



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 21, 2020 – 10:33 AM BST

PDB ID : 5D92
Title : Structure of a phosphatidylinositolphosphate (PIP) synthase from Renibacterium Salmoninarum
Authors : Clarke, O.B.; Tomasek, D.T.; Jorge, C.D.; Belcher Dufrisne, M.; Kim, M.; Banerjee, S.; Rajashankar, K.R.; Hendrickson, W.A.; Santos, H.; Mancina, F.
Deposited on : 2015-08-18
Resolution : 3.62 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 ⓘ symbol.

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 : 2.13.1
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) : 2.13.1

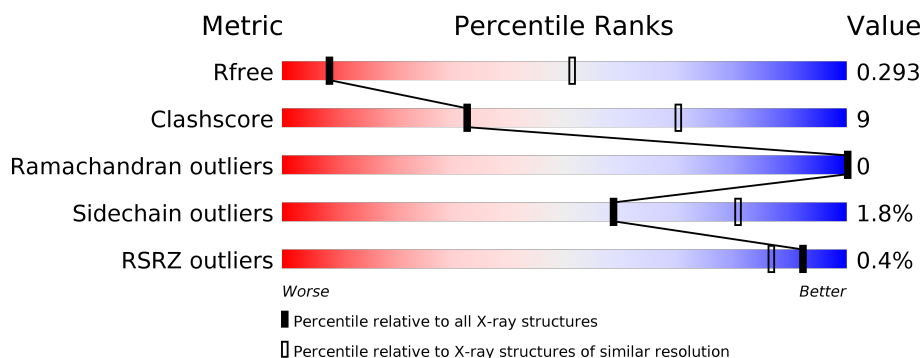
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.62 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	1290 (3.74-3.50)
Clashscore	141614	1387 (3.74-3.50)
Ramachandran outliers	138981	1339 (3.74-3.50)
Sidechain outliers	138945	1339 (3.74-3.50)
RSRZ outliers	127900	1191 (3.74-3.50)

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 on 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 $\leq 5\%$. 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	342	<div> <div style="width: 77%;"></div> <div style="width: 22%;"></div> <div style="width: 1%;"></div> </div> <div>77% 22% .</div>
1	B	342	<div> <div style="width: 81%;"></div> <div style="width: 18%;"></div> </div> <div>81% 18%</div>
1	C	342	<div> <div style="width: 79%;"></div> <div style="width: 18%;"></div> <div style="width: 3%;"></div> </div> <div>79% 18% ..</div>
1	D	342	<div> <div style="width: 76%;"></div> <div style="width: 23%;"></div> </div> <div>76% 23% .</div>

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
2	8K6	A	305	-	-	-	X
2	8K6	B	303	-	-	-	X
2	8K6	B	305	-	-	-	X
2	8K6	C	301	-	-	-	X
2	8K6	C	302	-	-	-	X
2	8K6	C	303	-	-	-	X
2	8K6	C	305	-	-	-	X
2	8K6	D	310	-	-	-	X
2	8K6	D	312	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10844 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 AF2299 protein, Phosphatidylinositol synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	342	Total	C	N	O	S	0	0	0
			2605	1716	414	470	5			
1	A	340	Total	C	N	O	S	0	0	0
			2591	1707	414	465	5			
1	B	342	Total	C	N	O	S	0	0	0
			2602	1715	413	469	5			
1	C	334	Total	C	N	O	S	0	0	0
			2551	1683	405	458	5			

There are 40 discrepancies between the modelled and reference sequences:

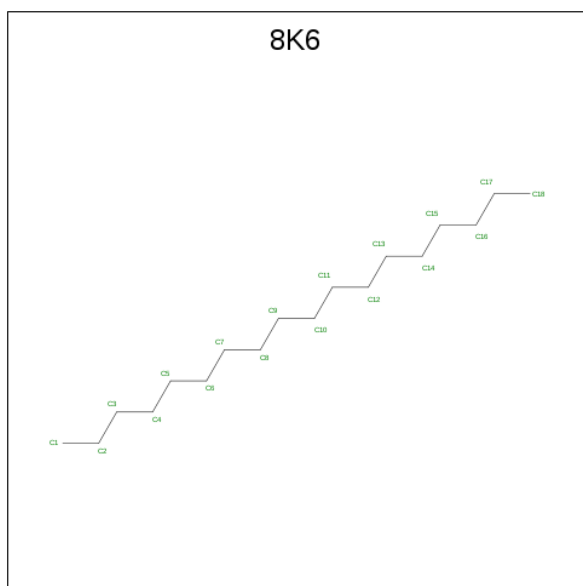
Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	GLY	-	linker	UNP O27985
D	-1	SER	-	linker	UNP O27985
D	0	GLY	-	linker	UNP O27985
D	1	SER	-	linker	UNP O27985
D	15	LEU	MET	conflict	UNP A9WSF5
D	22	ALA	VAL	conflict	UNP A9WSF5
D	23	ASP	ARG	conflict	UNP A9WSF5
D	75	LEU	GLN	conflict	UNP A9WSF5
D	77	PHE	ASP	conflict	UNP A9WSF5
D	79	GLU	PRO	conflict	UNP A9WSF5
A	-2	GLY	-	linker	UNP O27985
A	-1	SER	-	linker	UNP O27985
A	0	GLY	-	linker	UNP O27985
A	1	SER	-	linker	UNP O27985
A	15	LEU	MET	conflict	UNP A9WSF5
A	22	ALA	VAL	conflict	UNP A9WSF5
A	23	ASP	ARG	conflict	UNP A9WSF5
A	75	LEU	GLN	conflict	UNP A9WSF5
A	77	PHE	ASP	conflict	UNP A9WSF5
A	79	GLU	PRO	conflict	UNP A9WSF5
B	-2	GLY	-	linker	UNP O27985

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	SER	-	linker	UNP O27985
B	0	GLY	-	linker	UNP O27985
B	1	SER	-	linker	UNP O27985
B	15	LEU	MET	conflict	UNP A9WSF5
B	22	ALA	VAL	conflict	UNP A9WSF5
B	23	ASP	ARG	conflict	UNP A9WSF5
B	75	LEU	GLN	conflict	UNP A9WSF5
B	77	PHE	ASP	conflict	UNP A9WSF5
B	79	GLU	PRO	conflict	UNP A9WSF5
C	-2	GLY	-	linker	UNP O27985
C	-1	SER	-	linker	UNP O27985
C	0	GLY	-	linker	UNP O27985
C	1	SER	-	linker	UNP O27985
C	15	LEU	MET	conflict	UNP A9WSF5
C	22	ALA	VAL	conflict	UNP A9WSF5
C	23	ASP	ARG	conflict	UNP A9WSF5
C	75	LEU	GLN	conflict	UNP A9WSF5
C	77	PHE	ASP	conflict	UNP A9WSF5
C	79	GLU	PRO	conflict	UNP A9WSF5

- Molecule 2 is Octadecane (three-letter code: 8K6) (formula: C₁₈H₃₈).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total C 7 7	0	0
2	D	1	Total C 7 7	0	0

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

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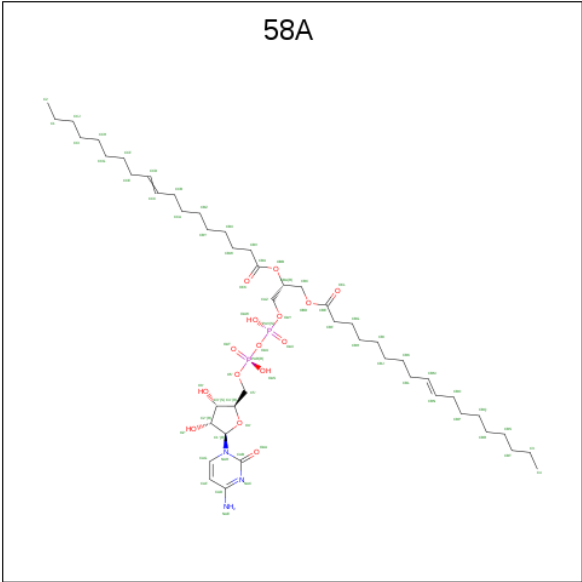
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total C 7 7	0	0
2	B	1	Total C 7 7	0	0
2	B	1	Total C 7 7	0	0
2	C	1	Total C 7 7	0	0
2	C	1	Total C 7 7	0	0
2	C	1	Total C 7 7	0	0
2	C	1	Total C 7 7	0	0
2	C	1	Total C 7 7	0	0
2	C	1	Total C 7 7	0	0
2	C	1	Total C 7 7	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	2	Total Mg 2 2	0	0
3	A	2	Total Mg 2 2	0	0
3	D	2	Total Mg 2 2	0	0
3	C	2	Total Mg 2 2	0	0

- Molecule 4 is 5'-O-[(R)-{[(S)-{(2R)-2,3-bis[(9E)-octadec-9-enoyloxy]propoxy}(hydroxy)phosphoryl]oxy}(hydroxy)phosphoryl]cytidine (three-letter code: 58A) (formula: C₄₈H₈₅N₃O₁₅P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	D	1	Total	C	N	O	P	0	0
			64	44	3	15	2		
4	A	1	Total	C	N	O	P	0	0
			64	44	3	15	2		
4	B	1	Total	C	N	O	P	0	0
			64	44	3	15	2		
4	C	1	Total	C	N	O	P	0	0
			64	44	3	15	2		

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.

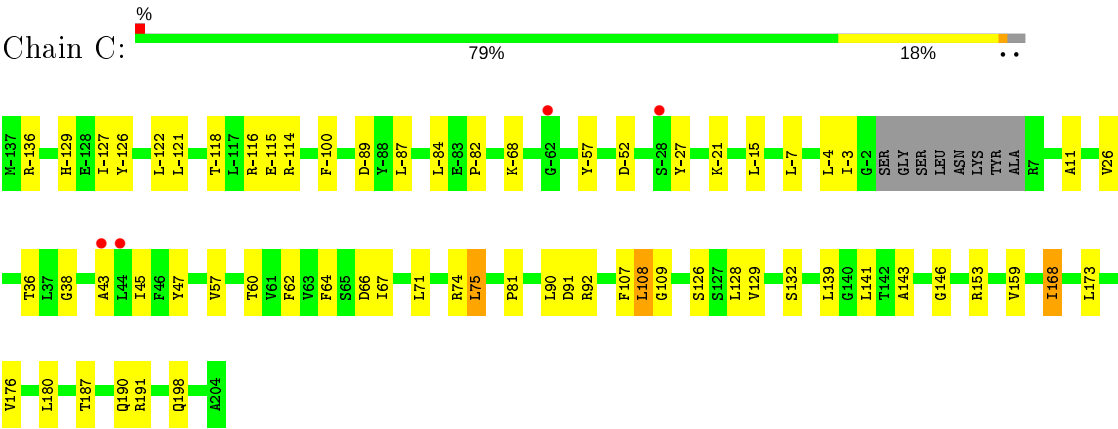
- Chain D: 76% 23%

R-137	R-136	I-127	Y-126	L-122	L-121	T-118	L-117	R-116	E-115	R-114	R-107	F-100	D-89	Y-88	R-69	K-68	F-56	G-53	D-52	Q-42	I-39	Y-27	L-15	E-11	L-4	I-3	G-2	S-1	L2	N3	R7	L9	I13	F14	L15	P16	S27	P28			
T32	V33	V34	G38	A43	L44	Y47	V57	T60	V61	F62	V63	D66	L71	R74	L75	L76	F77	R78	E79	L90	D91	R92	D95	S96	S97	F107	L108	G109	L118	I121	S126	V129	S130	E137	G138	L139	G140	L141	T142	A143	G146

- [illegible]

- Chain B:
-
- | Label | Color |
|-------|--------|
| N-137 | Green |
| K-131 | Green |
| N-130 | Green |
| H-129 | Green |
| Y-126 | Yellow |
| L-122 | Yellow |
| L-121 | Yellow |
| T-118 | Yellow |
| L-117 | Green |
| R-116 | Yellow |
| E-115 | Yellow |
| R-114 | Yellow |
| R-107 | Yellow |
| D-98 | Yellow |
| L-94 | Yellow |
| Y-88 | Yellow |
| L-87 | Yellow |
| L-84 | Yellow |
| E-83 | Yellow |
| P-82 | Yellow |
| L-78 | Yellow |
| K-68 | Yellow |
| Y-57 | Yellow |
| G-53 | Yellow |
| D-52 | Yellow |
| F-51 | Green |
| R-50 | Yellow |
| Y-27 | Yellow |
| T-22 | Yellow |
| K-21 | Yellow |
| E-11 | Yellow |
| K-10 | Green |
| L-9 | Yellow |
| L-8 | Yellow |
| L-4 | Yellow |
| I-3 | Yellow |
| L9 | Yellow |
| I13 | Yellow |
| P16 | Yellow |
-
- | Label | Color |
|-------|--------|
| T36 | Green |
| F46 | Green |
| L52 | Yellow |
| V57 | Yellow |
| V58 | Yellow |
| I59 | Green |
| T60 | Yellow |
| D66 | Yellow |
| I67 | Yellow |
| L71 | Yellow |
| R74 | Orange |
| L75 | Yellow |
| L76 | Green |
| F77 | Yellow |
| R78 | Yellow |
| F85 | Yellow |
| L86 | Green |
| D87 | Yellow |
| L90 | Yellow |
| D91 | Yellow |
| R92 | Yellow |
| F107 | Yellow |
| S126 | Yellow |
| V129 | Yellow |
| L139 | Yellow |
| A143 | Yellow |
| A143 | Red |
| L154 | Yellow |
| L163 | Yellow |
| V164 | Green |
| G165 | Yellow |
| L166 | Yellow |
| V186 | Yellow |
| Q190 | Yellow |
| R191 | Yellow |
| A204 | Green |

● Molecule 1: AF2299 protein,Phosphatidylinositol synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	89.00 Å 62.49 Å 169.76 Å 90.00° 99.77° 90.00°	Depositor
Resolution (Å)	166.97 – 3.62 167.30 – 3.61	Depositor EDS
% Data completeness (in resolution range)	98.4 (166.97-3.62) 98.6 (167.30-3.61)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.55 (at 3.58 Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.280 , 0.300 0.275 , 0.293	Depositor DCC
R_{free} test set	1045 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	72.9	Xtriage
Anisotropy	0.626	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 54.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	10844	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 20.91 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.8532e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: MG, 8K6, 58A

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	0.27	0/2641	0.55	1/3596 (0.0%)
1	B	0.26	0/2653	0.55	0/3616
1	C	0.27	0/2600	0.54	0/3542
1	D	0.27	0/2656	0.54	0/3620
All	All	0.27	0/10550	0.55	1/14374 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	80	GLY	N-CA-C	5.84	127.71	113.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2591	0	2635	54	0
1	B	2602	0	2646	41	0
1	C	2551	0	2603	42	0
1	D	2605	0	2650	52	0
2	A	56	0	80	2	0
2	B	42	0	60	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	49	0	70	3	0
2	D	84	0	120	1	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	A	64	0	68	5	0
4	B	64	0	68	1	0
4	C	64	0	68	5	0
4	D	64	0	68	7	0
All	All	10844	0	11136	191	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 9.

The worst 5 of 191 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)
4:C:310:58A:O4'	4:C:310:58A:C1'	1.65	1.29
4:A:311:58A:C1'	4:A:311:58A:O4'	1.65	1.27
4:B:309:58A:O4'	4:B:309:58A:C1'	1.65	1.21
4:D:315:58A:O4'	4:D:315:58A:C1'	1.65	1.15
1:D:66:ASP:OD1	4:D:315:58A:OAW	1.62	1.14

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	336/342 (98%)	329 (98%)	7 (2%)	0	100	100
1	B	340/342 (99%)	334 (98%)	6 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	330/342 (96%)	324 (98%)	6 (2%)	0	100	100
1	D	340/342 (99%)	334 (98%)	6 (2%)	0	100	100
All	All	1346/1368 (98%)	1321 (98%)	25 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	268/283 (95%)	265 (99%)	3 (1%)	73	87
1	B	270/283 (95%)	267 (99%)	3 (1%)	73	87
1	C	266/283 (94%)	261 (98%)	5 (2%)	57	80
1	D	271/283 (96%)	263 (97%)	8 (3%)	41	71
All	All	1075/1132 (95%)	1056 (98%)	19 (2%)	59	81

5 of 19 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-69	ARG
1	A	107	PHE
1	C	75	LEU
1	D	189	PHE
1	C	107	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 45 ligands modelled in this entry, 8 are monoatomic - leaving 37 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	$\# Z > 2$
2	8K6	C	302	-	6,6,17	0.31	0	5,5,16	0.63	0
2	8K6	B	305	-	6,6,17	0.31	0	5,5,16	0.68	0
2	8K6	A	305	-	6,6,17	0.31	0	5,5,16	0.66	0
2	8K6	D	309	-	6,6,17	0.32	0	5,5,16	0.61	0
2	8K6	C	303	-	6,6,17	0.32	0	5,5,16	0.67	0
2	8K6	A	304	-	6,6,17	0.30	0	5,5,16	0.69	0
2	8K6	B	302	-	6,6,17	0.31	0	5,5,16	0.66	0
2	8K6	D	305	-	6,6,17	0.32	0	5,5,16	0.62	0
2	8K6	D	311	-	6,6,17	0.30	0	5,5,16	0.68	0
2	8K6	B	306	-	6,6,17	0.31	0	5,5,16	0.66	0
2	8K6	D	312	-	6,6,17	0.32	0	5,5,16	0.68	0
2	8K6	C	301	-	6,6,17	0.31	0	5,5,16	0.65	0
2	8K6	C	305	-	6,6,17	0.31	0	5,5,16	0.67	0
2	8K6	C	306	-	6,6,17	0.30	0	5,5,16	0.70	0
2	8K6	A	302	-	6,6,17	0.30	0	5,5,16	0.66	0
2	8K6	B	304	-	6,6,17	0.30	0	5,5,16	0.70	0
2	8K6	A	306	-	6,6,17	0.31	0	5,5,16	0.66	0
2	8K6	A	303	-	6,6,17	0.31	0	5,5,16	0.68	0
2	8K6	D	310	-	6,6,17	0.30	0	5,5,16	0.67	0
2	8K6	C	307	-	6,6,17	0.30	0	5,5,16	0.71	0
2	8K6	D	306	-	6,6,17	0.31	0	5,5,16	0.65	0
2	8K6	D	308	-	6,6,17	0.32	0	5,5,16	0.66	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	8K6	B	301	-	6,6,17	0.31	0	5,5,16	0.64	0
2	8K6	D	304	-	6,6,17	0.31	0	5,5,16	0.68	0
4	58A	B	309	3	60,65,69	3.38	14 (23%)	66,82,86	1.32	7 (10%)
2	8K6	D	302	-	6,6,17	0.31	0	5,5,16	0.66	0
2	8K6	C	304	-	6,6,17	0.31	0	5,5,16	0.67	0
2	8K6	D	301	-	6,6,17	0.31	0	5,5,16	0.65	0
2	8K6	A	301	-	6,6,17	0.31	0	5,5,16	0.65	0
4	58A	D	315	3	60,65,69	3.37	14 (23%)	66,82,86	1.32	7 (10%)
2	8K6	A	308	-	6,6,17	0.30	0	5,5,16	0.67	0
4	58A	C	310	3	60,65,69	3.36	14 (23%)	66,82,86	1.35	7 (10%)
2	8K6	D	307	-	6,6,17	0.31	0	5,5,16	0.65	0
2	8K6	A	307	-	6,6,17	0.31	0	5,5,16	0.67	0
2	8K6	D	303	-	6,6,17	0.31	0	5,5,16	0.64	0
4	58A	A	311	3	60,65,69	3.37	15 (25%)	66,82,86	1.32	7 (10%)
2	8K6	B	303	-	6,6,17	0.31	0	5,5,16	0.67	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	8K6	C	302	-	-	3/4/4/15	-
2	8K6	B	305	-	-	0/4/4/15	-
2	8K6	A	305	-	-	0/4/4/15	-
2	8K6	D	309	-	-	2/4/4/15	-
2	8K6	C	303	-	-	0/4/4/15	-
2	8K6	A	304	-	-	0/4/4/15	-
2	8K6	B	302	-	-	0/4/4/15	-
2	8K6	D	305	-	-	2/4/4/15	-
2	8K6	D	311	-	-	0/4/4/15	-
2	8K6	B	306	-	-	0/4/4/15	-
2	8K6	D	312	-	-	0/4/4/15	-
2	8K6	C	301	-	-	0/4/4/15	-
2	8K6	C	305	-	-	0/4/4/15	-
2	8K6	C	306	-	-	0/4/4/15	-
2	8K6	A	302	-	-	0/4/4/15	-
2	8K6	B	304	-	-	0/4/4/15	-
2	8K6	A	306	-	-	0/4/4/15	-
2	8K6	A	303	-	-	0/4/4/15	-
2	8K6	D	310	-	-	0/4/4/15	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	8K6	C	307	-	-	0/4/4/15	-
2	8K6	D	306	-	-	0/4/4/15	-
2	8K6	D	308	-	-	0/4/4/15	-
2	8K6	B	301	-	-	1/4/4/15	-
2	8K6	D	304	-	-	1/4/4/15	-
4	58A	B	309	3	-	30/59/77/81	0/2/2/2
2	8K6	D	302	-	-	1/4/4/15	-
2	8K6	C	304	-	-	0/4/4/15	-
2	8K6	D	301	-	-	1/4/4/15	-
2	8K6	A	301	-	-	0/4/4/15	-
4	58A	D	315	3	-	37/59/77/81	0/2/2/2
2	8K6	A	308	-	-	0/4/4/15	-
4	58A	C	310	3	-	30/59/77/81	0/2/2/2
2	8K6	D	307	-	-	0/4/4/15	-
2	8K6	A	307	-	-	0/4/4/15	-
2	8K6	D	303	-	-	0/4/4/15	-
4	58A	A	311	3	-	26/59/77/81	0/2/2/2
2	8K6	B	303	-	-	0/4/4/15	-

The worst 5 of 57 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	315	58A	O4'-C1'	17.46	1.65	1.41
4	A	311	58A	O4'-C1'	17.45	1.65	1.41
4	B	309	58A	O4'-C1'	17.45	1.65	1.41
4	C	310	58A	O4'-C1'	17.37	1.65	1.41
4	B	309	58A	C2'-C1'	-13.28	1.33	1.53

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	310	58A	CAB-NAC-CAD	4.65	121.06	116.34
4	B	309	58A	CAB-NAC-CAD	4.56	120.96	116.34
4	A	311	58A	CAB-NAC-CAD	4.36	120.76	116.34
4	D	315	58A	CAB-NAC-CAD	4.27	120.67	116.34
4	A	311	58A	OBB-CBU-CBV	4.09	120.32	111.50

There are no chirality outliers.

5 of 134 torsion outliers are listed below:

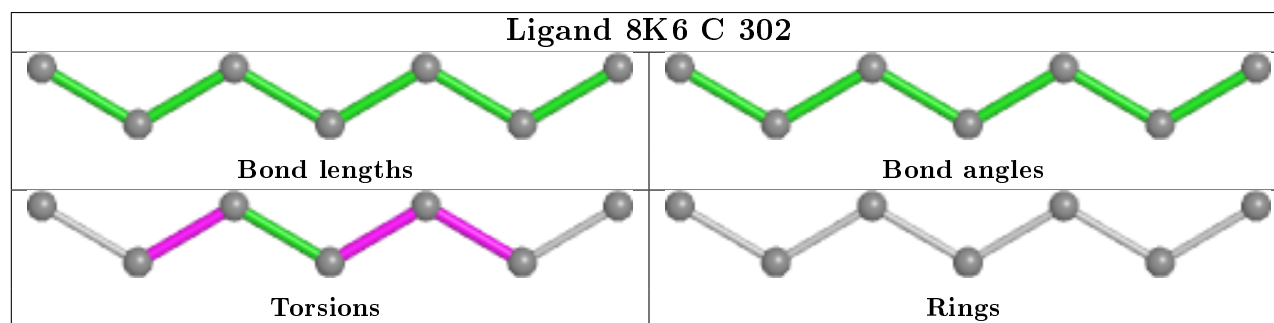
Mol	Chain	Res	Type	Atoms
4	B	309	58A	O4'-C4'-C5'-O5'
4	B	309	58A	C3'-C4'-C5'-O5'
4	B	309	58A	CAZ-OAY-PAV-OAX
4	B	309	58A	CAZ-OAY-PAV-OAW
4	B	309	58A	OBB-CBA-CBC-OB

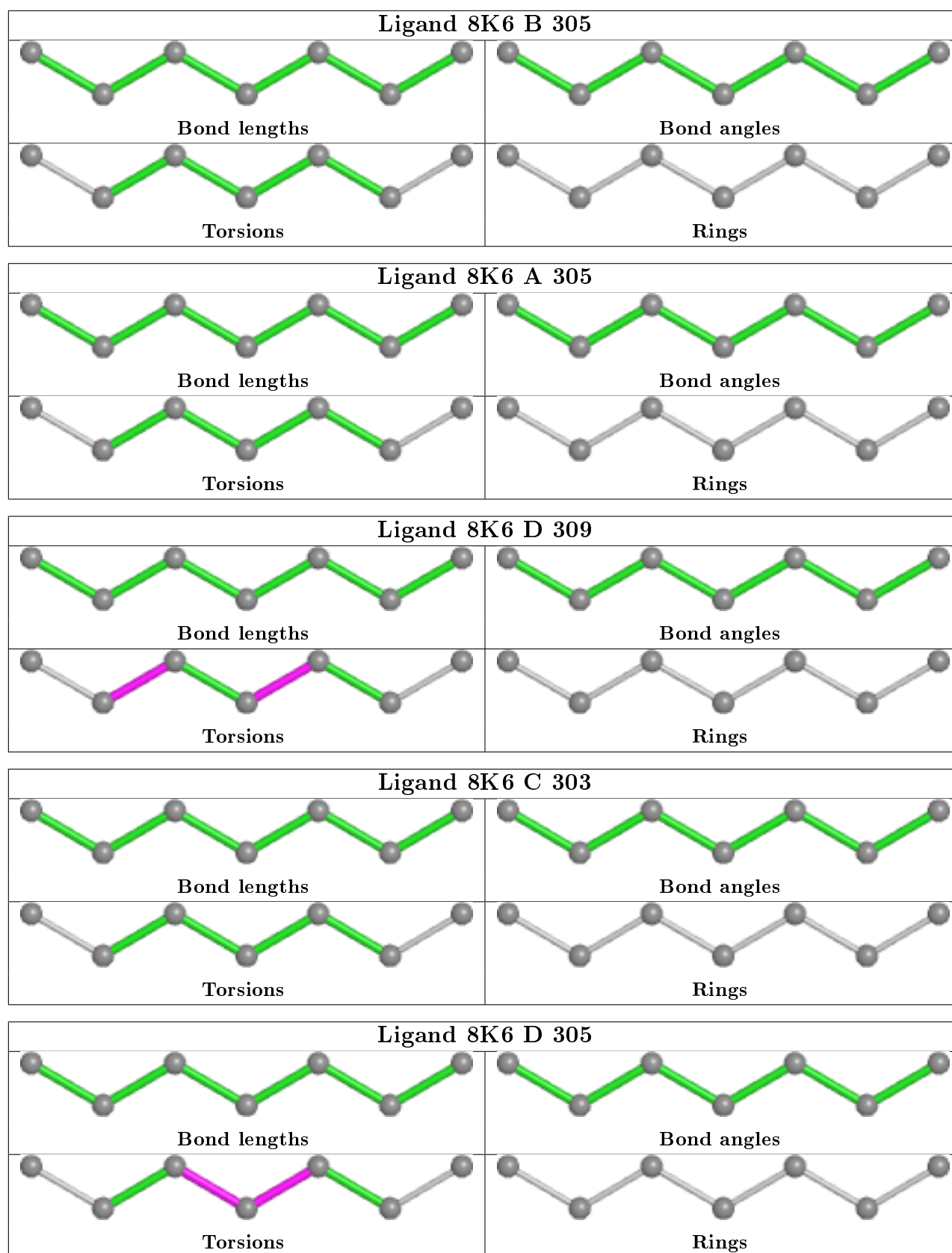
There are no ring outliers.

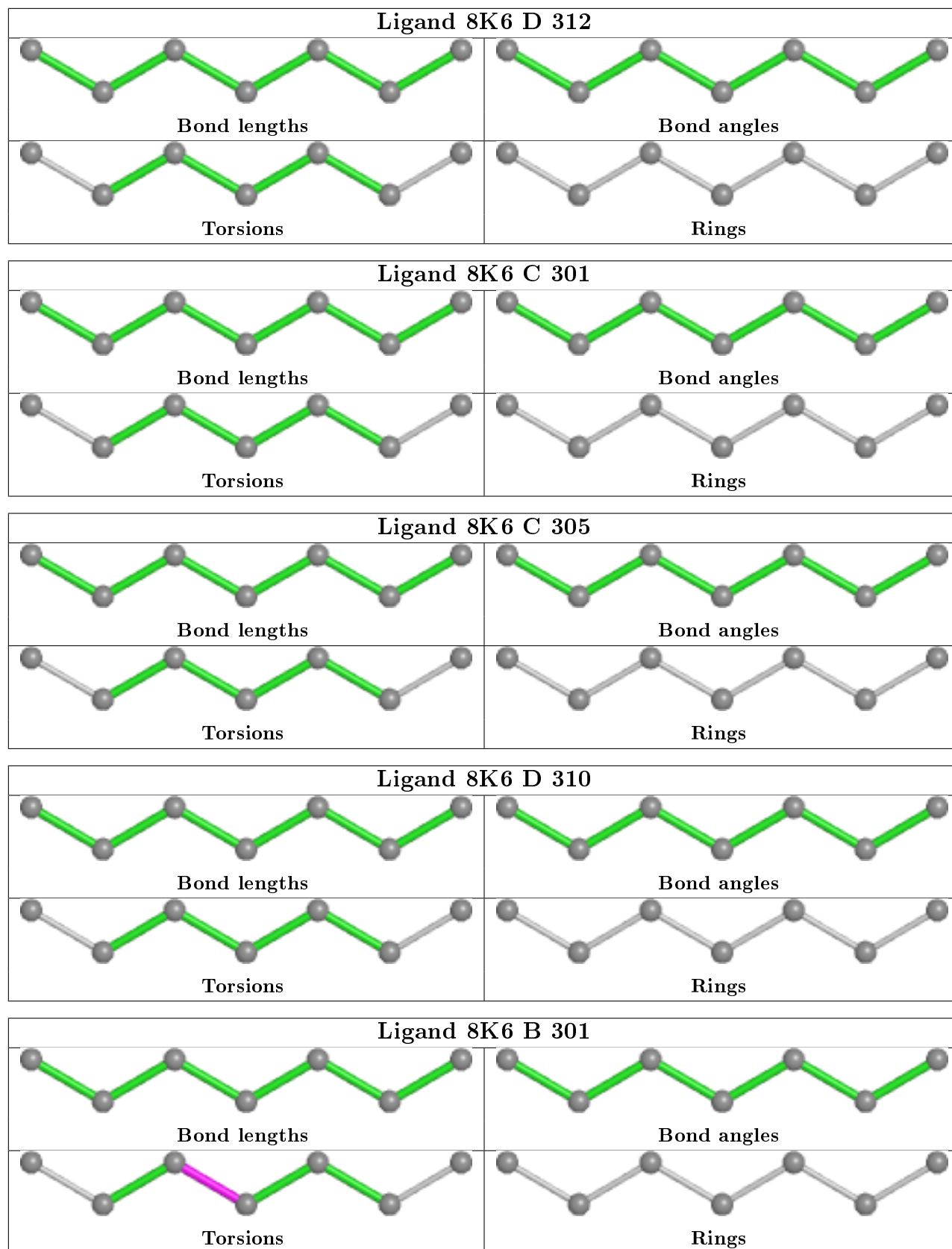
12 monomers are involved in 25 short contacts:

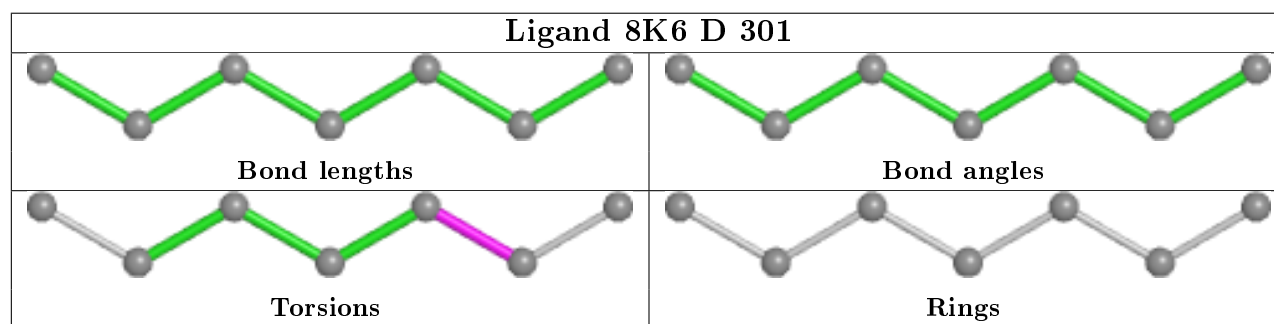
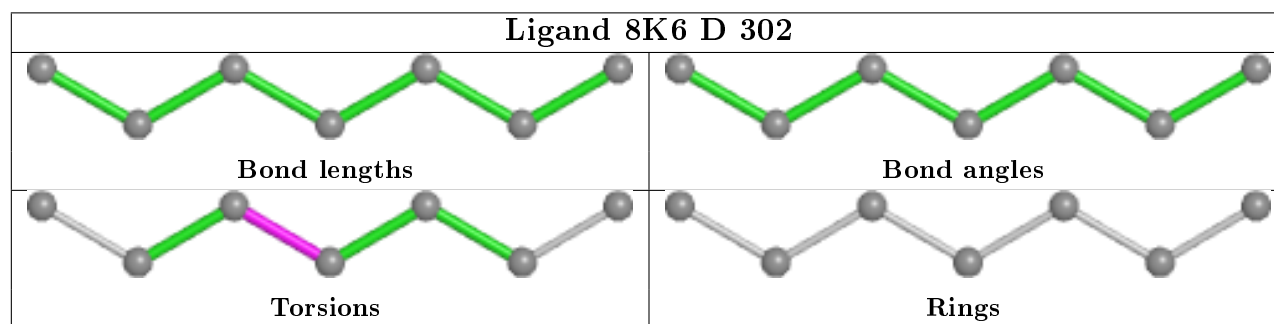
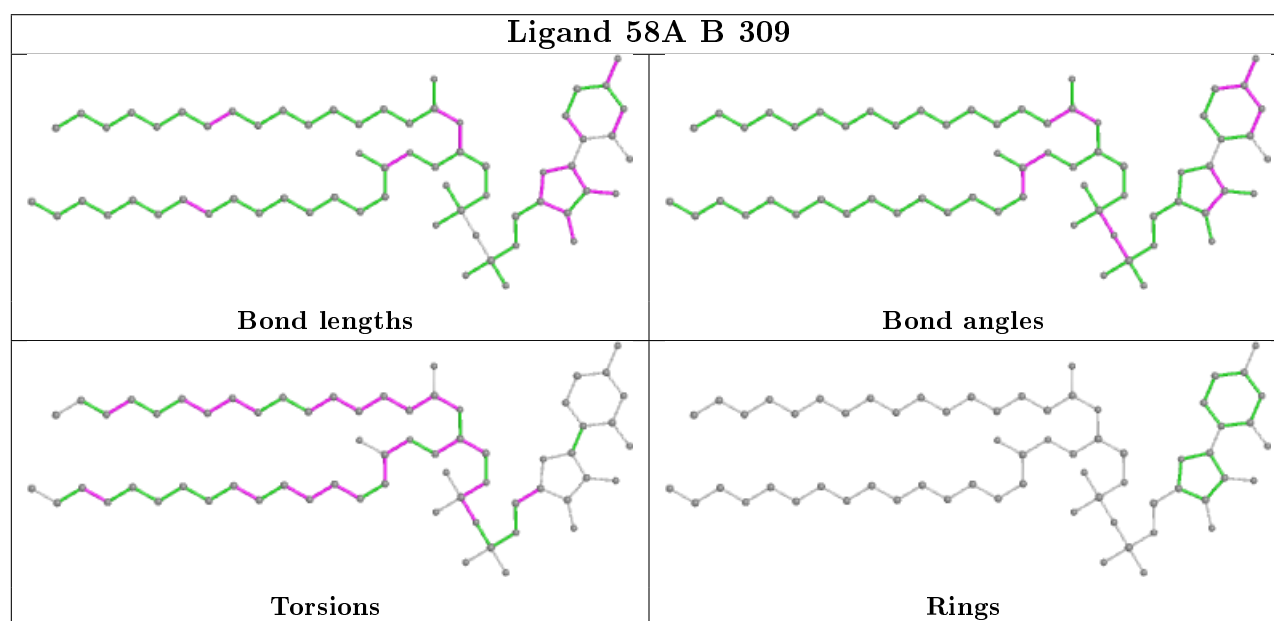
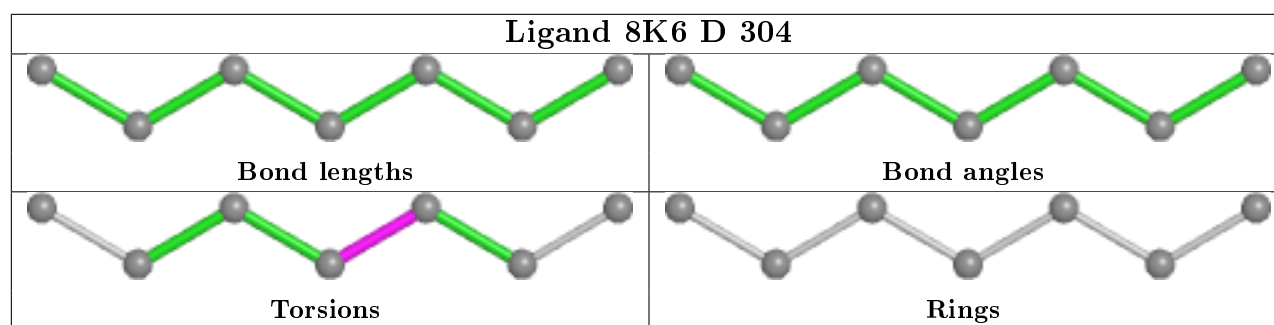
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	302	8K6	1	0
2	B	306	8K6	1	0
2	C	301	8K6	1	0
2	C	306	8K6	1	0
2	A	306	8K6	1	0
4	B	309	58A	1	0
2	C	304	8K6	1	0
2	A	301	8K6	1	0
4	D	315	58A	7	0
4	C	310	58A	5	0
2	D	307	8K6	1	0
4	A	311	58A	5	0

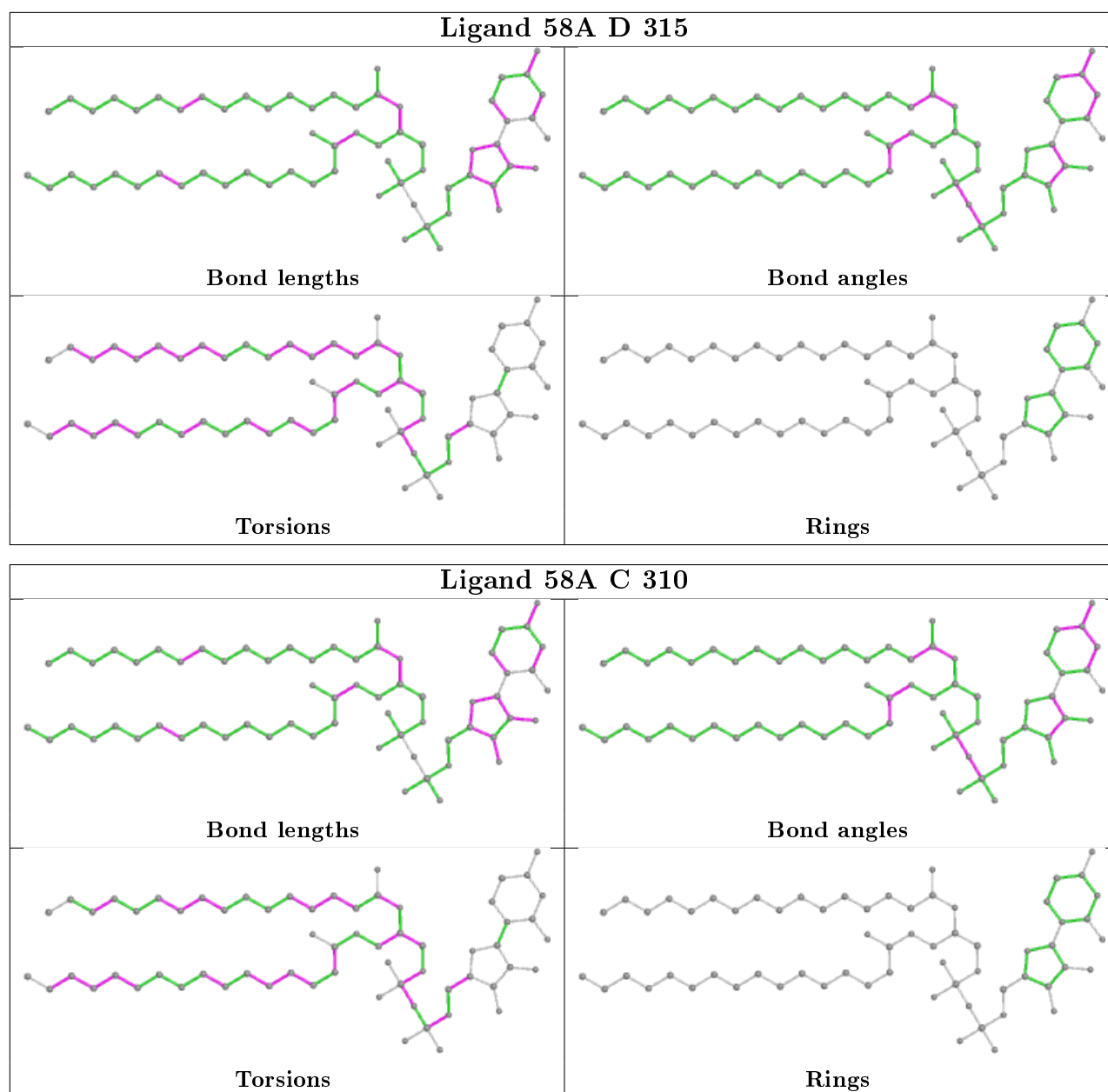
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

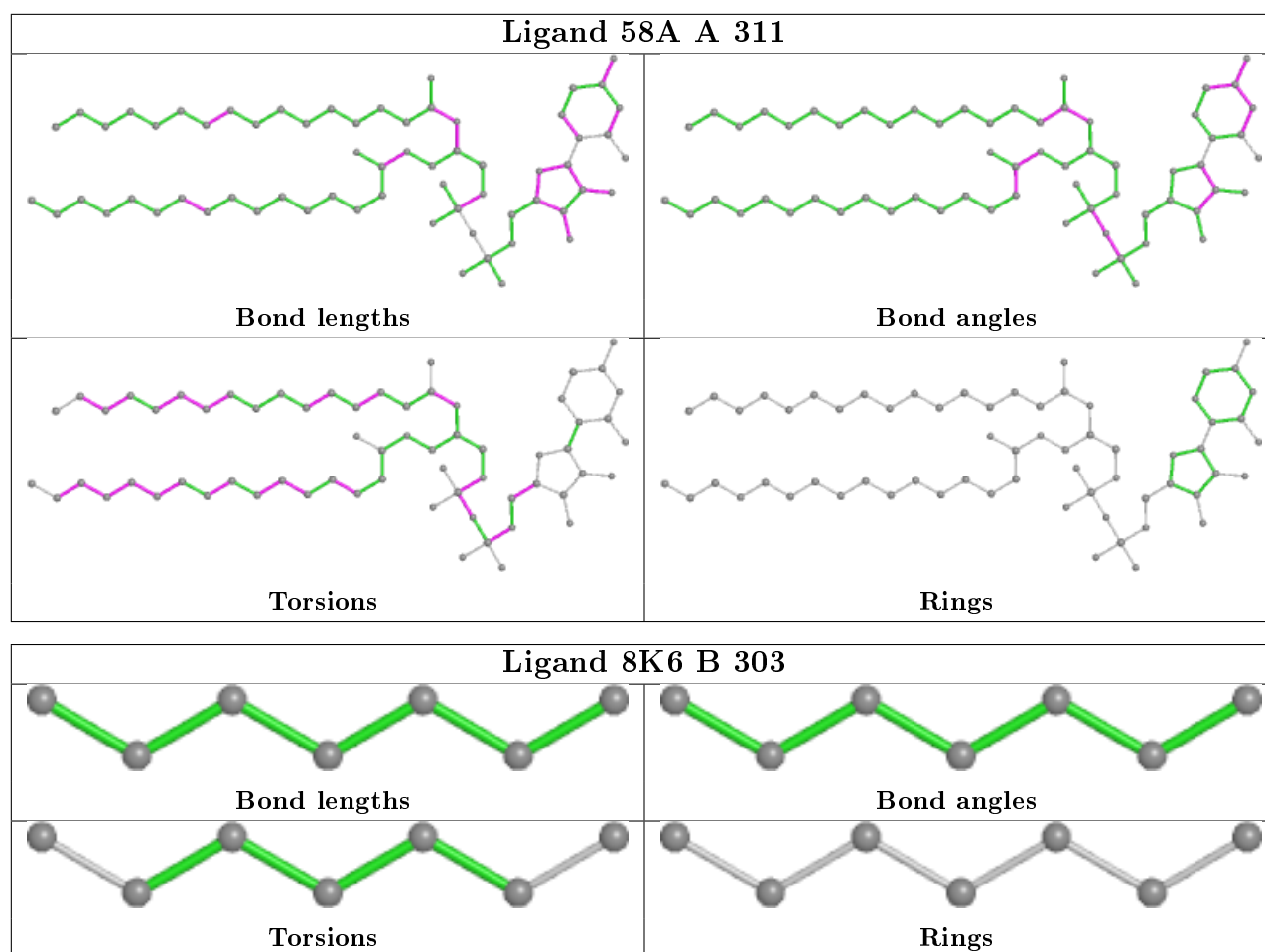












5.7 Other polymers [i](#)

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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, 95th 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	340/342 (99%)	-0.16	0 100 100	38, 68, 106, 154	0
1	B	342/342 (100%)	-0.10	1 (0%) 94 89	37, 69, 119, 151	0
1	C	334/342 (97%)	-0.06	4 (1%) 79 66	44, 87, 149, 176	0
1	D	342/342 (100%)	-0.18	1 (0%) 94 89	35, 66, 127, 152	0
All	All	1358/1368 (99%)	-0.12	6 (0%) 92 86	35, 70, 134, 176	0

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	-62	GLY	3.9
1	B	148	ALA	2.8
1	C	43	ALA	2.7
1	C	-28	SER	2.6
1	C	44	LEU	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, 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.

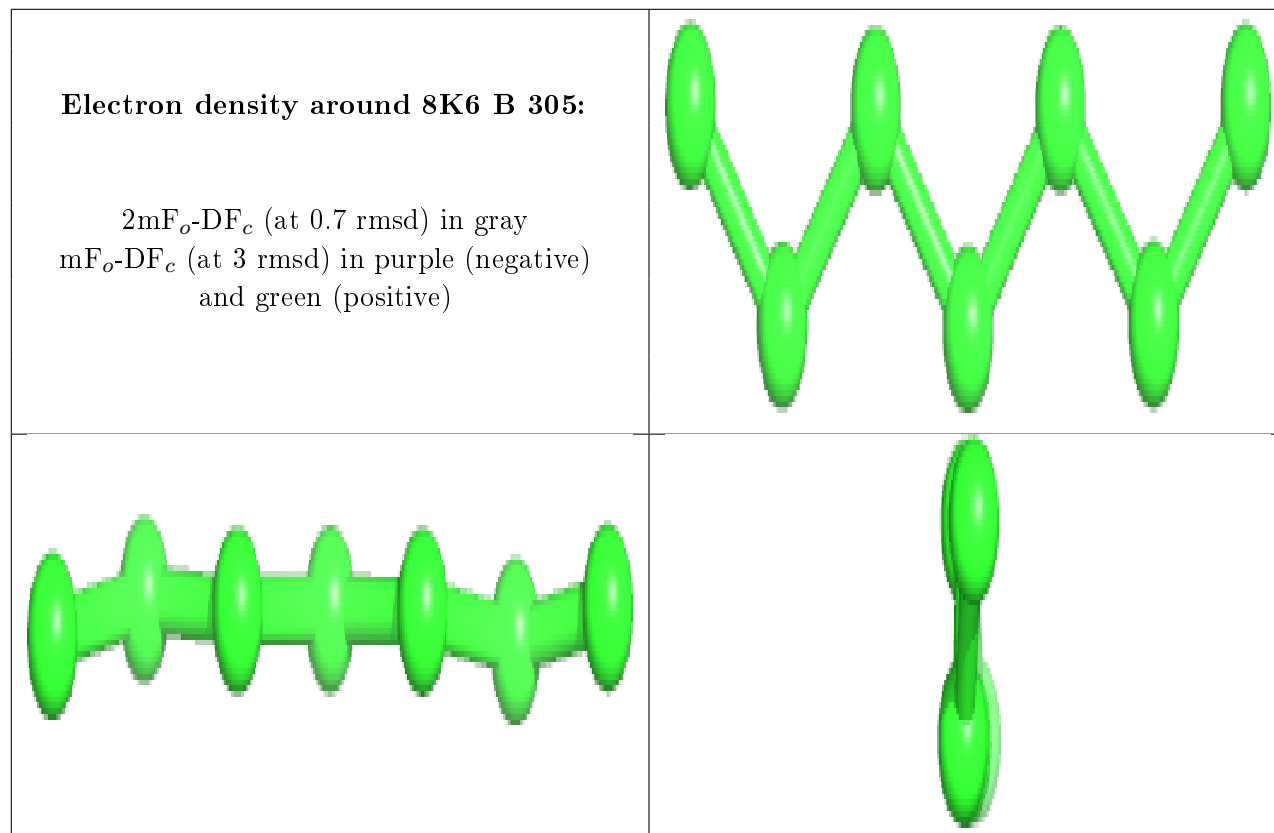
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	8K6	B	305	7/18	0.45	1.36	57,68,77,90	0
2	8K6	C	301	7/18	0.46	0.48	61,69,83,92	0
3	MG	D	313	1/1	0.65	0.16	64,64,64,64	0
2	8K6	B	303	7/18	0.67	0.50	50,51,57,64	0
2	8K6	D	310	7/18	0.69	0.78	63,73,75,90	0
2	8K6	A	305	7/18	0.71	0.91	45,48,50,56	0
3	MG	C	308	1/1	0.74	0.13	70,70,70,70	0
2	8K6	D	312	7/18	0.74	0.42	51,52,54,61	0
2	8K6	C	302	7/18	0.76	0.62	44,51,58,60	0
2	8K6	C	303	7/18	0.77	0.59	44,47,54,56	0
2	8K6	C	305	7/18	0.78	0.73	63,66,71,71	0
2	8K6	D	308	7/18	0.80	0.57	32,33,41,44	0
2	8K6	D	305	7/18	0.80	0.65	26,28,31,34	0
2	8K6	B	306	7/18	0.82	0.40	47,51,52,53	0
2	8K6	D	304	7/18	0.83	0.22	60,74,85,91	0
2	8K6	A	308	7/18	0.83	0.54	35,36,37,37	0
2	8K6	D	309	7/18	0.83	0.40	55,57,64,76	0
2	8K6	A	302	7/18	0.83	0.40	46,49,54,65	0
2	8K6	B	301	7/18	0.83	0.64	37,39,41,42	0
2	8K6	D	302	7/18	0.84	0.29	40,45,48,48	0
2	8K6	D	311	7/18	0.84	0.50	61,62,69,84	0
2	8K6	D	306	7/18	0.84	0.53	40,41,46,47	0
2	8K6	A	306	7/18	0.84	0.92	44,48,54,63	0
2	8K6	C	306	7/18	0.84	0.26	63,65,70,79	0
2	8K6	B	302	7/18	0.85	0.58	27,28,29,29	0
2	8K6	B	304	7/18	0.85	0.60	36,37,39,42	0
3	MG	B	308	1/1	0.85	0.09	63,63,63,63	0
2	8K6	C	304	7/18	0.85	0.82	51,53,55,57	0
2	8K6	A	303	7/18	0.86	0.46	35,37,40,41	0
2	8K6	D	301	7/18	0.86	0.62	36,36,40,43	0
2	8K6	A	307	7/18	0.88	0.45	33,35,39,39	0
2	8K6	D	303	7/18	0.88	0.23	37,38,40,40	0
4	58A	C	310	64/68	0.88	0.38	59,73,101,139	0
2	8K6	D	307	7/18	0.88	0.28	38,40,44,44	0
3	MG	B	307	1/1	0.89	0.21	63,63,63,63	0
2	8K6	A	301	7/18	0.89	0.42	40,40,44,46	0
4	58A	B	309	64/68	0.90	0.42	55,75,116,127	0
4	58A	D	315	64/68	0.90	0.40	56,67,84,126	0
2	8K6	C	307	7/18	0.91	0.25	46,50,56,60	0
4	58A	A	311	64/68	0.91	0.37	48,63,91,113	0
3	MG	A	309	1/1	0.92	0.21	59,59,59,59	0
2	8K6	A	304	7/18	0.92	1.05	36,38,41,44	0
3	MG	C	309	1/1	0.92	0.06	69,69,69,69	0

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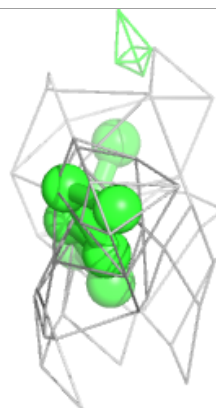
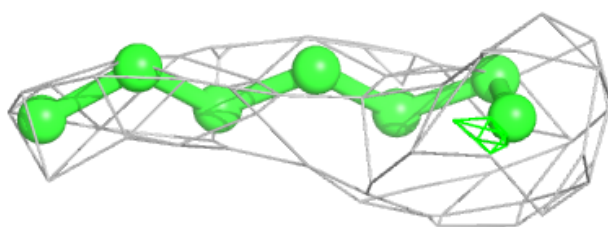
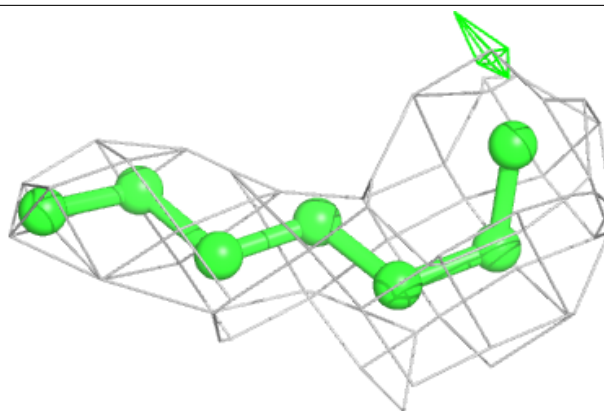
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	MG	D	314	1/1	0.93	0.11	63,63,63,63	0
3	MG	A	310	1/1	0.99	0.04	61,61,61,61	0

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.

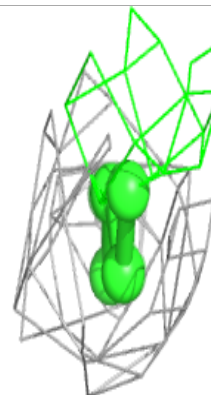
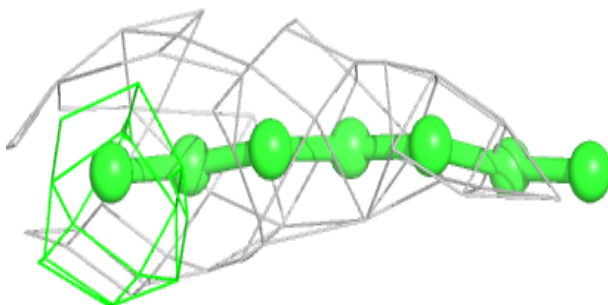
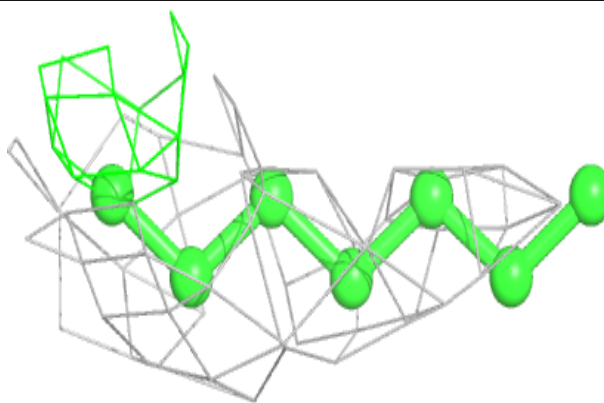


Electron density around 8K6 C 301:

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

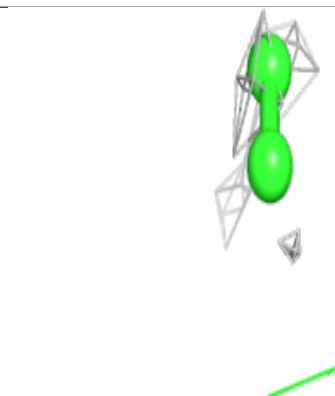
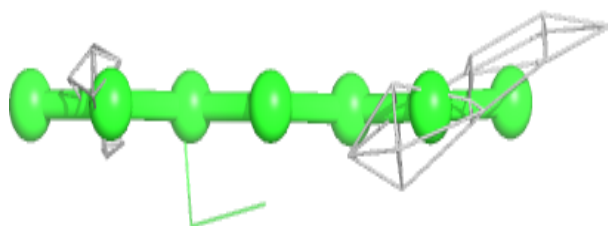
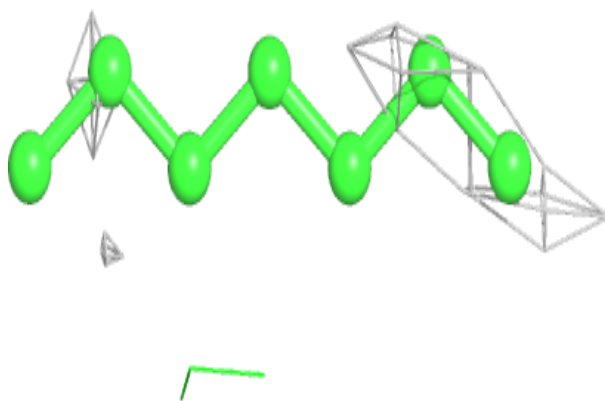
**Electron density around 8K6 B 303:**

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

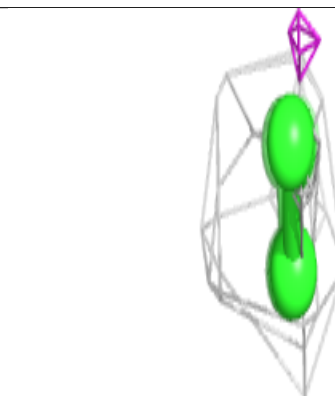
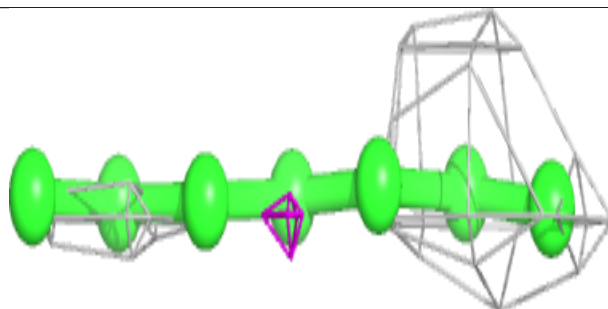
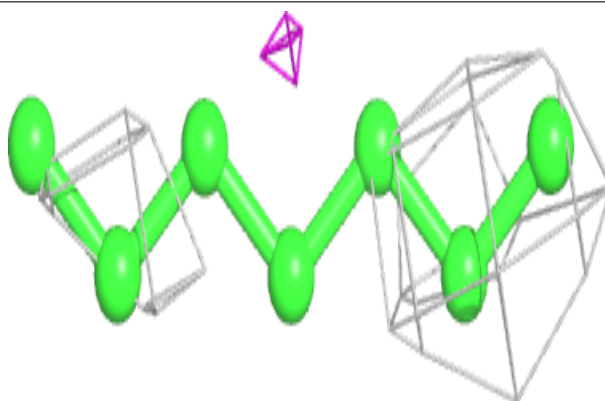


Electron density around 8K6 D 310:

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

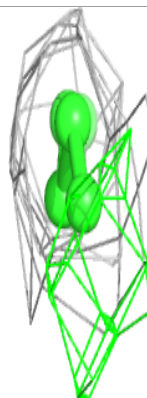
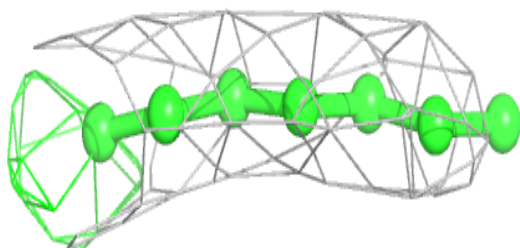
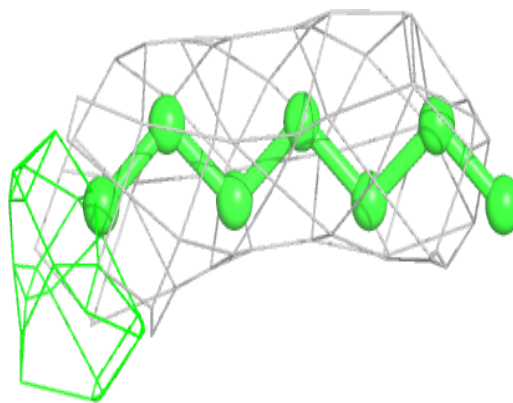
**Electron density around 8K6 A 305:**

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

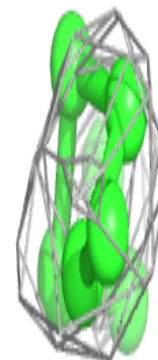
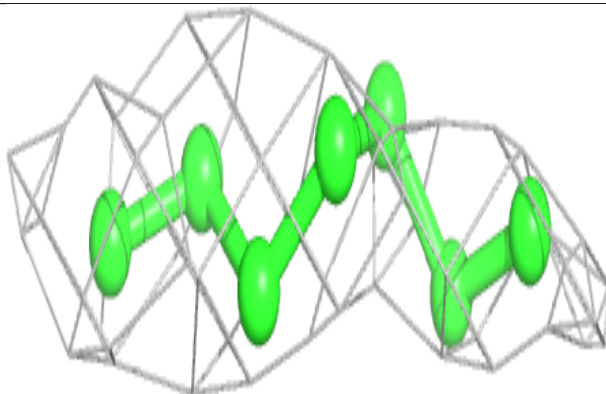
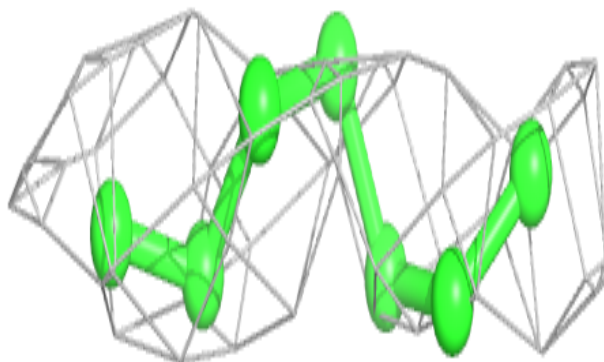


Electron density around 8K6 D 312:

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

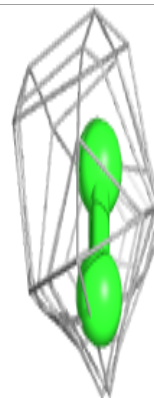
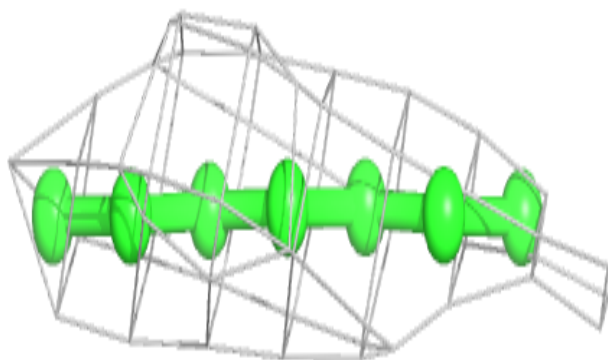
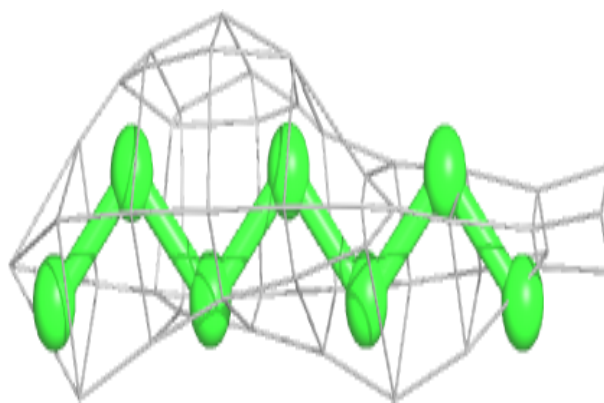
**Electron density around 8K6 C 302:**

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

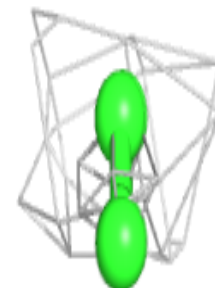
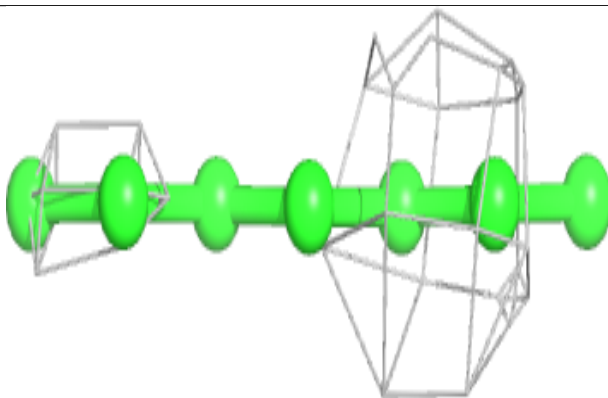
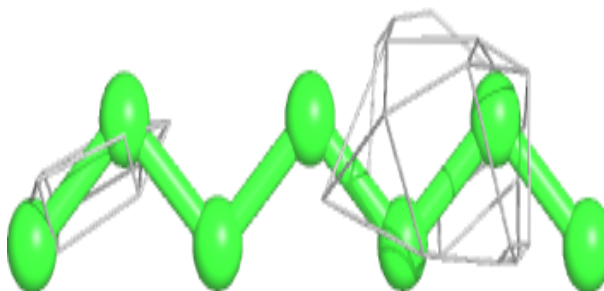


Electron density around 8K6 C 303:

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

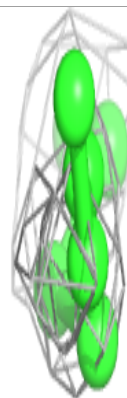
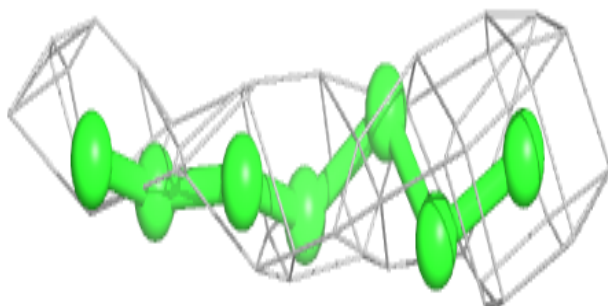
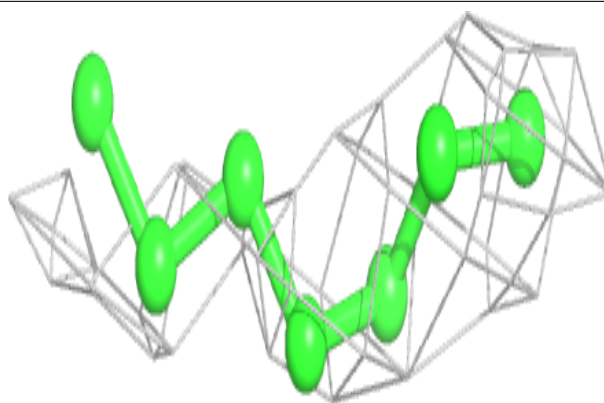
**Electron density around 8K6 C 305:**

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

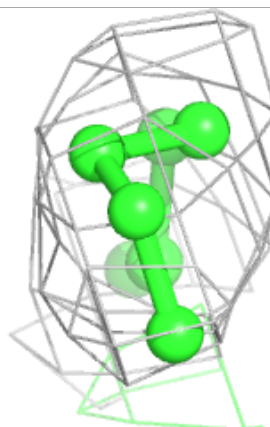
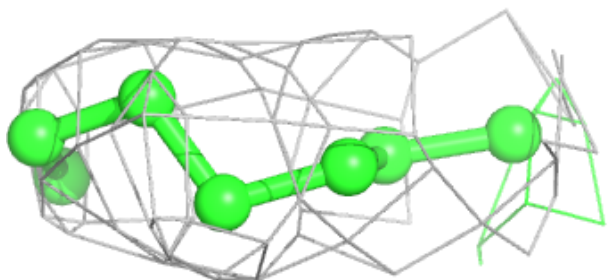
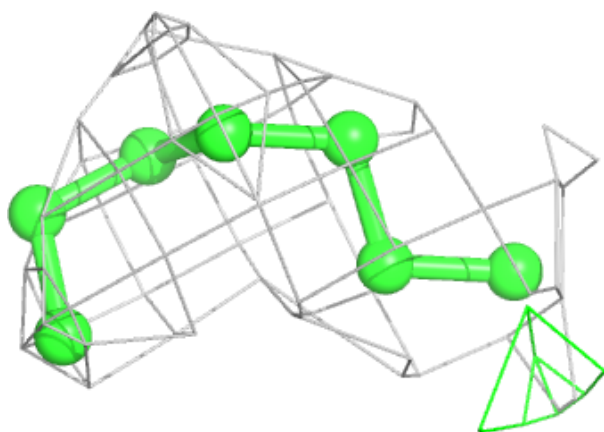


Electron density around 8K6 D 305:

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

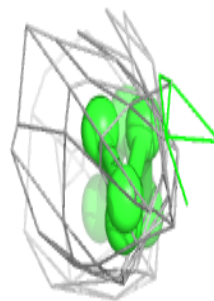
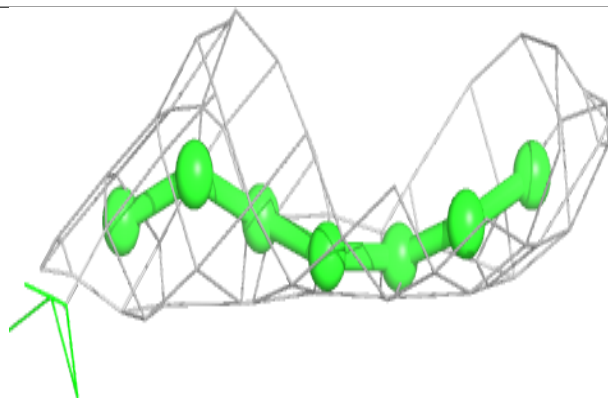
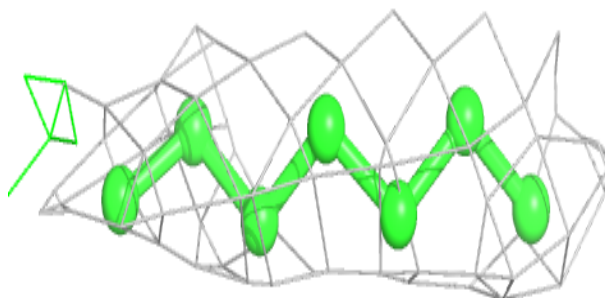
**Electron density around 8K6 D 304:**

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

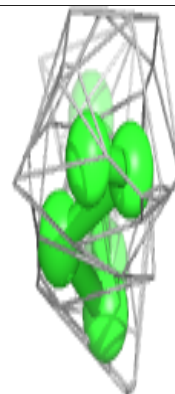
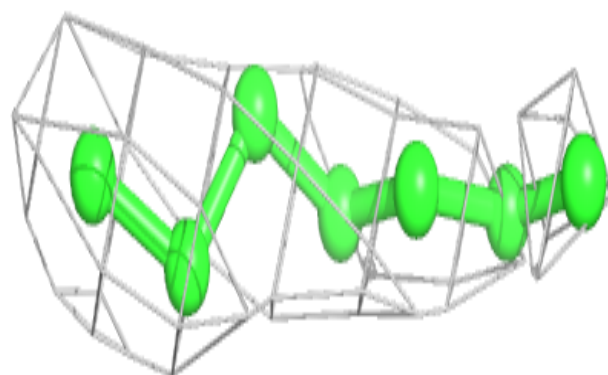
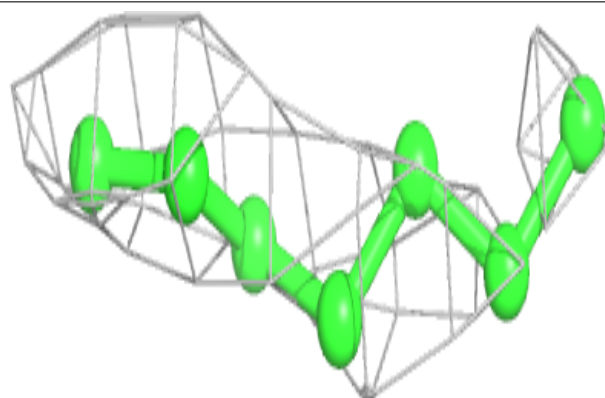


Electron density around 8K6 D 309:

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

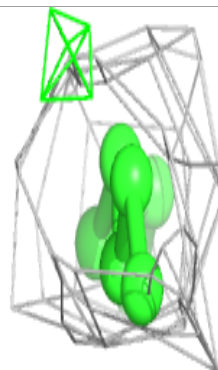
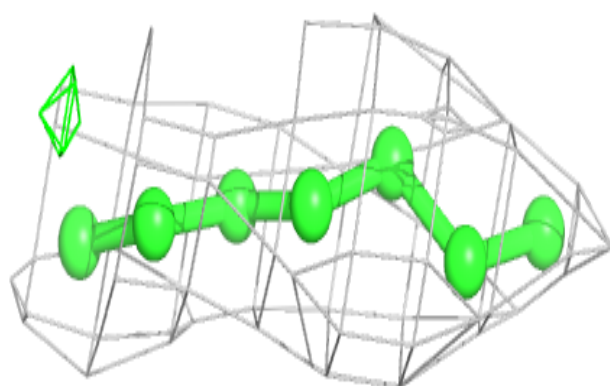
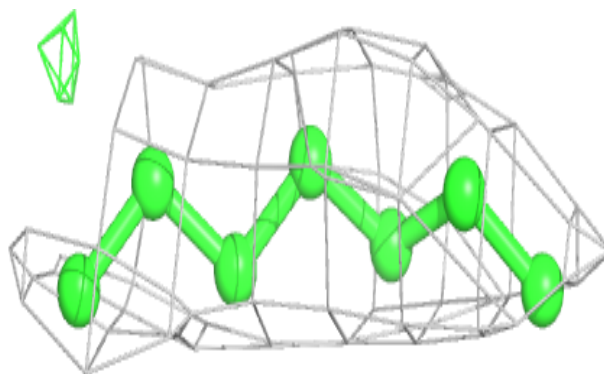
**Electron density around 8K6 B 301:**

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

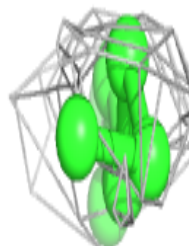
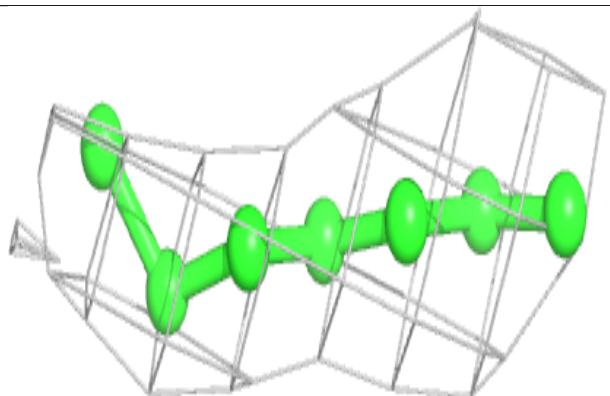
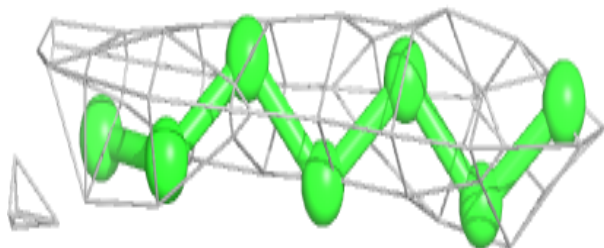


Electron density around 8K6 D 302:

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

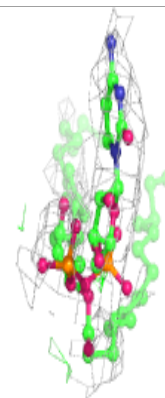
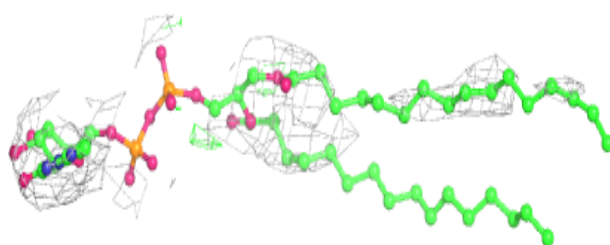
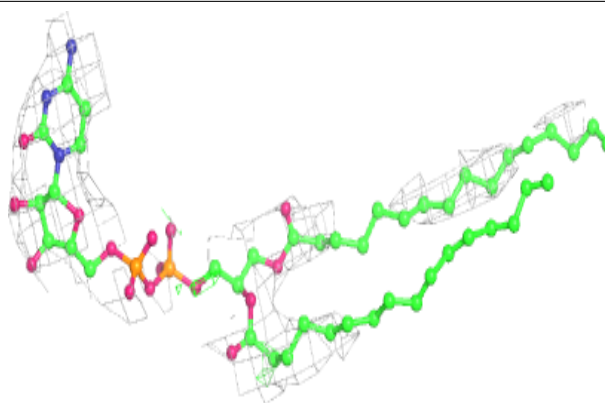
**Electron density around 8K6 D 301:**

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

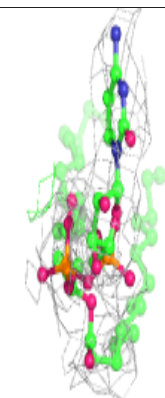
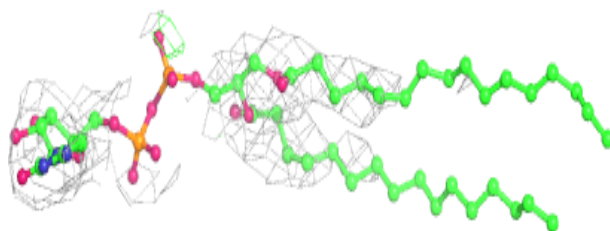
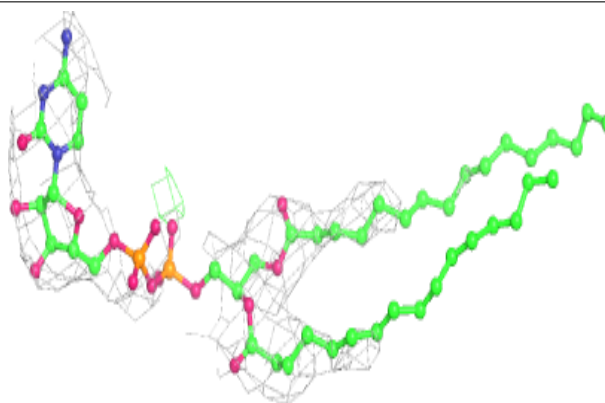


Electron density around 58A C 310:

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

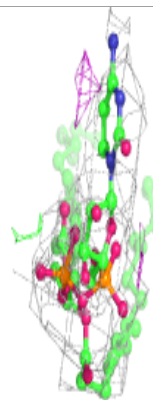
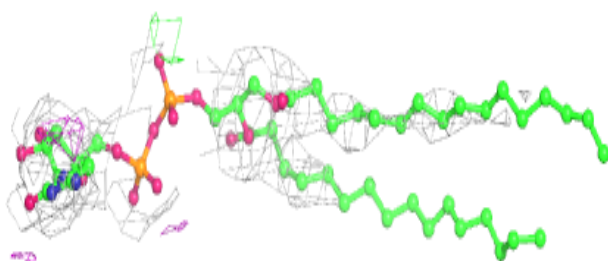
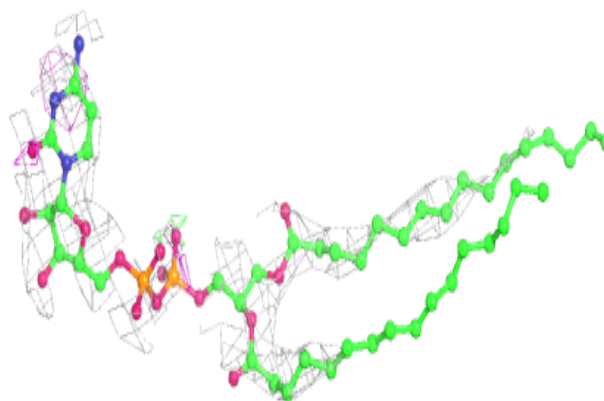
**Electron density around 58A B 309:**

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

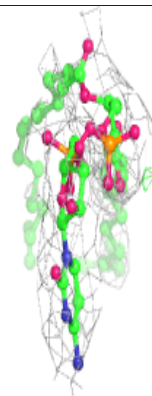
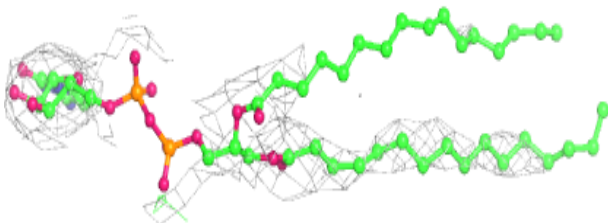
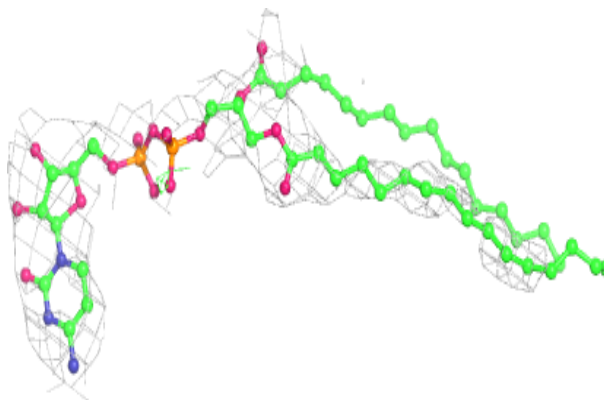


Electron density around 58A D 315:

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

**Electron density around 58A 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.