Full wwPDB X-ray Structure Validation Report ⓘ

Aug 28, 2023 – 02:49 PM JST

PDB ID	:	7VSO
Title	:	Serial Femtosecond Crystallography (SFX) of Ground State Bacteriorhodopsin Crystallized from Bicelles in Complex with HAD16 Determined Using 7-keV X-ray Free Electron Laser (XFEL) at SACLA
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Deposited on	:	2021-10-27
Resolution	:	2.35 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp
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:

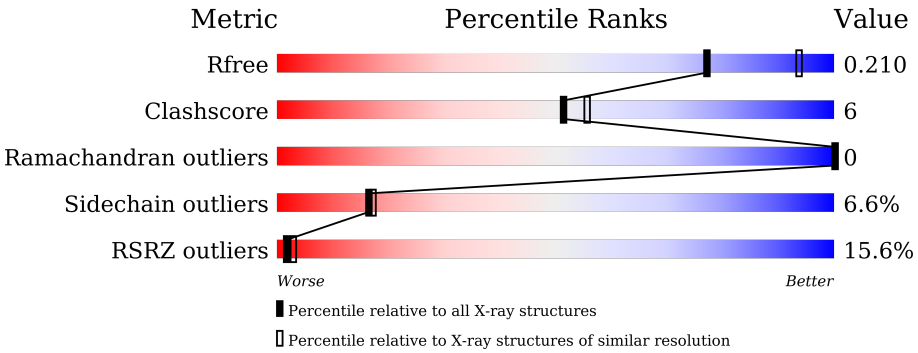
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance

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

The reported resolution of this entry is 2.35 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	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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	249	14% 78% 10% • 10%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	D10	A	312[B]	-	-	-	X
6	OCT	A	320	-	-	-	X
7	HP6	A	311	-	-	-	X
7	HP6	A	313	-	-	-	X
8	D12	A	307	-	-	-	X
8	D12	A	316	-	-	-	X
9	R16	A	318	-	-	-	X

2 Entry composition

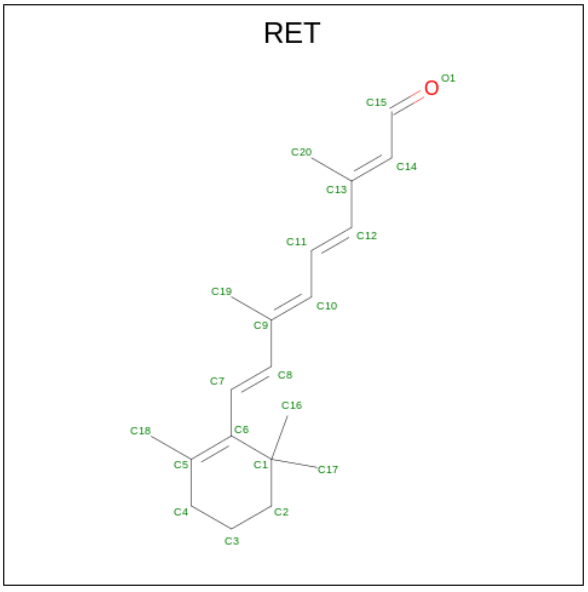
There are 12 unique types of molecules in this entry. The entry contains 2067 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Bacteriorhodopsin.

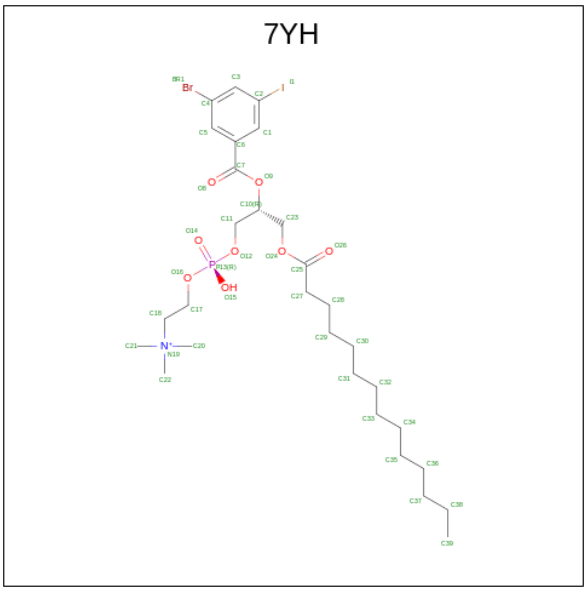
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	224	Total	C	N	O	S	0	0	0
			1741	1172	265	295	9			

- Molecule 2 is RETINAL (three-letter code: RET) (formula: $C_{20}H_{28}O$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	C	0	0
			20	20		

- Molecule 3 is 2-[[(2R)-2-(3-bromanyl-5-iodanyl-phenyl)carbonyloxy-3-tetradecanoyloxy-propoxy]-oxidanyl-phosphoryl]oxyethyl-trimethyl-azanium (three-letter code: 7YH) (formula: $C_{29}H_{49}BrINO_8P$) (labeled as "Ligand of Interest" by depositor).

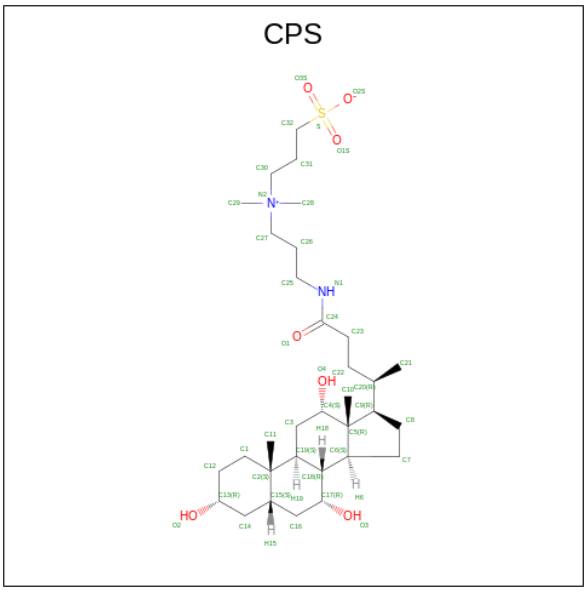


Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
3	A	1	Total	Br	C	I	N	O	P	0	1
			82	2	58	2	2	16	2		

- Molecule 4 is IODIDE ION (three-letter code: IOD) (formula: I) (labeled as "Ligand of Interest" by depositor).

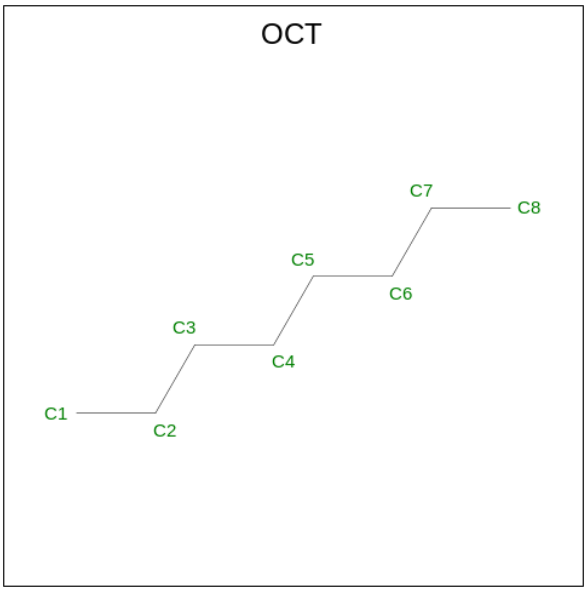
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	I	0	0
			1	1		

- Molecule 5 is 3-[(3-CHOLAMIDOPROPYL)DIMETHYLAMMONIO]-1-PROPANESULFONATE (three-letter code: CPS) (formula: $C_{32}H_{58}N_2O_7S$) (labeled as "Ligand of Interest" by depositor).



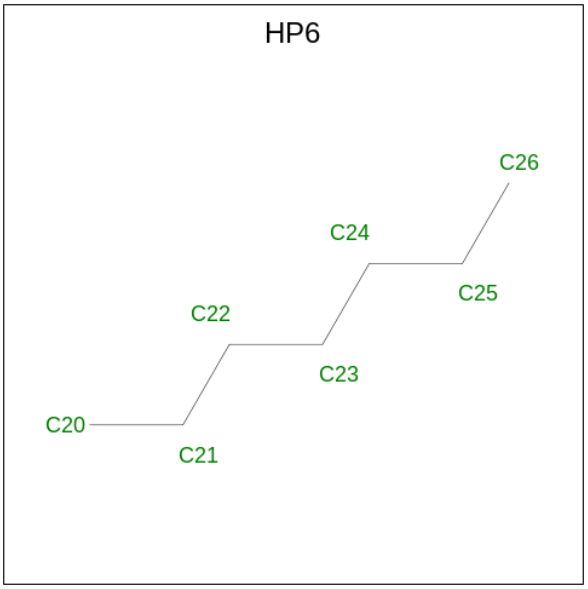
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 27 24 3	0	0

- Molecule 6 is N-OCTANE (three-letter code: OCT) (formula: C_8H_{18}) (labeled as "Ligand of Interest" by depositor).



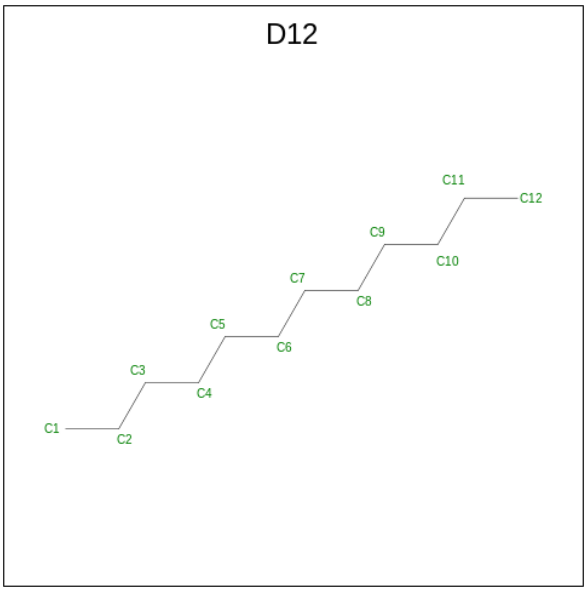
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C 8 8	0	0
6	A	1	Total C 8 8	0	0

- Molecule 7 is HEPTANE (three-letter code: HP6) (formula: C_7H_{16}) (labeled as "Ligand of Interest" by depositor).



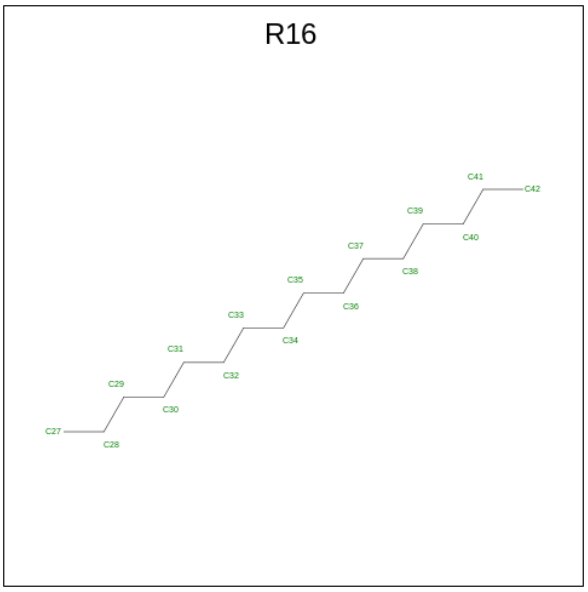
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C 7 7	0	0
7	A	1	Total C 7 7	0	0
7	A	1	Total C 7 7	0	0
7	A	1	Total C 7 7	0	1
7	A	1	Total C 7 7	0	0

- Molecule 8 is DODECANE (three-letter code: D12) (formula: $C_{12}H_{26}$) (labeled as "Ligand of Interest" by depositor).



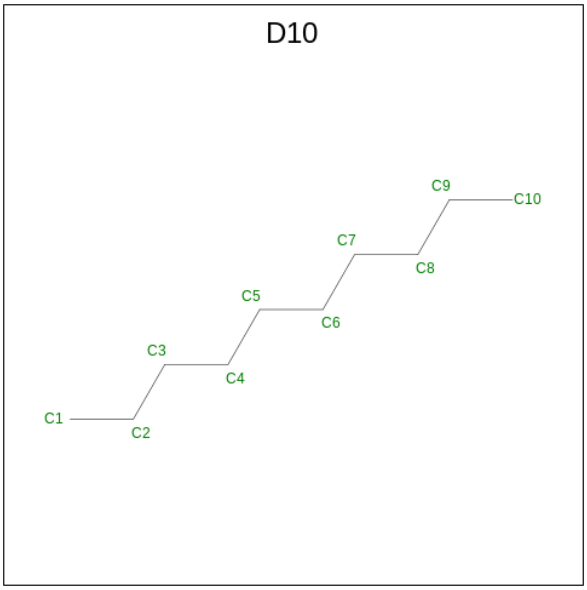
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C 12 12	0	0
8	A	1	Total C 12 12	0	0
8	A	1	Total C 12 12	0	0

- Molecule 9 is HEXADECANE (three-letter code: R16) (formula: $C_{16}H_{34}$) (labeled as "Ligand of Interest" by depositor).



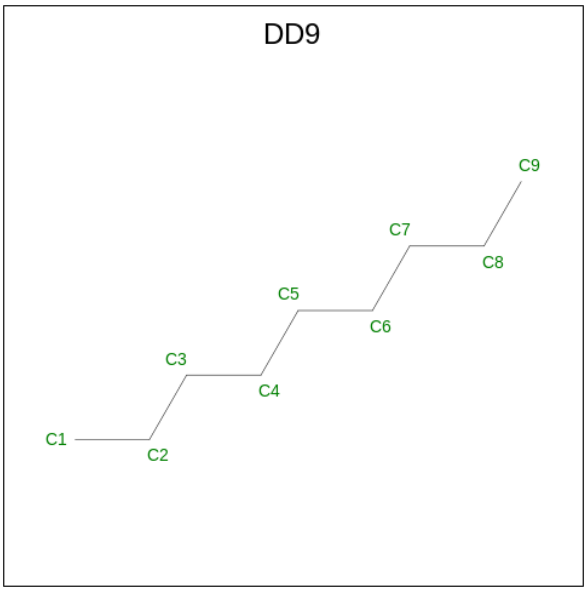
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total C 16 16	0	0
9	A	1	Total C 16 16	0	0
9	A	1	Total C 16 16	0	0

- Molecule 10 is DECANE (three-letter code: D10) (formula: $C_{10}H_{22}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	1	Total C 10 10	0	0
10	A	1	Total C 10 10	0	1

- Molecule 11 is nonane (three-letter code: DD9) (formula: C_9H_{20}) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	1	Total C 9 9	0	0

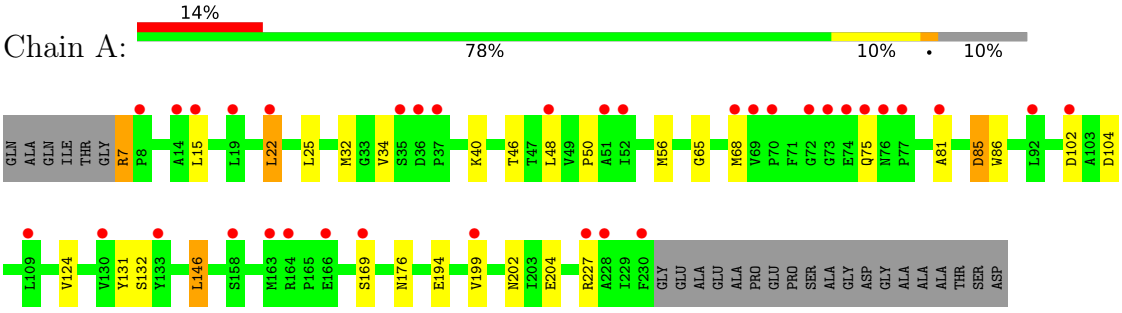
- Molecule 12 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	32	Total O 32 32	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: Bacteriorhodopsin



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	46.20Å 103.00Å 128.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.90 – 2.35 42.15 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.9 (42.90-2.35) 100.0 (42.15-2.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.18 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.8.0131	Depositor
R, R_{free}	0.158 , 0.210 0.158 , 0.210	Depositor DCC
R_{free} test set	650 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å^2)	65.5	Xtriage
Anisotropy	0.102	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 99.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	2067	wwPDB-VP
Average B, all atoms (Å^2)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.88% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HP6, OCT, RET, D10, IOD, R16, CPS, 7YH, DD9, D12

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	0.81	0/1789	0.85	6/2444 (0.2%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	85	ASP	CB-CG-OD1	7.53	125.08	118.30
1	A	32	MET	CG-SD-CE	-5.63	91.19	100.20
1	A	7	ARG	NE-CZ-NH1	5.47	123.04	120.30
1	A	7	ARG	NE-CZ-NH2	-5.35	117.62	120.30
1	A	146	LEU	CB-CG-CD1	5.24	119.91	111.00
1	A	22	LEU	CA-CB-CG	5.23	127.33	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1741	0	1800	11	0
2	A	20	0	27	5	0
3	A	82	0	0	3	0
4	A	1	0	0	0	0
5	A	27	0	39	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	16	0	36	1	0
7	A	35	0	80	5	0
8	A	36	0	78	2	0
9	A	48	0	102	5	0
10	A	20	0	44	0	0
11	A	9	0	20	0	0
12	A	32	0	0	1	0
All	All	2067	0	2226	24	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (24) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:301:RET:H8	2:A:301:RET:H161	1.50	0.93
3:A:302[B]:7YH:C28	3:A:302[B]:7YH:C23	2.53	0.87
8:A:307:D12:H52	8:A:307:D12:H13	1.75	0.68
3:A:302[A]:7YH:C27	7:A:314[A]:HP6:H201	2.26	0.66
7:A:306:HP6:H232	9:A:308:R16:C28	2.28	0.63
5:A:304:CPS:H21A	5:A:304:CPS:H10B	1.84	0.59
1:A:56:MET:HG3	1:A:85:ASP:HB2	1.86	0.57
7:A:306:HP6:H232	9:A:308:R16:H281	1.87	0.57
1:A:68:MET:HB3	1:A:75:GLN:HG3	1.86	0.56
7:A:306:HP6:H232	9:A:308:R16:H282	1.88	0.56
1:A:65:GLY:HA3	1:A:81:ALA:HB2	1.90	0.53
1:A:86:TRP:CD1	2:A:301:RET:H14	2.44	0.53
1:A:199:VAL:HG22	8:A:317:D12:H82	1.93	0.51
3:A:302[A]:7YH:C27	7:A:314[A]:HP6:C20	2.90	0.50
1:A:46:THR:O	1:A:50:PRO:HD2	2.13	0.49
2:A:301:RET:H8	2:A:301:RET:C16	2.32	0.48
1:A:176:ASN:HD22	9:A:308:R16:H312	1.78	0.48
2:A:301:RET:H161	2:A:301:RET:C8	2.34	0.47
1:A:7:ARG:HG2	12:A:416:HOH:O	2.16	0.45
9:A:308:R16:H291	9:A:308:R16:H322	1.70	0.44
1:A:34:VAL:O	1:A:40:LYS:HE3	2.17	0.44
1:A:194:GLU:OE1	1:A:204:GLU:OE2	2.36	0.43
2:A:301:RET:H7	2:A:301:RET:H181	1.72	0.43
1:A:124:VAL:HG21	6:A:320:OCT:H32	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	222/249 (89%)	220 (99%)	2 (1%)	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 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	181/195 (93%)	169 (93%)	12 (7%)	16 17

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	LEU
1	A	22	LEU
1	A	25	LEU
1	A	48	LEU
1	A	102	ASP
1	A	104	ASP
1	A	131	TYR
1	A	132	SER
1	A	146	LEU
1	A	169	SER
1	A	202	ASN
1	A	227	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	202	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 21 ligands modelled in this entry, 1 is monoatomic - leaving 20 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	$\#\|Z\| > 2$
7	HP6	A	306	-	6,6,6	0.36	0	5,5,5	0.34	0
6	OCT	A	320	-	7,7,7	0.52	0	6,6,6	0.24	0
9	R16	A	308	-	15,15,15	0.33	0	14,14,14	0.54	0
9	R16	A	318	-	15,15,15	0.42	0	14,14,14	0.61	0
7	HP6	A	319	-	6,6,6	0.39	0	5,5,5	0.22	0
10	D10	A	309	-	9,9,9	0.34	0	8,8,8	0.40	0
3	7YH	A	302[A]	-	41,41,41	1.35	2 (4%)	50,53,53	1.35	8 (16%)
7	HP6	A	311	-	6,6,6	0.38	0	5,5,5	0.26	0
7	HP6	A	314[A]	-	6,6,6	0.62	0	5,5,5	0.37	0
7	HP6	A	313	-	6,6,6	0.33	0	5,5,5	0.36	0
8	D12	A	307	-	11,11,11	0.37	0	10,10,10	0.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
11	DD9	A	315	-	8,8,8	0.39	0	7,7,7	0.39	0
8	D12	A	316	-	11,11,11	0.45	0	10,10,10	0.43	0
6	OCT	A	305	-	7,7,7	0.43	0	6,6,6	0.20	0
3	7YH	A	302[B]	-	41,41,41	1.31	2 (4%)	50,53,53	1.06	6 (12%)
2	RET	A	301	-	20,20,21	1.54	2 (10%)	27,27,28	1.56	6 (22%)
10	D10	A	312[B]	-	9,9,9	0.46	0	8,8,8	0.38	0
8	D12	A	317	-	11,11,11	0.44	0	10,10,10	0.75	0
9	R16	A	310	-	15,15,15	0.24	0	14,14,14	1.08	1 (7%)
5	CPS	A	304	-	30,30,45	0.60	0	47,48,70	1.31	5 (10%)

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
7	HP6	A	306	-	-	1/4/4/4	-
6	OCT	A	320	-	-	2/5/5/5	-
9	R16	A	308	-	-	9/13/13/13	-
9	R16	A	318	-	-	5/13/13/13	-
7	HP6	A	319	-	-	1/4/4/4	-
10	D10	A	309	-	-	3/7/7/7	-
3	7YH	A	302[A]	-	-	21/40/40/40	0/1/1/1
7	HP6	A	311	-	-	0/4/4/4	-
7	HP6	A	314[A]	-	-	1/4/4/4	-
7	HP6	A	313	-	-	3/4/4/4	-
8	D12	A	307	-	-	6/9/9/9	-
11	DD9	A	315	-	-	2/6/6/6	-
8	D12	A	316	-	-	6/9/9/9	-
6	OCT	A	305	-	-	5/5/5/5	-
3	7YH	A	302[B]	-	-	22/40/40/40	0/1/1/1
2	RET	A	301	-	-	0/13/30/31	0/1/1/1
10	D10	A	312[B]	-	-	4/7/7/7	-
8	D12	A	317	-	-	6/9/9/9	-
9	R16	A	310	-	-	5/13/13/13	-
5	CPS	A	304	-	-	1/7/72/90	0/4/4/4

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	302[B]	7YH	O9-C7	5.74	1.46	1.34
3	A	302[A]	7YH	O9-C7	5.51	1.45	1.34
2	A	301	RET	C15-C14	-4.63	1.32	1.49
3	A	302[B]	7YH	O24-C25	4.51	1.46	1.33
3	A	302[A]	7YH	O24-C25	4.43	1.46	1.33
2	A	301	RET	C14-C13	-3.83	1.30	1.33

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	304	CPS	C16-C17-C18	4.27	116.04	111.48
3	A	302[A]	7YH	O9-C7-C6	3.70	117.90	111.92
2	A	301	RET	C10-C11-C12	-3.65	111.83	123.22
3	A	302[A]	7YH	C23-C10-C11	-3.46	103.61	111.79
5	A	304	CPS	C7-C6-C5	3.39	106.88	103.55
2	A	301	RET	C7-C8-C9	-3.04	121.65	126.23
3	A	302[B]	7YH	BR1-C4-C5	2.79	123.15	119.27
3	A	302[B]	7YH	C1-C6-C7	-2.74	114.78	120.10
9	A	310	R16	C38-C37-C36	-2.72	100.63	114.42
3	A	302[A]	7YH	C10-O9-C7	-2.71	112.89	117.56
3	A	302[A]	7YH	O24-C25-C27	2.67	120.29	111.91
2	A	301	RET	C8-C9-C10	-2.61	114.94	118.94
5	A	304	CPS	C8-C9-C5	2.52	106.03	103.55
2	A	301	RET	C18-C5-C6	-2.43	121.80	124.53
3	A	302[B]	7YH	BR1-C4-C3	-2.39	115.95	119.27
2	A	301	RET	C11-C10-C9	-2.37	123.92	127.31
3	A	302[A]	7YH	C1-C2-I1	2.34	122.36	119.37
3	A	302[B]	7YH	C23-C10-C11	-2.27	106.43	111.79
3	A	302[A]	7YH	C5-C6-C7	-2.25	115.72	120.10
3	A	302[B]	7YH	O9-C7-C6	2.24	115.53	111.92
3	A	302[B]	7YH	C17-C18-N19	-2.19	108.45	115.78
3	A	302[A]	7YH	C17-C18-N19	-2.11	108.74	115.78
5	A	304	CPS	C15-C14-C13	-2.10	109.68	112.76
2	A	301	RET	C7-C6-C5	-2.05	116.50	121.46
5	A	304	CPS	C1-C2-C15	2.05	110.79	107.77
3	A	302[A]	7YH	C32-C31-C30	-2.02	104.16	114.42

There are no chirality outliers.

All (103) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	302[A]	7YH	O16-C17-C18-N19

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Mol	Chain	Res	Type	Atoms
3	A	302[A]	7YH	O9-C10-C11-O12
3	A	302[B]	7YH	O9-C10-C11-O12
3	A	302[B]	7YH	C6-C7-O9-C10
3	A	302[B]	7YH	O26-C25-O24-C23
3	A	302[B]	7YH	C27-C25-O24-C23
3	A	302[B]	7YH	O8-C7-O9-C10
9	A	308	R16	C29-C30-C31-C32
3	A	302[A]	7YH	C11-O12-P13-O16
3	A	302[B]	7YH	C17-O16-P13-O12
3	A	302[B]	7YH	C11-O12-P13-O16
3	A	302[B]	7YH	C25-C27-C28-C29
3	A	302[A]	7YH	C31-C32-C33-C34
9	A	308	R16	C37-C38-C39-C40
9	A	318	R16	C29-C30-C31-C32
8	A	316	D12	C4-C5-C6-C7
9	A	318	R16	C32-C33-C34-C35
9	A	310	R16	C32-C33-C34-C35
3	A	302[A]	7YH	C28-C29-C30-C31
3	A	302[B]	7YH	C32-C33-C34-C35
8	A	307	D12	C4-C5-C6-C7
8	A	307	D12	C7-C8-C9-C10
9	A	308	R16	C30-C31-C32-C33
3	A	302[B]	7YH	C34-C35-C36-C37
6	A	305	OCT	C3-C4-C5-C6
8	A	317	D12	C2-C3-C4-C5
10	A	309	D10	C6-C7-C8-C9
8	A	316	D12	C11-C10-C9-C8
7	A	313	HP6	C21-C22-C23-C24
8	A	316	D12	C3-C4-C5-C6
9	A	308	R16	C31-C32-C33-C34
8	A	307	D12	C2-C3-C4-C5
9	A	308	R16	C34-C35-C36-C37
10	A	312[B]	D10	C2-C3-C4-C5
3	A	302[A]	7YH	C27-C28-C29-C30
5	A	304	CPS	C21-C20-C9-C5
8	A	316	D12	C6-C7-C8-C9
7	A	319	HP6	C22-C23-C24-C25
8	A	316	D12	C7-C8-C9-C10
6	A	305	OCT	C5-C6-C7-C8
9	A	310	R16	C34-C35-C36-C37
10	A	312[B]	D10	C4-C5-C6-C7
6	A	305	OCT	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
9	A	318	R16	C27-C28-C29-C30
10	A	309	D10	C7-C8-C9-C10
3	A	302[B]	7YH	C29-C30-C31-C32
10	A	312[B]	D10	C3-C4-C5-C6
9	A	318	R16	C31-C32-C33-C34
3	A	302[B]	7YH	C31-C32-C33-C34
6	A	320	OCT	C3-C4-C5-C6
3	A	302[A]	7YH	C23-C10-C11-O12
3	A	302[B]	7YH	C23-C10-C11-O12
10	A	309	D10	C3-C4-C5-C6
3	A	302[A]	7YH	C33-C34-C35-C36
7	A	313	HP6	C23-C24-C25-C26
9	A	310	R16	C27-C28-C29-C30
3	A	302[A]	7YH	O24-C25-C27-C28
9	A	308	R16	C38-C39-C40-C41
8	A	307	D12	C1-C2-C3-C4
3	A	302[A]	7YH	C35-C36-C37-C38
3	A	302[B]	7YH	C28-C29-C30-C31
8	A	317	D12	C6-C7-C8-C9
3	A	302[A]	7YH	C30-C31-C32-C33
9	A	318	R16	C37-C38-C39-C40
9	A	308	R16	C28-C29-C30-C31
3	A	302[B]	7YH	C35-C36-C37-C38
3	A	302[A]	7YH	C11-O12-P13-O14
3	A	302[A]	7YH	C11-O12-P13-O15
3	A	302[A]	7YH	C17-C18-N19-C22
3	A	302[A]	7YH	C17-C18-N19-C21
3	A	302[B]	7YH	C17-O16-P13-O15
3	A	302[B]	7YH	C11-O12-P13-O14
3	A	302[B]	7YH	C11-O12-P13-O15
10	A	312[B]	D10	C7-C8-C9-C10
11	A	315	DD9	C2-C3-C4-C5
3	A	302[B]	7YH	O16-C17-C18-N19
6	A	305	OCT	C1-C2-C3-C4
3	A	302[B]	7YH	C17-C18-N19-C22
8	A	317	D12	C11-C10-C9-C8
3	A	302[A]	7YH	C29-C30-C31-C32
7	A	306	HP6	C20-C21-C22-C23
8	A	307	D12	C11-C10-C9-C8
7	A	313	HP6	C20-C21-C22-C23
11	A	315	DD9	C1-C2-C3-C4
3	A	302[A]	7YH	C17-O16-P13-O12

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Mol	Chain	Res	Type	Atoms
6	A	320	OCT	C2-C3-C4-C5
8	A	317	D12	C5-C6-C7-C8
3	A	302[A]	7YH	C32-C33-C34-C35
3	A	302[A]	7YH	C17-C18-N19-C20
3	A	302[B]	7YH	C17-C18-N19-C21
9	A	310	R16	C37-C38-C39-C40
8	A	307	D12	C3-C4-C5-C6
8	A	317	D12	C4-C5-C6-C7
9	A	308	R16	C36-C37-C38-C39
6	A	305	OCT	C4-C5-C6-C7
8	A	317	D12	C1-C2-C3-C4
3	A	302[A]	7YH	O26-C25-C27-C28
9	A	308	R16	C35-C36-C37-C38
7	A	314[A]	HP6	C22-C23-C24-C25
9	A	310	R16	C31-C32-C33-C34
3	A	302[A]	7YH	C36-C37-C38-C39
3	A	302[B]	7YH	C17-C18-N19-C20
8	A	316	D12	C1-C2-C3-C4

There are no ring outliers.

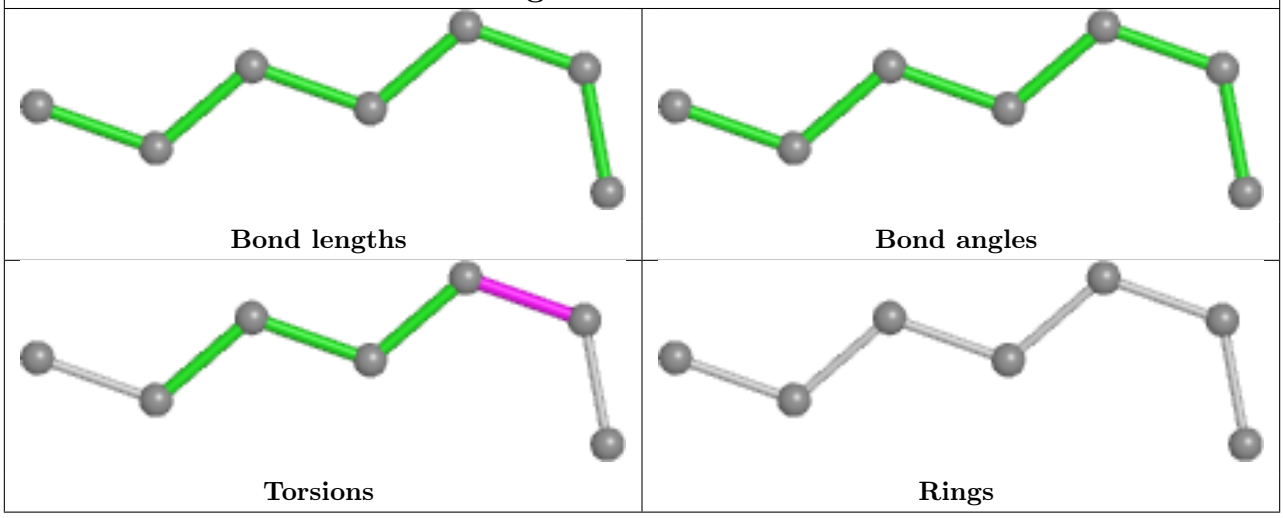
10 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	306	HP6	3	0
6	A	320	OCT	1	0
9	A	308	R16	5	0
3	A	302[A]	7YH	2	0
7	A	314[A]	HP6	2	0
8	A	307	D12	1	0
3	A	302[B]	7YH	1	0
2	A	301	RET	5	0
8	A	317	D12	1	0
5	A	304	CPS	1	0

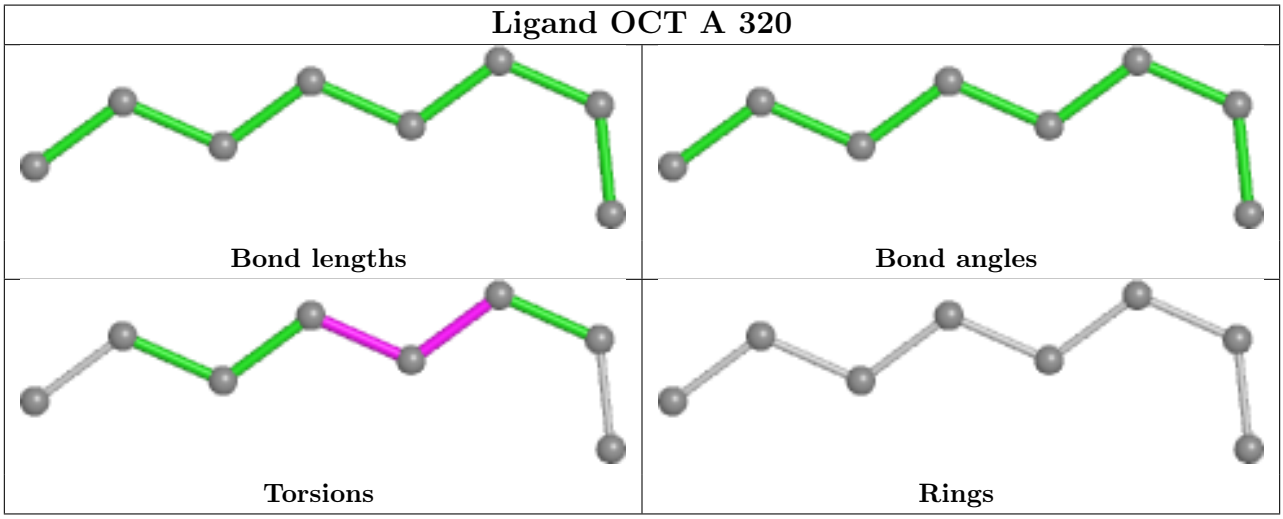
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

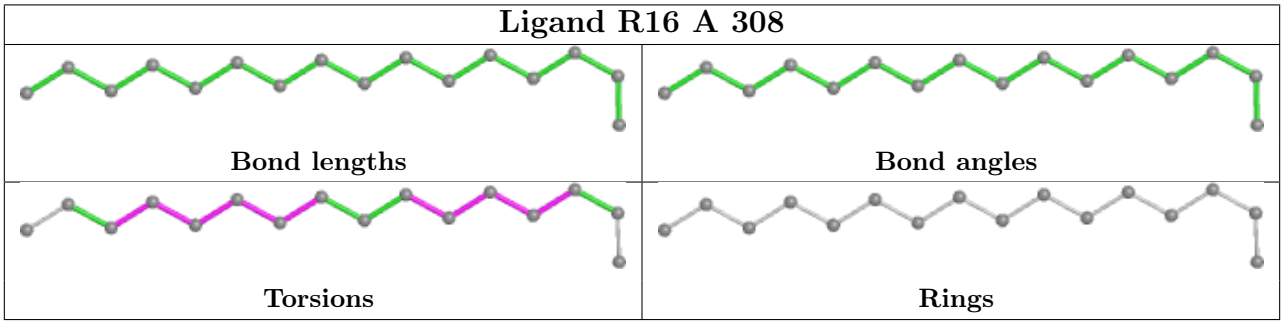
Ligand HP6 A 306



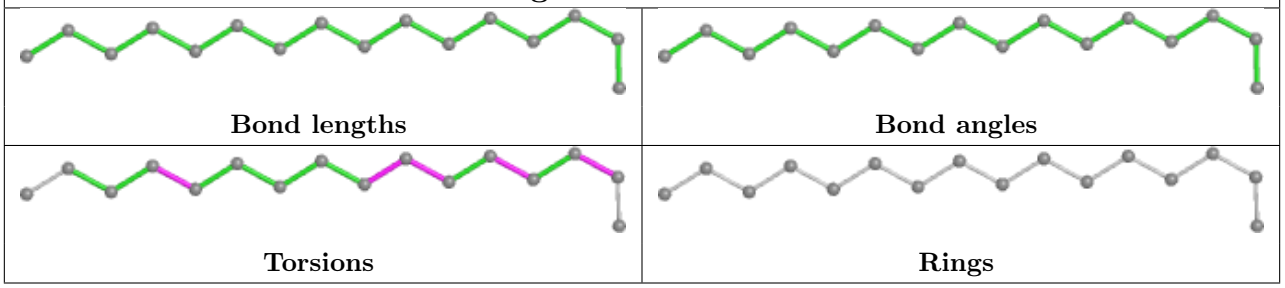
Ligand OCT A 320



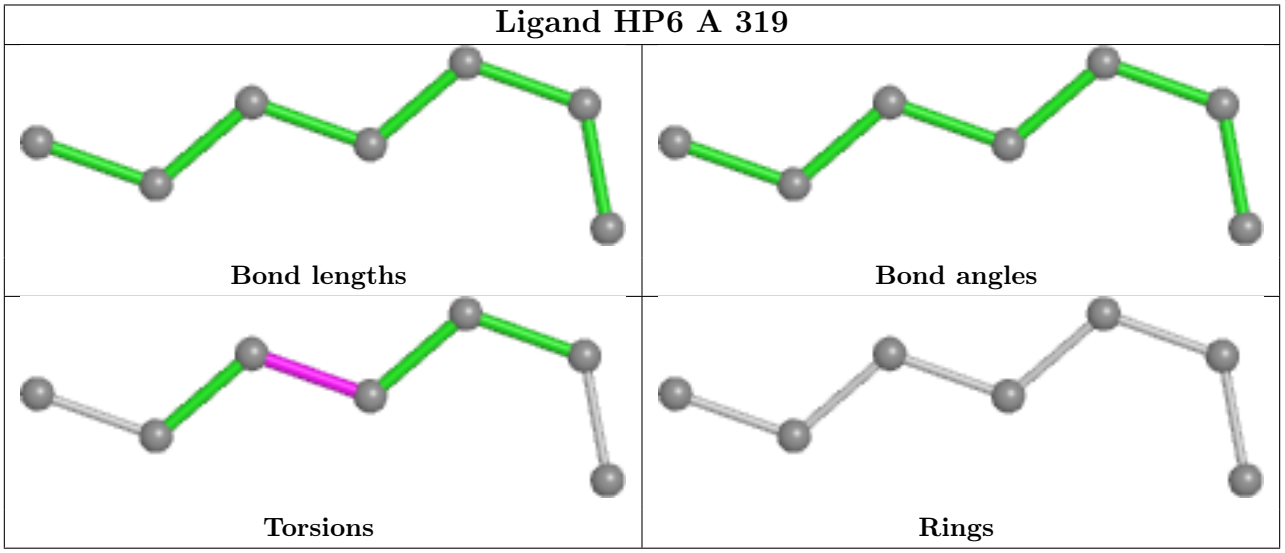
Ligand R16 A 308



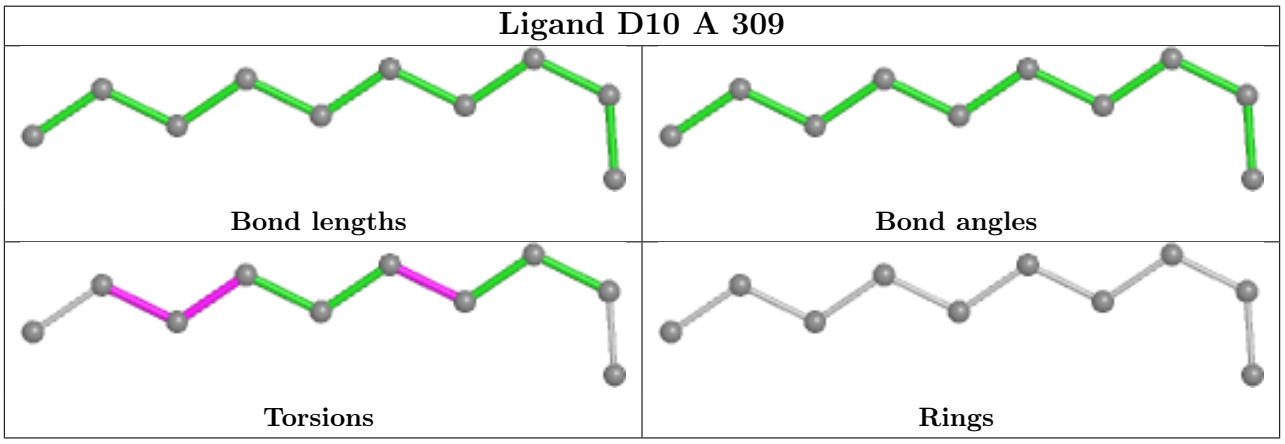
Ligand R16 A 318



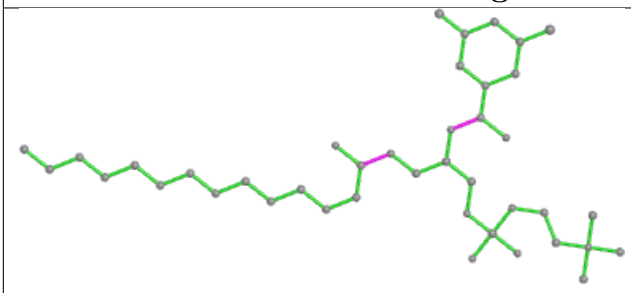
Ligand HP6 A 319



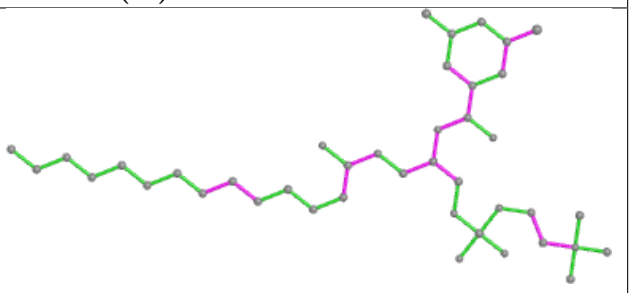
Ligand D10 A 309



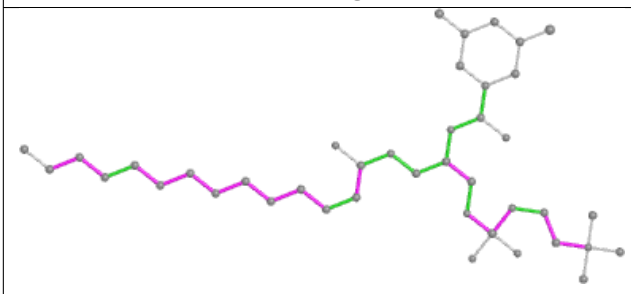
Ligand 7YH A 302 (A)



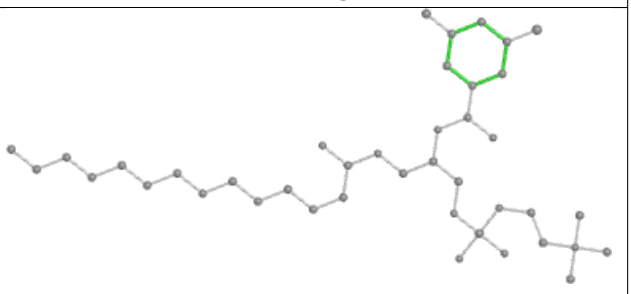
Bond lengths



Bond angles

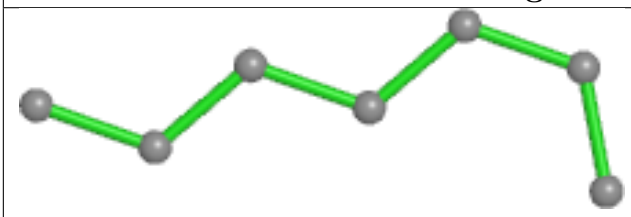


Torsions

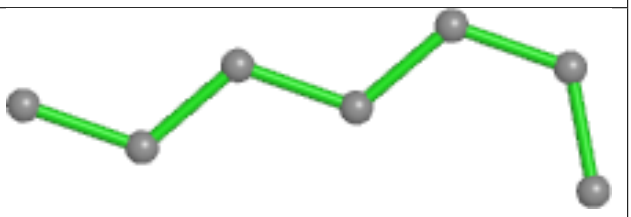


Rings

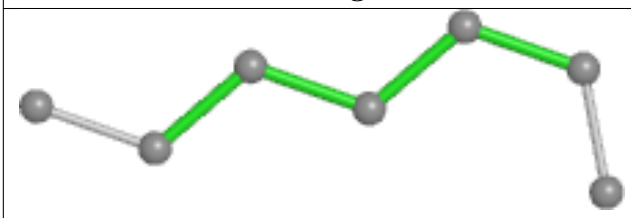
Ligand HP6 A 311



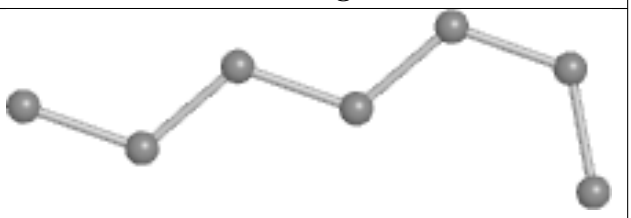
Bond lengths



Bond angles

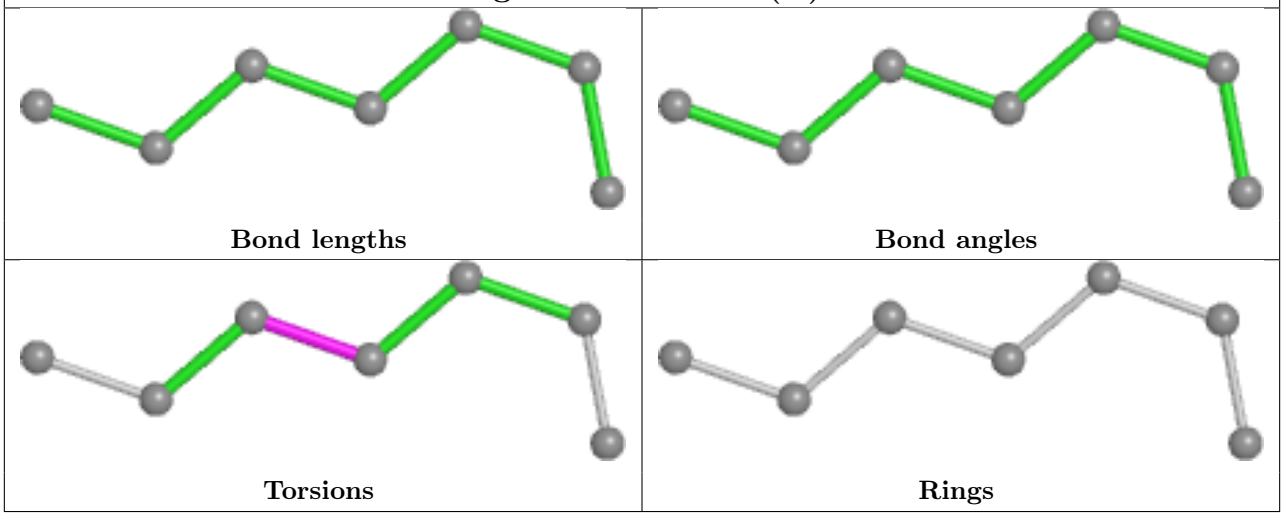


Torsions

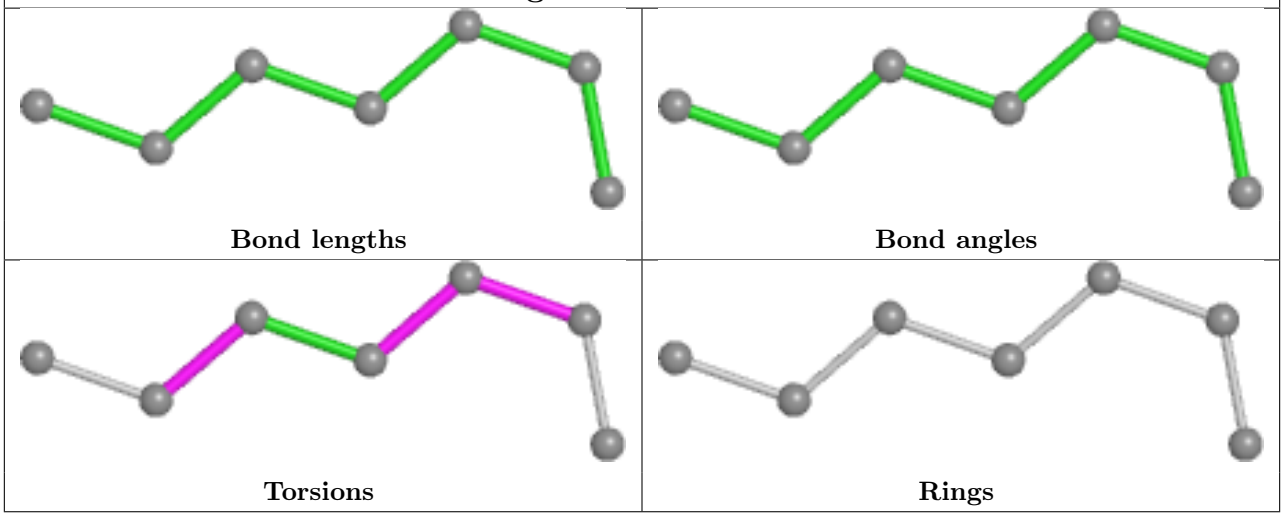


Rings

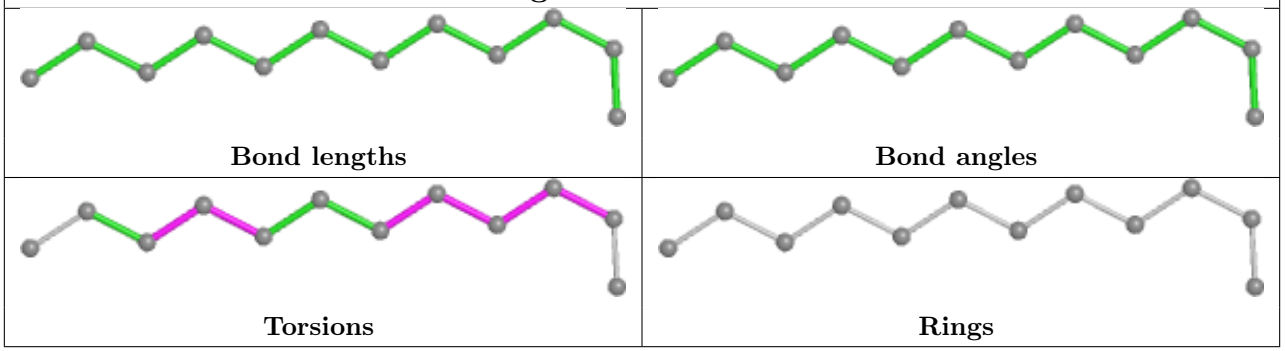
Ligand HP6 A 314 (A)



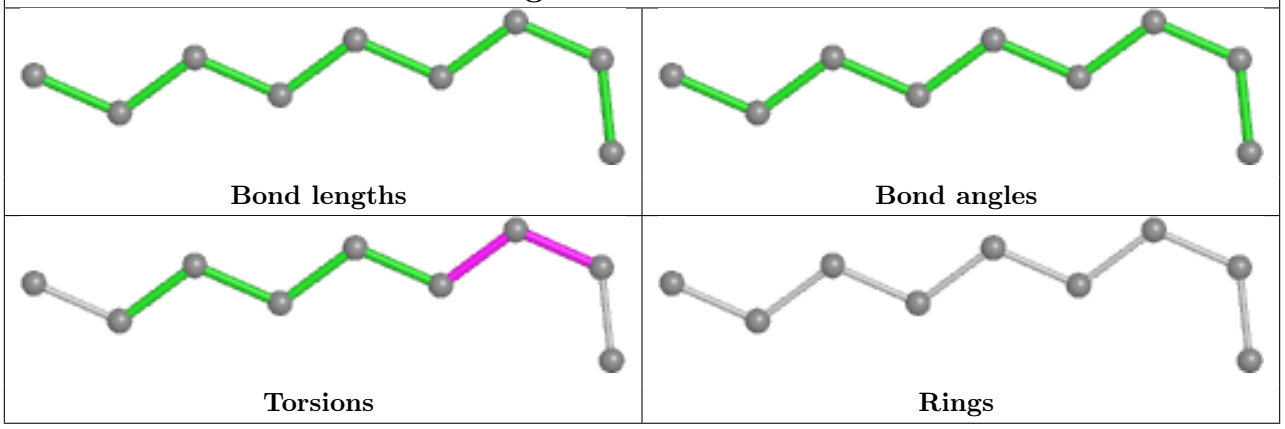
Ligand HP6 A 313



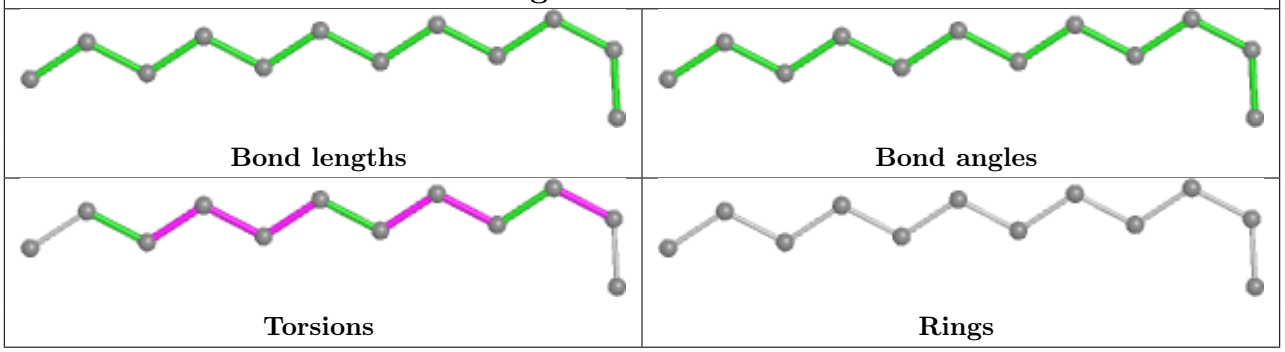
Ligand D12 A 307



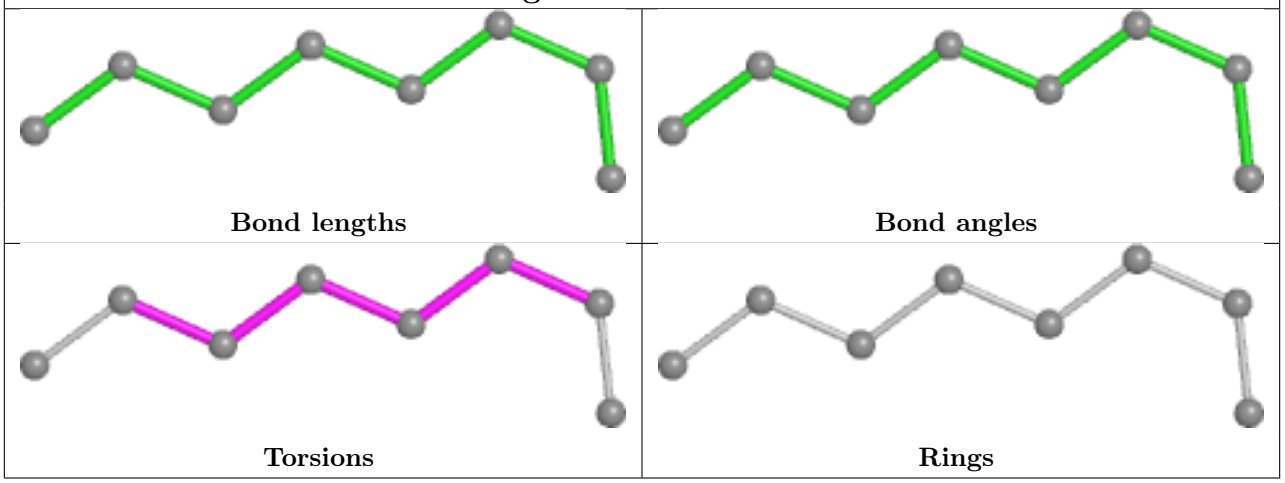
Ligand DD9 A 315



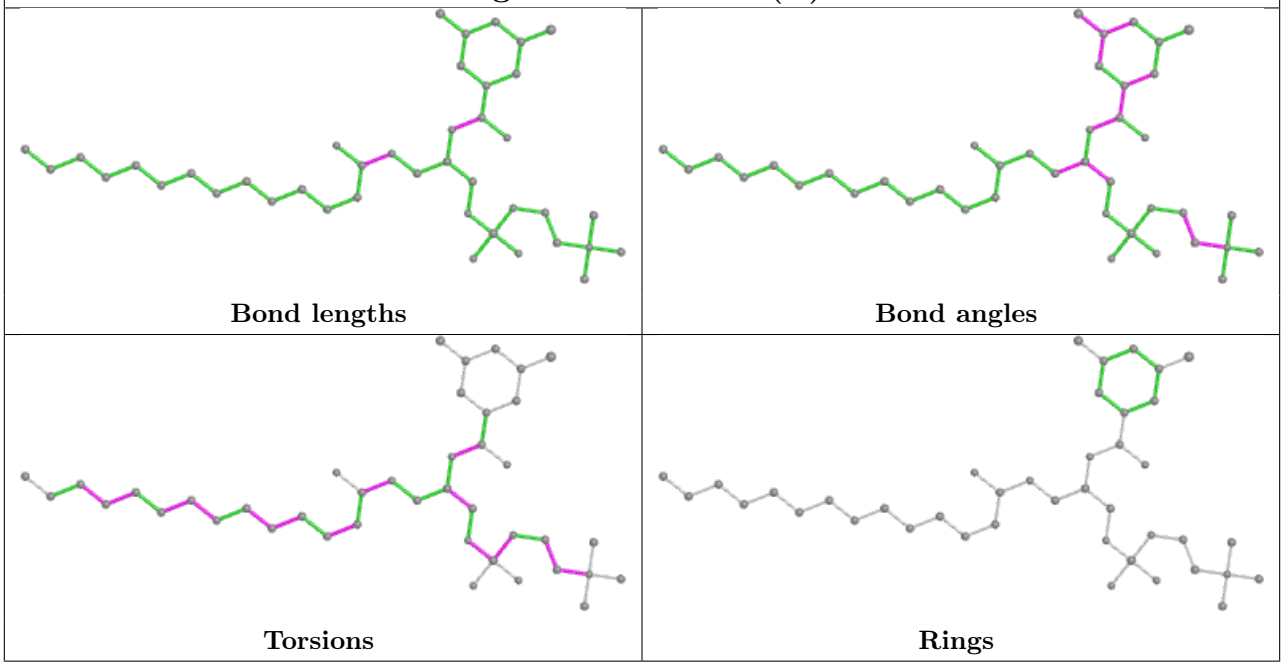
Ligand D12 A 316



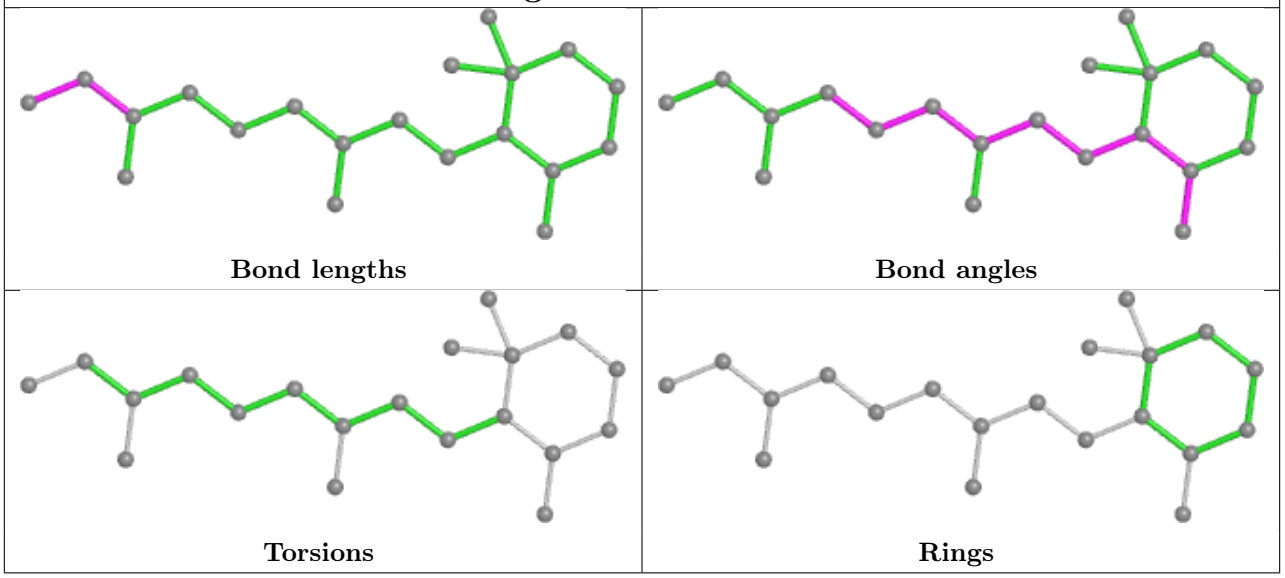
Ligand OCT A 305



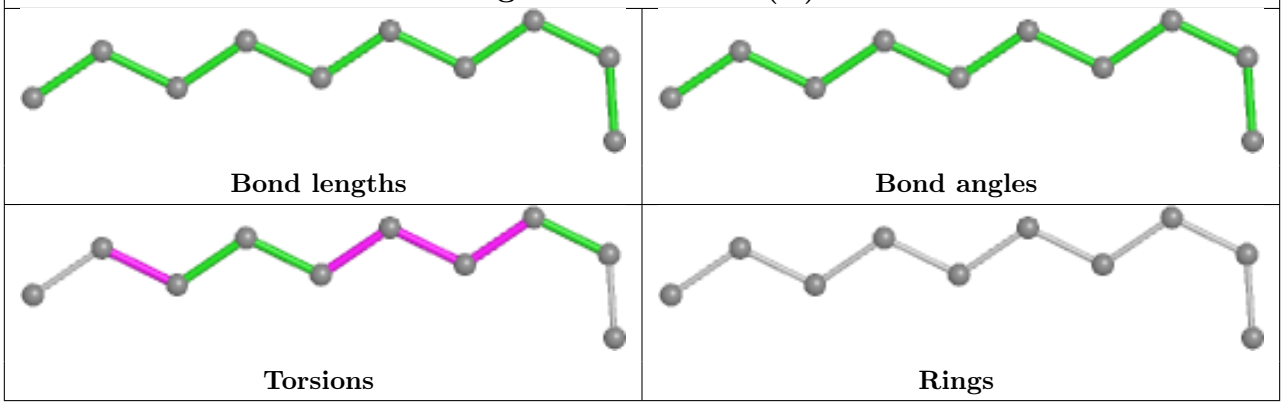
Ligand 7YH A 302 (B)

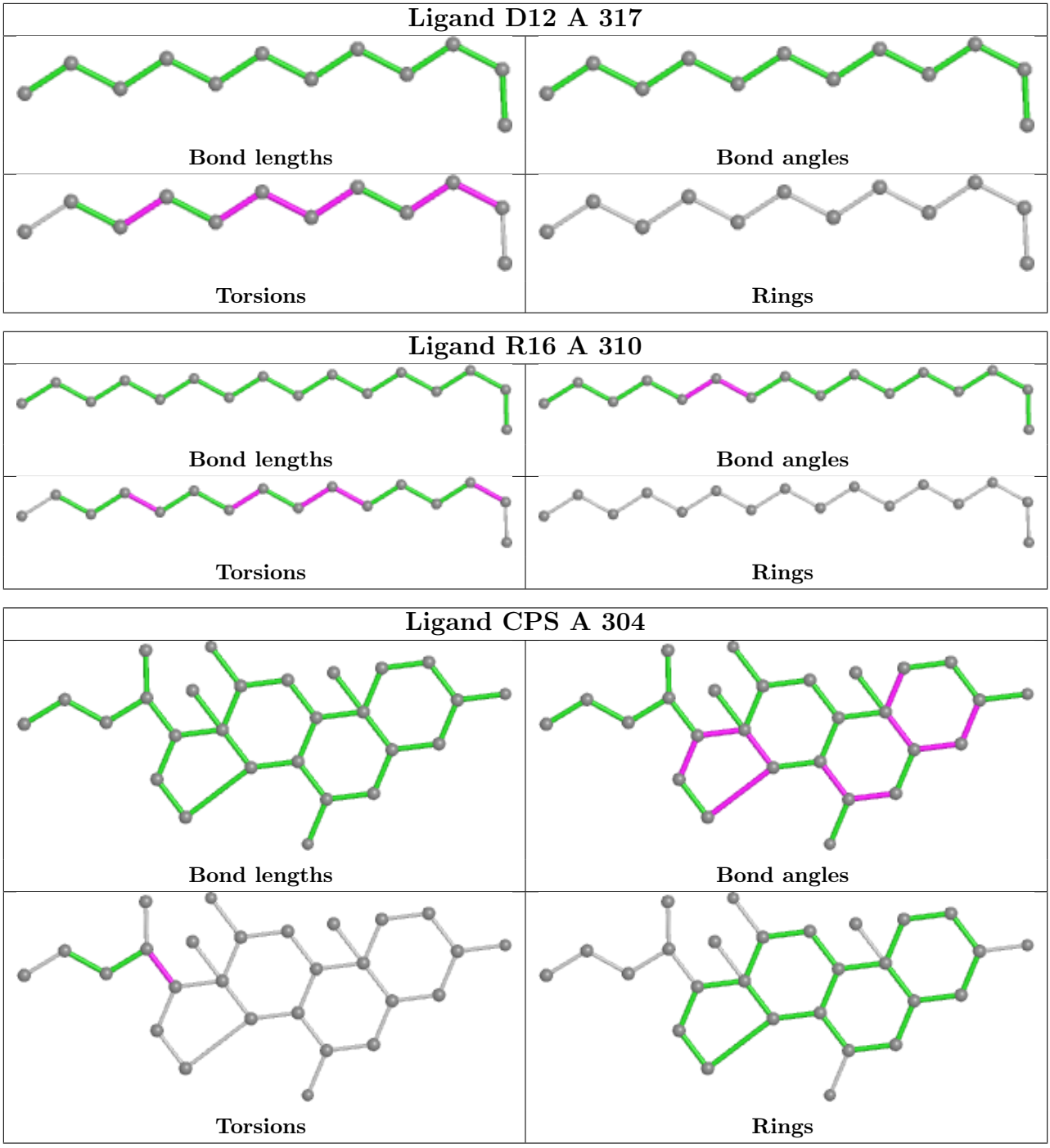


Ligand RET A 301



Ligand D10 A 312 (B)





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	224/249 (89%)	1.02	35 (15%)	2	3	64, 72, 95, 119	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	35	SER	5.6
1	A	73	GLY	4.9
1	A	227	ARG	4.9
1	A	74	GLU	4.7
1	A	228	ALA	4.4
1	A	70	PRO	4.3
1	A	72	GLY	4.3
1	A	36	ASP	3.9
1	A	69	VAL	3.6
1	A	158	SER	3.6
1	A	15	LEU	3.2
1	A	8	PRO	3.0
1	A	130	VAL	2.9
1	A	163	MET	2.9
1	A	102	ASP	2.8
1	A	37	PRO	2.7
1	A	68	MET	2.7
1	A	133	TYR	2.7
1	A	166	GLU	2.6
1	A	52	ILE	2.6
1	A	76	ASN	2.6
1	A	77	PRO	2.5
1	A	19	LEU	2.4
1	A	22	LEU	2.3
1	A	164	ARG	2.3
1	A	199	VAL	2.2
1	A	92	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	48	LEU	2.2
1	A	109	LEU	2.2
1	A	230	PHE	2.2
1	A	81	ALA	2.2
1	A	169	SER	2.1
1	A	75	GLN	2.1
1	A	51	ALA	2.1
1	A	14	ALA	2.0

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, 95^{th} 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
8	D12	A	316	12/12	0.38	0.53	100,118,126,127	0
7	HP6	A	306	7/7	0.40	0.27	124,135,141,143	0
6	OCT	A	305	8/8	0.52	0.30	90,120,137,145	0
7	HP6	A	313	7/7	0.61	0.49	106,119,132,139	0
5	CPS	A	304	27/42	0.61	0.29	97,111,121,125	27
10	D10	A	312[B]	10/10	0.62	0.93	97,107,114,115	10
7	HP6	A	311	7/7	0.64	0.50	114,120,130,136	0
6	OCT	A	320	8/8	0.66	0.52	87,108,132,145	0
8	D12	A	307	12/12	0.67	0.42	88,106,118,119	0
9	R16	A	308	16/16	0.70	0.28	84,108,131,131	0
9	R16	A	318	16/16	0.77	0.53	83,113,126,130	0
8	D12	A	317	12/12	0.78	0.34	102,111,116,125	0
7	HP6	A	319	7/7	0.79	0.35	91,110,125,129	0
3	7YH	A	302[B]	41/41	0.85	0.56	70,85,104,107	41
7	HP6	A	314[A]	7/7	0.85	1.15	128,133,153,163	7

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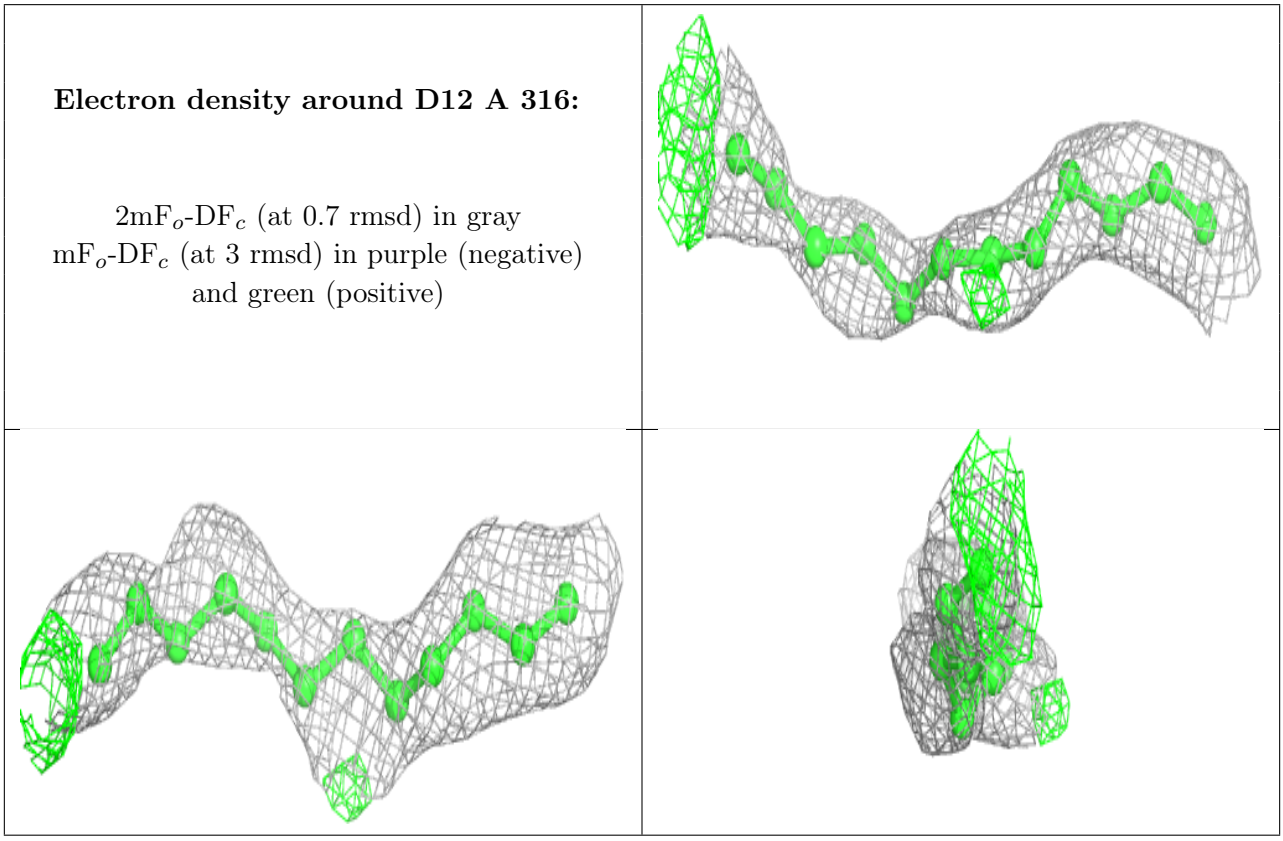
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	7YH	A	302[A]	41/41	0.85	0.56	81,98,112,117	41
10	D10	A	309	10/10	0.86	0.22	89,96,105,113	0
11	DD9	A	315	9/9	0.86	0.43	100,109,114,121	0
4	IOD	A	303	1/1	0.87	0.29	132,132,132,132	1
2	RET	A	301	20/21	0.90	0.22	57,69,75,77	0
9	R16	A	310	16/16	0.90	0.23	74,90,114,117	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.

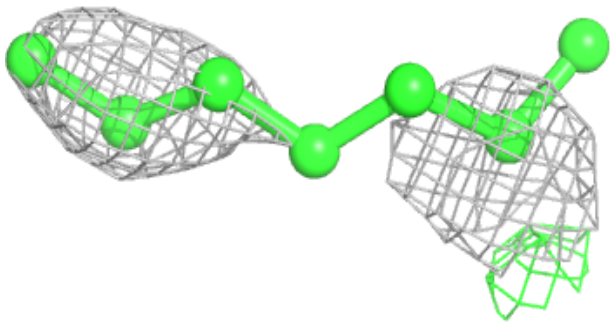
Electron density around D12 A 316:

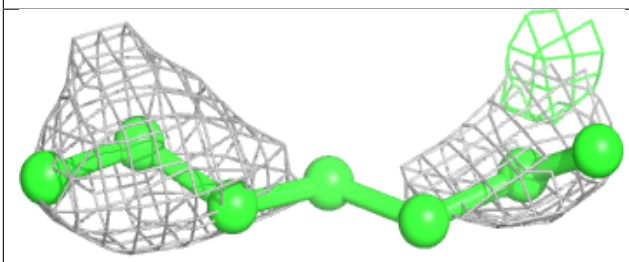
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

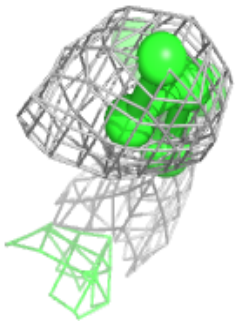


Electron density around HP6 A 306:

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

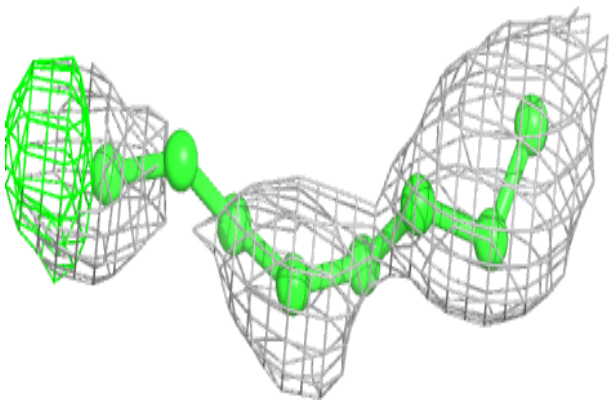


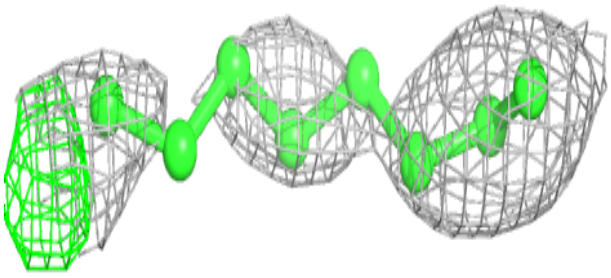


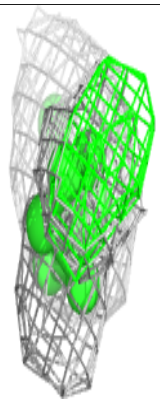


Electron density around OCT A 305:

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

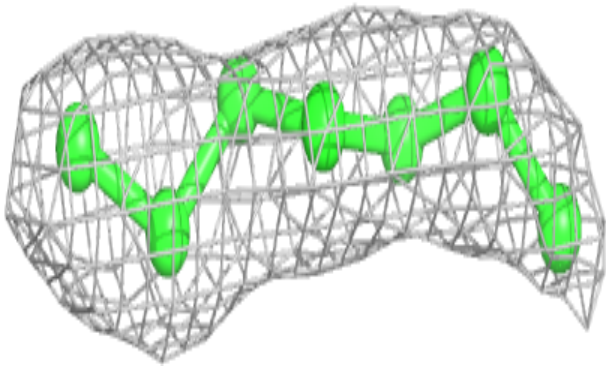


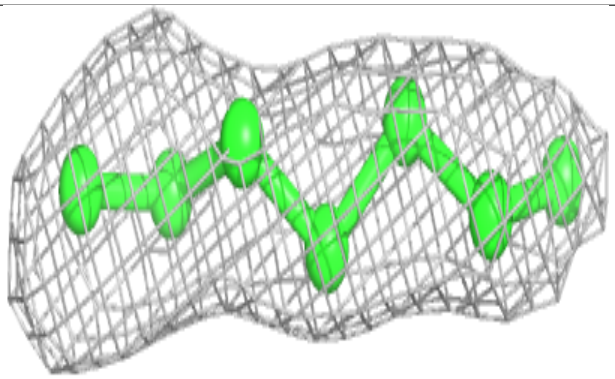


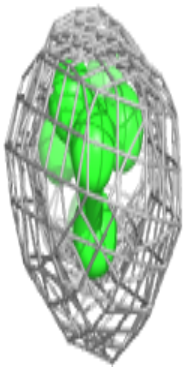


Electron density around HP6 A 313:

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

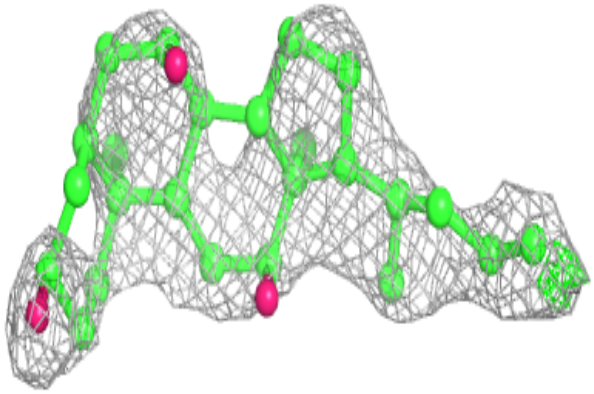


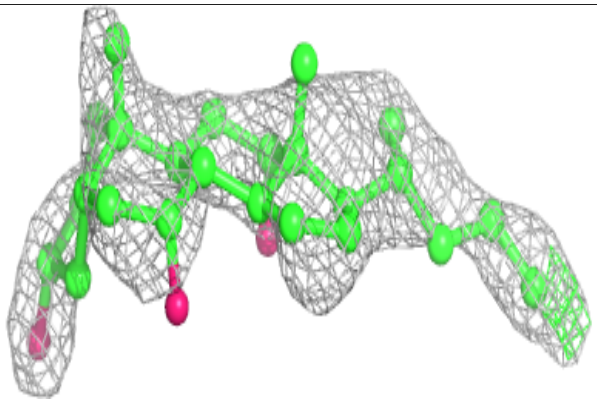


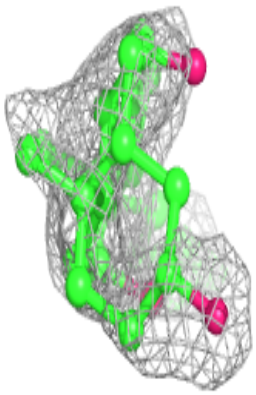


Electron density around CPS A 304:

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

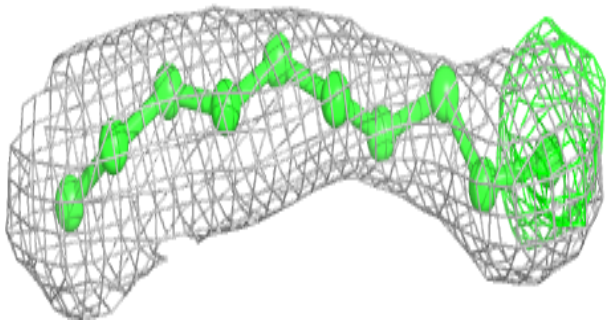


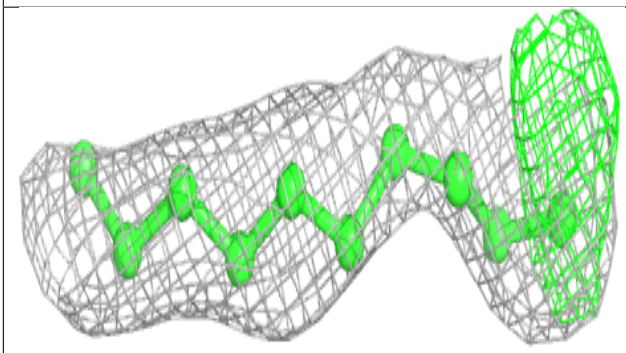


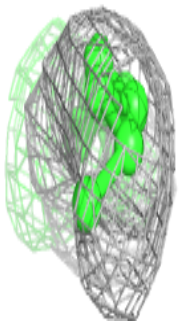


Electron density around D10 A 312 (B):

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

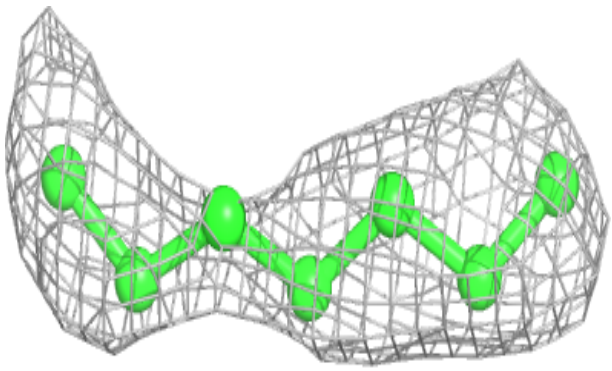


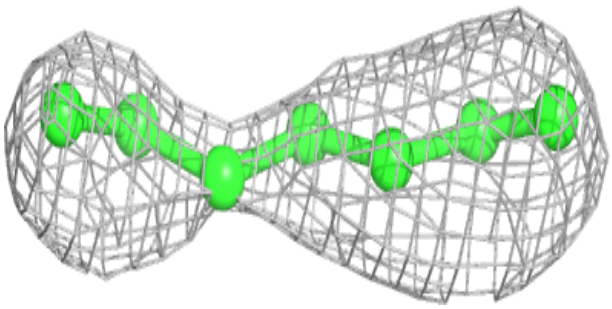


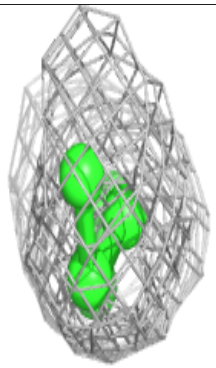


Electron density around HP6 A 311:

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

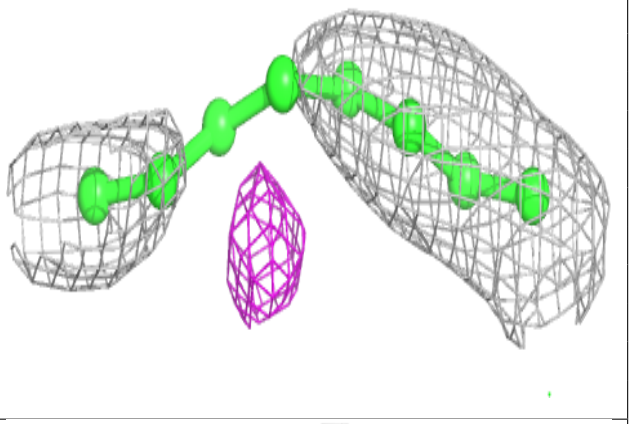


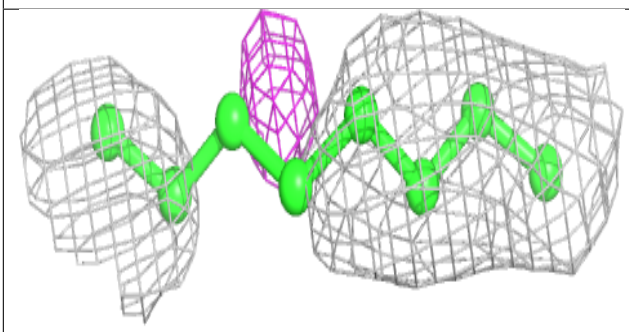


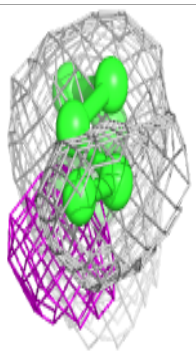


Electron density around OCT A 320:

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

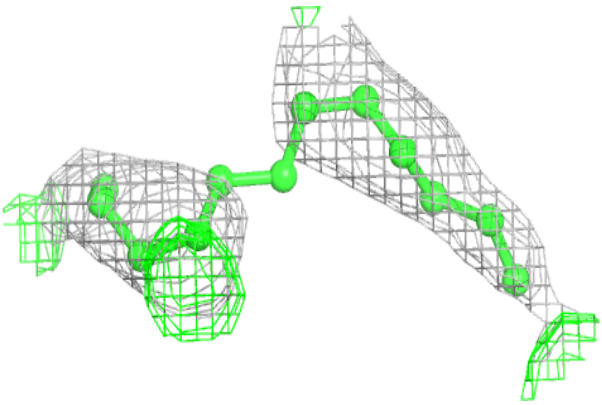


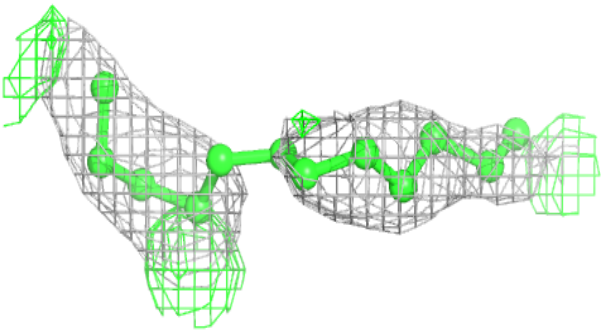


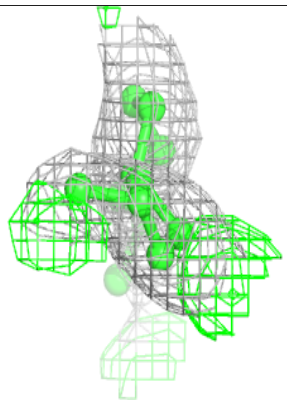


Electron density around D12 A 307:

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

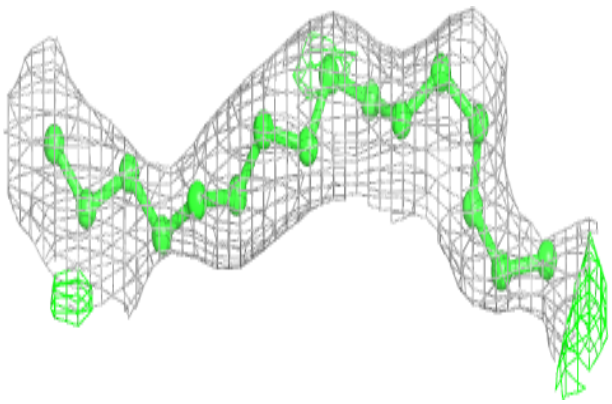


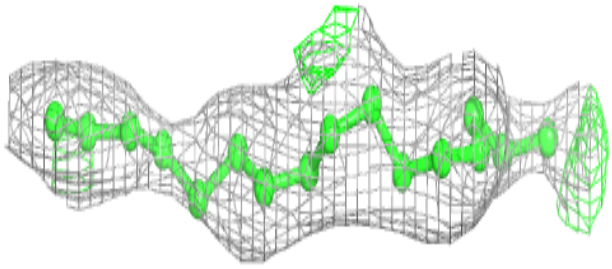


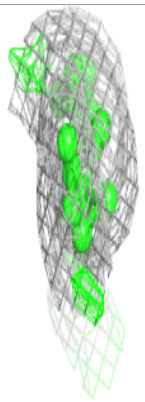


Electron density around R16 A 308:

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

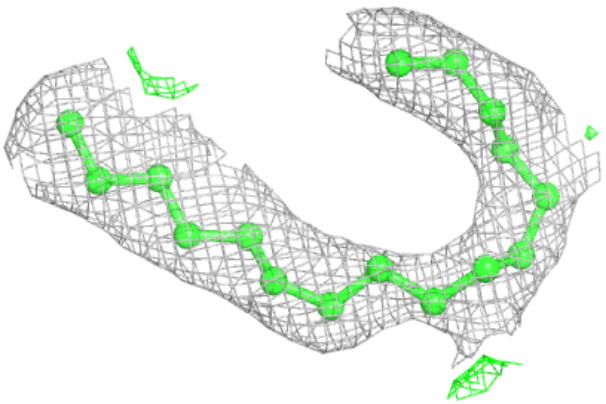


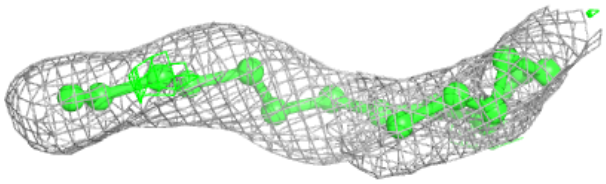


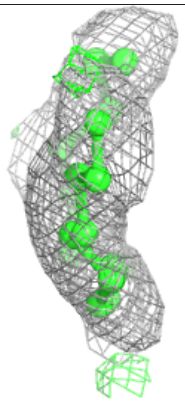


Electron density around R16 A 318:

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

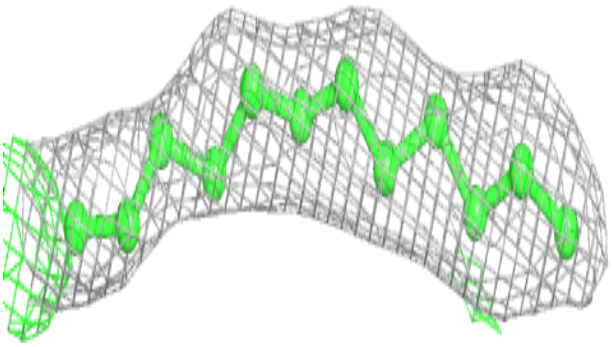


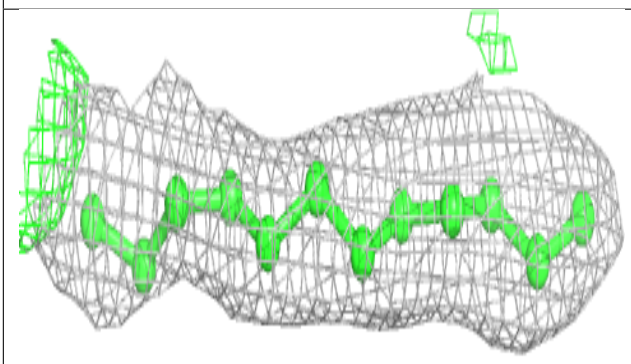


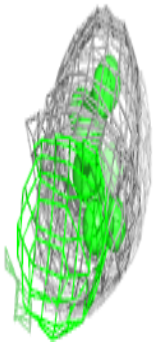


Electron density around D12 A 317:

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

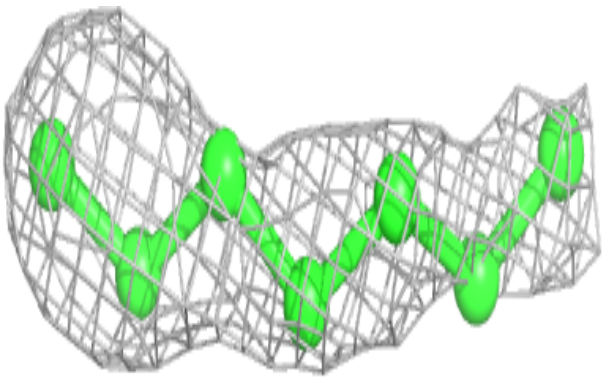


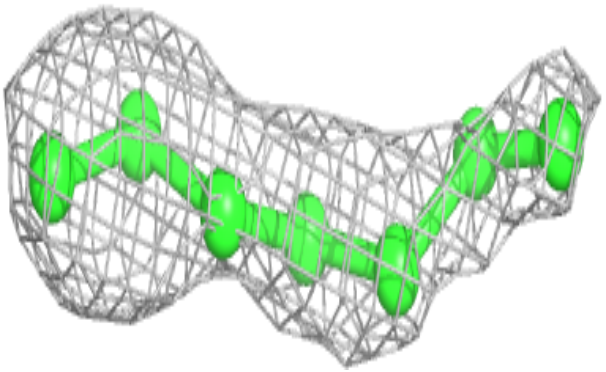


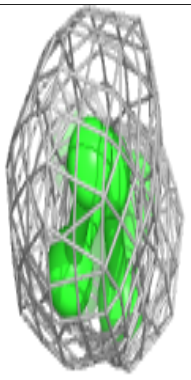


Electron density around HP6 A 319:

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

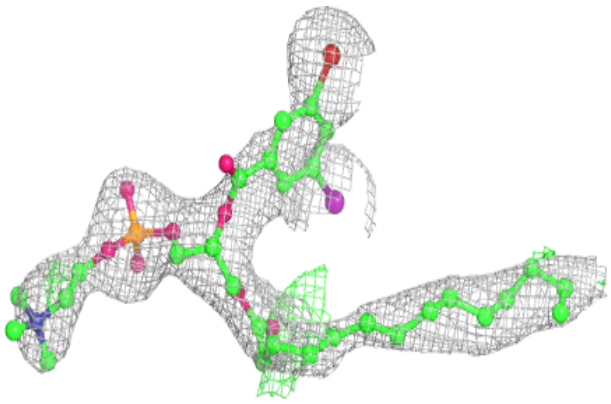


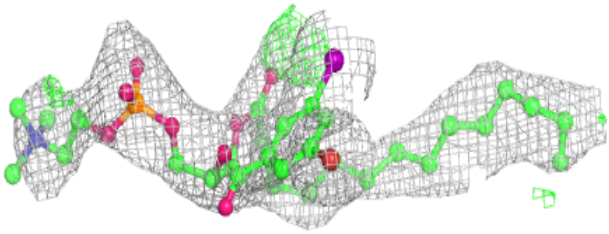


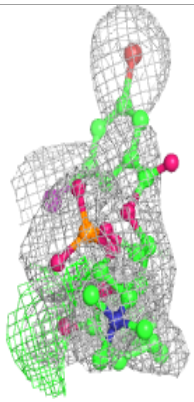


Electron density around 7YH A 302 (B):

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

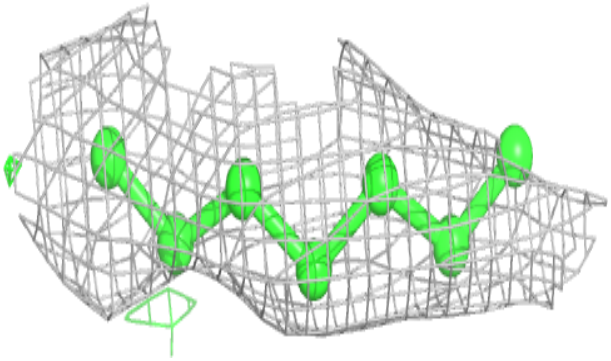


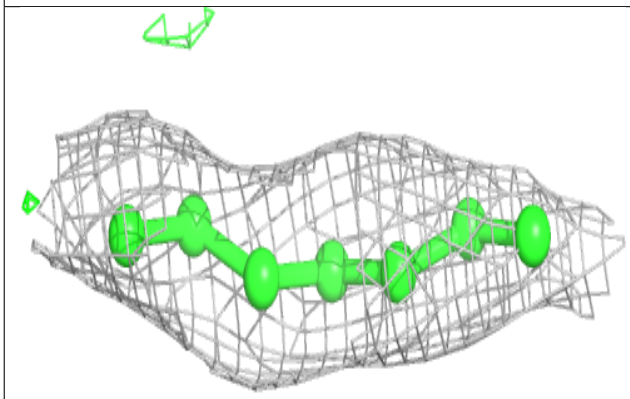


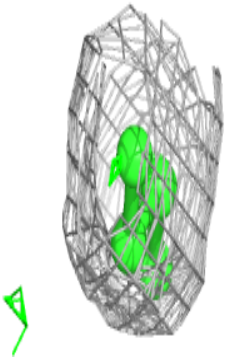


Electron density around HP6 A 314 (A):

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

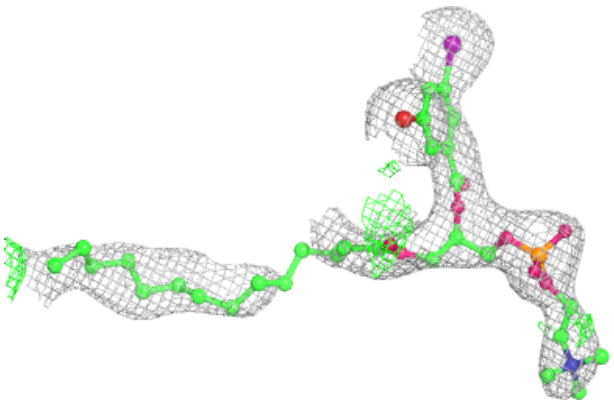


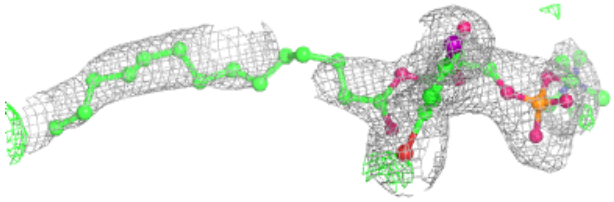


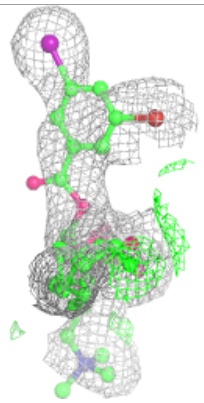


Electron density around 7YH A 302 (A):

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

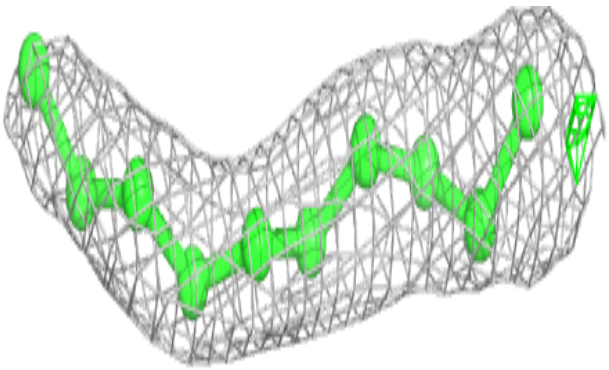


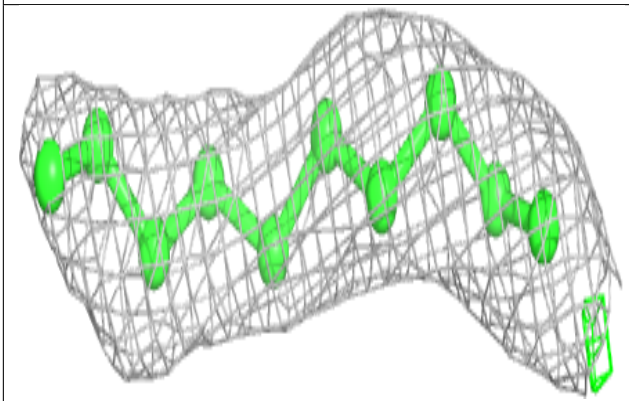


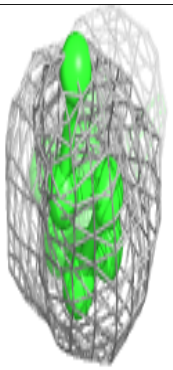


Electron density around D10 A 309:

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

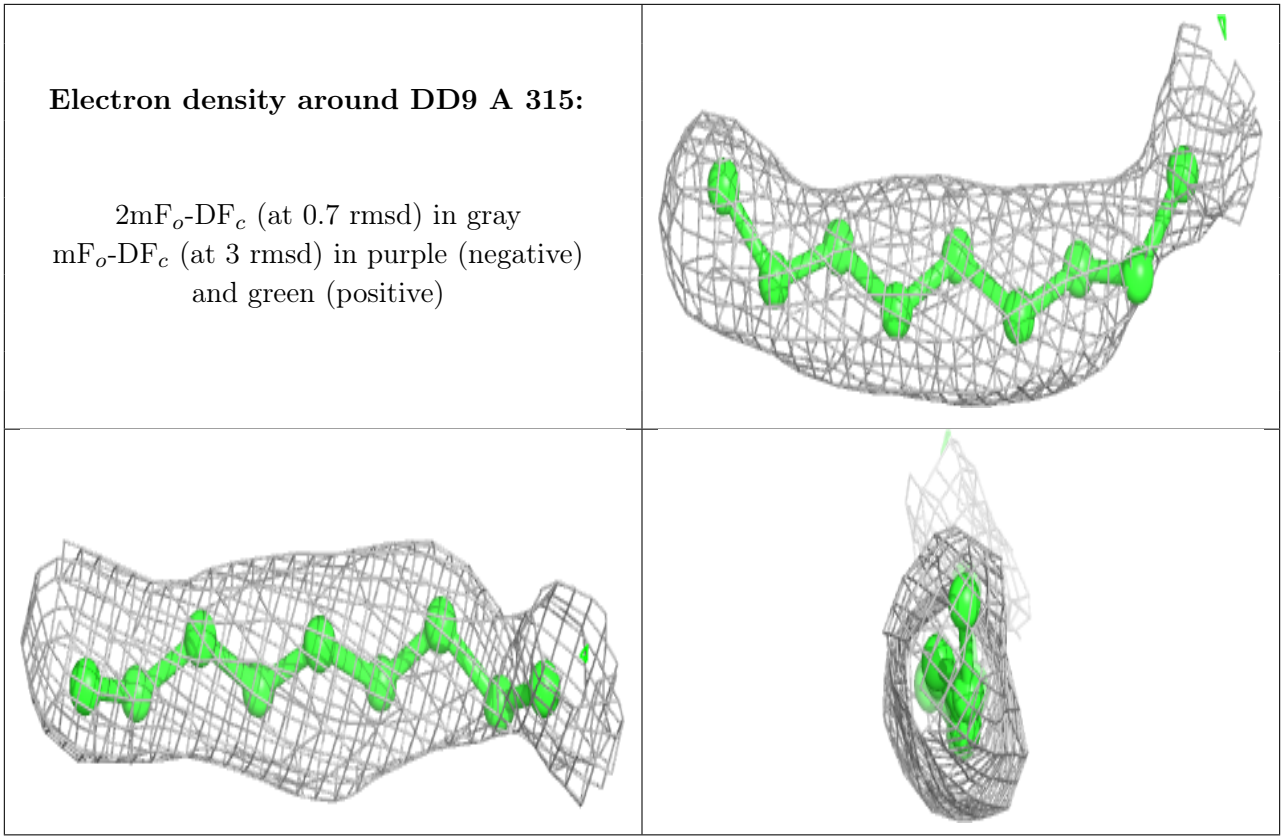






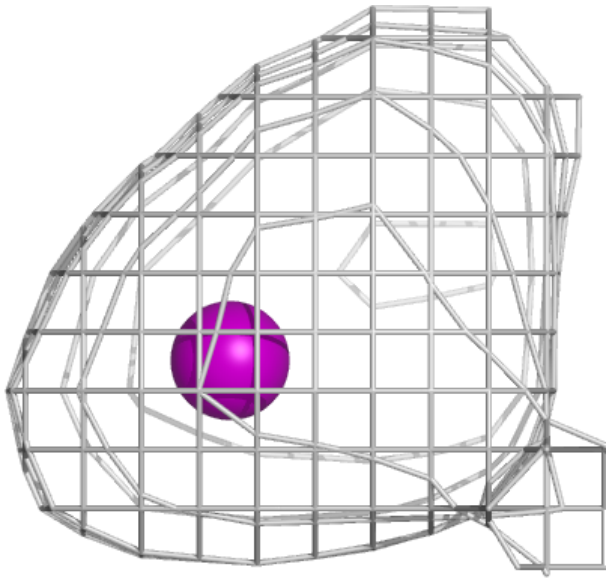
Electron density around DD9 A 315:

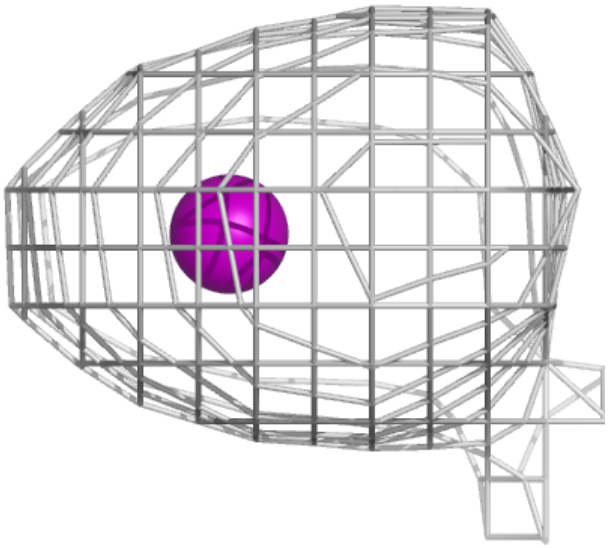
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

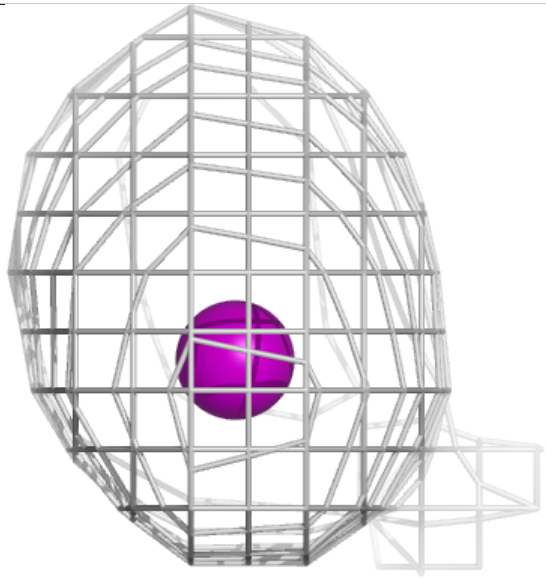


Electron density around IOD A 303:

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

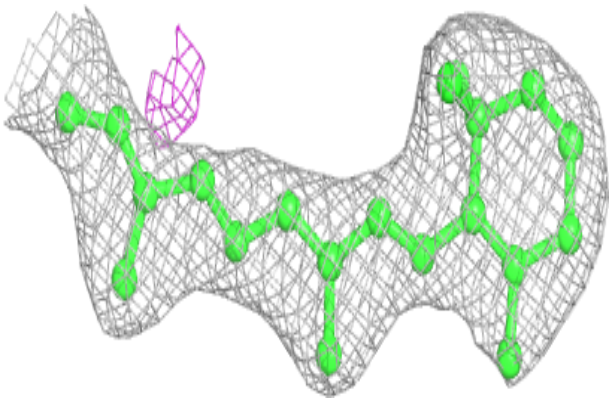


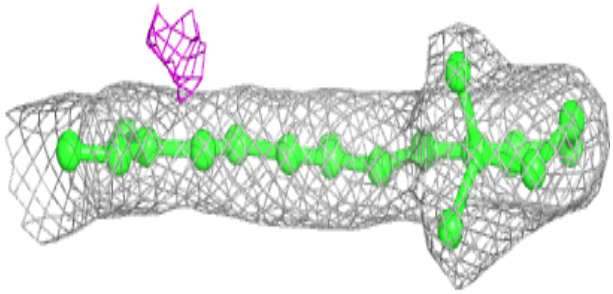


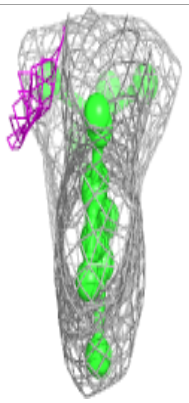


Electron density around RET A 301:

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

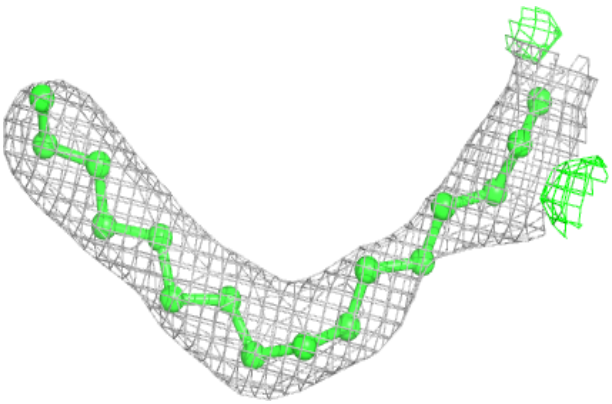


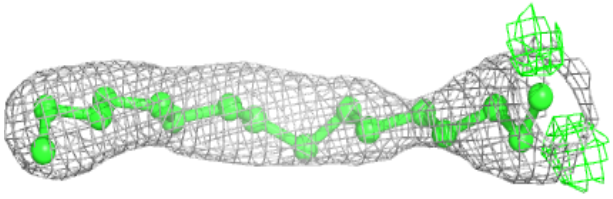


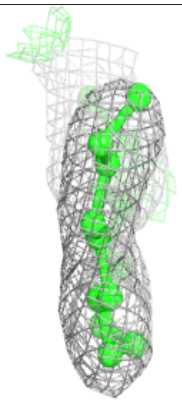


Electron density around R16 A 310:

$2mF_o$-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.