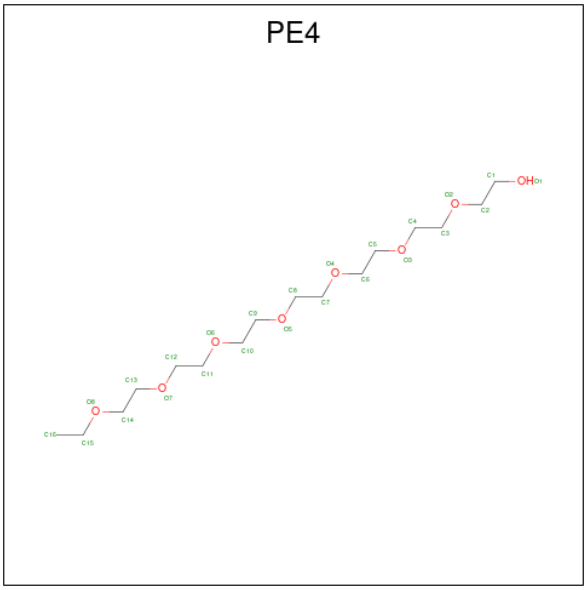
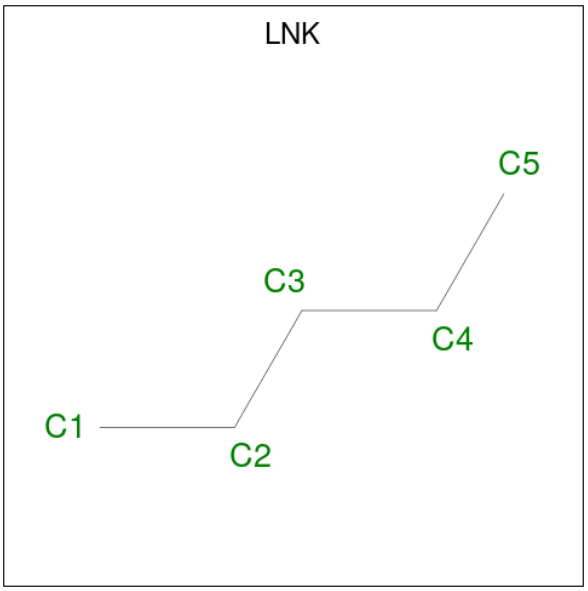
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	W	1	Total C 8 8	0	0
6	X	1	Total C 8 8	0	0
6	a	1	Total C 8 8	0	0
6	l	1	Total C 8 8	0	0
6	o	1	Total C 8 8	0	0
6	h	1	Total C 8 8	0	0

- Molecule 7 is 2-{2-[2-(2-{2-[2-(2-ETHOXY-ETHOXY)-ETHOXY]-ETHOXY}-ETHOXY)-ETHOXY]-ETHOXY}-ETHANOL (three-letter code: PE4) (formula: $C_{16}H_{34}O_8$).



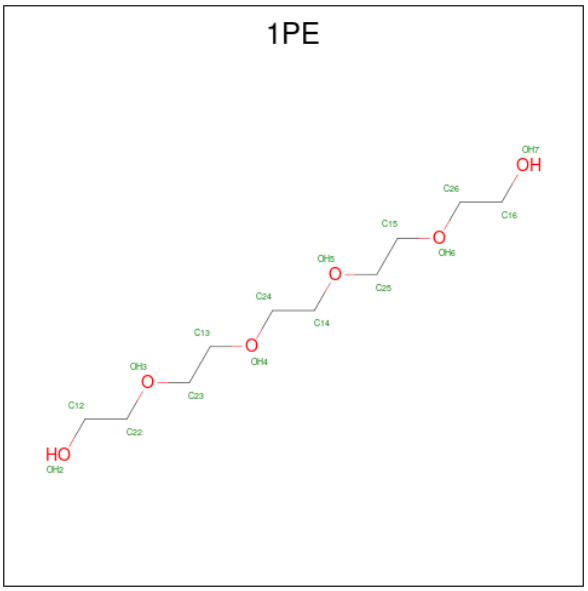
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	H	1	Total C O 24 16 8	0	0

- Molecule 8 is PENTANE (three-letter code: LNK) (formula: C_5H_{12}).



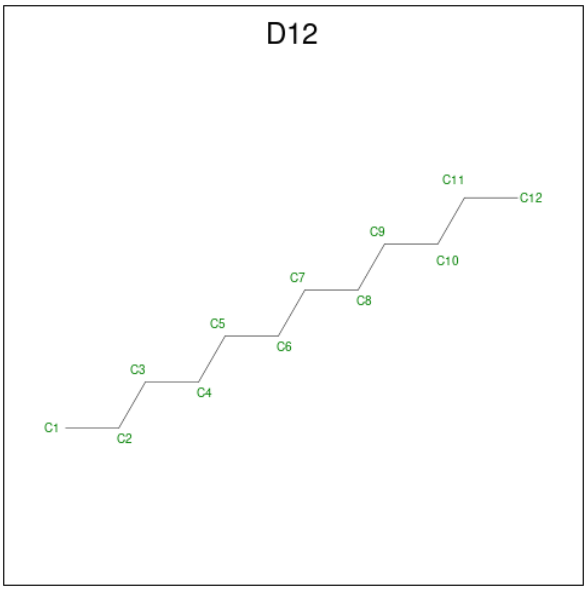
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	c	1	Total C 5 5	0	0
8	T	1	Total C 5 5	0	0
8	W	1	Total C 5 5	0	0
8	W	1	Total C 5 5	0	0
8	Z	1	Total C 5 5	0	0
8	Z	1	Total C 5 5	0	0
8	d	1	Total C 5 5	0	0
8	d	1	Total C 5 5	0	0
8	l	1	Total C 5 5	0	0
8	h	1	Total C 5 5	0	0
8	e	1	Total C 5 5	0	0
8	e	1	Total C 5 5	0	0
8	e	1	Total C 5 5	0	0

- Molecule 9 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).



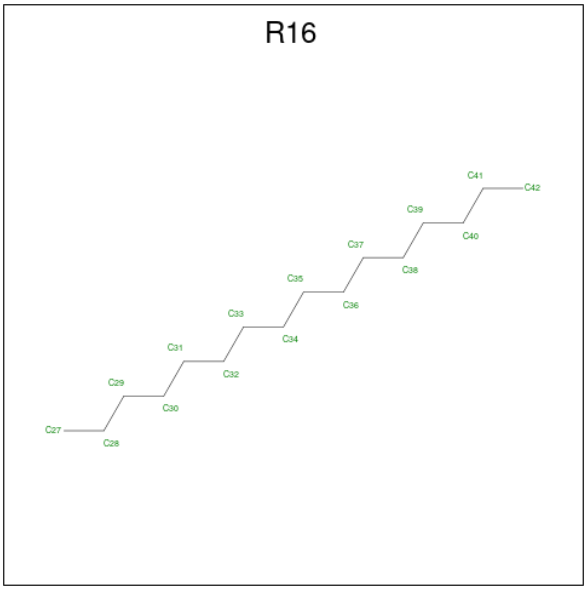
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total C O 16 10 6	0	0
9	R	1	Total C O 16 10 6	0	0
9	l	1	Total C O 16 10 6	0	0
9	h	1	Total C O 16 10 6	0	0

- Molecule 10 is DODECANE (three-letter code: D12) (formula: $C_{12}H_{26}$).



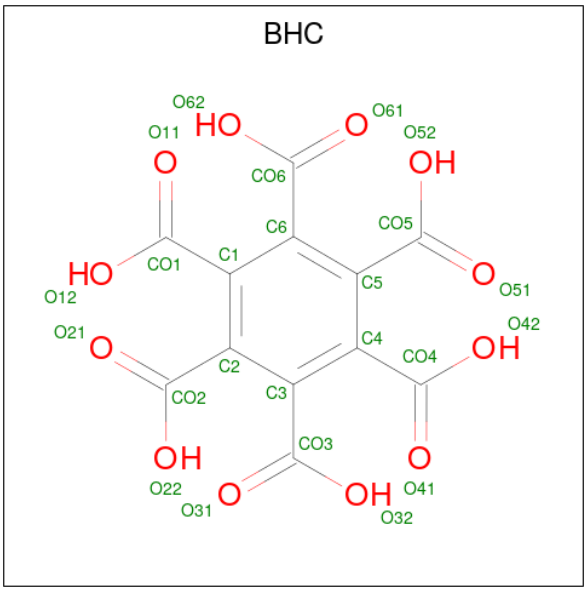
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	a	1	Total C 12 12	0	0
10	o	1	Total C 12 12	0	0
10	e	1	Total C 12 12	0	0

- Molecule 11 is HEXADECANE (three-letter code: R16) (formula: $C_{16}H_{34}$).



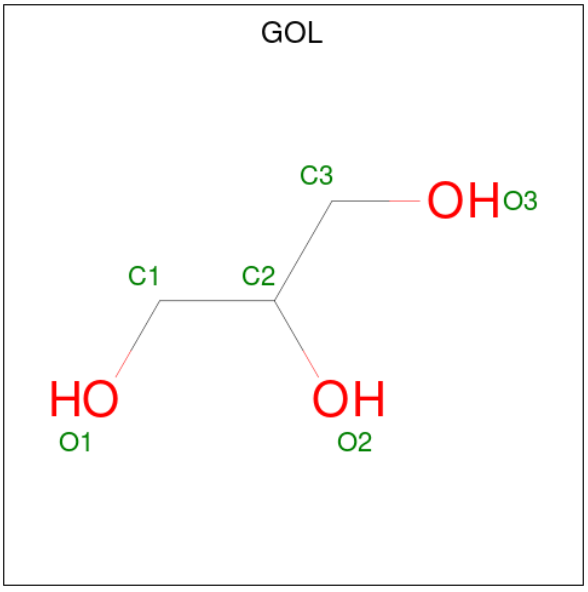
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	p	1	Total C 16 16	0	0

- Molecule 12 is BENZENE HEXACARBOXYLIC ACID (three-letter code: BHC) (formula: $C_{12}H_6O_{12}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	h	1	Total C O 24 12 12	0	0

- Molecule 13 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	h	1	Total C O 6 3 3	0	0

- Molecule 14 is water.

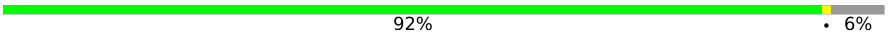
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	L	1	Total O 1 1	0	0
14	B	1	Total O 1 1	0	0
14	S	1	Total O 1 1	0	0
14	Y	1	Total O 1 1	0	0
14	b	1	Total O 1 1	0	0
14	n	1	Total O 1 1	0	0
14	q	1	Total O 1 1	0	0
14	g	1	Total O 1 1	0	0
14	k	1	Total O 1 1	0	0

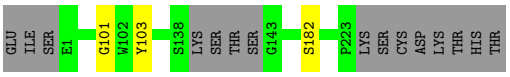
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron 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 dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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: SAT09 fab fragment, heavy chain

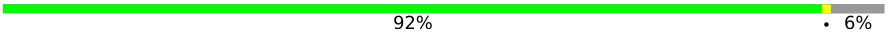
Chain H:

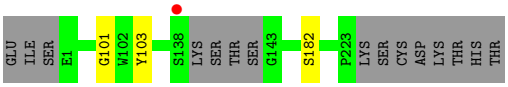




• Molecule 1: SAT09 fab fragment, heavy chain

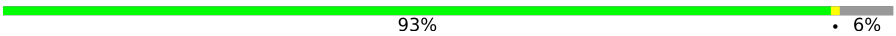
Chain A:

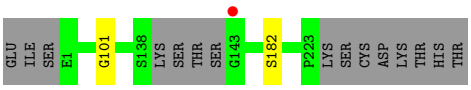




• Molecule 1: SAT09 fab fragment, heavy chain

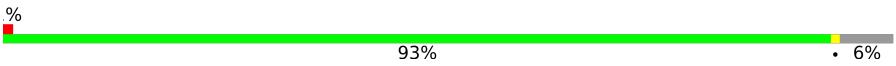
Chain R:

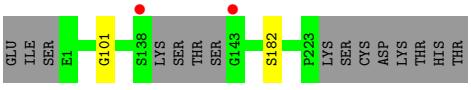




• Molecule 1: SAT09 fab fragment, heavy chain

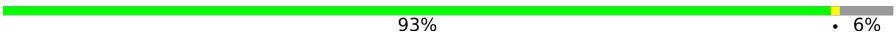
Chain U:

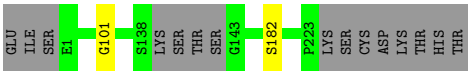




• Molecule 1: SAT09 fab fragment, heavy chain

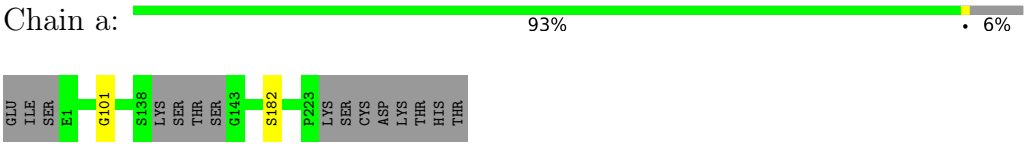
Chain X:





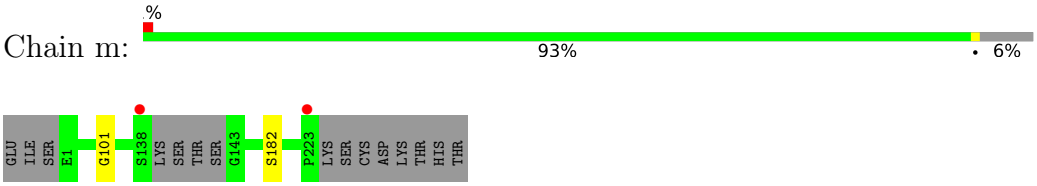
• Molecule 1: SAT09 fab fragment, heavy chain

Chain a:



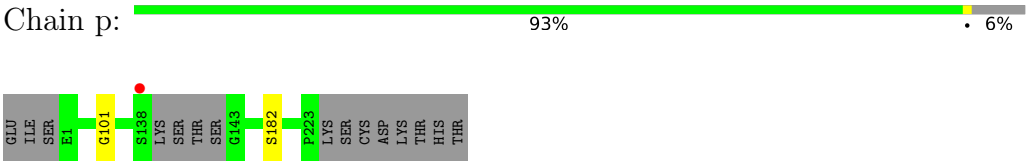
• Molecule 1: SAT09 fab fragment, heavy chain

Chain m:



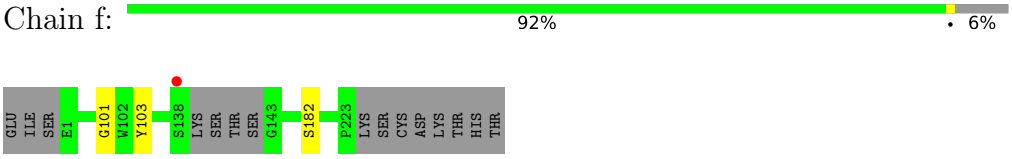
• Molecule 1: SAT09 fab fragment, heavy chain

Chain p:



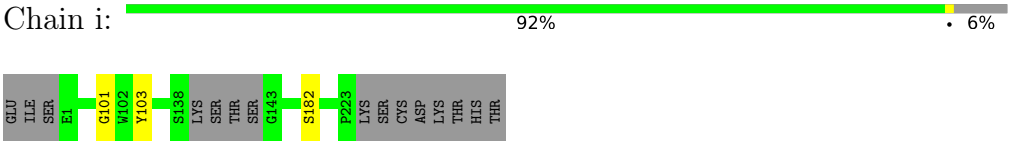
• Molecule 1: SAT09 fab fragment, heavy chain

Chain f:



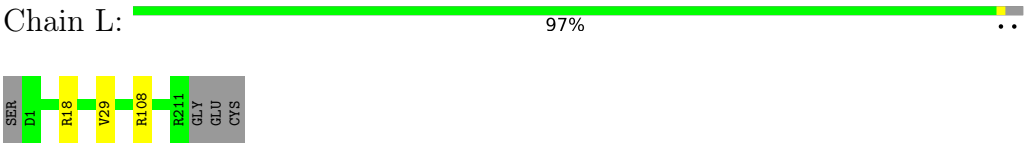
• Molecule 1: SAT09 fab fragment, heavy chain

Chain i:



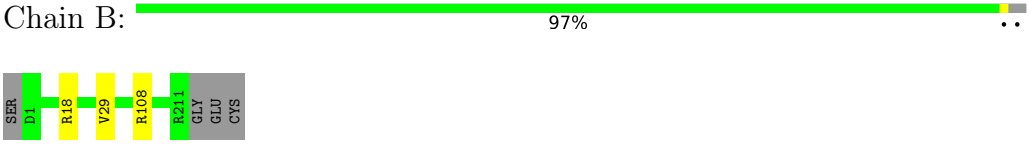
• Molecule 2: SAT09 fab fragment, light chain

Chain L:



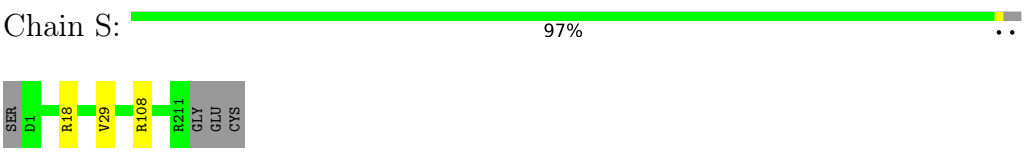
• Molecule 2: SAT09 fab fragment, light chain

Chain B:



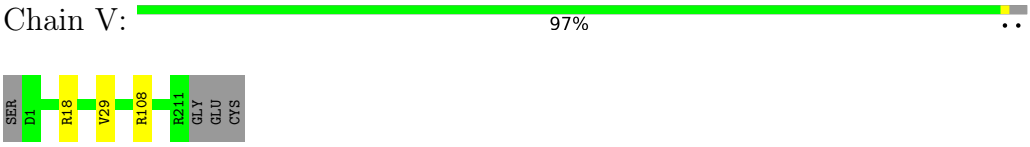
• Molecule 2: SAT09 fab fragment, light chain

Chain S:



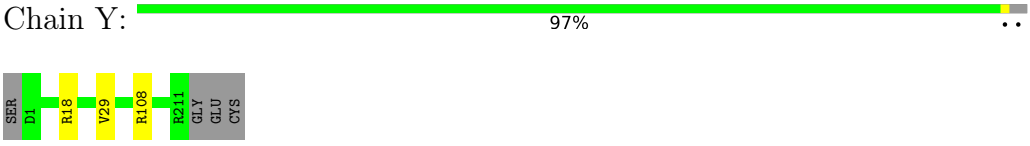
• Molecule 2: SAT09 fab fragment, light chain

Chain V:



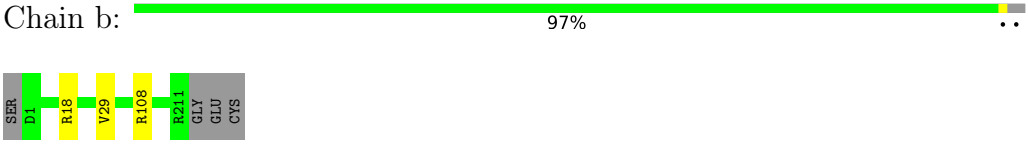
• Molecule 2: SAT09 fab fragment, light chain

Chain Y:



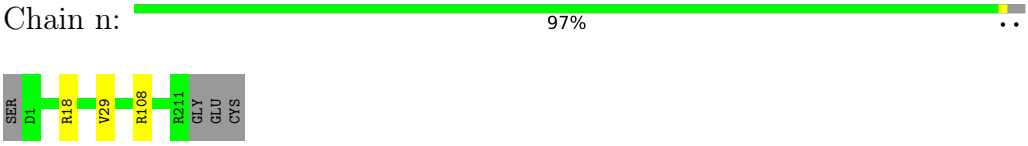
• Molecule 2: SAT09 fab fragment, light chain

Chain b:



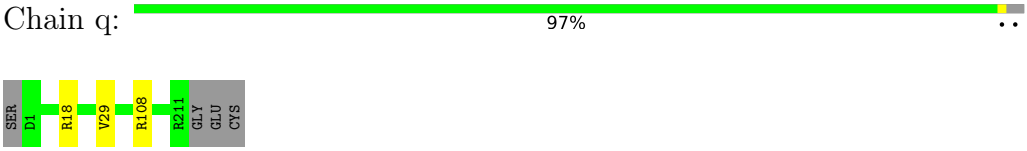
• Molecule 2: SAT09 fab fragment, light chain

Chain n:



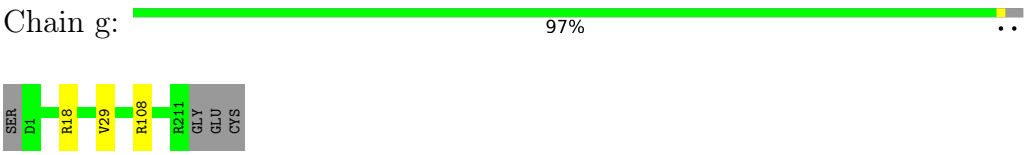
• Molecule 2: SAT09 fab fragment, light chain

Chain q:



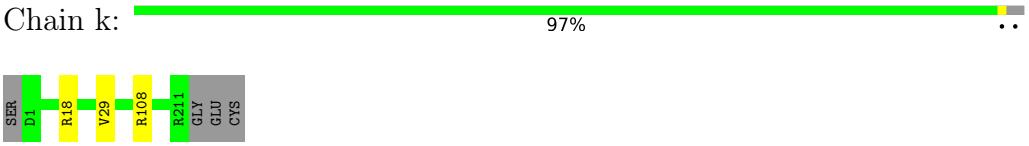
• Molecule 2: SAT09 fab fragment, light chain

Chain g:



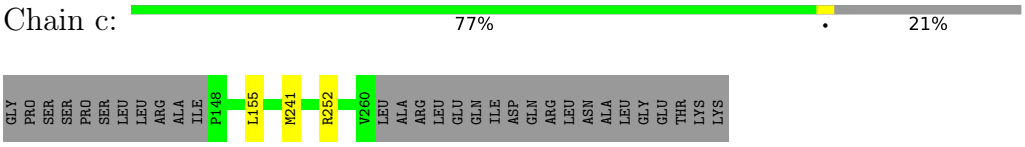
• Molecule 2: SAT09 fab fragment, light chain

Chain k:



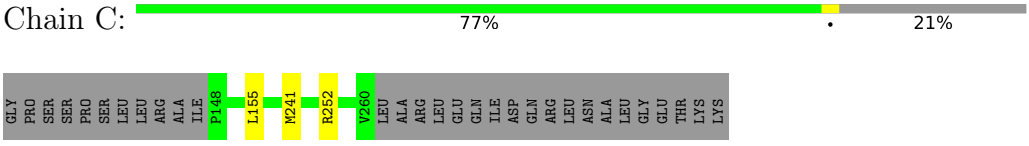
• Molecule 3: Ion transport protein,Voltage-gated sodium channel

Chain c:



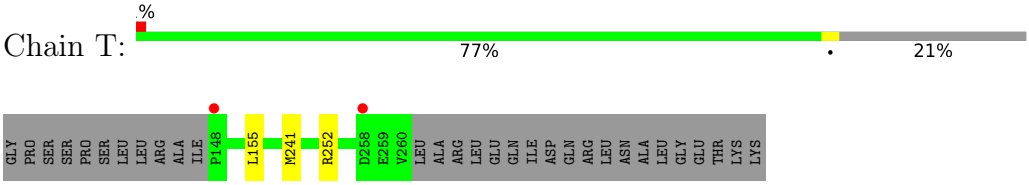
• Molecule 3: Ion transport protein,Voltage-gated sodium channel

Chain C:



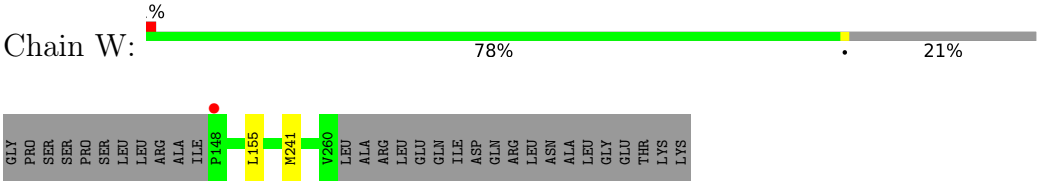
• Molecule 3: Ion transport protein,Voltage-gated sodium channel

Chain T:



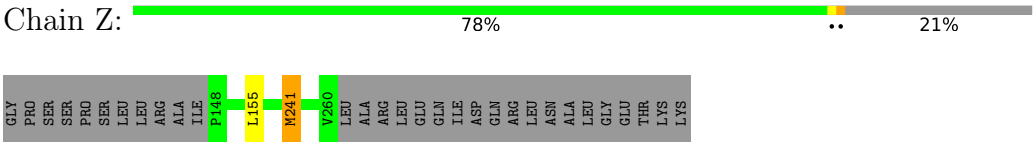
• Molecule 3: Ion transport protein,Voltage-gated sodium channel

Chain W:



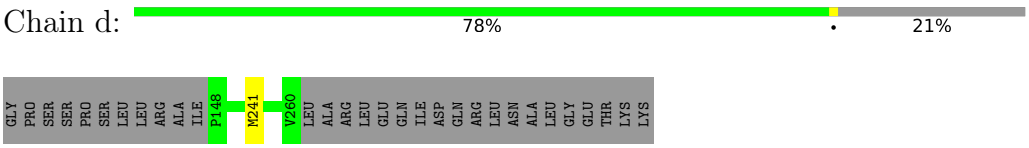
• Molecule 3: Ion transport protein,Voltage-gated sodium channel

Chain Z:



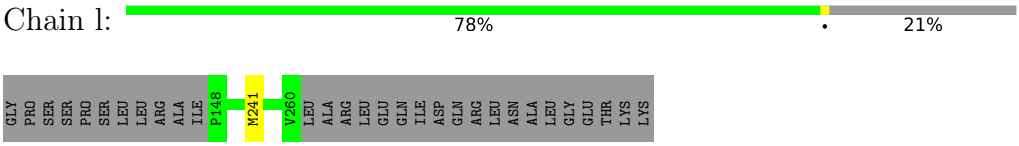
• Molecule 3: Ion transport protein,Voltage-gated sodium channel

Chain d:



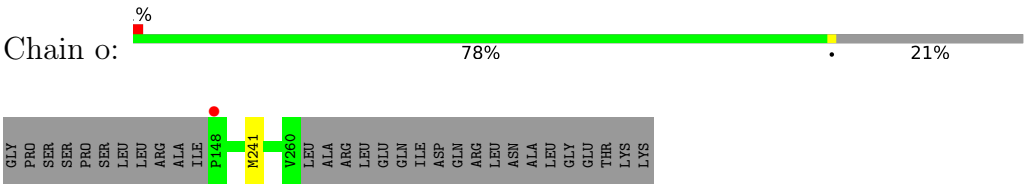
• Molecule 3: Ion transport protein,Voltage-gated sodium channel

Chain l:



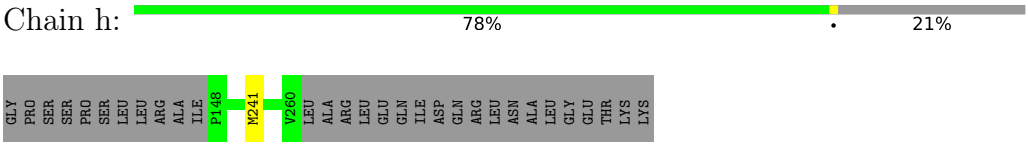
• Molecule 3: Ion transport protein,Voltage-gated sodium channel

Chain o:



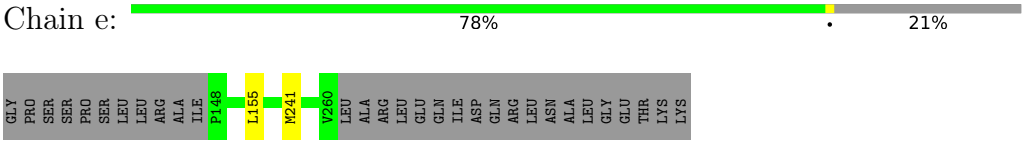
• Molecule 3: Ion transport protein,Voltage-gated sodium channel

Chain h:



• Molecule 3: Ion transport protein,Voltage-gated sodium channel

Chain e:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α, β, γ	200.87Å 200.87Å 327.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 3.60 15.00 – 3.60	Depositor EDS
% Data completeness (in resolution range)	99.9 (15.00-3.60) 99.9 (15.00-3.60)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.06 (at 3.57Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.207 , 0.232 0.207 , 0.232	Depositor DCC
R_{free} test set	7391 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	156.8	Xtriage
Anisotropy	0.076	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	0.377 for h,-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	42734	wwPDB-VP
Average B, all atoms (Å^2)	190.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.60% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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: D12, 1PE, LHG, PE4, OCT, BHC, 4NB, GOL, R16, LNK

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	0.25	0/1686	0.53	0/2303
1	H	0.26	0/1686	0.53	0/2303
1	R	0.26	0/1686	0.52	0/2303
1	U	0.26	0/1686	0.52	0/2303
1	X	0.26	0/1686	0.52	0/2303
1	a	0.26	0/1686	0.52	0/2303
1	f	0.26	0/1686	0.53	0/2303
1	i	0.26	0/1686	0.53	0/2303
1	m	0.25	0/1686	0.53	0/2303
1	p	0.26	0/1686	0.52	0/2303
2	B	0.28	0/1645	0.48	0/2233
2	L	0.28	0/1645	0.48	0/2233
2	S	0.28	0/1645	0.48	0/2233
2	V	0.28	0/1645	0.48	0/2233
2	Y	0.28	0/1645	0.48	0/2233
2	b	0.28	0/1645	0.48	0/2233
2	g	0.28	0/1645	0.48	0/2233
2	k	0.27	0/1645	0.48	0/2233
2	n	0.28	0/1645	0.48	0/2233
2	q	0.27	0/1645	0.48	0/2233
3	C	0.28	0/936	0.47	0/1277
3	T	0.26	0/929	0.46	1/1269 (0.1%)
3	W	0.26	0/929	0.47	1/1269 (0.1%)
3	Z	0.27	0/929	0.69	2/1269 (0.2%)
3	c	0.27	0/940	0.47	1/1282 (0.1%)
3	d	0.27	0/929	0.47	1/1269 (0.1%)
3	e	0.26	0/929	0.47	1/1269 (0.1%)
3	h	0.27	0/929	0.46	1/1269 (0.1%)
3	l	0.27	0/929	0.47	1/1269 (0.1%)
3	o	0.26	0/929	0.45	0/1269
All	All	0.27	0/42618	0.50	9/58071 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	H	0	1
1	R	0	1
1	U	0	1
1	X	0	1
1	a	0	1
1	f	0	1
1	i	0	1
1	m	0	1
1	p	0	1
2	B	0	1
2	L	0	1
2	S	0	1
2	V	0	1
2	Y	0	1
2	b	0	1
2	g	0	1
2	k	0	1
2	n	0	1
2	q	0	1
All	All	0	20

There are no bond length outliers.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	Z	241	MET	CA-CB-CG	14.59	138.11	113.30
3	Z	241	MET	CB-CG-SD	11.83	147.88	112.40
3	d	241	MET	CA-CB-CG	5.31	122.33	113.30
3	T	241	MET	CA-CB-CG	5.27	122.26	113.30
3	e	241	MET	CA-CB-CG	5.25	122.22	113.30

There are no chirality outliers.

5 of 20 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	101	GLY	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
2	B	29	VAL	Peptide
1	H	101	GLY	Peptide
2	L	29	VAL	Peptide
1	R	101	GLY	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 X-ray entries followed by that with respect to entries of similar resolution.

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	215/234 (92%)	200 (93%)	14 (6%)	1 (0%)	29	68
1	H	215/234 (92%)	200 (93%)	14 (6%)	1 (0%)	29	68
1	R	215/234 (92%)	199 (93%)	15 (7%)	1 (0%)	29	68
1	U	215/234 (92%)	199 (93%)	15 (7%)	1 (0%)	29	68
1	X	215/234 (92%)	200 (93%)	14 (6%)	1 (0%)	29	68
1	a	215/234 (92%)	200 (93%)	14 (6%)	1 (0%)	29	68
1	f	215/234 (92%)	200 (93%)	14 (6%)	1 (0%)	29	68
1	i	215/234 (92%)	198 (92%)	16 (7%)	1 (0%)	29	68
1	m	215/234 (92%)	199 (93%)	15 (7%)	1 (0%)	29	68
1	p	215/234 (92%)	198 (92%)	16 (7%)	1 (0%)	29	68
2	B	209/215 (97%)	197 (94%)	12 (6%)	0	100	100
2	L	209/215 (97%)	197 (94%)	12 (6%)	0	100	100
2	S	209/215 (97%)	197 (94%)	12 (6%)	0	100	100
2	V	209/215 (97%)	197 (94%)	12 (6%)	0	100	100
2	Y	209/215 (97%)	197 (94%)	12 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	b	209/215 (97%)	197 (94%)	12 (6%)	0	100	100
2	g	209/215 (97%)	197 (94%)	12 (6%)	0	100	100
2	k	209/215 (97%)	197 (94%)	12 (6%)	0	100	100
2	n	209/215 (97%)	198 (95%)	11 (5%)	0	100	100
2	q	209/215 (97%)	197 (94%)	12 (6%)	0	100	100
3	C	111/143 (78%)	106 (96%)	5 (4%)	0	100	100
3	T	111/143 (78%)	106 (96%)	5 (4%)	0	100	100
3	W	111/143 (78%)	106 (96%)	5 (4%)	0	100	100
3	Z	111/143 (78%)	106 (96%)	5 (4%)	0	100	100
3	c	111/143 (78%)	105 (95%)	6 (5%)	0	100	100
3	d	111/143 (78%)	106 (96%)	5 (4%)	0	100	100
3	e	111/143 (78%)	106 (96%)	5 (4%)	0	100	100
3	h	111/143 (78%)	107 (96%)	4 (4%)	0	100	100
3	l	111/143 (78%)	106 (96%)	5 (4%)	0	100	100
3	o	111/143 (78%)	106 (96%)	5 (4%)	0	100	100
All	All	5350/5920 (90%)	5024 (94%)	316 (6%)	10 (0%)	47	79

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	182	SER
1	A	182	SER
1	R	182	SER
1	U	182	SER
1	X	182	SER

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 X-ray entries followed by that with respect to entries of similar resolution.

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	181/196 (92%)	180 (99%)	1 (1%)	86	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	181/196 (92%)	180 (99%)	1 (1%)	86	94
1	R	181/196 (92%)	181 (100%)	0	100	100
1	U	181/196 (92%)	181 (100%)	0	100	100
1	X	181/196 (92%)	181 (100%)	0	100	100
1	a	181/196 (92%)	181 (100%)	0	100	100
1	f	181/196 (92%)	180 (99%)	1 (1%)	86	94
1	i	181/196 (92%)	180 (99%)	1 (1%)	86	94
1	m	181/196 (92%)	181 (100%)	0	100	100
1	p	181/196 (92%)	181 (100%)	0	100	100
2	B	186/189 (98%)	184 (99%)	2 (1%)	73	88
2	L	186/189 (98%)	184 (99%)	2 (1%)	73	88
2	S	186/189 (98%)	184 (99%)	2 (1%)	73	88
2	V	186/189 (98%)	184 (99%)	2 (1%)	73	88
2	Y	186/189 (98%)	184 (99%)	2 (1%)	73	88
2	b	186/189 (98%)	184 (99%)	2 (1%)	73	88
2	g	186/189 (98%)	184 (99%)	2 (1%)	73	88
2	k	186/189 (98%)	184 (99%)	2 (1%)	73	88
2	n	186/189 (98%)	184 (99%)	2 (1%)	73	88
2	q	186/189 (98%)	184 (99%)	2 (1%)	73	88
3	C	94/120 (78%)	91 (97%)	3 (3%)	39	70
3	T	92/120 (77%)	90 (98%)	2 (2%)	52	77
3	W	92/120 (77%)	91 (99%)	1 (1%)	73	88
3	Z	92/120 (77%)	90 (98%)	2 (2%)	52	77
3	c	95/120 (79%)	93 (98%)	2 (2%)	53	78
3	d	92/120 (77%)	92 (100%)	0	100	100
3	e	92/120 (77%)	91 (99%)	1 (1%)	73	88
3	h	92/120 (77%)	92 (100%)	0	100	100
3	l	92/120 (77%)	92 (100%)	0	100	100
3	o	92/120 (77%)	91 (99%)	1 (1%)	73	88
All	All	4595/5050 (91%)	4559 (99%)	36 (1%)	81	91

5 of 36 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	o	241	MET
3	e	155	LEU
1	f	103	TYR
1	i	103	TYR
2	S	108	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
3	d	245	HIS
1	p	28	ASN
2	k	166	GLN
2	n	166	GLN
2	q	160	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

77 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	$\#\|Z\|>2$
8	LNK	T	305	-	4,4,4	0.34	0	3,3,3	0.50	0
6	OCT	U	303	-	7,7,7	0.34	0	6,6,6	0.69	0
5	LHG	m	302	-	48,48,48	0.58	1 (2%)	51,54,54	1.20	6 (11%)
4	4NB	e	303	-	9,12,12	2.30	2 (22%)	11,16,16	0.67	0
4	4NB	H	302	-	9,12,12	2.22	2 (22%)	11,16,16	0.70	0
5	LHG	H	303	-	48,48,48	0.62	1 (2%)	51,54,54	1.21	6 (11%)
7	PE4	H	305	-	23,23,23	0.55	0	22,22,22	0.22	0
9	1PE	h	306	-	15,15,15	0.54	0	14,14,14	0.20	0
5	LHG	a	302	-	48,48,48	0.62	1 (2%)	51,54,54	1.24	6 (11%)
12	BHC	h	304	-	12,24,24	4.41	6 (50%)	18,36,36	0.35	0
4	4NB	h	301	-	9,12,12	2.16	2 (22%)	11,16,16	0.71	0
4	4NB	T	303	-	9,12,12	2.18	2 (22%)	11,16,16	0.72	0
4	4NB	C	302	-	9,12,12	2.24	2 (22%)	11,16,16	0.66	0
8	LNK	h	307	-	4,4,4	0.35	0	3,3,3	0.48	0
4	4NB	f	301	-	9,12,12	2.20	2 (22%)	11,16,16	0.67	0
10	D12	a	301	-	11,11,11	0.32	0	10,10,10	0.78	0
8	LNK	W	304	-	4,4,4	0.32	0	3,3,3	0.52	0
4	4NB	o	302	-	9,12,12	2.13	2 (22%)	11,16,16	0.71	0
4	4NB	d	301	-	9,12,12	2.19	2 (22%)	11,16,16	0.71	0
4	4NB	l	303	-	9,12,12	2.21	2 (22%)	11,16,16	0.67	0
4	4NB	Z	302	-	9,12,12	2.20	2 (22%)	11,16,16	0.72	0
6	OCT	C	303	-	7,7,7	0.31	0	6,6,6	0.72	0
4	4NB	l	304	-	9,12,12	2.32	2 (22%)	11,16,16	1.21	1 (9%)
4	4NB	C	301	-	9,12,12	2.24	2 (22%)	11,16,16	0.79	0
5	LHG	A	301	-	48,48,48	0.67	1 (2%)	51,54,54	1.22	7 (13%)
4	4NB	W	301	-	9,12,12	2.14	2 (22%)	11,16,16	0.73	0
4	4NB	T	301	-	9,12,12	2.16	2 (22%)	11,16,16	0.72	0
8	LNK	Z	304	-	4,4,4	0.34	0	3,3,3	0.52	0
6	OCT	h	303	-	7,7,7	0.33	0	6,6,6	0.68	0
4	4NB	d	302	-	9,12,12	2.25	2 (22%)	11,16,16	0.74	0
4	4NB	H	301	-	9,12,12	2.16	2 (22%)	11,16,16	0.67	0
8	LNK	W	303	-	4,4,4	0.34	0	3,3,3	0.51	0
10	D12	e	304	-	11,11,11	0.31	0	10,10,10	0.78	0
8	LNK	e	306	-	4,4,4	0.33	0	3,3,3	0.52	0
8	LNK	e	305	-	4,4,4	0.34	0	3,3,3	0.52	0
4	4NB	p	301	-	9,12,12	2.19	2 (22%)	11,16,16	0.71	0
6	OCT	T	304	-	7,7,7	0.31	0	6,6,6	0.71	0
4	4NB	R	301	-	9,12,12	2.14	2 (22%)	11,16,16	0.83	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
9	1PE	A	302	-	15,15,15	0.54	0	14,14,14	0.30	0
9	1PE	R	303	-	15,15,15	0.55	0	14,14,14	0.30	0
4	4NB	i	301	-	9,12,12	2.29	2 (22%)	11,16,16	0.71	0
4	4NB	X	302	-	9,12,12	2.24	2 (22%)	11,16,16	0.82	0
6	OCT	a	303	-	7,7,7	0.31	0	6,6,6	0.73	0
4	4NB	e	301	-	9,12,12	2.17	2 (22%)	11,16,16	0.71	0
5	LHG	p	302	-	48,48,48	0.64	0	51,54,54	1.25	6 (11%)
11	R16	p	303	-	15,15,15	0.33	0	14,14,14	0.77	0
5	LHG	i	302	-	48,48,48	0.63	1 (2%)	51,54,54	1.25	6 (11%)
4	4NB	l	302	-	9,12,12	2.30	2 (22%)	11,16,16	0.83	1 (9%)
6	OCT	l	305	-	7,7,7	0.35	0	6,6,6	0.63	0
6	OCT	c	301	-	7,7,7	0.33	0	6,6,6	0.65	0
5	LHG	R	302	-	48,48,48	0.62	0	51,54,54	1.25	6 (11%)
6	OCT	W	302	-	7,7,7	0.31	0	6,6,6	0.69	0
6	OCT	X	304	-	7,7,7	0.31	0	6,6,6	0.74	0
8	LNK	e	307	-	4,4,4	0.33	0	3,3,3	0.53	0
4	4NB	o	301	-	9,12,12	2.22	2 (22%)	11,16,16	0.70	0
5	LHG	f	302	-	48,48,48	0.61	1 (2%)	51,54,54	1.22	6 (11%)
8	LNK	Z	305	-	4,4,4	0.34	0	3,3,3	0.49	0
13	GOL	h	305	-	5,5,5	0.94	0	5,5,5	0.96	0
4	4NB	X	301	-	9,12,12	2.22	2 (22%)	11,16,16	0.69	0
5	LHG	X	303	-	48,48,48	0.59	1 (2%)	51,54,54	1.23	6 (11%)
4	4NB	Z	301	-	9,12,12	2.21	2 (22%)	11,16,16	0.65	0
4	4NB	Z	303	-	9,12,12	2.16	2 (22%)	11,16,16	0.77	0
6	OCT	H	304	-	7,7,7	0.30	0	6,6,6	0.73	0
4	4NB	U	301	-	9,12,12	2.24	2 (22%)	11,16,16	0.65	0
4	4NB	h	302	-	9,12,12	2.21	2 (22%)	11,16,16	0.74	0
8	LNK	l	307	-	4,4,4	0.33	0	3,3,3	0.52	0
4	4NB	l	301	-	9,12,12	2.39	2 (22%)	11,16,16	0.73	0
9	1PE	l	306	-	15,15,15	0.53	0	14,14,14	0.25	0
8	LNK	c	302	-	4,4,4	0.34	0	3,3,3	0.52	0
5	LHG	U	302	-	48,48,48	0.62	0	51,54,54	1.22	6 (11%)
4	4NB	m	301	-	9,12,12	2.27	2 (22%)	11,16,16	0.72	0
10	D12	o	303	-	11,11,11	0.31	0	10,10,10	0.77	0
4	4NB	e	302	-	9,12,12	2.18	2 (22%)	11,16,16	0.69	0
8	LNK	d	303	-	4,4,4	0.35	0	3,3,3	0.49	0
8	LNK	d	304	-	4,4,4	0.34	0	3,3,3	0.50	0
4	4NB	T	302	-	9,12,12	2.39	2 (22%)	11,16,16	0.70	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	OCT	o	304	-	7,7,7	0.33	0	6,6,6	0.68	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	LNK	T	305	-	-	0/2/2/2	-
6	OCT	U	303	-	-	2/5/5/5	-
5	LHG	m	302	-	-	24/53/53/53	-
4	4NB	e	303	-	-	0/2/8/8	0/1/1/1
4	4NB	H	302	-	-	0/2/8/8	0/1/1/1
5	LHG	H	303	-	-	30/53/53/53	-
7	PE4	H	305	-	-	14/21/21/21	-
9	1PE	h	306	-	-	6/13/13/13	-
5	LHG	a	302	-	-	29/53/53/53	-
12	BHC	h	304	-	-	0/0/24/24	0/1/1/1
4	4NB	h	301	-	-	2/2/8/8	0/1/1/1
4	4NB	T	303	-	-	2/2/8/8	0/1/1/1
4	4NB	C	302	-	-	0/2/8/8	0/1/1/1
8	LNK	h	307	-	-	0/2/2/2	-
4	4NB	f	301	-	-	2/2/8/8	0/1/1/1
10	D12	a	301	-	-	1/9/9/9	-
8	LNK	W	304	-	-	1/2/2/2	-
4	4NB	o	302	-	-	0/2/8/8	0/1/1/1
4	4NB	d	301	-	-	0/2/8/8	0/1/1/1
4	4NB	l	303	-	-	2/2/8/8	0/1/1/1
4	4NB	Z	302	-	-	0/2/8/8	0/1/1/1
6	OCT	C	303	-	-	0/5/5/5	-
4	4NB	l	304	-	-	2/2/8/8	0/1/1/1
4	4NB	C	301	-	-	0/2/8/8	0/1/1/1
5	LHG	A	301	-	-	26/53/53/53	-
4	4NB	W	301	-	-	0/2/8/8	0/1/1/1
4	4NB	T	301	-	-	2/2/8/8	0/1/1/1
8	LNK	Z	304	-	-	0/2/2/2	-
6	OCT	h	303	-	-	0/5/5/5	-
4	4NB	d	302	-	-	2/2/8/8	0/1/1/1
4	4NB	H	301	-	-	0/2/8/8	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	LNK	W	303	-	-	0/2/2/2	-
10	D12	e	304	-	-	2/9/9/9	-
8	LNK	e	306	-	-	1/2/2/2	-
8	LNK	e	305	-	-	0/2/2/2	-
4	4NB	p	301	-	-	0/2/8/8	0/1/1/1
6	OCT	T	304	-	-	0/5/5/5	-
4	4NB	R	301	-	-	0/2/8/8	0/1/1/1
9	1PE	A	302	-	-	6/13/13/13	-
9	1PE	R	303	-	-	6/13/13/13	-
4	4NB	i	301	-	-	0/2/8/8	0/1/1/1
4	4NB	X	302	-	-	2/2/8/8	0/1/1/1
6	OCT	a	303	-	-	2/5/5/5	-
4	4NB	e	301	-	-	0/2/8/8	0/1/1/1
5	LHG	p	302	-	-	28/53/53/53	-
11	R16	p	303	-	-	6/13/13/13	-
5	LHG	i	302	-	-	32/53/53/53	-
4	4NB	l	302	-	-	0/2/8/8	0/1/1/1
6	OCT	l	305	-	-	0/5/5/5	-
6	OCT	c	301	-	-	0/5/5/5	-
5	LHG	R	302	-	-	27/53/53/53	-
6	OCT	W	302	-	-	3/5/5/5	-
6	OCT	X	304	-	-	1/5/5/5	-
8	LNK	e	307	-	-	0/2/2/2	-
4	4NB	o	301	-	-	0/2/8/8	0/1/1/1
5	LHG	f	302	-	-	28/53/53/53	-
8	LNK	Z	305	-	-	0/2/2/2	-
13	GOL	h	305	-	-	2/4/4/4	-
4	4NB	X	301	-	-	0/2/8/8	0/1/1/1
5	LHG	X	303	-	-	22/53/53/53	-
4	4NB	Z	301	-	-	2/2/8/8	0/1/1/1
4	4NB	Z	303	-	-	0/2/8/8	0/1/1/1
6	OCT	H	304	-	-	2/5/5/5	-
4	4NB	U	301	-	-	0/2/8/8	0/1/1/1
4	4NB	h	302	-	-	2/2/8/8	0/1/1/1
8	LNK	l	307	-	-	1/2/2/2	-
4	4NB	l	301	-	-	2/2/8/8	0/1/1/1
9	1PE	l	306	-	-	7/13/13/13	-
8	LNK	c	302	-	-	0/2/2/2	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	LHG	U	302	-	-	26/53/53/53	-
4	4NB	m	301	-	-	0/2/8/8	0/1/1/1
10	D12	o	303	-	-	2/9/9/9	-
4	4NB	e	302	-	-	2/2/8/8	0/1/1/1
8	LNK	d	303	-	-	1/2/2/2	-
8	LNK	d	304	-	-	0/2/2/2	-
4	4NB	T	302	-	-	0/2/8/8	0/1/1/1
6	OCT	o	304	-	-	3/5/5/5	-

The worst 5 of 77 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	T	302	4NB	C1-C	6.60	1.53	1.47
4	l	301	4NB	C1-C	6.59	1.53	1.47
12	h	304	BHC	C1-CO1	6.34	1.53	1.47
4	l	302	4NB	C1-C	6.29	1.53	1.47
4	i	301	4NB	C1-C	6.29	1.53	1.47

The worst 5 of 63 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	X	303	LHG	O4-P-O5	4.20	133.02	112.24
5	a	302	LHG	O4-P-O5	4.19	132.95	112.24
5	A	301	LHG	O4-P-O5	4.18	132.90	112.24
5	p	302	LHG	O4-P-O5	4.15	132.74	112.24
5	R	302	LHG	O4-P-O5	4.14	132.71	112.24

There are no chirality outliers.

5 of 365 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	T	301	4NB	C3-C4-N-O2'
4	T	301	4NB	C5-C4-N-O2'
4	T	303	4NB	C3-C4-N-O2'
4	X	302	4NB	C3-C4-N-O2'
4	X	302	4NB	C5-C4-N-O2'

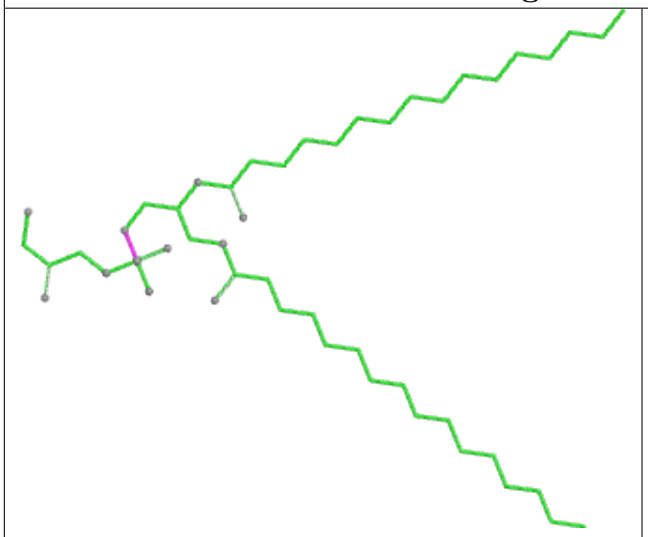
There are no ring outliers.

No monomer is involved in short contacts.

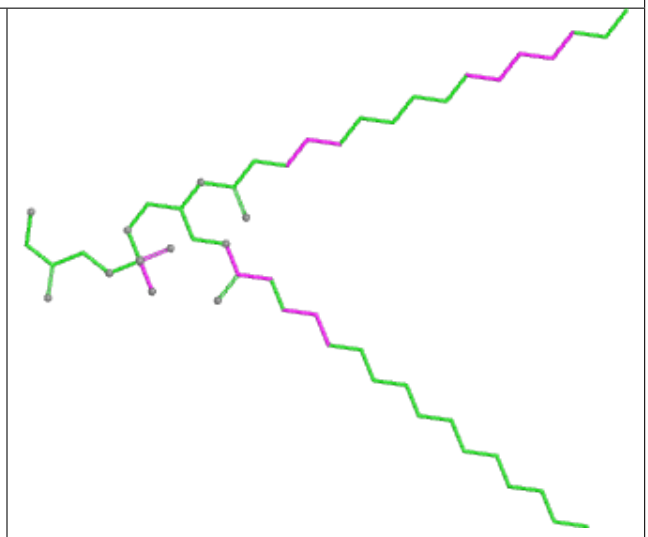
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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.

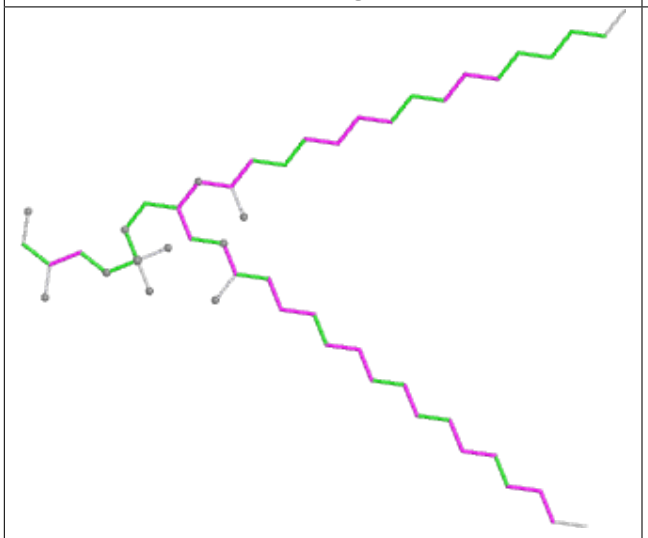
Ligand LHG m 302



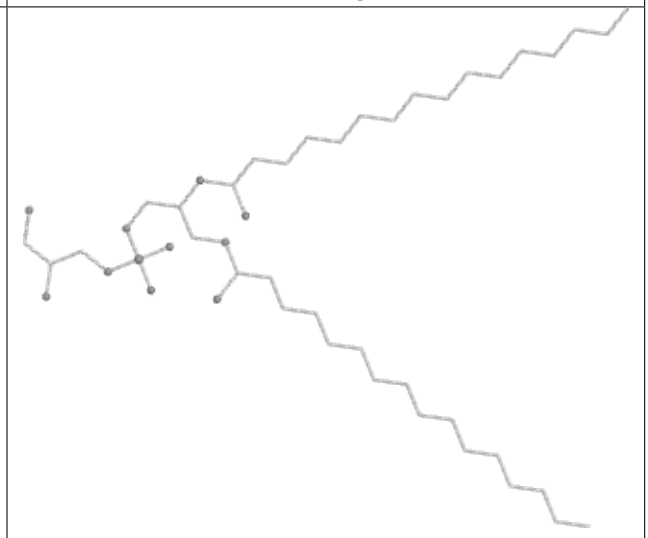
Bond lengths



Bond angles

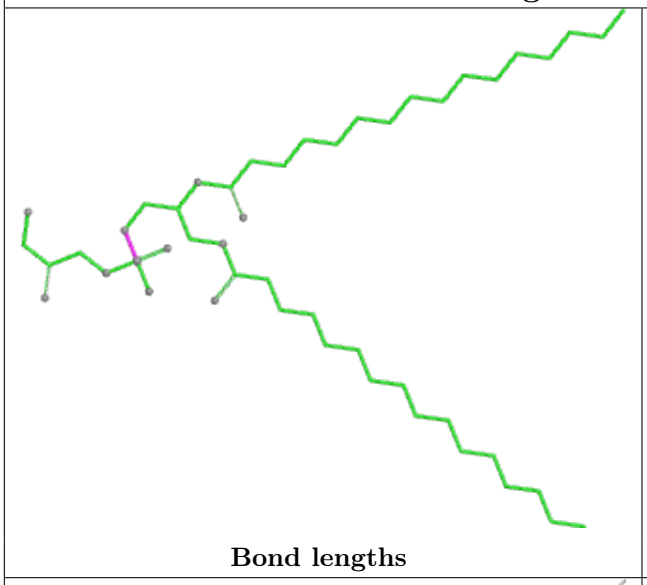


Torsions

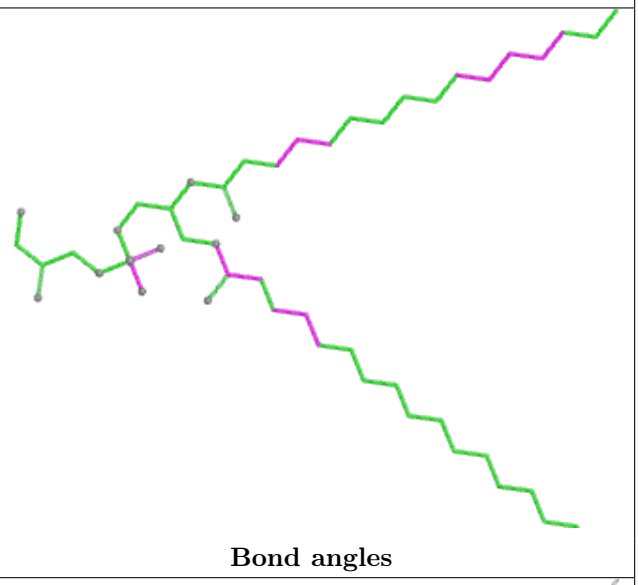


Rings

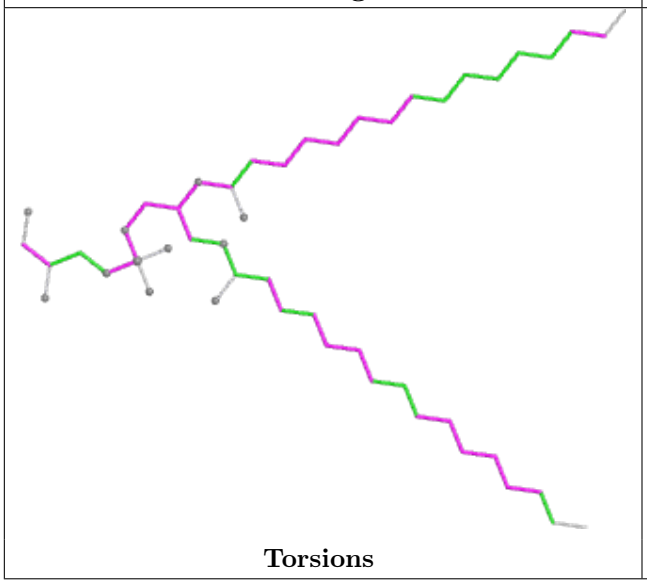
Ligand LHG H 303



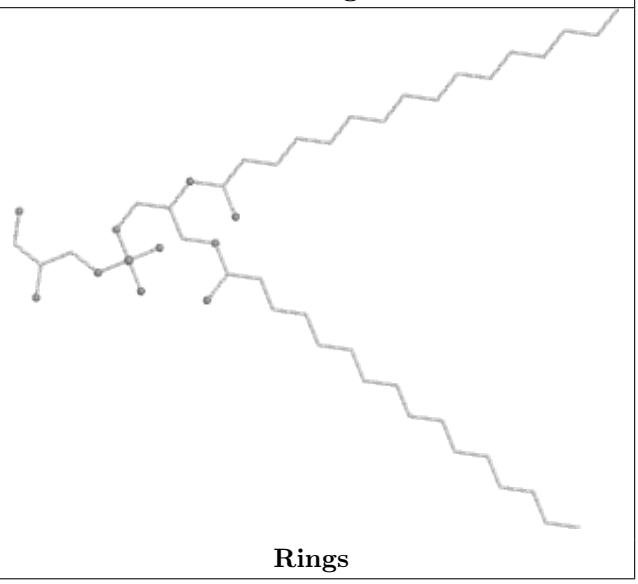
Bond lengths



Bond angles

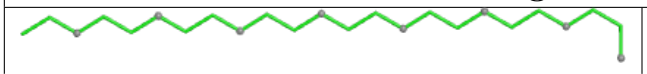


Torsions

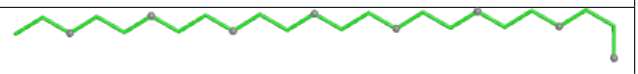


Rings

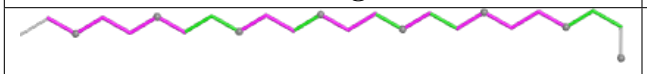
Ligand PE4 H 305



Bond lengths



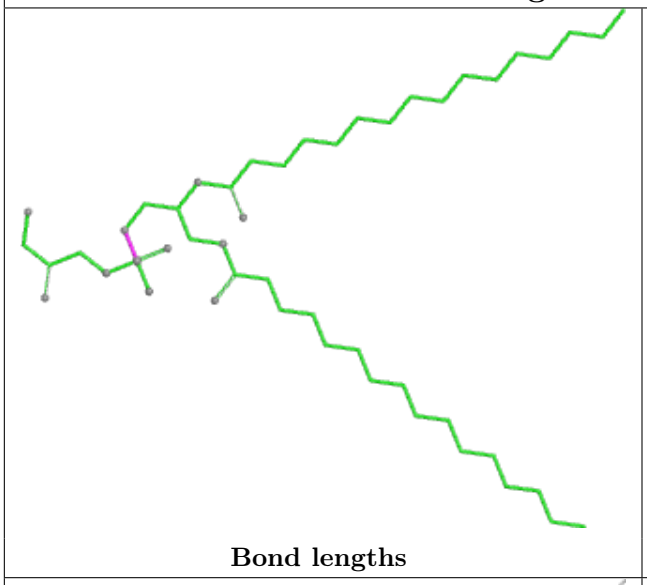
Bond angles



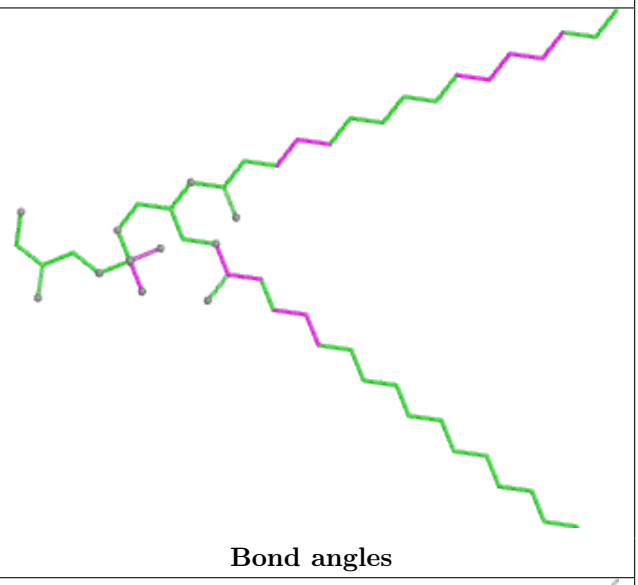
Torsions

Rings

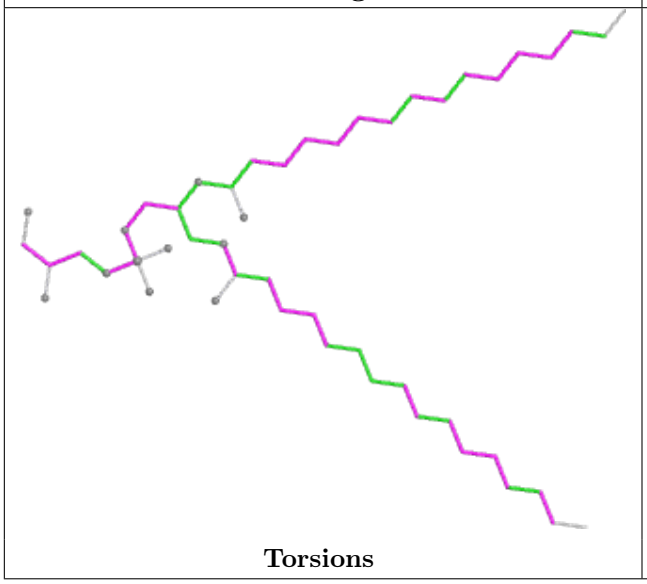
Ligand LHG a 302



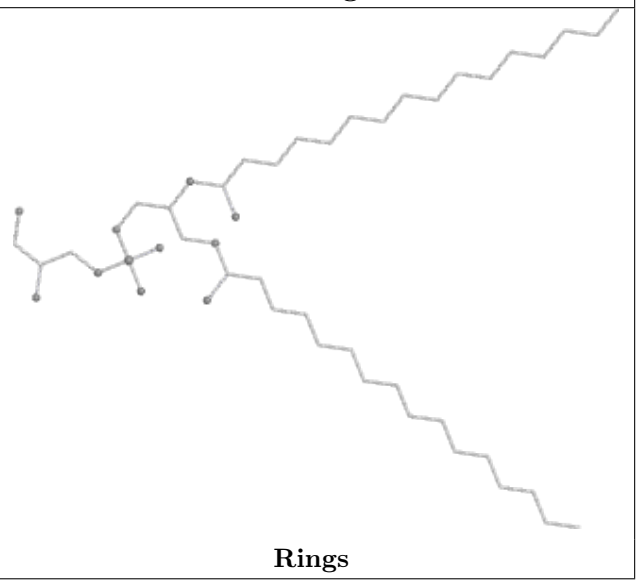
Bond lengths



Bond angles

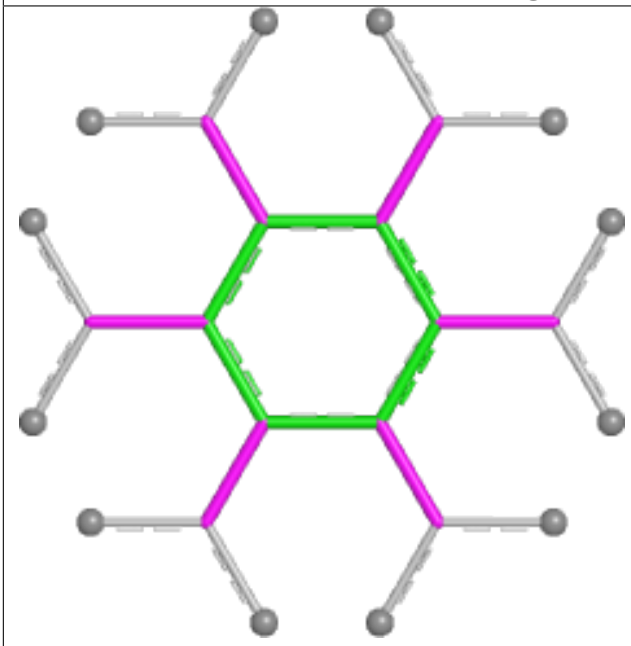


Torsions

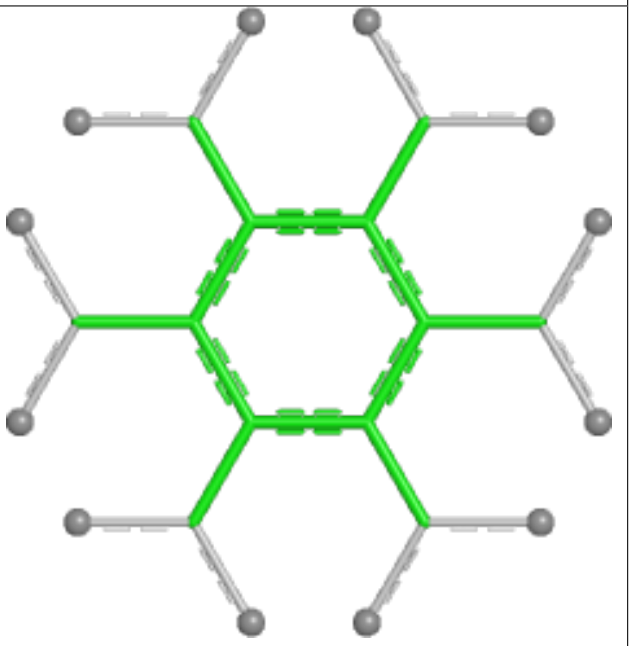


Rings

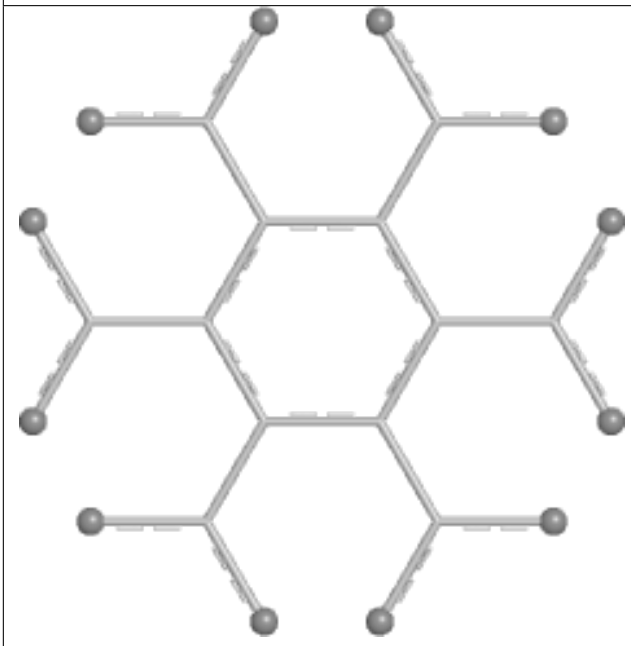
Ligand BHC h 304



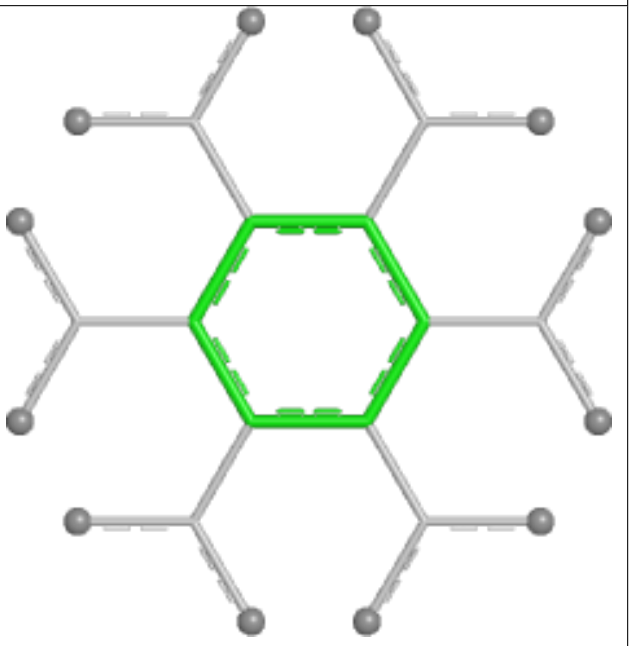
Bond lengths



Bond angles

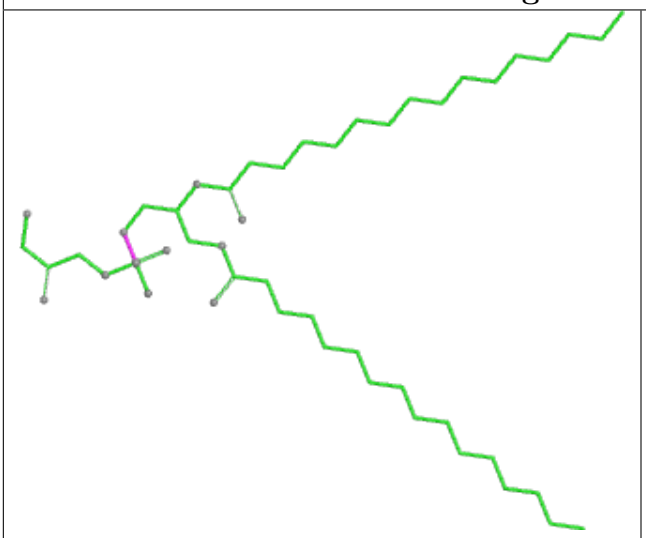


Torsions

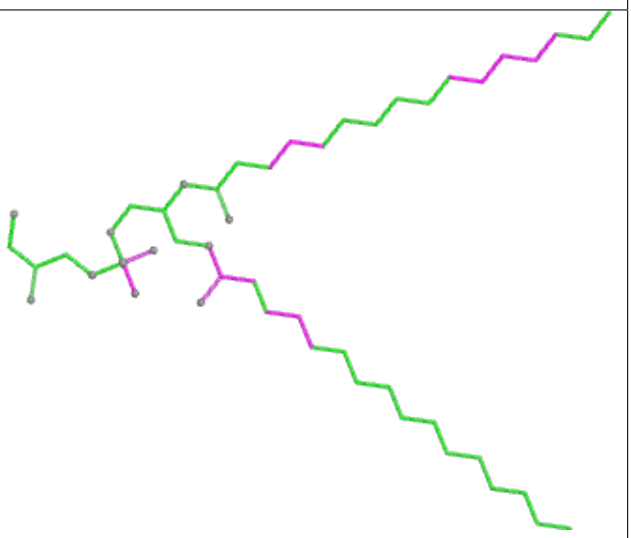


Rings

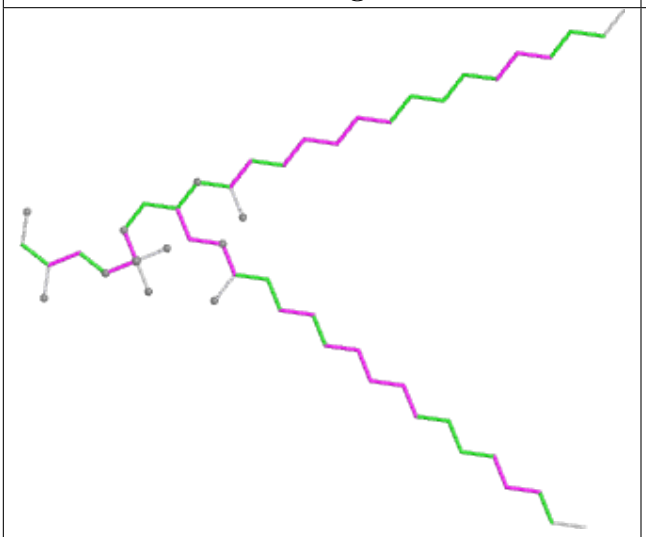
Ligand LHG A 301



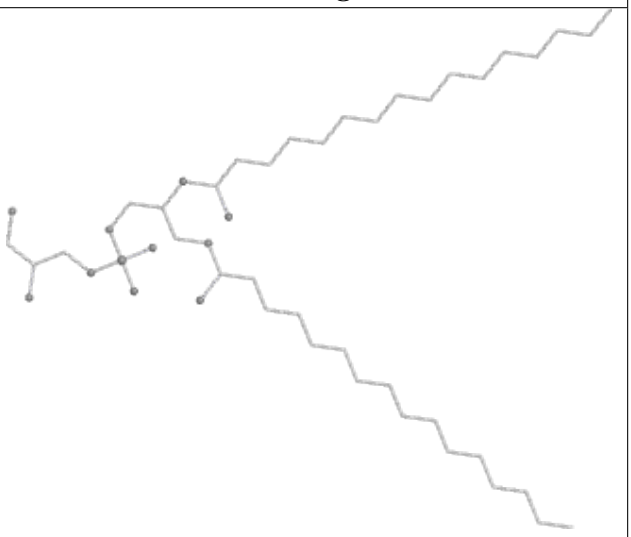
Bond lengths



Bond angles

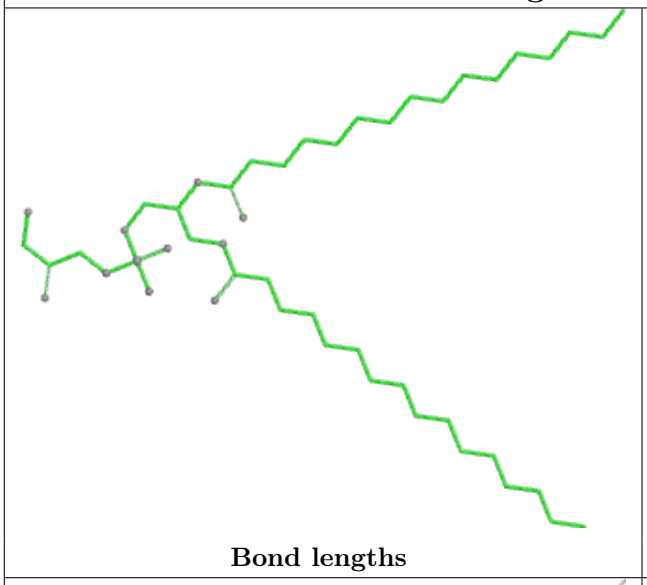


Torsions

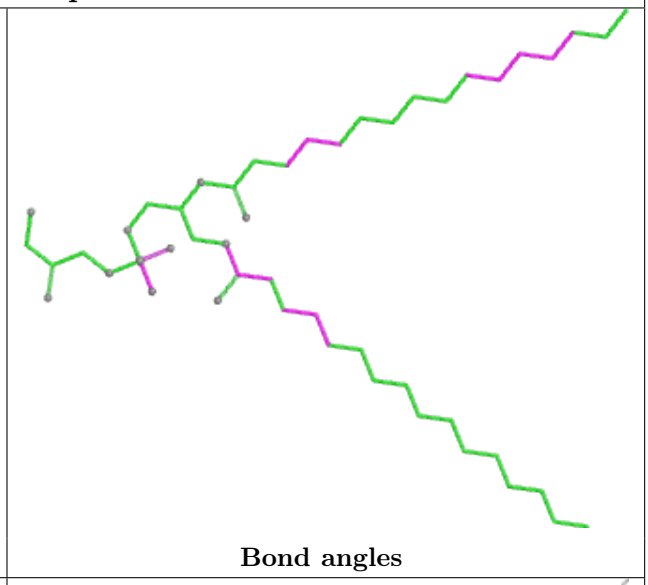


Rings

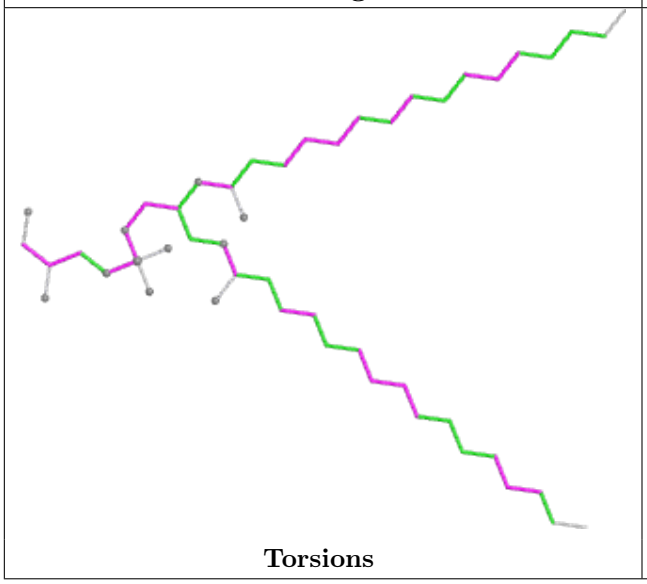
Ligand LHG p 302



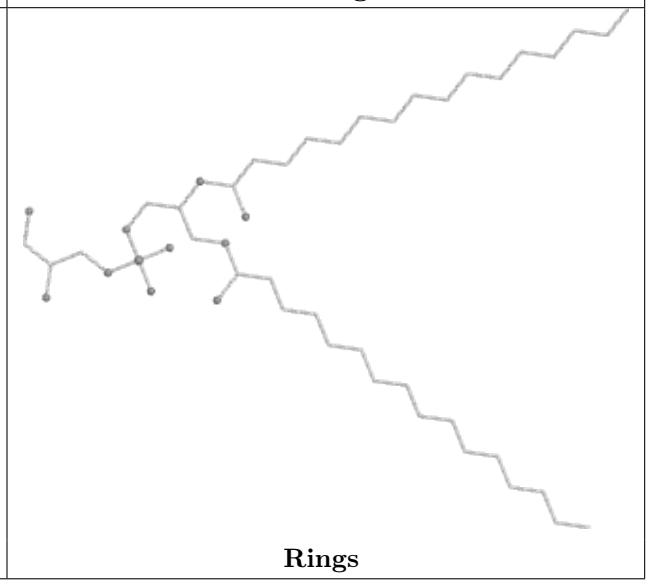
Bond lengths



Bond angles

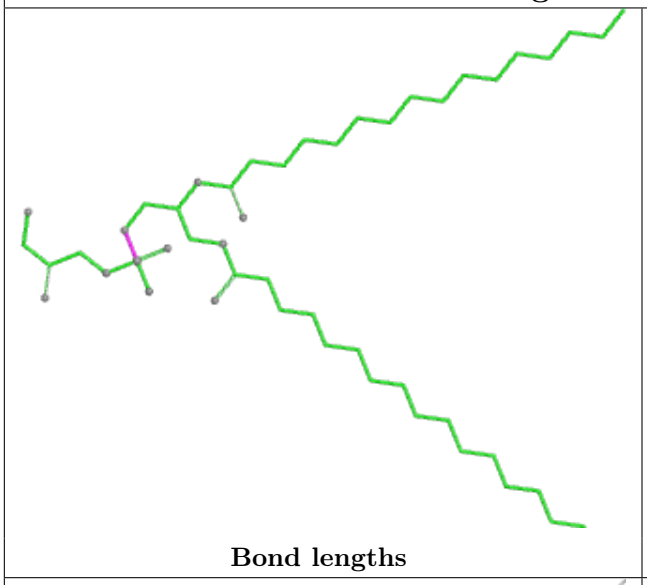


Torsions

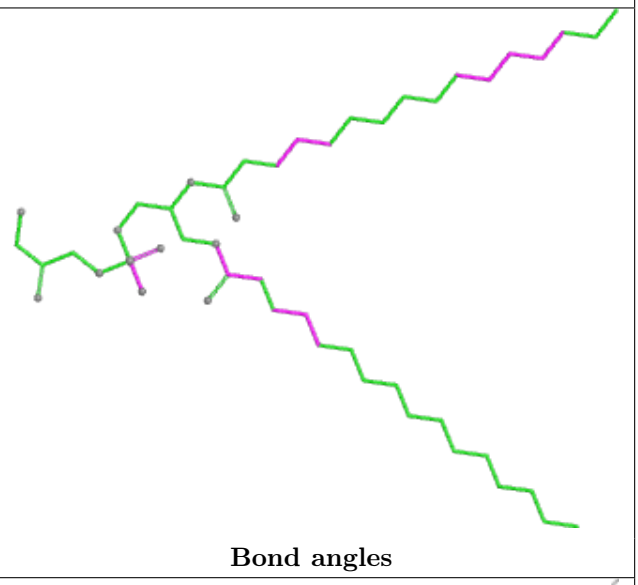


Rings

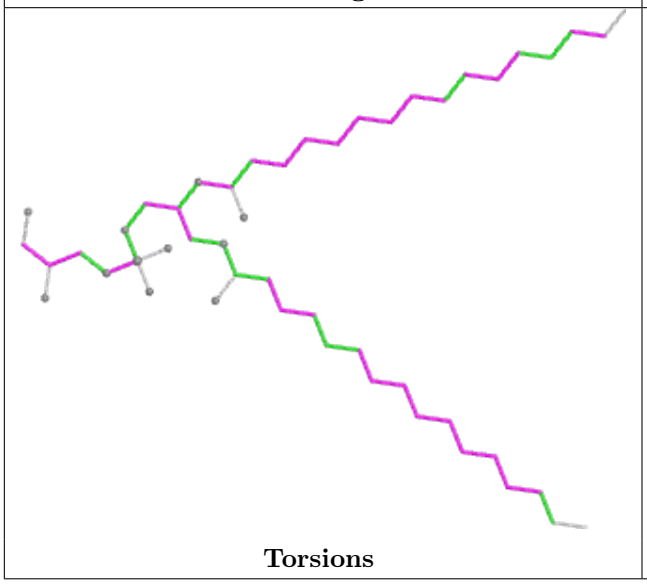
Ligand LHG i 302



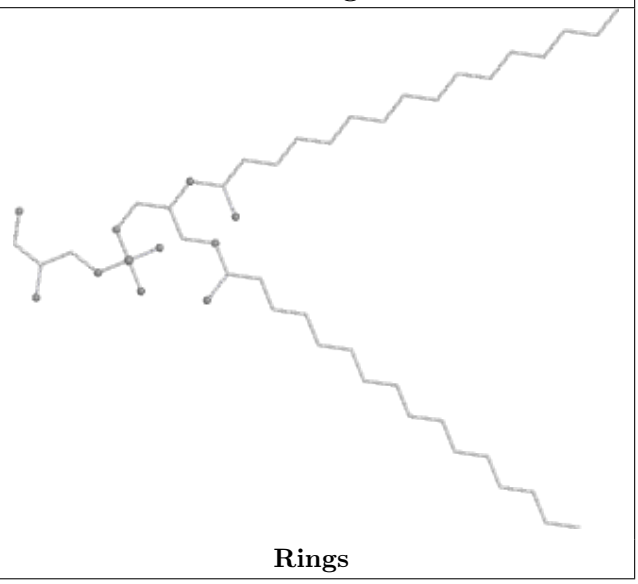
Bond lengths



Bond angles

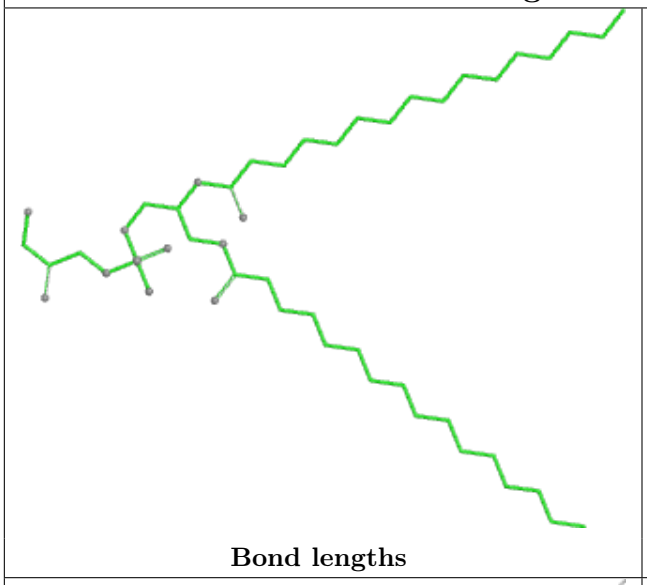


Torsions

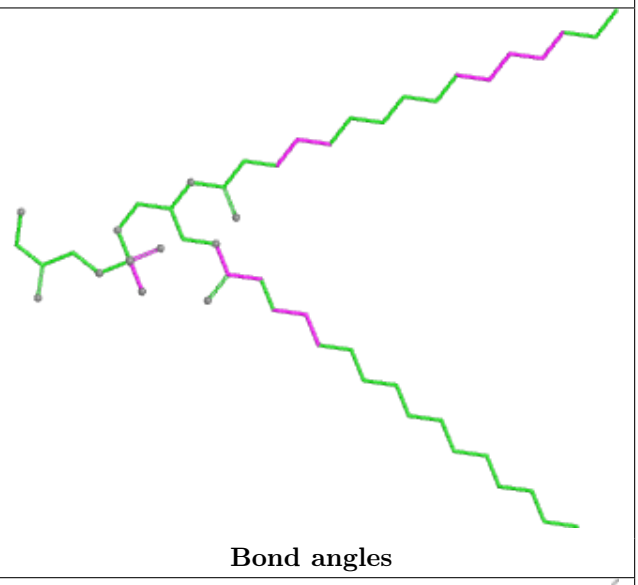


Rings

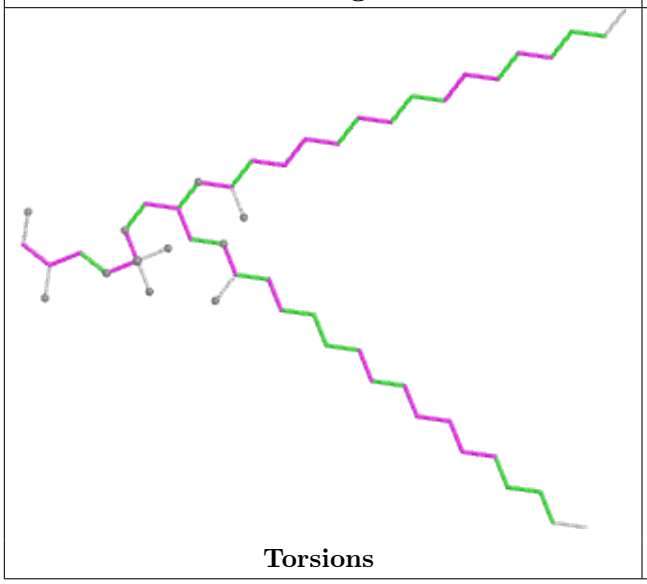
Ligand LHG R 302



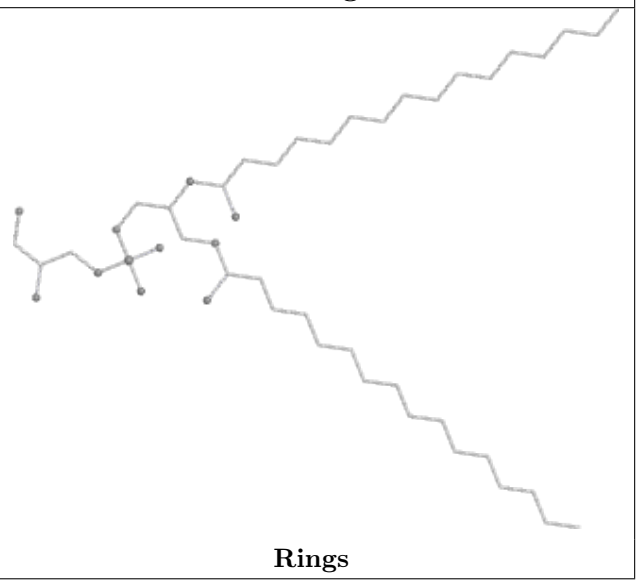
Bond lengths



Bond angles

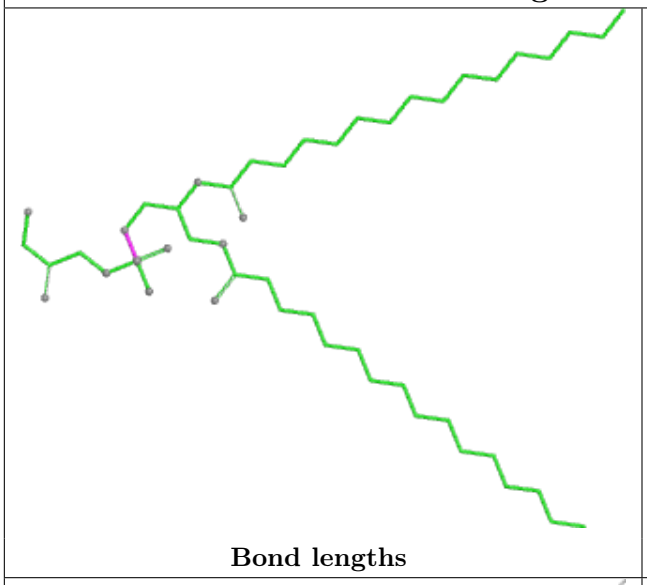


Torsions

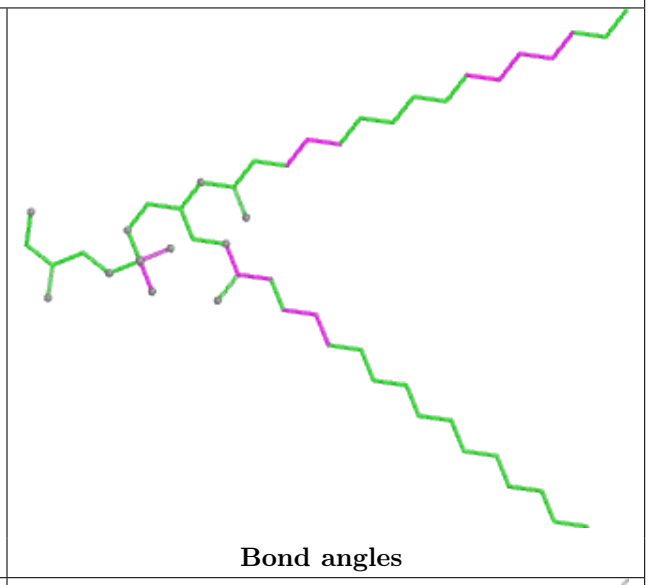


Rings

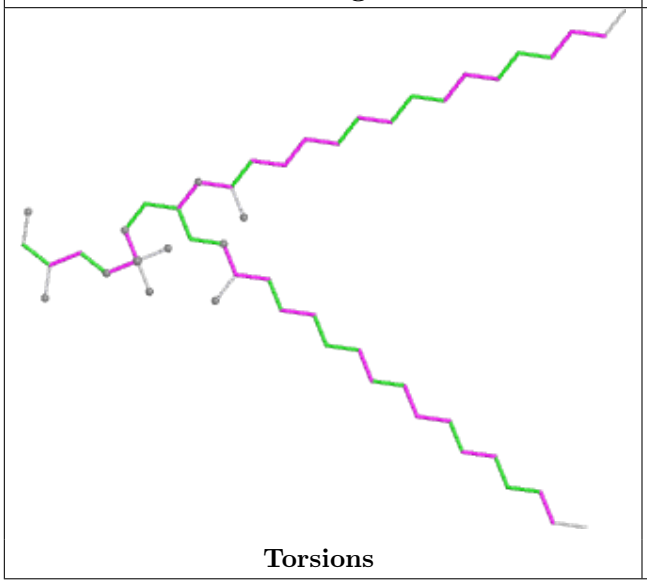
Ligand LHG f 302



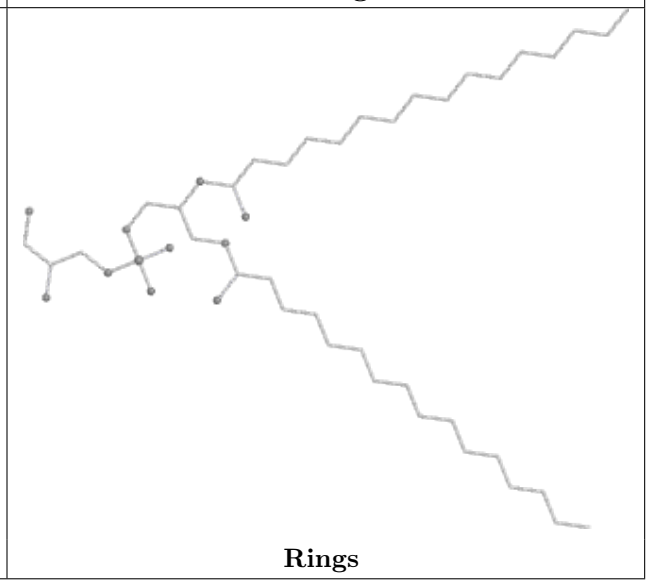
Bond lengths



Bond angles

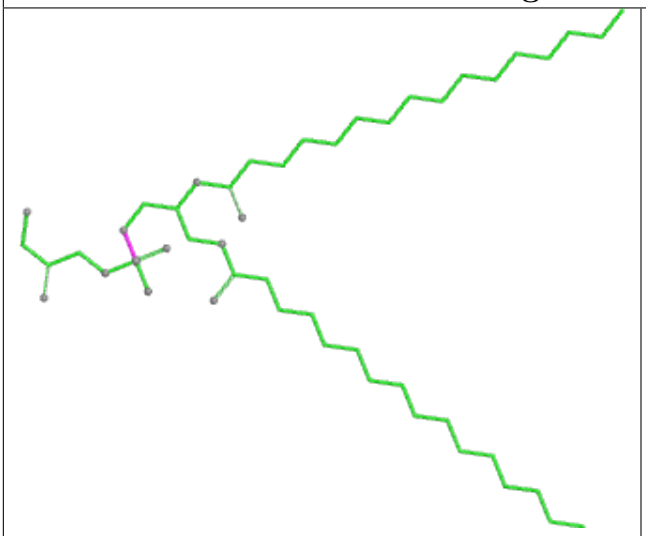


Torsions

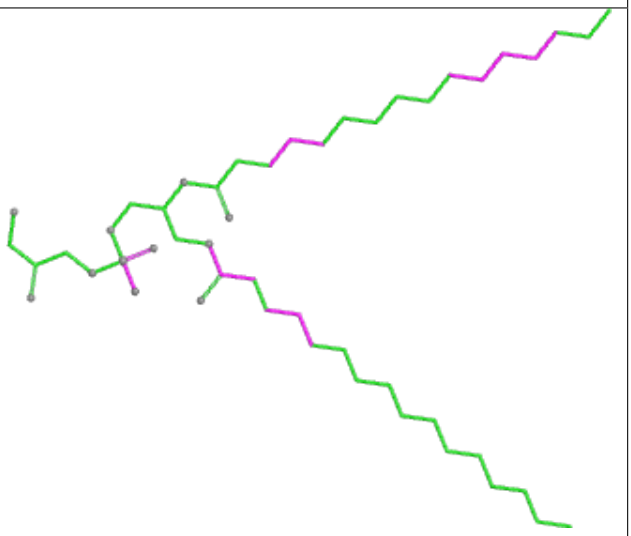


Rings

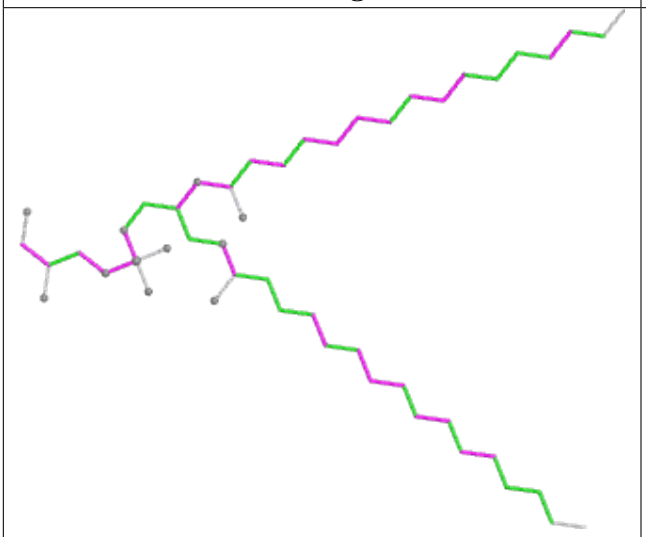
Ligand LHG X 303



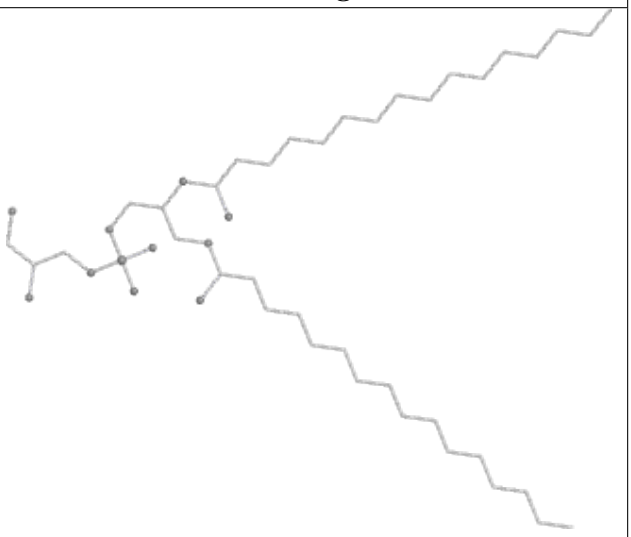
Bond lengths



Bond angles

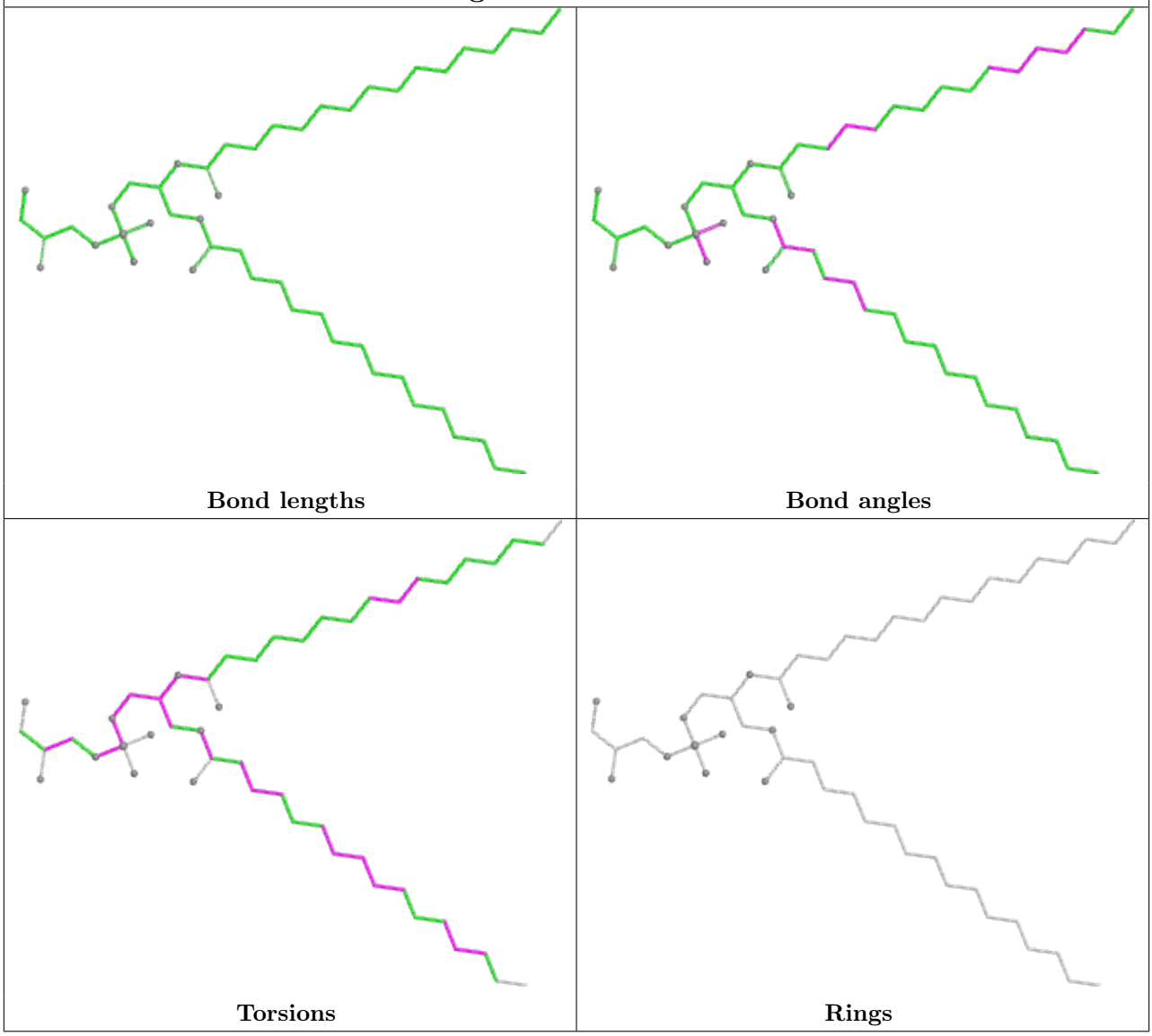


Torsions



Rings

Ligand LHG U 302



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 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	219/234 (93%)	-0.41	1 (0%) 91 83	107, 179, 262, 295	0
1	H	219/234 (93%)	-0.40	0 100 100	104, 180, 263, 293	0
1	R	219/234 (93%)	-0.60	1 (0%) 91 83	120, 195, 265, 287	0
1	U	219/234 (93%)	-0.57	2 (0%) 84 73	123, 194, 264, 289	0
1	X	219/234 (93%)	-0.64	0 100 100	118, 196, 266, 294	0
1	a	219/234 (93%)	-0.64	0 100 100	123, 196, 266, 299	0
1	f	219/234 (93%)	-0.43	1 (0%) 91 83	102, 184, 267, 289	0
1	i	219/234 (93%)	-0.57	0 100 100	117, 191, 263, 294	0
1	m	219/234 (93%)	-0.44	2 (0%) 84 73	105, 183, 268, 289	0
1	p	219/234 (93%)	-0.56	1 (0%) 91 83	120, 190, 265, 292	0
2	B	211/215 (98%)	-0.54	0 100 100	110, 180, 254, 283	0
2	L	211/215 (98%)	-0.53	0 100 100	112, 180, 257, 284	0
2	S	211/215 (98%)	-0.64	0 100 100	122, 193, 258, 293	0
2	V	211/215 (98%)	-0.65	0 100 100	122, 192, 257, 296	0
2	Y	211/215 (98%)	-0.65	0 100 100	121, 194, 263, 280	0
2	b	211/215 (98%)	-0.63	0 100 100	122, 195, 262, 286	0
2	g	211/215 (98%)	-0.56	0 100 100	112, 186, 258, 278	0
2	k	211/215 (98%)	-0.64	0 100 100	118, 186, 260, 284	0
2	n	211/215 (98%)	-0.54	0 100 100	112, 185, 254, 276	0
2	q	211/215 (98%)	-0.61	0 100 100	117, 186, 260, 283	0
3	C	113/143 (79%)	-0.27	0 100 100	103, 152, 379, 425	0
3	T	113/143 (79%)	-0.29	2 (1%) 68 53	107, 154, 376, 416	0
3	W	113/143 (79%)	-0.28	1 (0%) 84 73	109, 151, 378, 415	0
3	Z	113/143 (79%)	-0.35	0 100 100	106, 154, 379, 411	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
3	c	113/143 (79%)	-0.25	0	100	100	100, 150, 381, 429	0
3	d	113/143 (79%)	-0.34	0	100	100	111, 155, 371, 412	0
3	e	113/143 (79%)	-0.29	0	100	100	106, 150, 360, 414	0
3	h	113/143 (79%)	-0.33	0	100	100	107, 149, 380, 419	0
3	l	113/143 (79%)	-0.30	0	100	100	109, 150, 359, 409	0
3	o	113/143 (79%)	-0.32	1 (0%)	84	73	108, 149, 375, 415	0
All	All	5430/5920 (91%)	-0.51	12 (0%)	95	91	100, 181, 274, 429	0

The worst 5 of 12 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	f	138	SER	4.0
1	m	138	SER	3.4
3	W	148	PRO	3.3
1	U	143	GLY	3.1
1	m	223	PRO	2.7

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	4NB	H	302	12/12	0.40	0.29	174,251,316,316	0
13	GOL	h	305	6/6	0.54	0.84	117,159,262,272	0
6	OCT	a	303	8/8	0.63	1.48	76,169,186,249	0
10	D12	e	304	12/12	0.64	0.58	123,160,210,223	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	4NB	e	302	12/12	0.70	0.36	160,239,271,278	0
4	4NB	h	302	12/12	0.71	0.57	171,234,297,299	0
9	1PE	R	303	16/16	0.72	0.33	78,158,266,281	0
6	OCT	X	304	8/8	0.72	1.36	112,166,179,198	0
6	OCT	l	305	8/8	0.72	0.80	62,142,179,203	0
4	4NB	X	302	12/12	0.73	0.23	116,167,206,211	0
8	LNK	d	303	5/5	0.74	1.16	95,116,153,210	0
4	4NB	T	302	12/12	0.74	0.46	96,197,233,242	0
10	D12	a	301	12/12	0.74	0.29	90,137,174,189	0
4	4NB	Z	302	12/12	0.74	0.53	126,221,305,306	0
5	LHG	a	302	49/49	0.74	0.32	105,192,317,371	0
12	BHC	h	304	24/24	0.75	0.19	169,324,353,375	0
4	4NB	d	302	12/12	0.75	0.38	144,220,269,290	0
6	OCT	U	303	8/8	0.76	0.51	53,136,163,177	0
6	OCT	c	301	8/8	0.77	0.94	87,127,161,162	0
4	4NB	l	303	12/12	0.78	0.33	148,225,276,278	0
5	LHG	p	302	49/49	0.78	0.32	89,210,335,393	0
4	4NB	i	301	12/12	0.78	0.25	101,172,193,202	0
11	R16	p	303	16/16	0.78	0.38	97,126,189,191	0
5	LHG	U	302	49/49	0.78	0.33	102,228,327,371	0
9	1PE	A	302	16/16	0.78	0.28	87,128,184,210	0
9	1PE	h	306	16/16	0.79	0.34	80,121,214,217	0
6	OCT	o	304	8/8	0.79	0.91	62,185,210,237	0
4	4NB	Z	303	12/12	0.79	0.17	136,171,199,222	0
8	LNK	d	304	5/5	0.79	0.48	90,90,166,167	0
5	LHG	X	303	49/49	0.79	0.28	114,208,325,364	0
4	4NB	U	301	12/12	0.79	0.23	111,149,206,214	0
5	LHG	i	302	49/49	0.80	0.31	73,205,321,347	0
8	LNK	Z	304	5/5	0.80	1.06	95,98,133,208	0
5	LHG	A	301	49/49	0.80	0.32	76,195,306,325	0
5	LHG	f	302	49/49	0.80	0.26	97,176,318,364	0
4	4NB	l	302	12/12	0.81	0.22	91,129,203,207	0
8	LNK	Z	305	5/5	0.81	0.52	78,90,140,149	0
5	LHG	H	303	49/49	0.81	0.24	104,185,277,344	0
4	4NB	p	301	12/12	0.81	0.23	103,164,189,201	0
7	PE4	H	305	24/24	0.82	0.27	95,136,250,269	0
8	LNK	e	305	5/5	0.82	0.43	107,108,149,178	0
4	4NB	H	301	12/12	0.82	0.22	84,147,190,203	0
4	4NB	l	301	12/12	0.82	0.19	91,139,211,227	0
5	LHG	R	302	49/49	0.82	0.30	118,209,304,343	0
4	4NB	X	301	12/12	0.83	0.16	89,141,206,216	0
4	4NB	R	301	12/12	0.83	0.19	110,158,191,197	0

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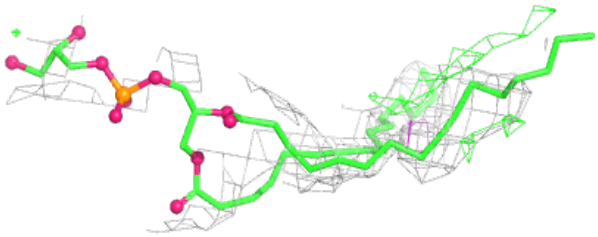
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	4NB	l	304	12/12	0.83	0.45	142,158,247,273	0
5	LHG	m	302	49/49	0.84	0.31	99,192,299,357	0
4	4NB	C	302	12/12	0.84	0.23	80,143,206,214	0
4	4NB	f	301	12/12	0.85	0.23	97,132,198,201	0
4	4NB	m	301	12/12	0.85	0.17	71,104,194,215	0
4	4NB	T	301	12/12	0.86	0.20	135,182,217,249	0
4	4NB	C	301	12/12	0.86	0.16	88,149,219,220	0
8	LNK	W	304	5/5	0.87	0.62	77,100,116,183	0
4	4NB	T	303	12/12	0.87	0.15	154,180,223,230	0
8	LNK	T	305	5/5	0.88	0.42	92,103,133,179	0
10	D12	o	303	12/12	0.88	0.52	75,114,189,211	0
4	4NB	h	301	12/12	0.88	0.14	146,173,206,206	0
4	4NB	e	303	12/12	0.88	0.57	121,181,261,278	0
6	OCT	W	302	8/8	0.88	0.59	73,105,145,206	0
4	4NB	o	301	12/12	0.88	0.14	146,165,196,205	0
6	OCT	H	304	8/8	0.89	0.53	71,123,146,147	0
9	1PE	l	306	16/16	0.89	0.27	139,179,232,259	0
8	LNK	l	307	5/5	0.89	0.95	73,90,153,189	0
8	LNK	h	307	5/5	0.90	0.78	74,82,114,153	0
6	OCT	C	303	8/8	0.90	0.96	76,112,191,215	0
4	4NB	W	301	12/12	0.90	0.19	116,175,198,244	0
4	4NB	o	302	12/12	0.90	0.17	129,159,218,219	0
8	LNK	c	302	5/5	0.91	0.85	72,73,125,171	0
4	4NB	d	301	12/12	0.91	0.12	128,187,211,247	0
8	LNK	W	303	5/5	0.92	0.56	96,102,119,145	0
6	OCT	h	303	8/8	0.92	0.86	83,111,142,144	0
6	OCT	T	304	8/8	0.92	0.24	125,163,196,202	0
8	LNK	e	306	5/5	0.92	1.09	110,125,156,174	0
8	LNK	e	307	5/5	0.92	0.89	76,95,155,168	0
4	4NB	e	301	12/12	0.93	0.14	120,158,213,228	0
4	4NB	Z	301	12/12	0.93	0.14	152,183,209,253	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

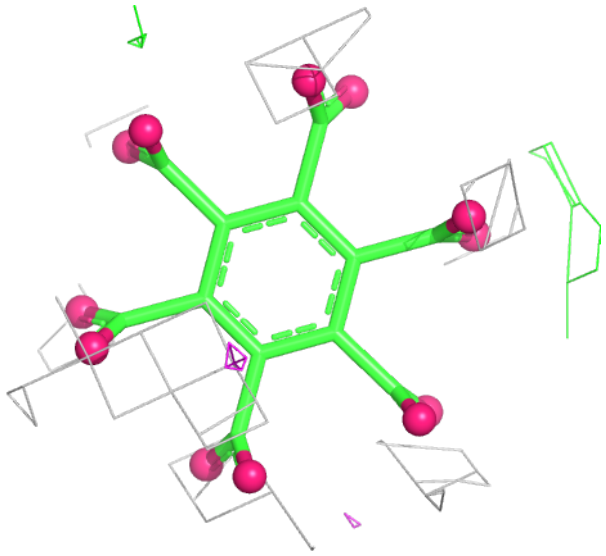
Electron density around LHG a 302:

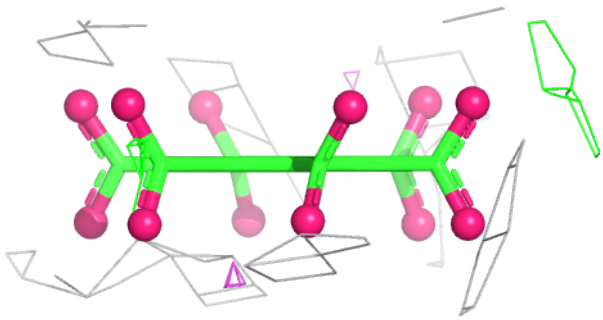
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

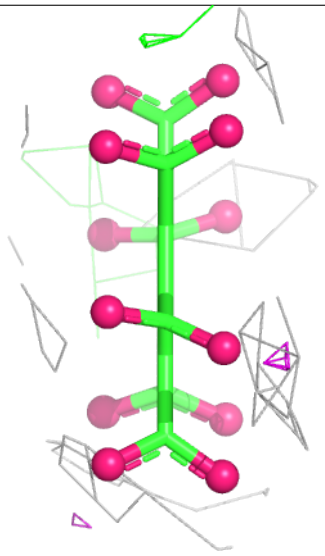


Electron density around BHC h 304:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

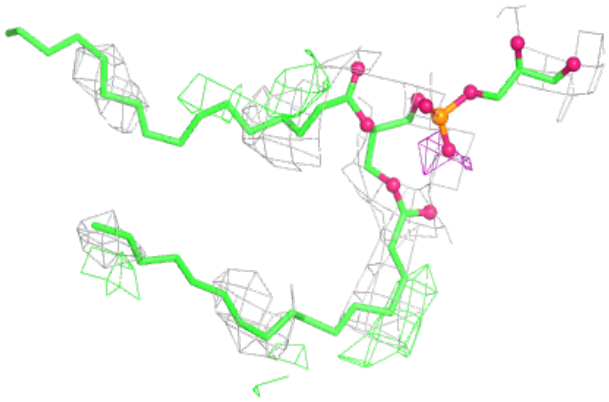


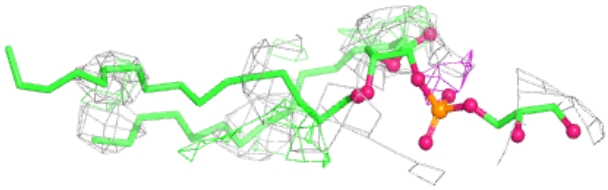




Electron density around LHG p 302:

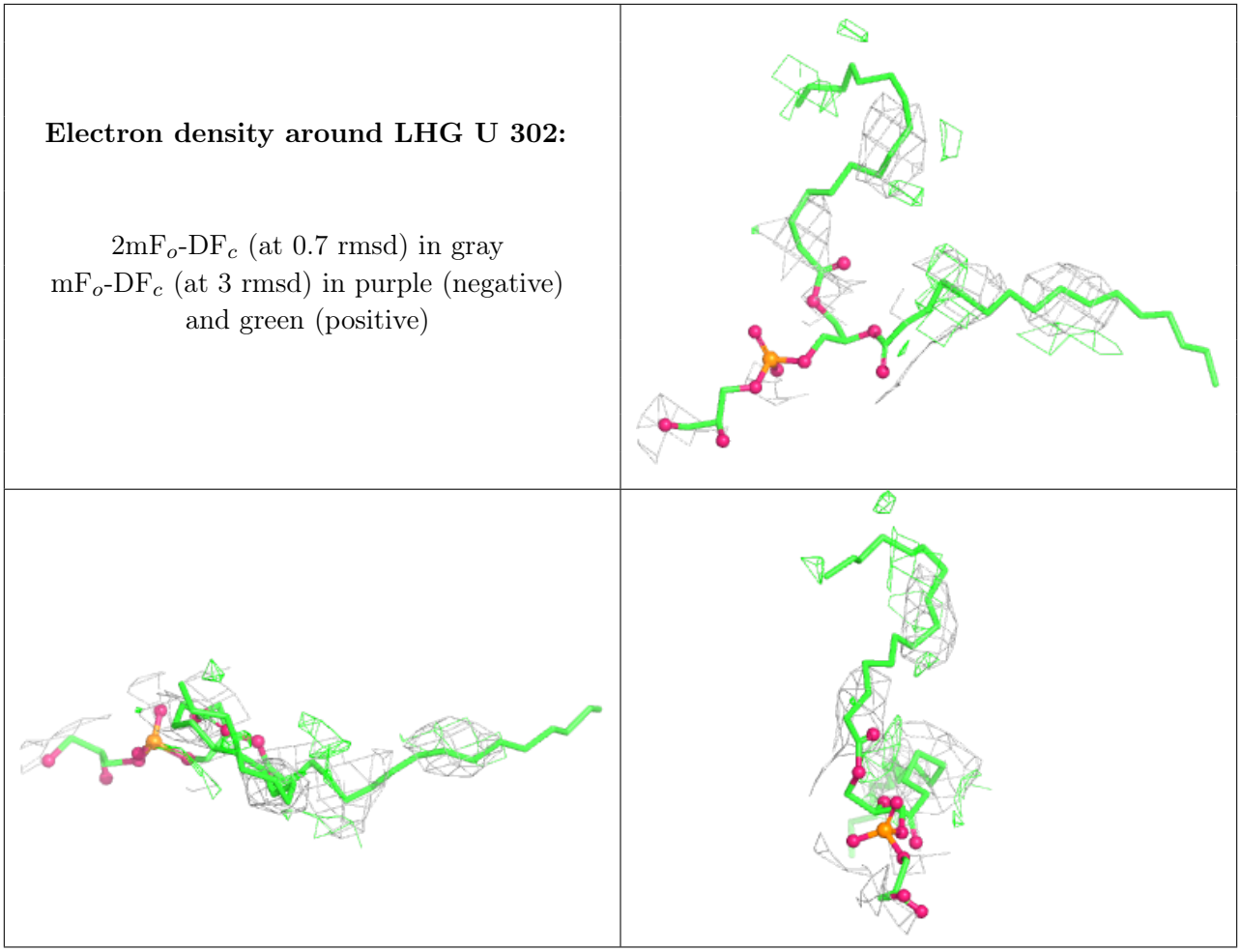
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





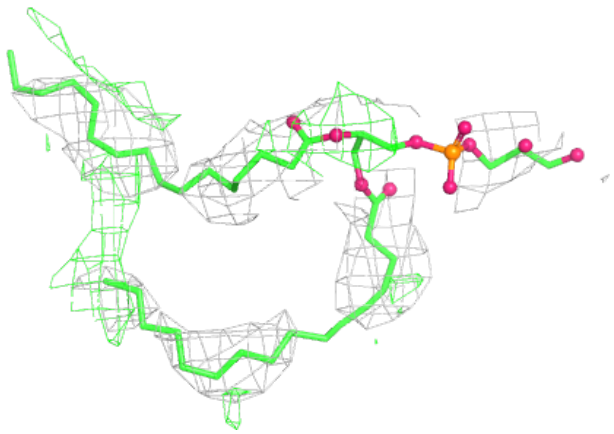
Electron density around LHG U 302:

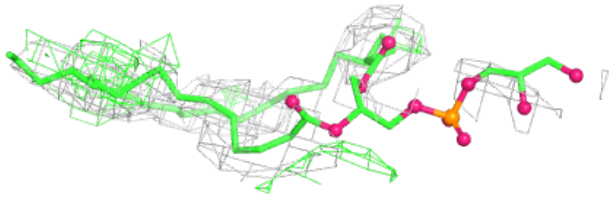
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around LHG X 303:

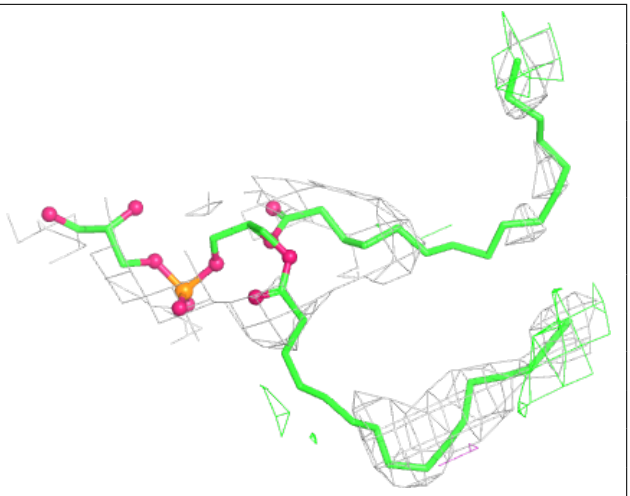
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

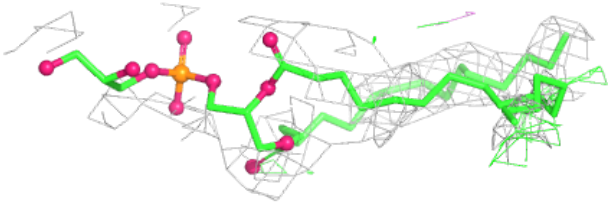


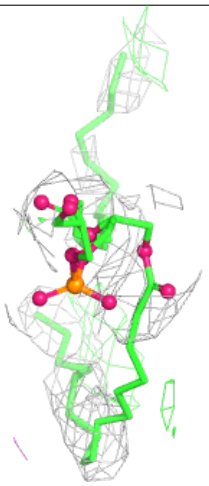


Electron density around LHG i 302:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

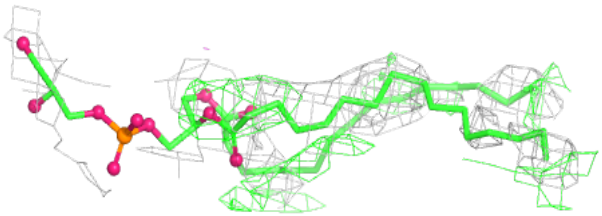






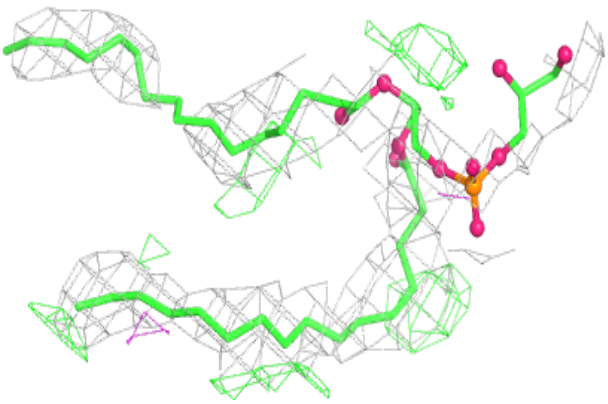
Electron density around LHG A 301:

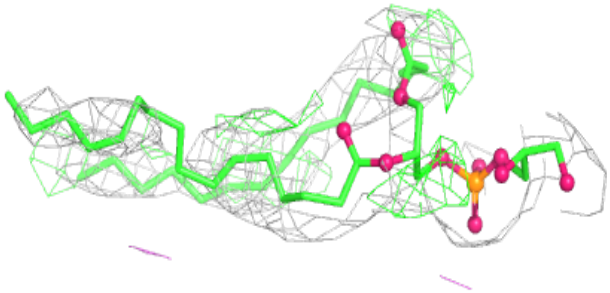
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

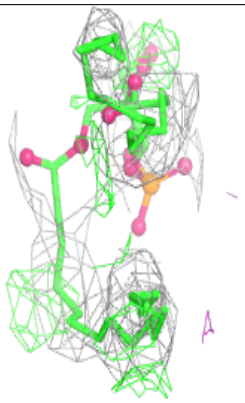


Electron density around LHG f 302:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

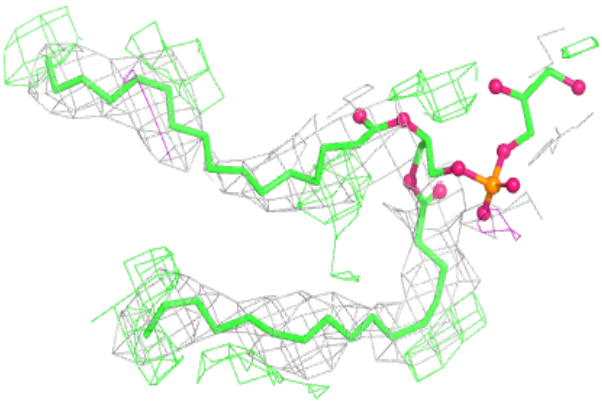


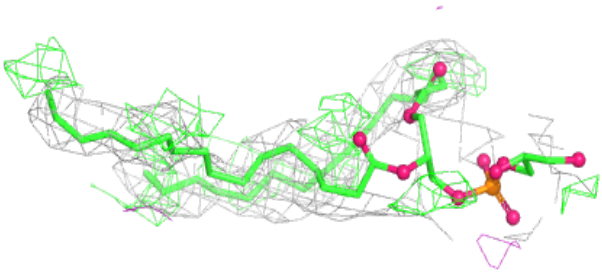




Electron density around LHG H 303:

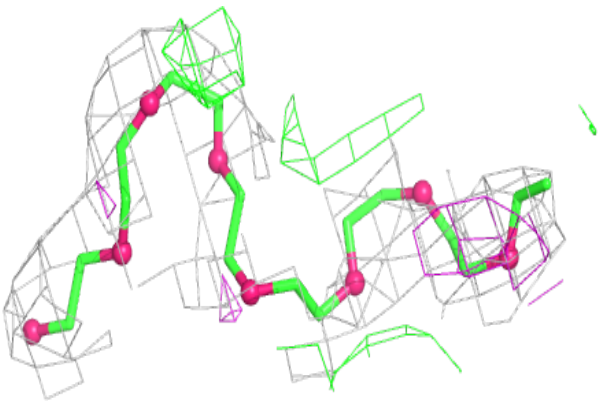
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

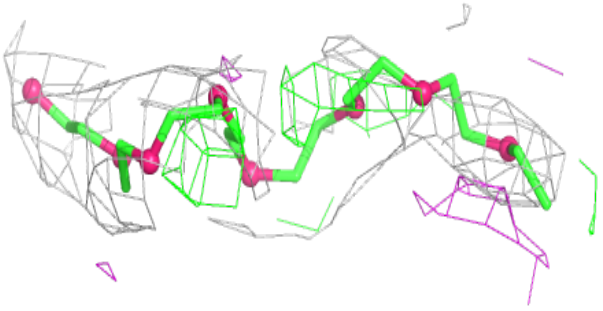


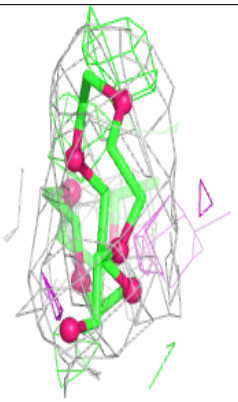


Electron density around PE4 H 305:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

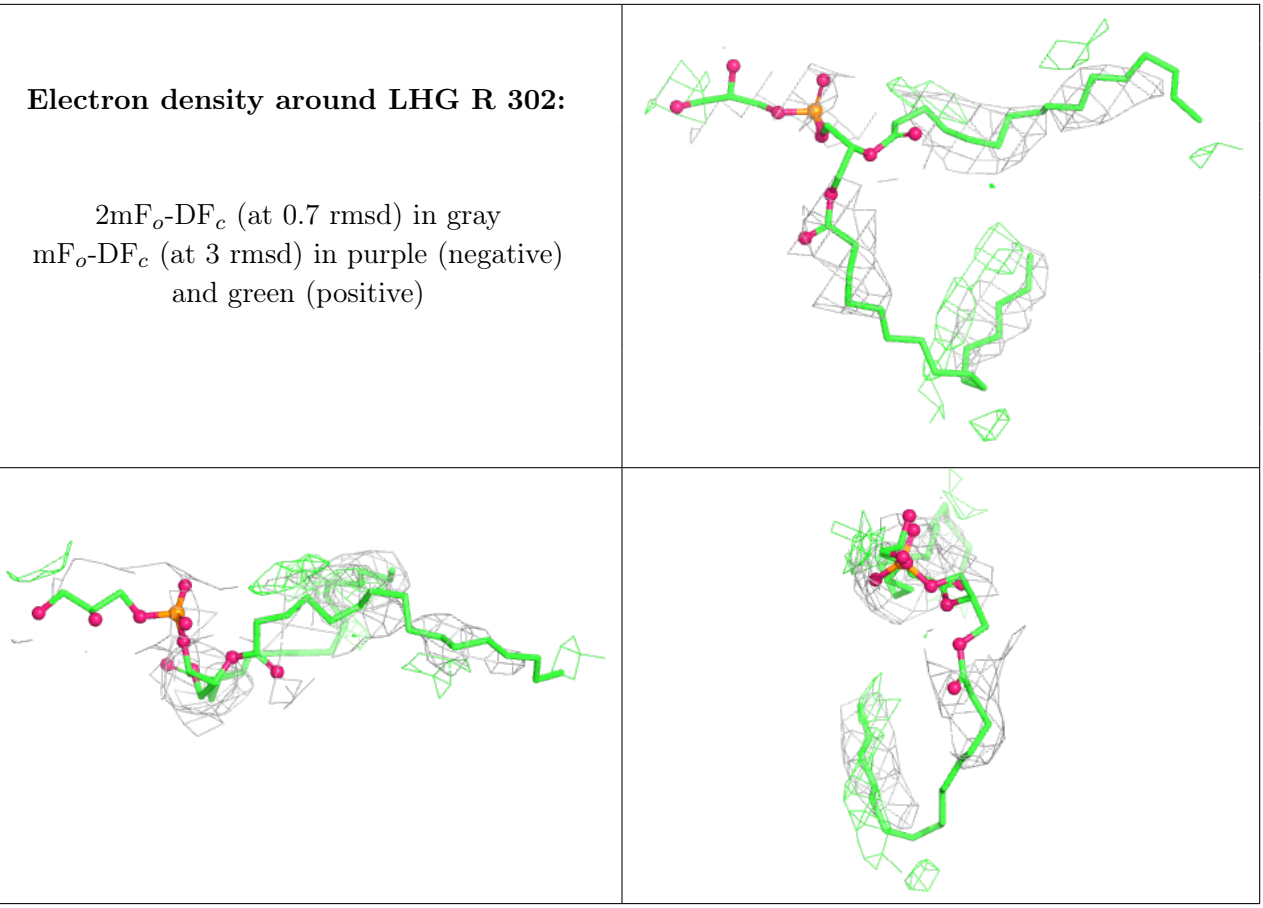






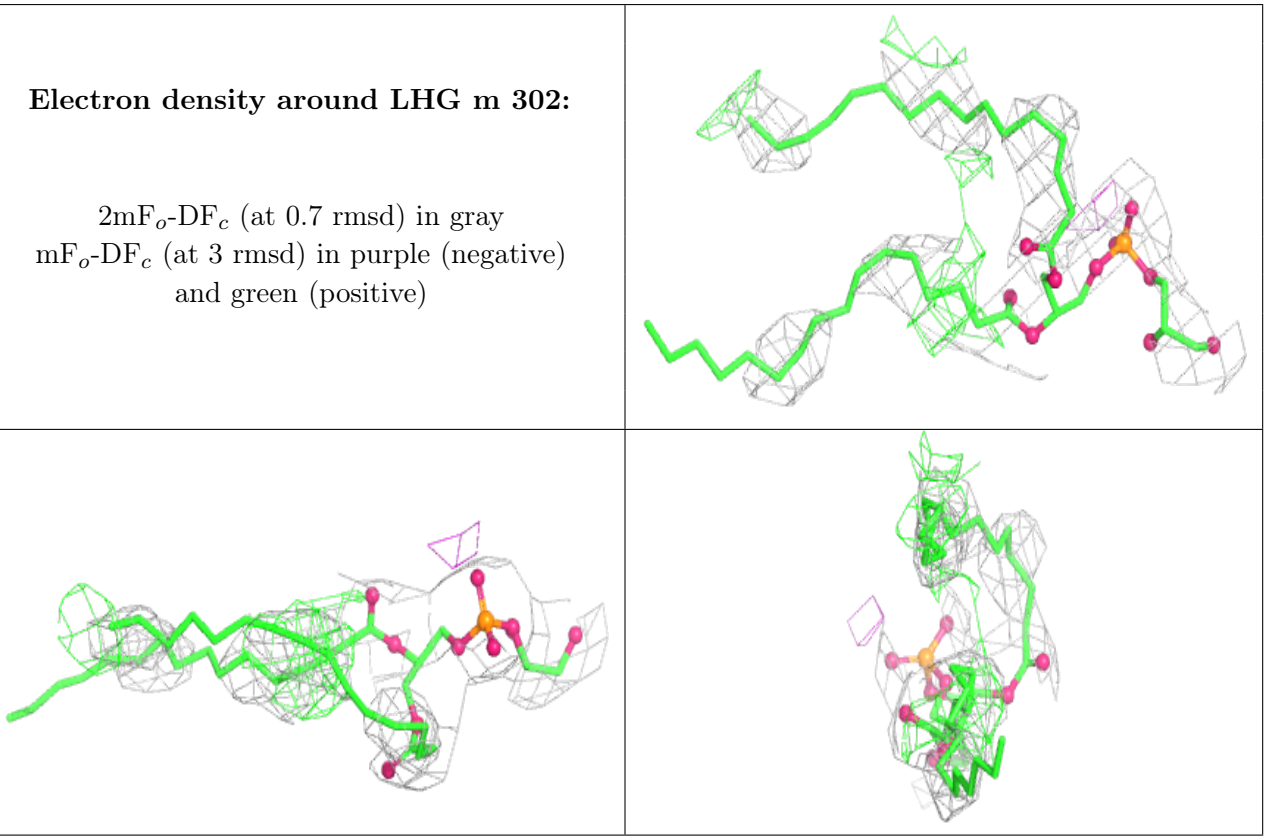
Electron density around LHG R 302:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around LHG m 302:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.