



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 8, 2020 – 02:11 AM BST

PDB ID : 6KHM
Title : Lipase (Open form)
Authors : Kim, H.J.; Kwon, A.R.
Deposited on : 2019-07-16
Resolution : 2.40 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

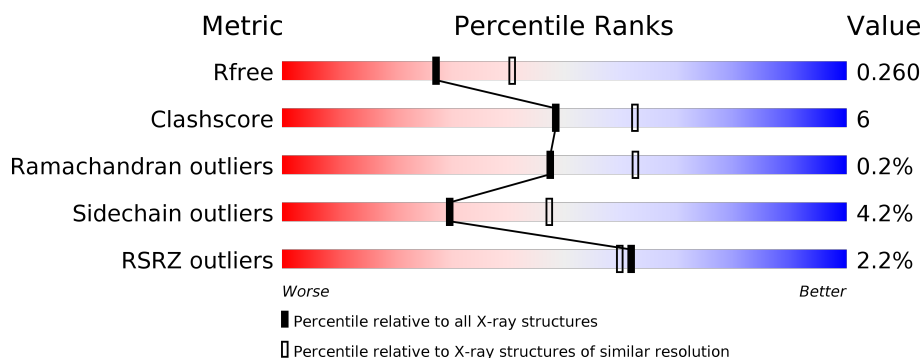
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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.







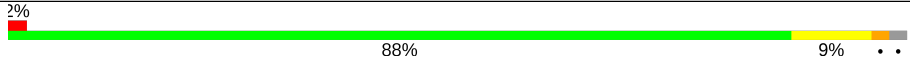
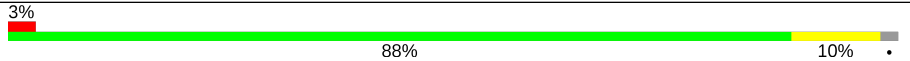
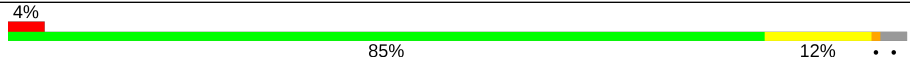
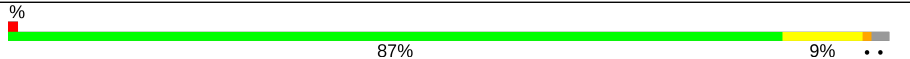
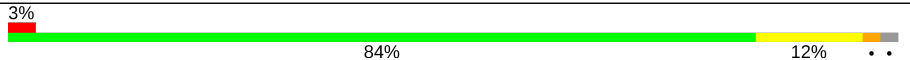
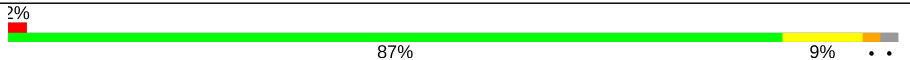
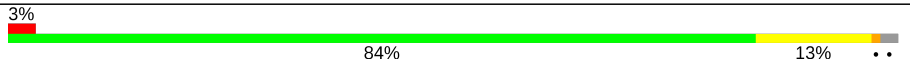
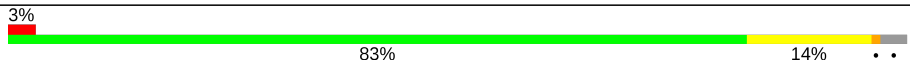
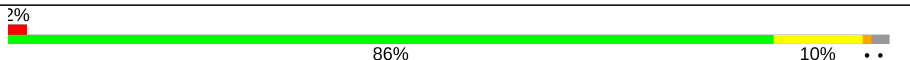



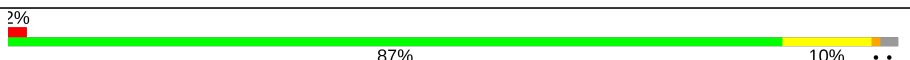
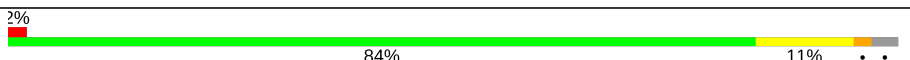
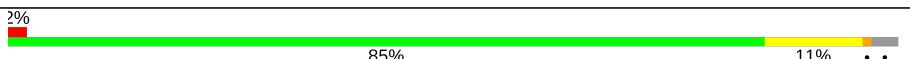
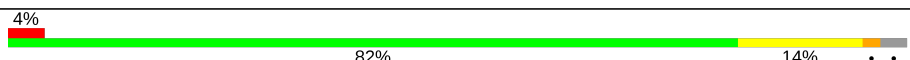
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	317	<div> <div>3%</div> <div> <div></div> <div>81%</div> <div>15%</div> <div>• •</div> </div> </div>
1	B	317	<div> <div>%</div> <div> <div></div> <div>83%</div> <div>13%</div> <div>• •</div> </div> </div>
1	C	317	<div> <div>2%</div> <div> <div></div> <div>87%</div> <div>10%</div> <div>• •</div> </div> </div>
1	D	317	<div> <div>3%</div> <div> <div></div> <div>86%</div> <div>10%</div> <div>• •</div> </div> </div>
1	E	317	<div> <div>2%</div> <div> <div></div> <div>84%</div> <div>14%</div> <div>• •</div> </div> </div>
1	F	317	<div> <div></div> <div> <div></div> <div>88%</div> <div>9%</div> <div>•</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	317	
1	H	317	
1	I	317	
1	J	317	
1	K	317	
1	L	317	
1	M	317	
1	N	317	
1	O	317	
1	P	317	
1	Q	317	
1	R	317	
1	S	317	
1	T	317	
1	U	317	
1	V	317	
1	W	317	
1	X	317	
1	Y	317	
1	Z	317	

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
2	DKL	A	900	-	X	-	-
2	DKL	C	900	-	-	X	X
2	DKL	X	900	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	DKO	B	900	-	X	-	-
4	DK6	D	900	-	-	-	X
4	DK6	H	900	-	X	X	-
4	DK6	S	900	-	X	-	X
4	DK6	Z	900	-	X	X	-
5	DKF	E	900	-	-	X	-
5	DKF	G	900	-	-	-	X
5	DKF	M	900	-	-	-	X
5	DKF	U	900	-	X	-	X
5	DKF	W	900	-	X	-	X
6	DK9	O	900	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 64002 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 Hydrolase, alpha/beta domain protein.

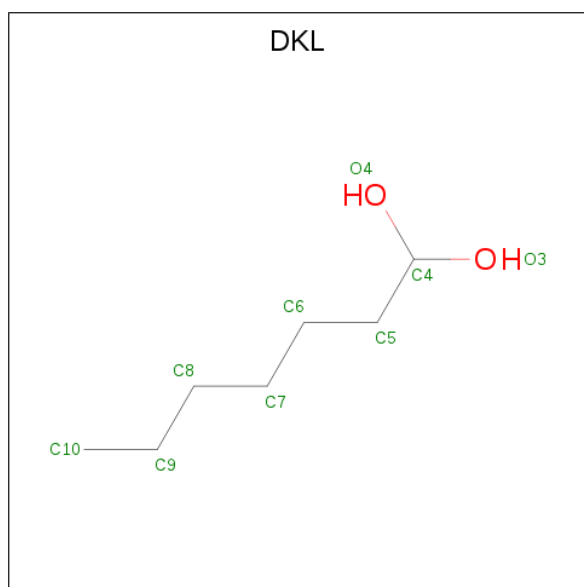
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	310	Total	C	N	O	S	0	0	0
			2360	1476	421	453	10			
1	B	309	Total	C	N	O	S	0	0	0
			2349	1470	417	452	10			
1	C	309	Total	C	N	O	S	0	0	0
			2349	1470	417	452	10			
1	D	308	Total	C	N	O	S	0	0	0
			2341	1466	415	450	10			
1	E	311	Total	C	N	O	S	0	0	0
			2371	1482	425	454	10			
1	F	308	Total	C	N	O	S	0	0	0
			2341	1466	415	450	10			
1	G	310	Total	C	N	O	S	0	0	0
			2360	1476	421	453	10			
1	H	309	Total	C	N	O	S	0	0	0
			2349	1470	417	452	10			
1	I	311	Total	C	N	O	S	0	0	0
			2371	1482	425	454	10			
1	J	310	Total	C	N	O	S	0	0	0
			2360	1476	421	453	10			
1	K	312	Total	C	N	O	S	0	0	0
			2379	1488	426	455	10			
1	L	312	Total	C	N	O	S	0	0	0
			2379	1488	426	455	10			
1	M	309	Total	C	N	O	S	0	0	0
			2349	1470	417	452	10			
1	N	310	Total	C	N	O	S	0	0	0
			2360	1476	421	453	10			
1	O	310	Total	C	N	O	S	0	0	0
			2360	1476	421	453	10			
1	P	310	Total	C	N	O	S	0	0	0
			2360	1476	421	453	10			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	311	Total	C	N	O	S	0	0	0
			2371	1482	425	454	10			
1	R	309	Total	C	N	O	S	0	0	0
			2349	1470	417	452	10			
1	S	310	Total	C	N	O	S	0	0	0
			2360	1476	421	453	10			
1	T	309	Total	C	N	O	S	0	0	0
			2349	1470	417	452	10			
1	U	310	Total	C	N	O	S	0	0	0
			2360	1476	421	453	10			
1	V	309	Total	C	N	O	S	0	0	0
			2349	1470	417	452	10			
1	X	309	Total	C	N	O	S	0	0	0
			2349	1470	417	452	10			
1	Y	309	Total	C	N	O	S	0	0	0
			2349	1470	417	452	10			
1	W	310	Total	C	N	O	S	0	0	0
			2360	1476	421	453	10			
1	Z	309	Total	C	N	O	S	0	0	0
			2349	1470	417	452	10			

- Molecule 2 is heptane-1,1-diol (three-letter code: DKL) (formula: C₇H₁₆O₂) (labeled as "Ligand of Interest" by author).



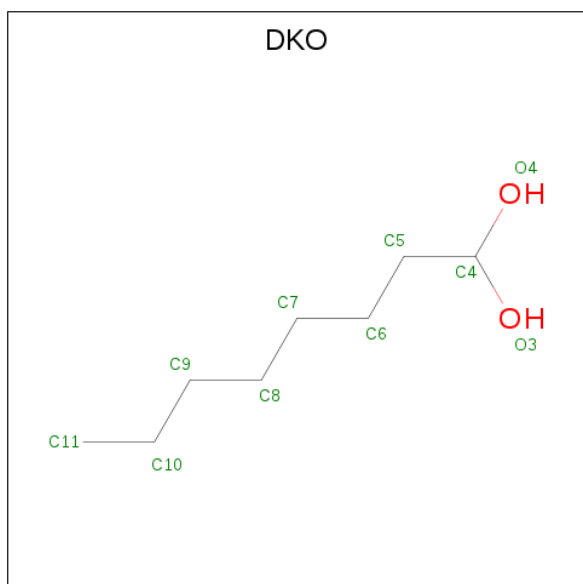
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			9	7	2		

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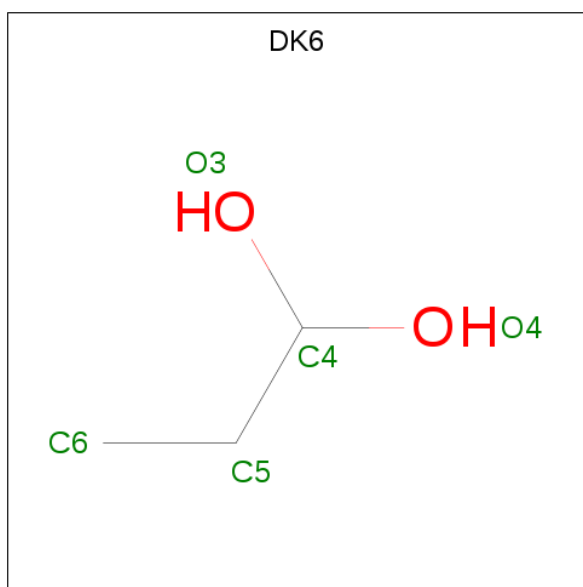
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	C	O	0	0
			9	7	2		
2	Q	1	Total	C	O	0	0
			9	7	2		
2	T	1	Total	C	O	0	0
			9	7	2		
2	X	1	Total	C	O	0	0
			9	7	2		

- Molecule 3 is octane-1,1-diol (three-letter code: DKO) (formula: $C_8H_{18}O_2$) (labeled as "Ligand of Interest" by author).



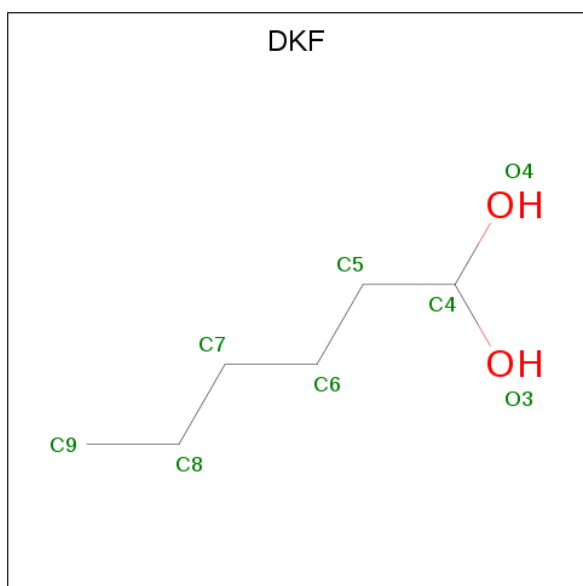
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			10	8	2		
3	N	1	Total	C	O	0	0
			10	8	2		
3	R	1	Total	C	O	0	0
			10	8	2		

- Molecule 4 is propane-1,1-diol (three-letter code: DK6) (formula: $C_3H_8O_2$) (labeled as "Ligand of Interest" by author).



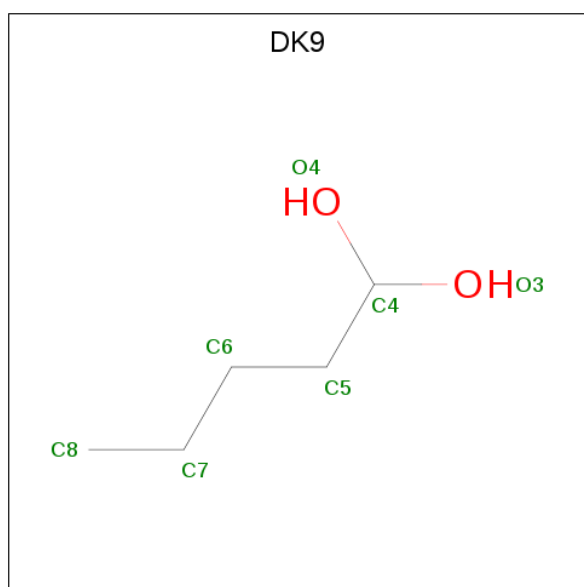
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	C	O	0	0
			5	3	2		
4	H	1	Total	C	O	0	0
			5	3	2		
4	S	1	Total	C	O	0	0
			5	3	2		
4	Z	1	Total	C	O	0	0
			5	3	2		

- Molecule 5 is hexane-1,1-diol (three-letter code: DKF) (formula: $C_6H_{14}O_2$) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	E	1	Total C O 8 6 2	0	0
5	G	1	Total C O 8 6 2	0	0
5	I	1	Total C O 8 6 2	0	0
5	J	1	Total C O 8 6 2	0	0
5	K	1	Total C O 8 6 2	0	0
5	L	1	Total C O 8 6 2	0	0
5	M	1	Total C O 8 6 2	0	0
5	U	1	Total C O 8 6 2	0	0
5	V	1	Total C O 8 6 2	0	0
5	Y	1	Total C O 8 6 2	0	0
5	W	1	Total C O 8 6 2	0	0

- Molecule 6 is pentane-1,1-diol (three-letter code: DK9) (formula: $C_5H_{12}O_2$) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	F	1	Total C O 7 5 2	0	0
6	O	1	Total C O 7 5 2	0	0
6	P	1	Total C O 7 5 2	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	103	Total O 103 103	0	0
7	B	121	Total O 121 121	0	0
7	C	108	Total O 108 108	0	0
7	D	140	Total O 140 140	0	0
7	E	126	Total O 126 126	0	0
7	F	131	Total O 131 131	0	0
7	G	130	Total O 130 130	0	0
7	H	113	Total O 113 113	0	0
7	I	82	Total O 82 82	0	0
7	J	87	Total O 87 87	0	0
7	K	116	Total O 116 116	0	0
7	L	147	Total O 147 147	0	0
7	M	69	Total O 69 69	0	0
7	N	85	Total O 85 85	0	0
7	O	108	Total O 108 108	0	0
7	P	36	Total O 36 36	0	0
7	Q	105	Total O 105 105	0	0

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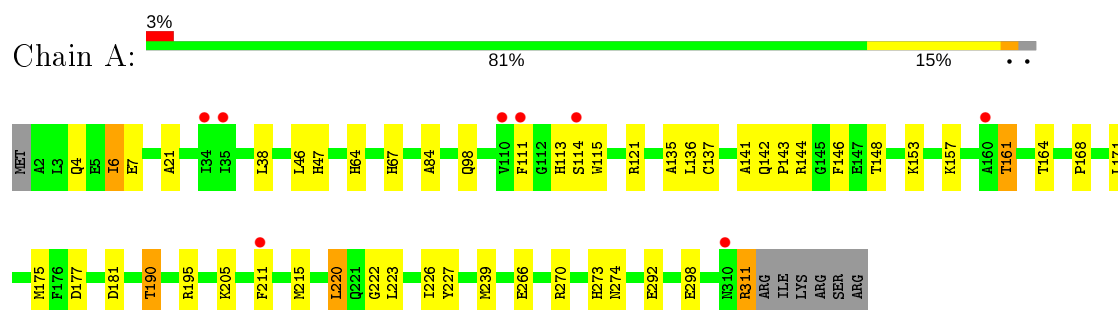
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	R	75	Total 75	O 75	0	0
7	S	128	Total 128	O 128	0	0
7	T	79	Total 79	O 79	0	0
7	U	80	Total 80	O 80	0	0
7	V	83	Total 83	O 83	0	0
7	X	63	Total 63	O 63	0	0
7	Y	82	Total 82	O 82	0	0
7	W	71	Total 71	O 71	0	0
7	Z	47	Total 47	O 47	0	0

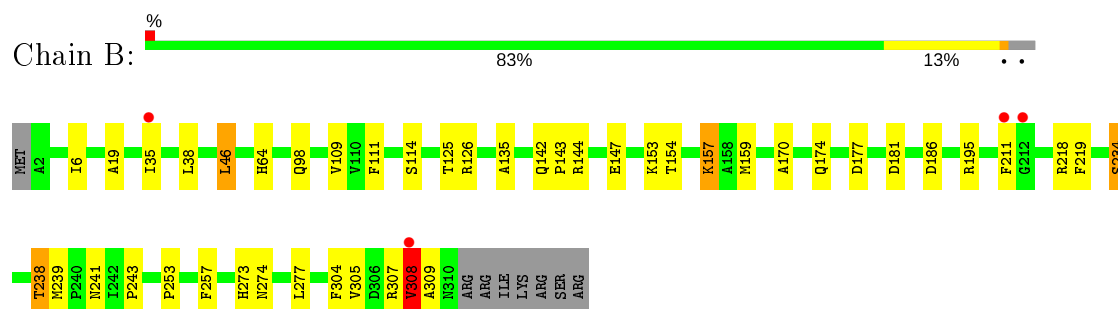
3 Residue-property plots

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.

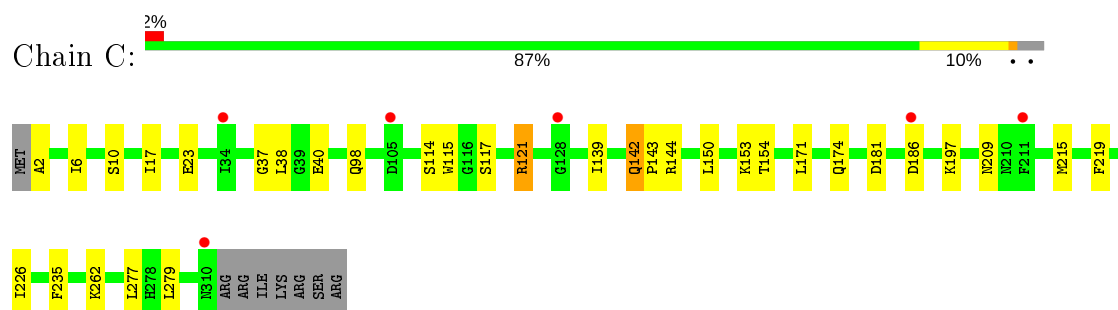
- Molecule 1: Hydrolase, alpha/beta domain protein



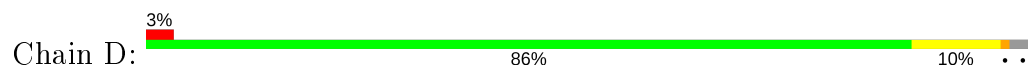
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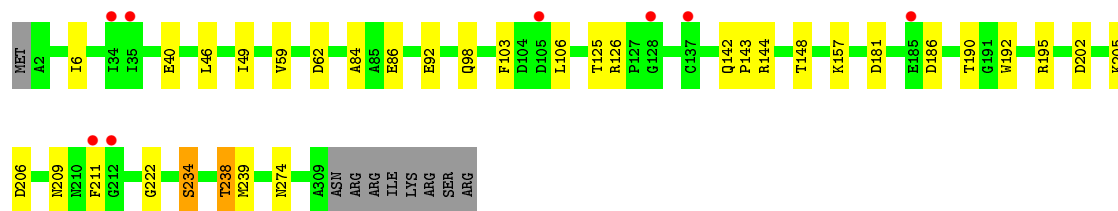


- Molecule 1: Hydrolase, alpha/beta domain protein

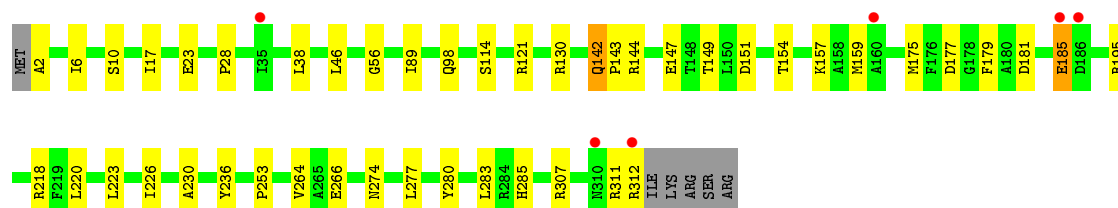
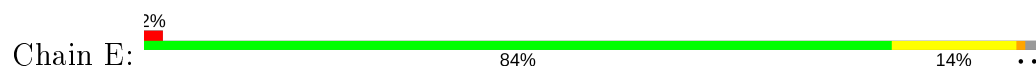


- Molecule 1: Hydrolase, alpha/beta domain protein

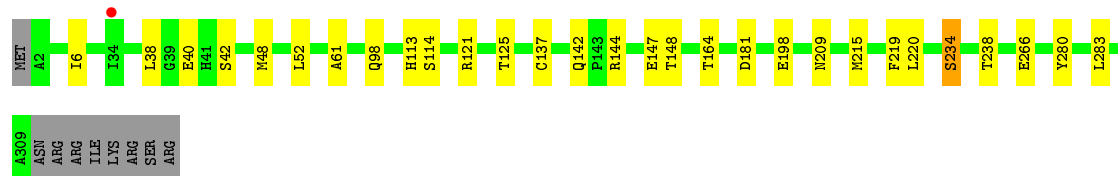
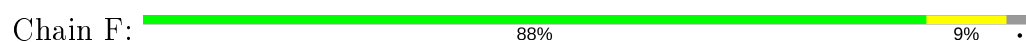




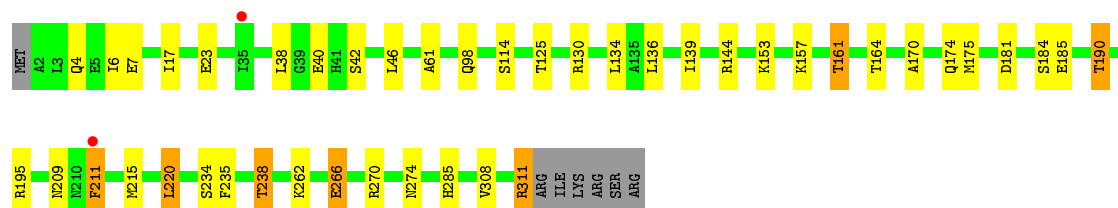
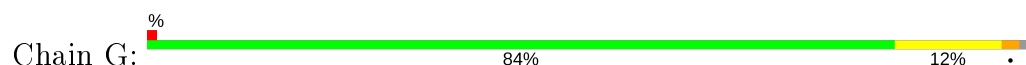
- Molecule 1: Hydrolase, alpha/beta domain protein



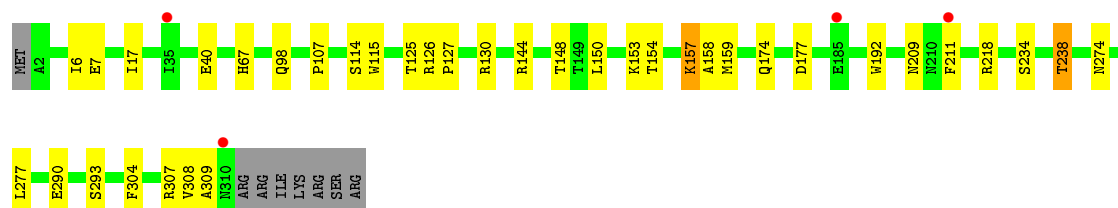
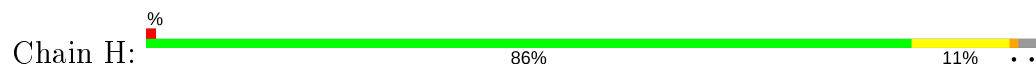
- Molecule 1: Hydrolase, alpha/beta domain protein



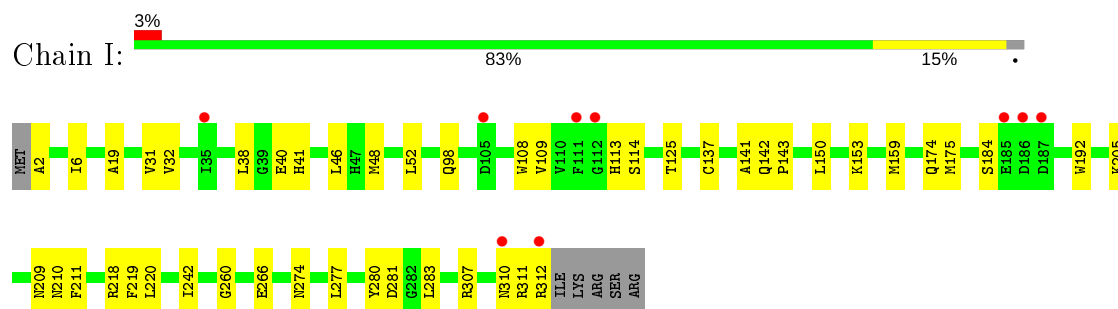
- Molecule 1: Hydrolase, alpha/beta domain protein



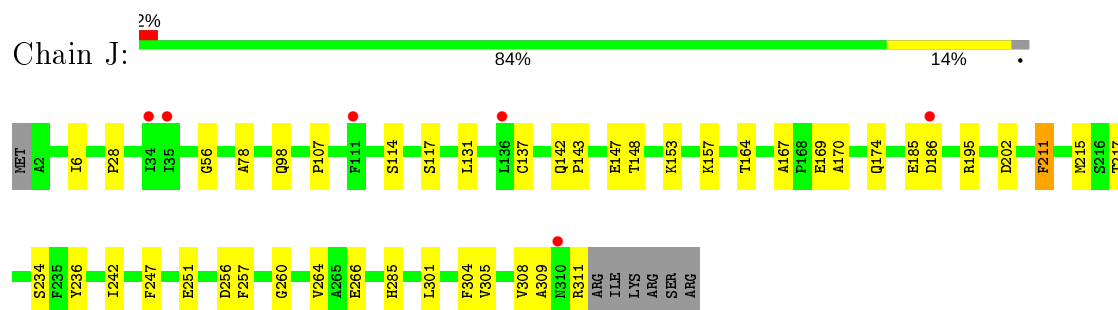
- Molecule 1: Hydrolase, alpha/beta domain protein



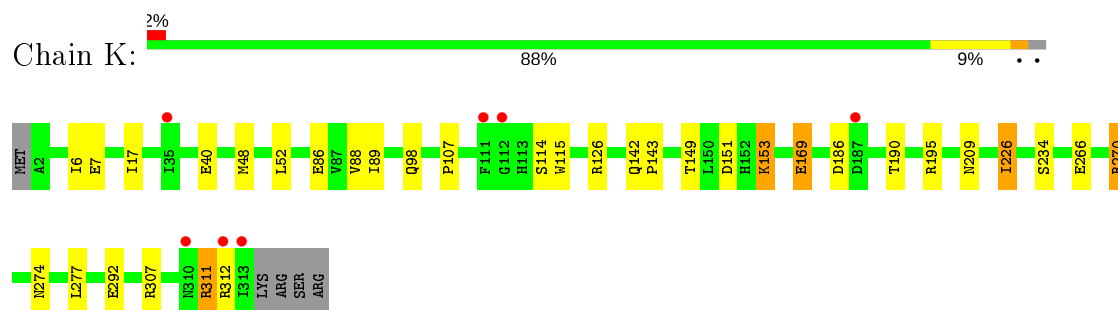
- Molecule 1: Hydrolase, alpha/beta domain protein



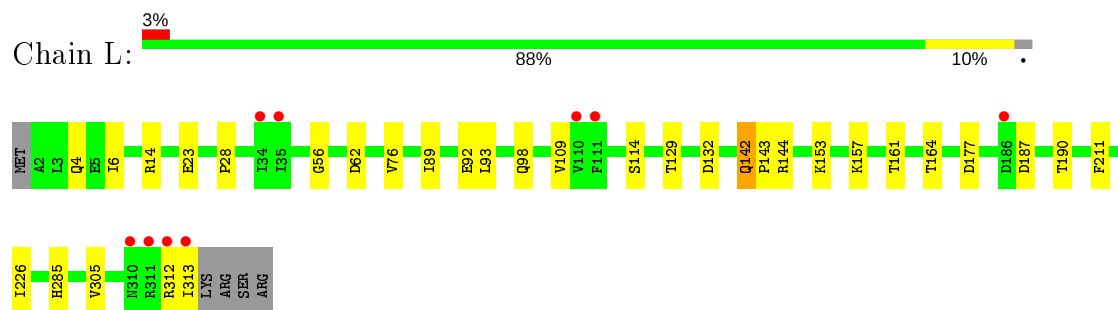
- Molecule 1: Hydrolase, alpha/beta domain protein



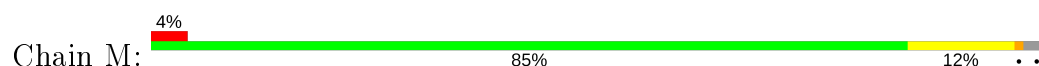
- Molecule 1: Hydrolase, alpha/beta domain protein

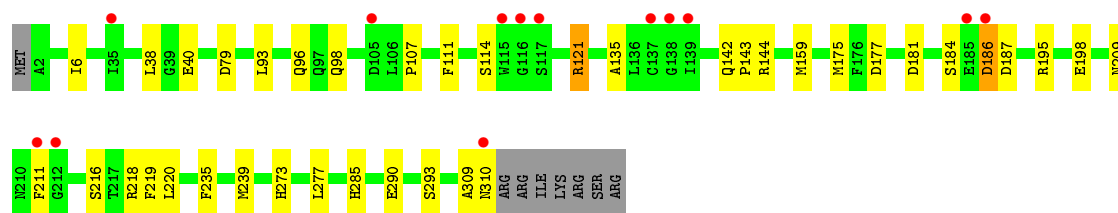


- Molecule 1: Hydrolase, alpha/beta domain protein

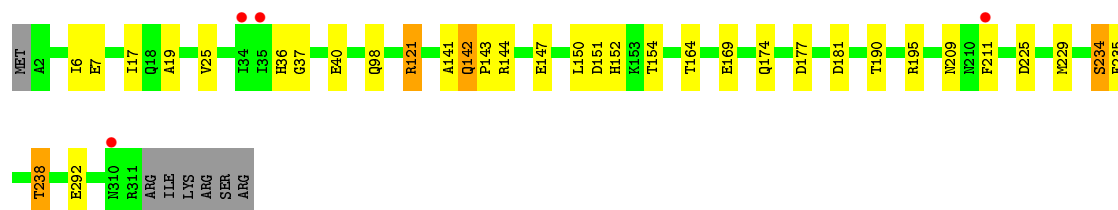
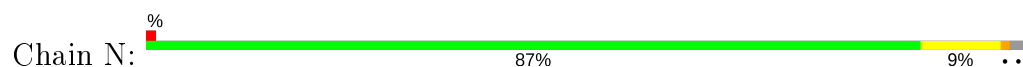


- Molecule 1: Hydrolase, alpha/beta domain protein

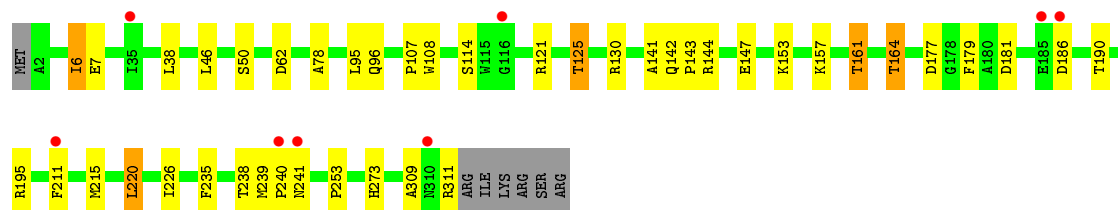
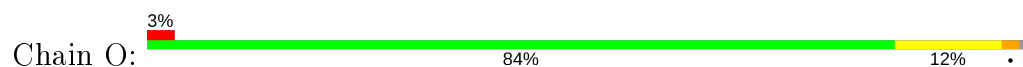




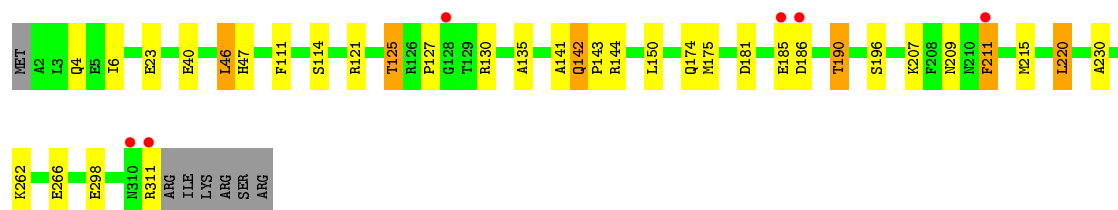
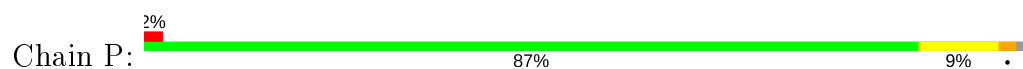
- Molecule 1: Hydrolase, alpha/beta domain protein



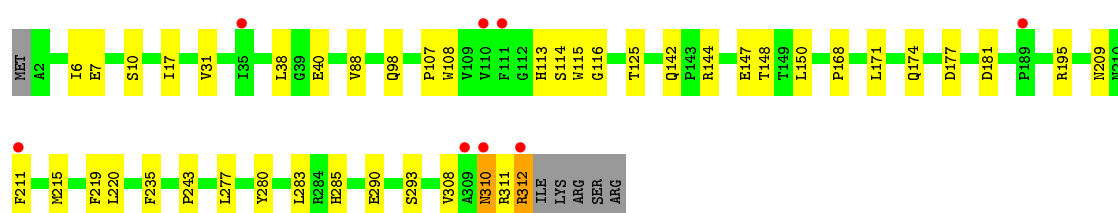
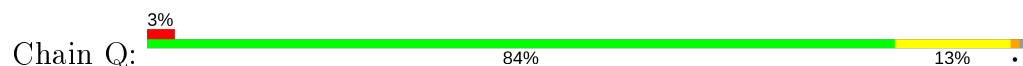
- Molecule 1: Hydrolase, alpha/beta domain protein




- Molecule 1: Hydrolase, alpha/beta domain protein

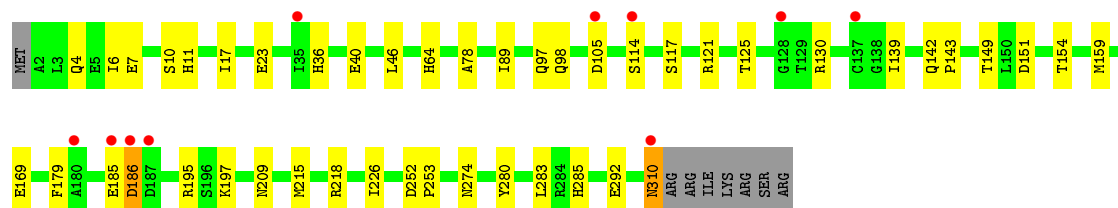


- Molecule 1: Hydrolase, alpha/beta domain protein




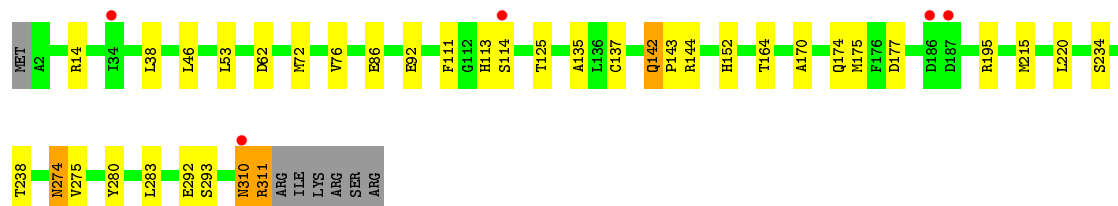
- Molecule 1: Hydrolase, alpha/beta domain protein

Chain R:  3% 83% 14% ..




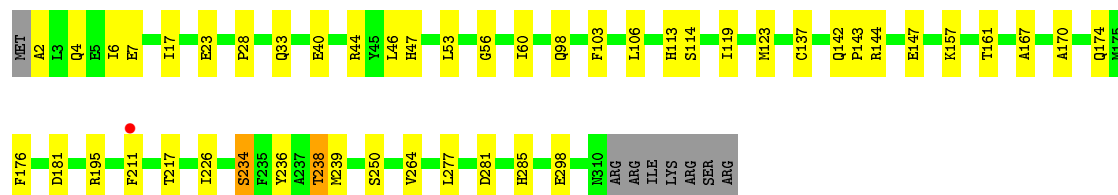
- Molecule 1: Hydrolase, alpha/beta domain protein

Chain S:  2% 86% 10% ..




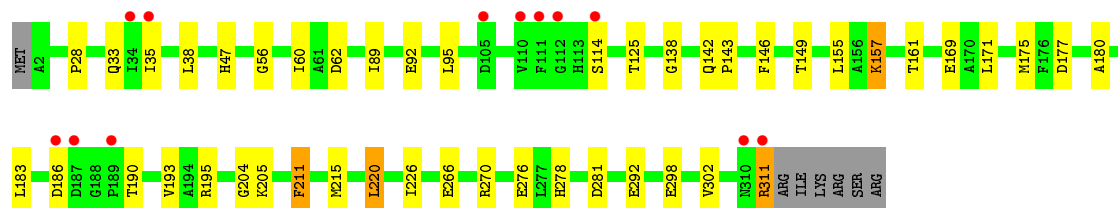
- Molecule 1: Hydrolase, alpha/beta domain protein

Chain T:  82% 15% ..




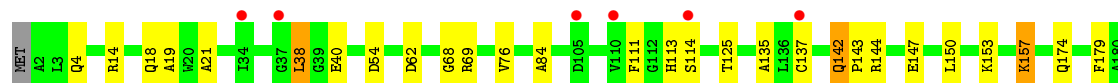
- Molecule 1: Hydrolase, alpha/beta domain protein

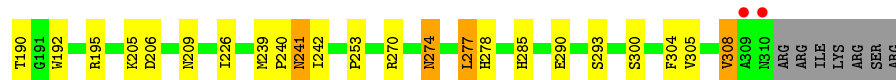
Chain U:  4% 83% 13% ..



- Molecule 1: Hydrolase, alpha/beta domain protein

Chain V:  2% 83% 14% ..





4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	185.86Å 185.86Å 205.10Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	28.64 – 2.40 28.63 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.5 (28.64-2.40) 99.6 (28.63-2.40)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.43 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.185 , 0.256 0.194 , 0.260	Depositor DCC
R_{free} test set	15636 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	30.0	Xtriage
Anisotropy	0.001	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 39.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.37$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l 0.000 for h,-h-k,-l 0.000 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	64002	wwPDB-VP
Average B, all atoms (Å ²)	32.0	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 25.20 % 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 3.3158e-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: DK6, DKF, DKL, DKO, DK9

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	0/2415	0.90	0/3284
1	B	0.77	0/2404	0.95	0/3270
1	C	0.78	0/2404	0.92	0/3270
1	D	0.78	0/2396	0.92	0/3259
1	E	0.78	0/2426	0.91	0/3298
1	F	0.79	0/2396	0.89	0/3259
1	G	0.79	0/2415	0.95	0/3284
1	H	0.78	0/2404	0.93	0/3270
1	I	0.76	0/2426	0.90	0/3298
1	J	0.77	0/2415	0.91	0/3284
1	K	0.79	0/2434	0.92	0/3309
1	L	0.77	0/2434	0.93	0/3309
1	M	0.79	0/2404	0.91	0/3270
1	N	0.79	0/2415	0.90	0/3284
1	O	0.80	0/2415	0.90	0/3284
1	P	0.80	0/2415	0.94	0/3284
1	Q	0.77	0/2426	0.90	0/3298
1	R	0.79	0/2404	0.90	0/3270
1	S	0.78	0/2415	0.91	0/3284
1	T	0.80	0/2404	0.92	0/3270
1	U	0.77	0/2415	0.90	0/3284
1	V	0.77	0/2404	0.92	0/3270
1	W	0.76	0/2415	0.88	0/3284
1	X	0.76	0/2404	0.90	0/3270
1	Y	0.76	0/2404	0.91	0/3270
1	Z	0.77	0/2404	0.90	0/3270
All	All	0.78	0/62713	0.91	0/85286

There are no bond length outliers.

There are no bond angle outliers.

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	2360	0	2253	39	0
1	B	2349	0	2240	38	0
1	C	2349	0	2240	28	0
1	D	2341	0	2233	17	0
1	E	2371	0	2265	27	0
1	F	2341	0	2234	19	0
1	G	2360	0	2253	34	0
1	H	2349	0	2239	21	0
1	I	2371	0	2266	31	0
1	J	2360	0	2253	26	0
1	K	2379	0	2277	29	0
1	L	2379	0	2276	21	0
1	M	2349	0	2240	25	0
1	N	2360	0	2252	22	0
1	O	2360	0	2253	43	0
1	P	2360	0	2253	25	0
1	Q	2371	0	2266	28	0
1	R	2349	0	2240	26	0
1	S	2360	0	2253	31	0
1	T	2349	0	2240	31	0
1	U	2360	0	2253	31	0
1	V	2349	0	2240	28	0
1	W	2360	0	2253	23	0
1	X	2349	0	2240	34	0
1	Y	2349	0	2240	21	0
1	Z	2349	0	2240	28	0
2	A	9	0	0	4	0
2	C	9	0	0	8	0
2	Q	9	0	0	4	0
2	T	9	0	0	5	0
2	X	9	0	0	3	0
3	B	10	0	0	3	0
3	N	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	R	10	0	0	3	0
4	D	5	0	0	2	0
4	H	5	0	0	4	0
4	S	5	0	0	2	0
4	Z	5	0	0	5	0
5	E	8	0	0	6	0
5	G	8	0	0	5	0
5	I	8	0	0	5	0
5	J	8	0	0	4	0
5	K	8	0	0	3	0
5	L	8	0	0	0	0
5	M	8	0	0	4	0
5	U	8	0	0	3	0
5	V	8	0	0	2	0
5	W	8	0	0	4	0
5	Y	8	0	0	5	0
6	F	7	0	0	3	0
6	O	7	0	0	4	0
6	P	7	0	0	3	0
7	A	103	0	0	3	0
7	B	121	0	0	1	0
7	C	108	0	0	0	0
7	D	140	0	0	0	0
7	E	126	0	0	0	0
7	F	131	0	0	1	0
7	G	130	0	0	1	0
7	H	113	0	0	0	0
7	I	82	0	0	1	0
7	J	87	0	0	0	0
7	K	116	0	0	1	0
7	L	147	0	0	1	0
7	M	69	0	0	0	0
7	N	85	0	0	2	0
7	O	108	0	0	3	0
7	P	36	0	0	0	0
7	Q	105	0	0	0	0
7	R	75	0	0	0	0
7	S	128	0	0	2	0
7	T	79	0	0	0	0
7	U	80	0	0	1	0
7	V	83	0	0	0	0
7	W	71	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	X	63	0	0	1	0
7	Y	82	0	0	1	0
7	Z	47	0	0	1	0
All	All	64002	0	58492	720	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.

The worst 5 of 720 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:114:SER:OG	3:B:900:DKO:C4	1.69	1.40
1:H:114:SER:OG	4:H:900:DK6:C4	1.68	1.40
1:E:114:SER:OG	5:E:900:DKF:C4	1.67	1.39
1:K:114:SER:OG	5:K:900:DKF:C4	1.71	1.37
1:C:114:SER:OG	2:C:900:DKL:C4	1.73	1.36

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	308/317 (97%)	292 (95%)	16 (5%)	0	100	100
1	B	307/317 (97%)	292 (95%)	14 (5%)	1 (0%)	41	55
1	C	307/317 (97%)	295 (96%)	11 (4%)	1 (0%)	41	55
1	D	306/317 (96%)	296 (97%)	10 (3%)	0	100	100
1	E	309/317 (98%)	296 (96%)	12 (4%)	1 (0%)	41	55
1	F	306/317 (96%)	294 (96%)	12 (4%)	0	100	100
1	G	308/317 (97%)	289 (94%)	18 (6%)	1 (0%)	41	55

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	307/317 (97%)	297 (97%)	10 (3%)	0	100	100
1	I	309/317 (98%)	298 (96%)	11 (4%)	0	100	100
1	J	308/317 (97%)	296 (96%)	12 (4%)	0	100	100
1	K	310/317 (98%)	298 (96%)	12 (4%)	0	100	100
1	L	310/317 (98%)	301 (97%)	8 (3%)	1 (0%)	41	55
1	M	307/317 (97%)	286 (93%)	21 (7%)	0	100	100
1	N	308/317 (97%)	302 (98%)	5 (2%)	1 (0%)	41	55
1	O	308/317 (97%)	293 (95%)	15 (5%)	0	100	100
1	P	308/317 (97%)	290 (94%)	16 (5%)	2 (1%)	25	36
1	Q	309/317 (98%)	298 (96%)	11 (4%)	0	100	100
1	R	307/317 (97%)	295 (96%)	11 (4%)	1 (0%)	41	55
1	S	308/317 (97%)	300 (97%)	7 (2%)	1 (0%)	41	55
1	T	307/317 (97%)	298 (97%)	9 (3%)	0	100	100
1	U	308/317 (97%)	287 (93%)	20 (6%)	1 (0%)	41	55
1	V	307/317 (97%)	298 (97%)	8 (3%)	1 (0%)	41	55
1	W	308/317 (97%)	296 (96%)	11 (4%)	1 (0%)	41	55
1	X	307/317 (97%)	290 (94%)	15 (5%)	2 (1%)	22	32
1	Y	307/317 (97%)	293 (95%)	13 (4%)	1 (0%)	41	55
1	Z	307/317 (97%)	290 (94%)	15 (5%)	2 (1%)	22	32
All	All	8001/8242 (97%)	7660 (96%)	323 (4%)	18 (0%)	47	62

5 of 18 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	211	PHE
1	P	211	PHE
1	C	142	GLN
1	N	142	GLN
1	U	211	PHE

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	240/247 (97%)	224 (93%)	16 (7%)	16	26
1	B	239/247 (97%)	227 (95%)	12 (5%)	24	40
1	C	239/247 (97%)	231 (97%)	8 (3%)	38	57
1	D	238/247 (96%)	229 (96%)	9 (4%)	33	51
1	E	241/247 (98%)	231 (96%)	10 (4%)	30	48
1	F	238/247 (96%)	234 (98%)	4 (2%)	60	78
1	G	240/247 (97%)	226 (94%)	14 (6%)	20	32
1	H	239/247 (97%)	231 (97%)	8 (3%)	38	57
1	I	241/247 (98%)	231 (96%)	10 (4%)	30	48
1	J	240/247 (97%)	228 (95%)	12 (5%)	24	40
1	K	242/247 (98%)	230 (95%)	12 (5%)	24	40
1	L	242/247 (98%)	239 (99%)	3 (1%)	71	85
1	M	239/247 (97%)	232 (97%)	7 (3%)	42	62
1	N	240/247 (97%)	232 (97%)	8 (3%)	38	57
1	O	240/247 (97%)	228 (95%)	12 (5%)	24	40
1	P	240/247 (97%)	230 (96%)	10 (4%)	30	47
1	Q	241/247 (98%)	233 (97%)	8 (3%)	38	57
1	R	239/247 (97%)	230 (96%)	9 (4%)	33	51
1	S	240/247 (97%)	231 (96%)	9 (4%)	33	51
1	T	239/247 (97%)	233 (98%)	6 (2%)	47	67
1	U	240/247 (97%)	228 (95%)	12 (5%)	24	40
1	V	239/247 (97%)	231 (97%)	8 (3%)	38	57
1	W	240/247 (97%)	230 (96%)	10 (4%)	30	47
1	X	239/247 (97%)	225 (94%)	14 (6%)	19	32
1	Y	239/247 (97%)	226 (95%)	13 (5%)	22	36
1	Z	239/247 (97%)	223 (93%)	16 (7%)	16	26
All	All	6233/6422 (97%)	5973 (96%)	260 (4%)	30	47

5 of 260 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	313	ILE
1	P	46	LEU
1	W	266	GLU
1	M	187	ASP
1	N	292	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 55 such sidechains are listed below:

Mol	Chain	Res	Type
1	K	274	ASN
1	Q	152	HIS
1	Y	273	HIS
1	M	152	HIS
1	M	274	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

26 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	DKO	R	900	-	9,9,9	3.25	1 (11%)	9,9,9	2.20	4 (44%)
4	DK6	S	900	-	4,4,4	2.64	1 (25%)	4,4,4	4.88	2 (50%)
5	DKF	E	900	-	7,7,7	0.79	0	7,7,7	0.30	0
3	DKO	B	900	-	9,9,9	1.66	1 (11%)	9,9,9	3.38	5 (55%)
6	DK9	O	900	-	6,6,6	0.81	0	6,6,6	1.40	1 (16%)
4	DK6	H	900	-	4,4,4	1.08	1 (25%)	4,4,4	1.43	1 (25%)
3	DKO	N	900	-	9,9,9	0.79	0	9,9,9	0.99	1 (11%)
2	DKL	Q	900	-	8,8,8	0.55	0	8,8,8	1.50	1 (12%)
5	DKF	M	900	-	7,7,7	0.82	0	7,7,7	1.08	1 (14%)
2	DKL	C	900	-	8,8,8	1.94	2 (25%)	8,8,8	2.41	2 (25%)
5	DKF	J	900	-	7,7,7	0.67	0	7,7,7	1.98	3 (42%)
2	DKL	A	900	-	8,8,8	3.48	2 (25%)	8,8,8	3.78	5 (62%)
5	DKF	W	900	-	7,7,7	1.17	1 (14%)	7,7,7	4.96	5 (71%)
5	DKF	U	900	-	7,7,7	0.93	0	7,7,7	1.98	3 (42%)
5	DKF	K	900	-	7,7,7	1.68	1 (14%)	7,7,7	1.45	1 (14%)
5	DKF	I	900	-	7,7,7	0.16	0	7,7,7	1.95	1 (14%)
2	DKL	T	900	-	8,8,8	0.64	0	8,8,8	0.93	0
6	DK9	P	900	-	6,6,6	0.98	0	6,6,6	1.40	2 (33%)
5	DKF	V	900	-	7,7,7	1.26	1 (14%)	7,7,7	1.97	2 (28%)
5	DKF	G	900	-	7,7,7	0.92	1 (14%)	7,7,7	3.59	2 (28%)
5	DKF	L	900	1	7,7,7	0.79	0	7,7,7	4.05	3 (42%)
6	DK9	F	900	-	6,6,6	0.69	0	6,6,6	1.56	2 (33%)
2	DKL	X	900	-	8,8,8	0.64	0	8,8,8	1.85	2 (25%)
4	DK6	D	900	-	4,4,4	0.91	0	4,4,4	1.74	1 (25%)
4	DK6	Z	900	-	4,4,4	1.49	2 (50%)	4,4,4	3.14	3 (75%)
5	DKF	Y	900	-	7,7,7	0.96	1 (14%)	7,7,7	0.94	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
3	DKO	R	900	-	-	3/7/7/7	-
4	DK6	S	900	-	-	1/2/2/2	-
5	DKF	E	900	-	-	3/5/5/5	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	DKO	B	900	-	-	5/7/7/7	-
6	DK9	O	900	-	-	3/4/4/4	-
4	DK6	H	900	-	-	2/2/2/2	-
3	DKO	N	900	-	-	3/7/7/7	-
2	DKL	Q	900	-	-	6/6/6/6	-
5	DKF	M	900	-	-	4/5/5/5	-
2	DKL	C	900	-	-	2/6/6/6	-
5	DKF	J	900	-	-	2/5/5/5	-
2	DKL	A	900	-	-	4/6/6/6	-
5	DKF	W	900	-	-	2/5/5/5	-
5	DKF	U	900	-	-	5/5/5/5	-
5	DKF	K	900	-	-	4/5/5/5	-
5	DKF	I	900	-	-	4/5/5/5	-
2	DKL	T	900	-	-	2/6/6/6	-
6	DK9	P	900	-	-	3/4/4/4	-
5	DKF	V	900	-	-	3/5/5/5	-
5	DKF	G	900	-	-	4/5/5/5	-
5	DKF	L	900	1	-	4/5/5/5	-
6	DK9	F	900	-	-	0/4/4/4	-
2	DKL	X	900	-	-	5/6/6/6	-
4	DK6	D	900	-	-	2/2/2/2	-
4	DK6	Z	900	-	-	2/2/2/2	-
5	DKF	Y	900	-	-	4/5/5/5	-

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	R	900	DKO	C5-C4	9.61	1.70	1.50
2	A	900	DKL	C5-C4	9.37	1.69	1.50
2	C	900	DKL	C5-C4	5.05	1.60	1.50
4	S	900	DK6	C5-C4	5.01	1.60	1.50
3	B	900	DKO	C5-C4	4.71	1.60	1.50

The worst 5 of 53 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	W	900	DKF	O3-C4-O4	-11.24	90.67	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	900	DKF	O3-C4-O4	-8.65	95.45	111.36
4	S	900	DK6	O4-C4-O3	-8.58	95.58	111.36
5	L	900	DKF	O4-C4-C5	8.30	127.36	109.17
3	B	900	DKO	O3-C4-C5	-6.67	94.56	109.17

There are no chirality outliers.

5 of 82 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	S	900	DK6	O3-C4-C5-C6
5	E	900	DKF	O3-C4-C5-C6
3	B	900	DKO	O3-C4-C5-C6
6	O	900	DK9	O3-C4-C5-C6
4	H	900	DK6	O3-C4-C5-C6

There are no ring outliers.

24 monomers are involved in 94 short contacts:

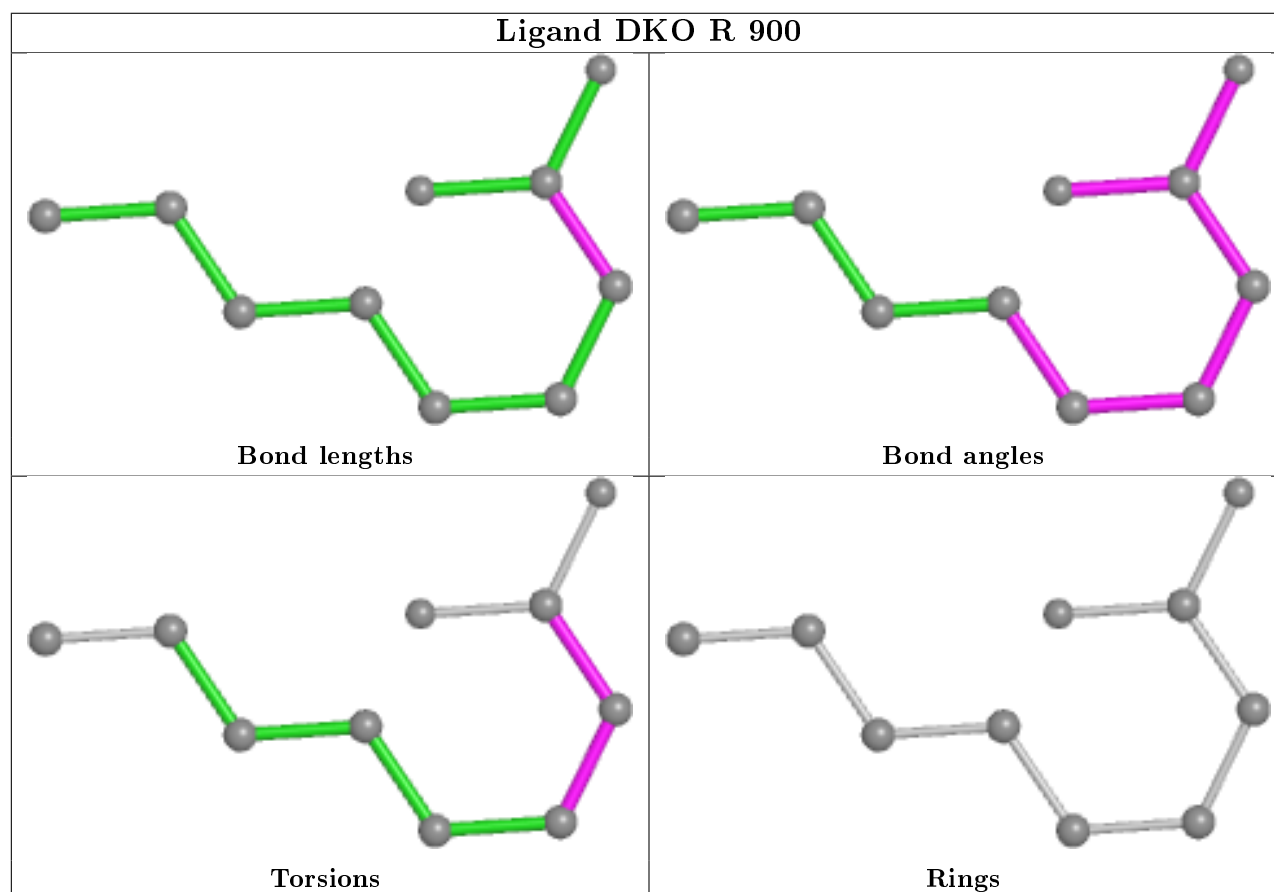
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	R	900	DKO	3	0
4	S	900	DK6	2	0
5	E	900	DKF	6	0
3	B	900	DKO	3	0
6	O	900	DK9	4	0
4	H	900	DK6	4	0
2	Q	900	DKL	4	0
5	M	900	DKF	4	0
2	C	900	DKL	8	0
5	J	900	DKF	4	0
2	A	900	DKL	4	0
5	W	900	DKF	4	0
5	U	900	DKF	3	0
5	K	900	DKF	3	0
5	I	900	DKF	5	0
2	T	900	DKL	5	0
6	P	900	DK9	3	0
5	V	900	DKF	2	0
5	G	900	DKF	5	0
6	F	900	DK9	3	0
2	X	900	DKL	3	0
4	D	900	DK6	2	0

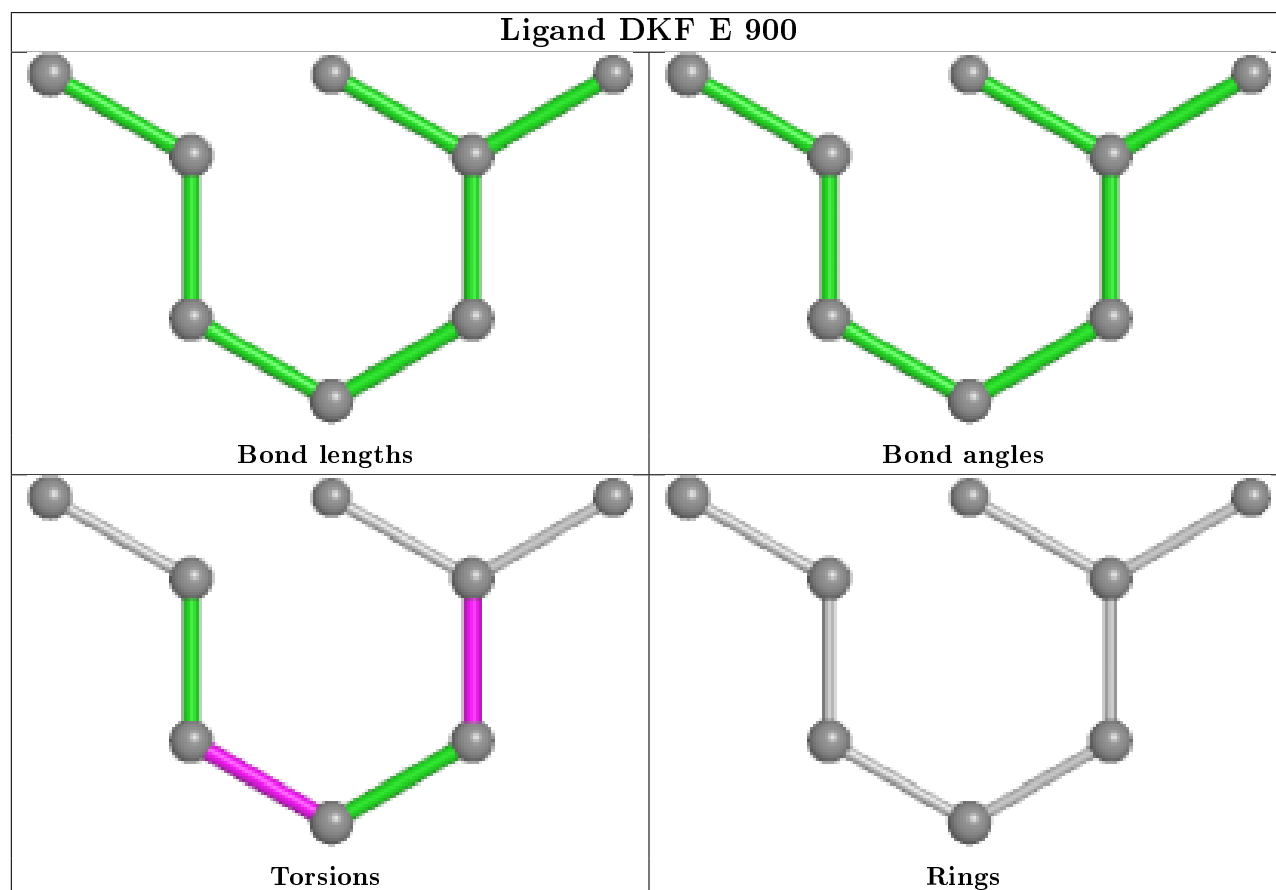
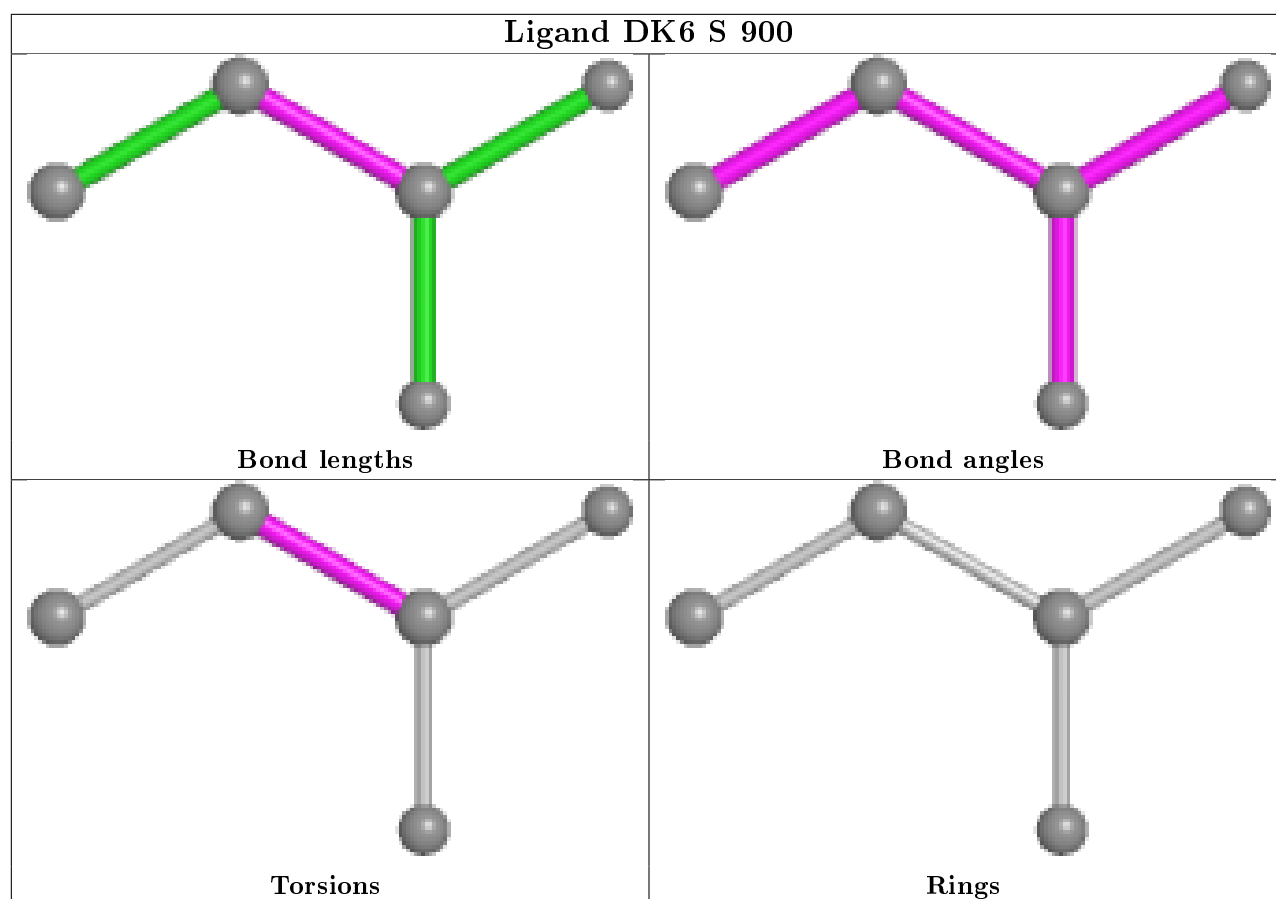
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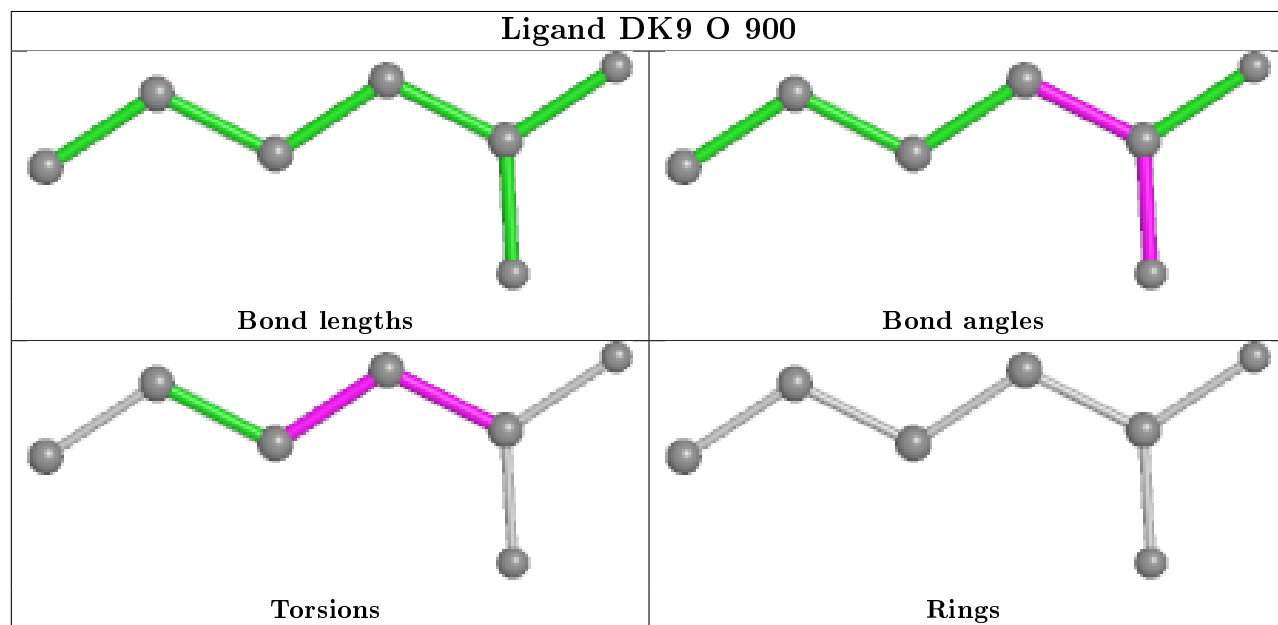
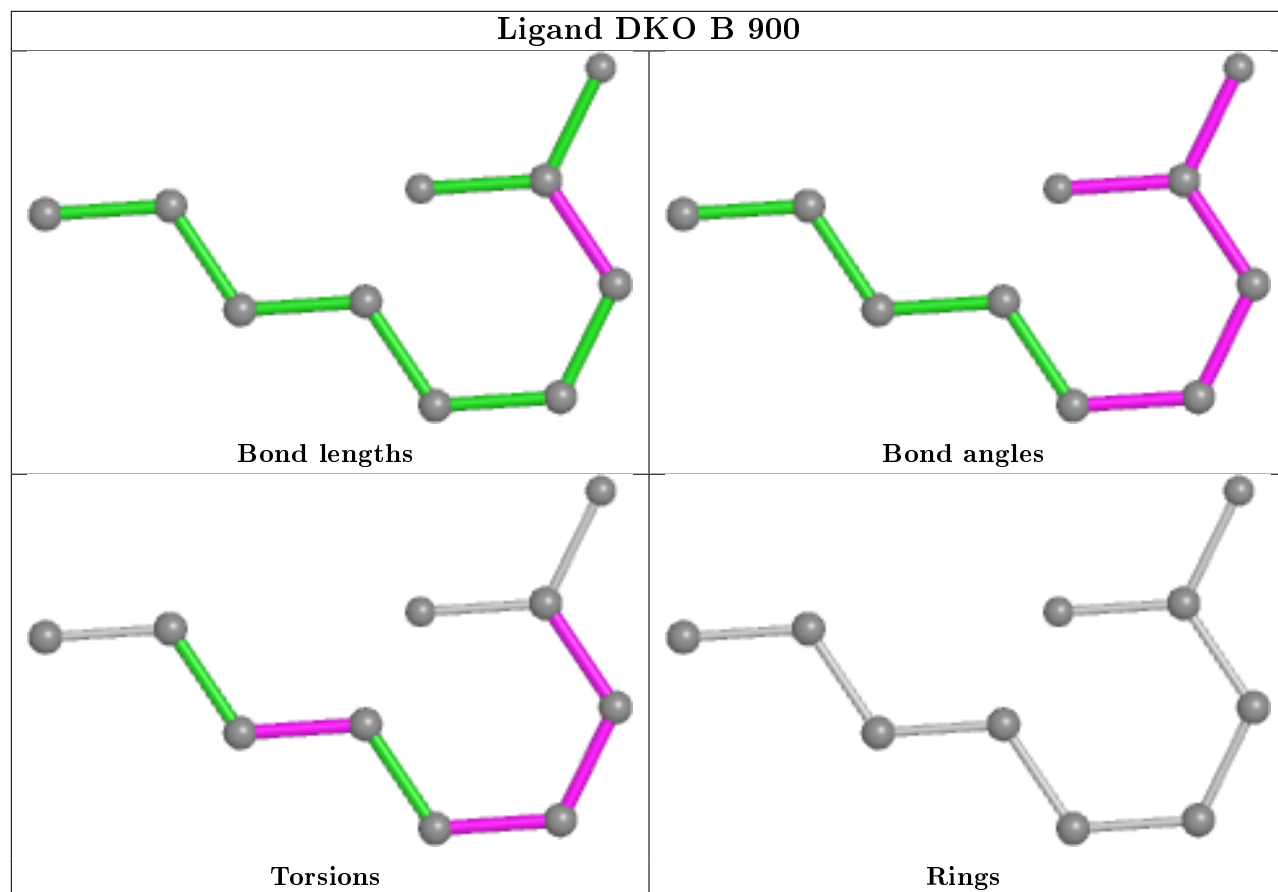
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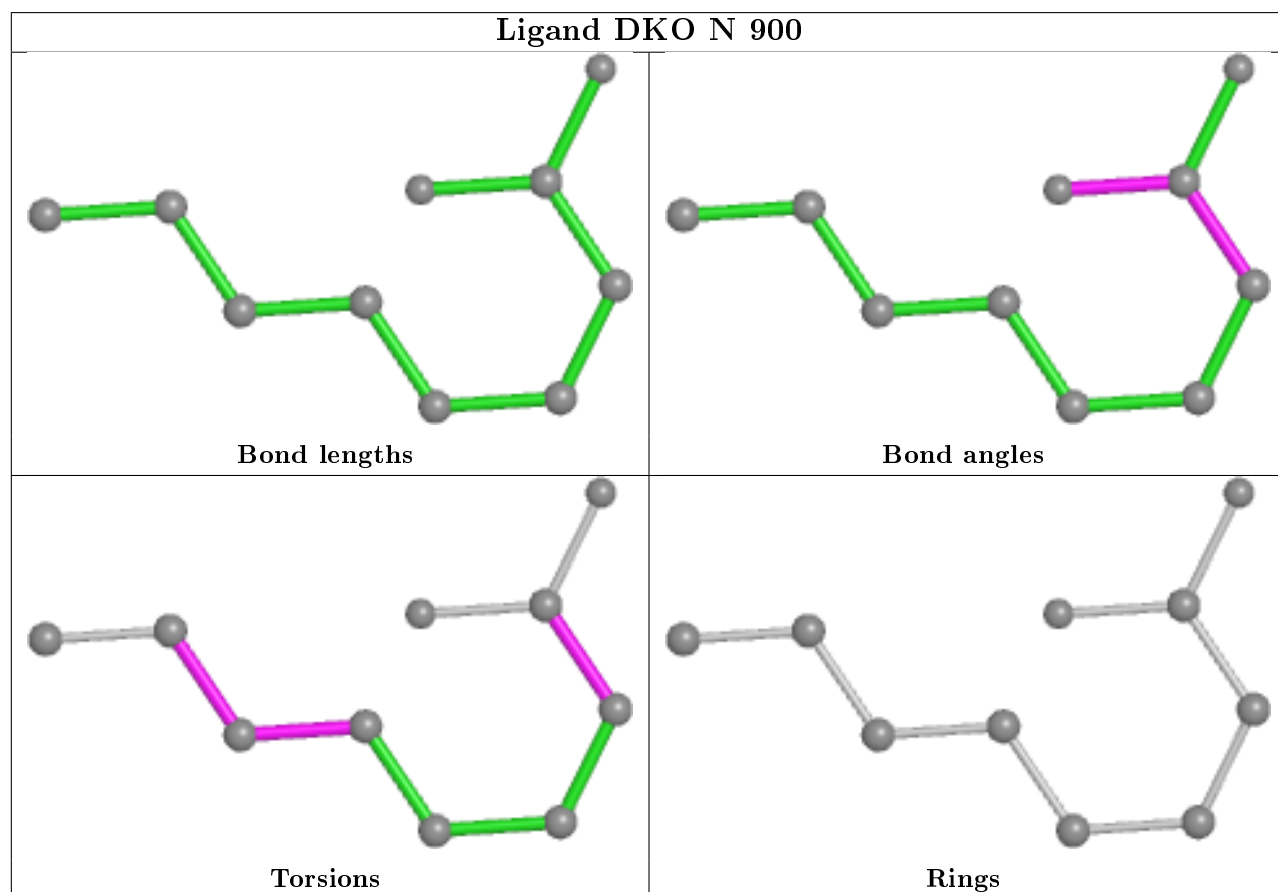
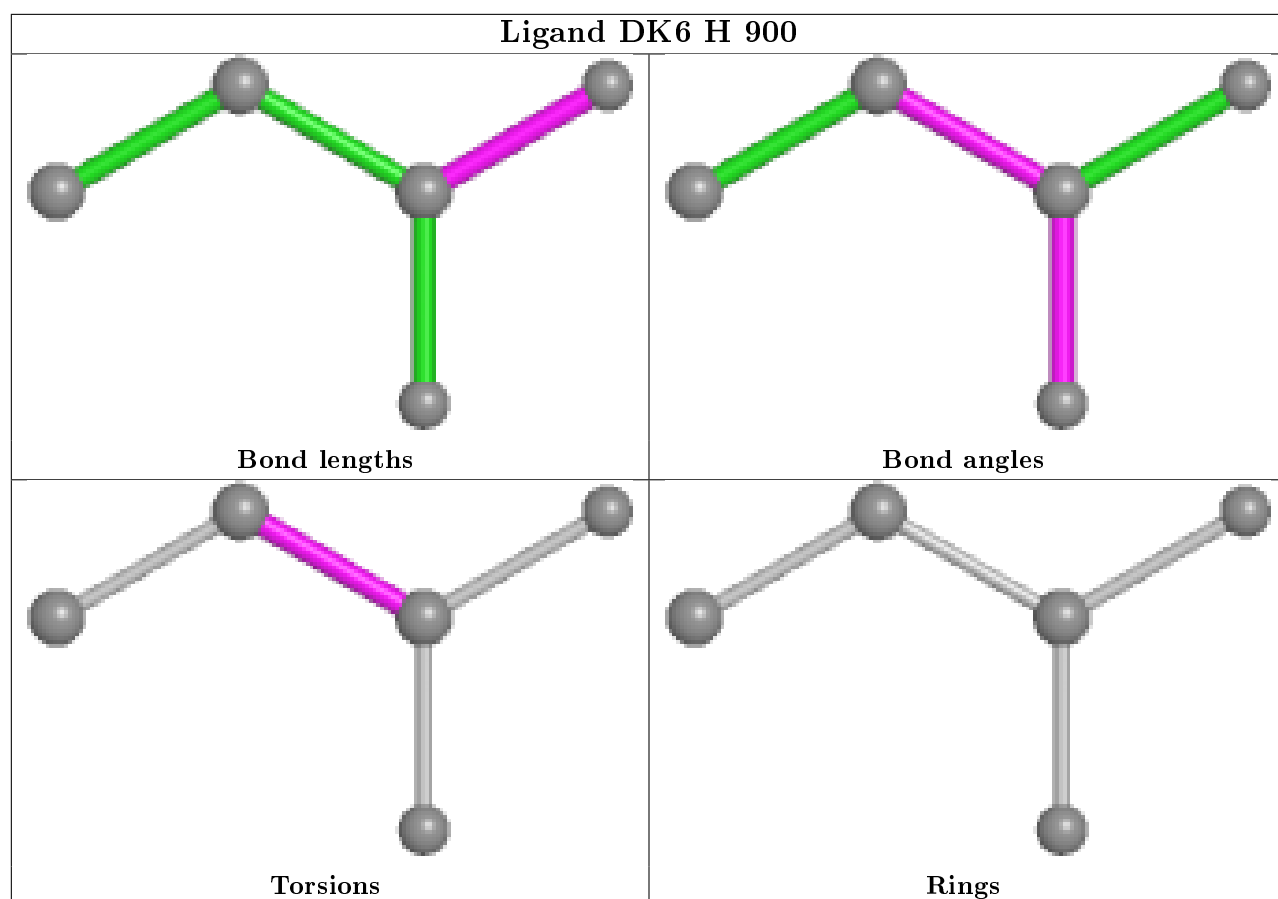
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	Z	900	DK6	5	0
5	Y	900	DKF	5	0

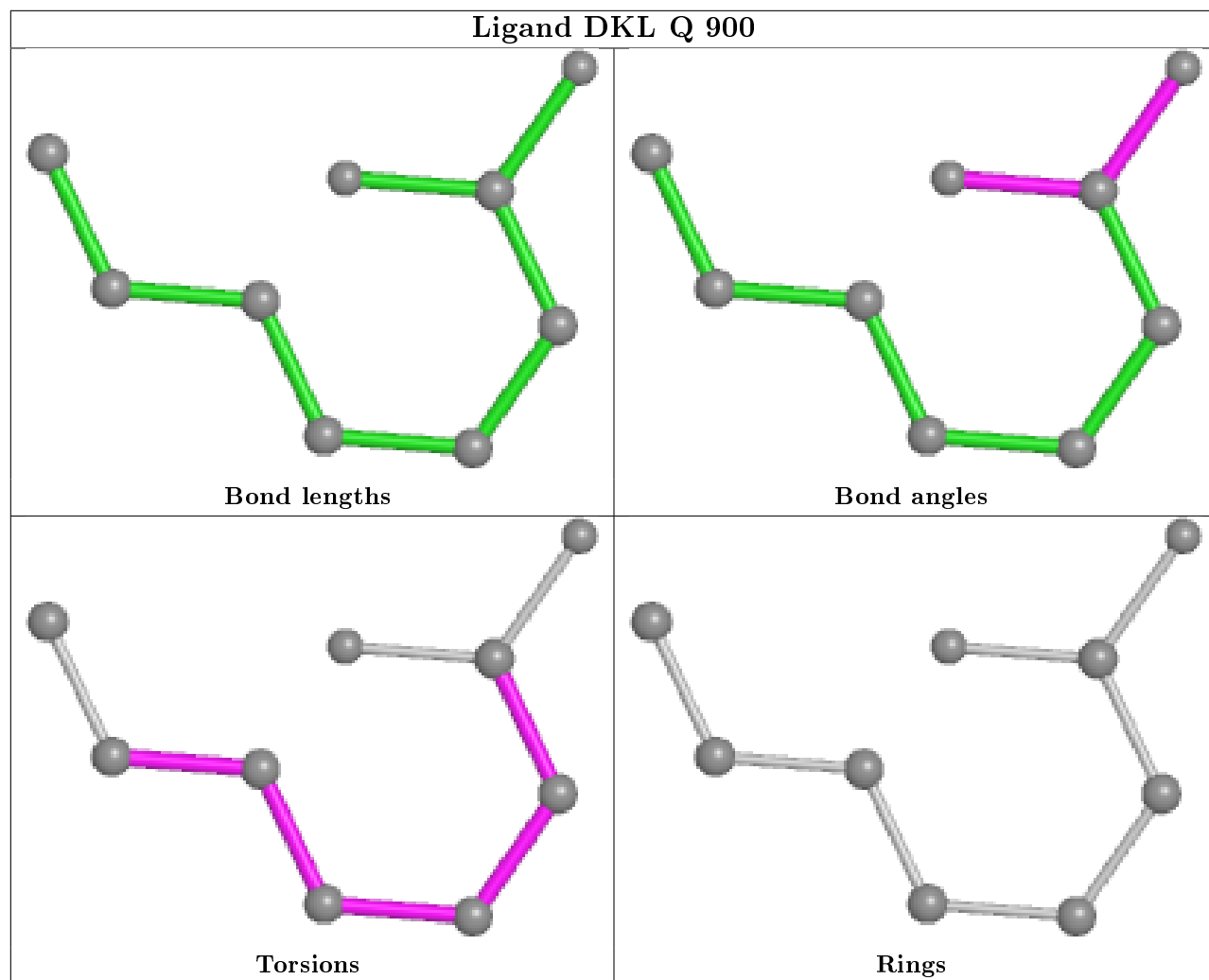
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

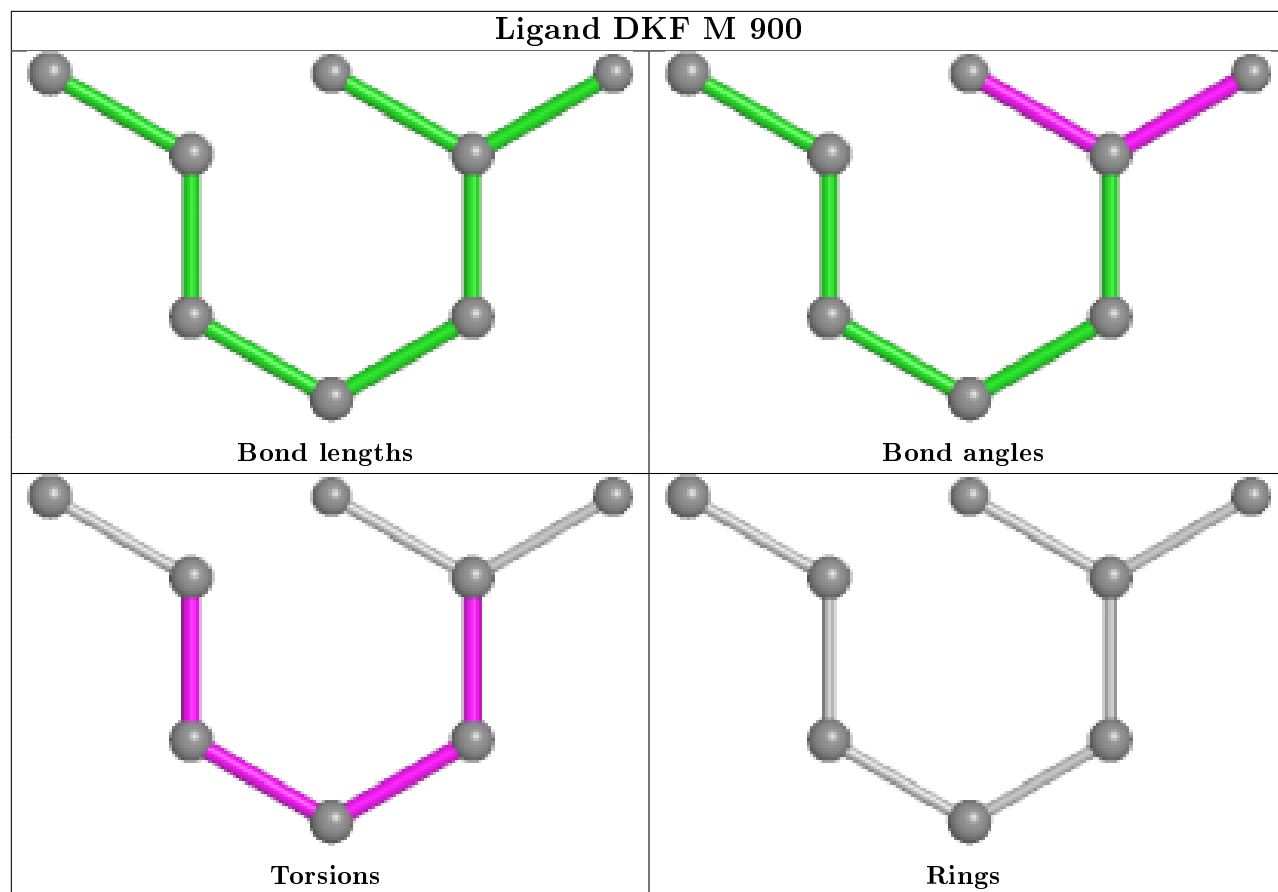


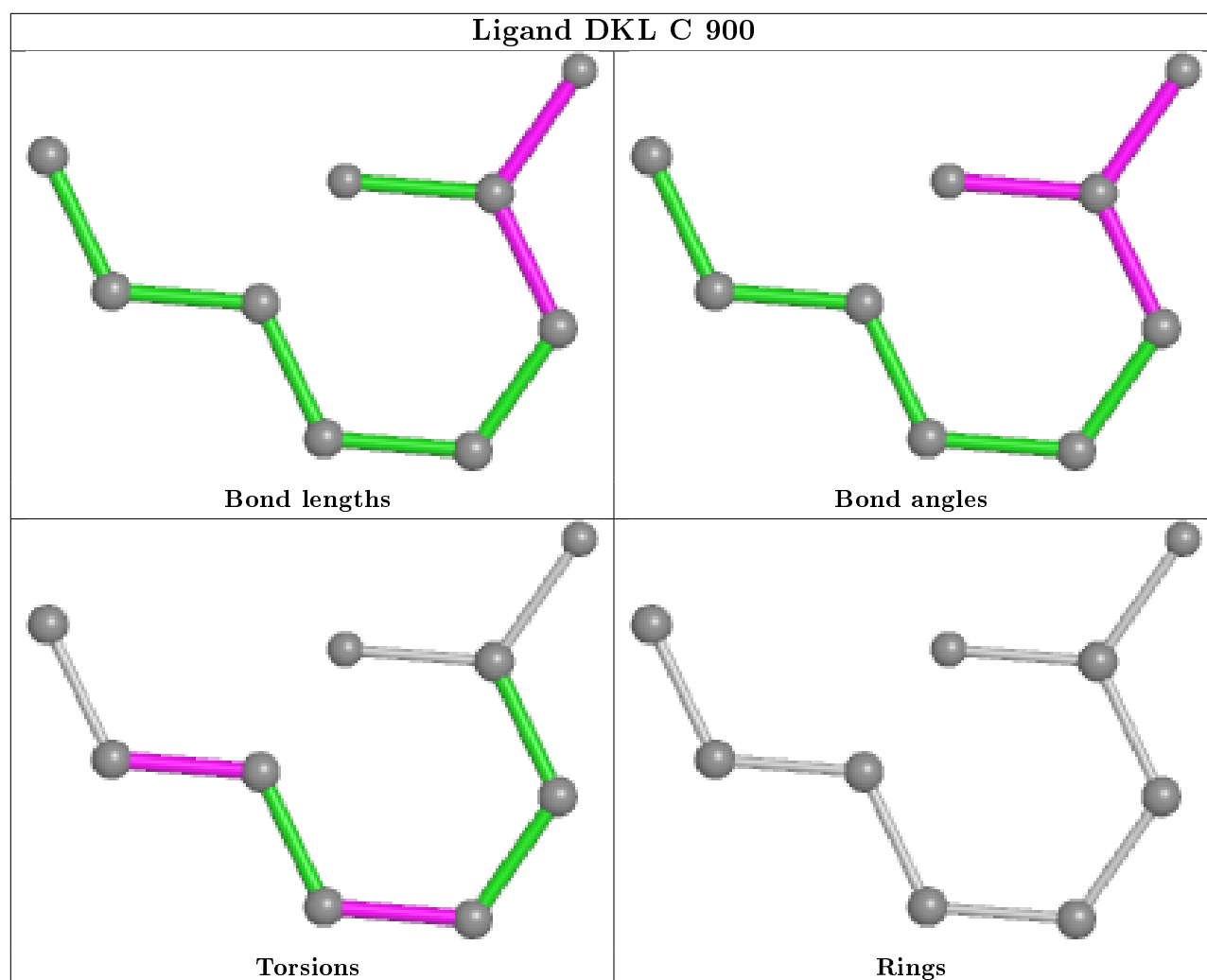


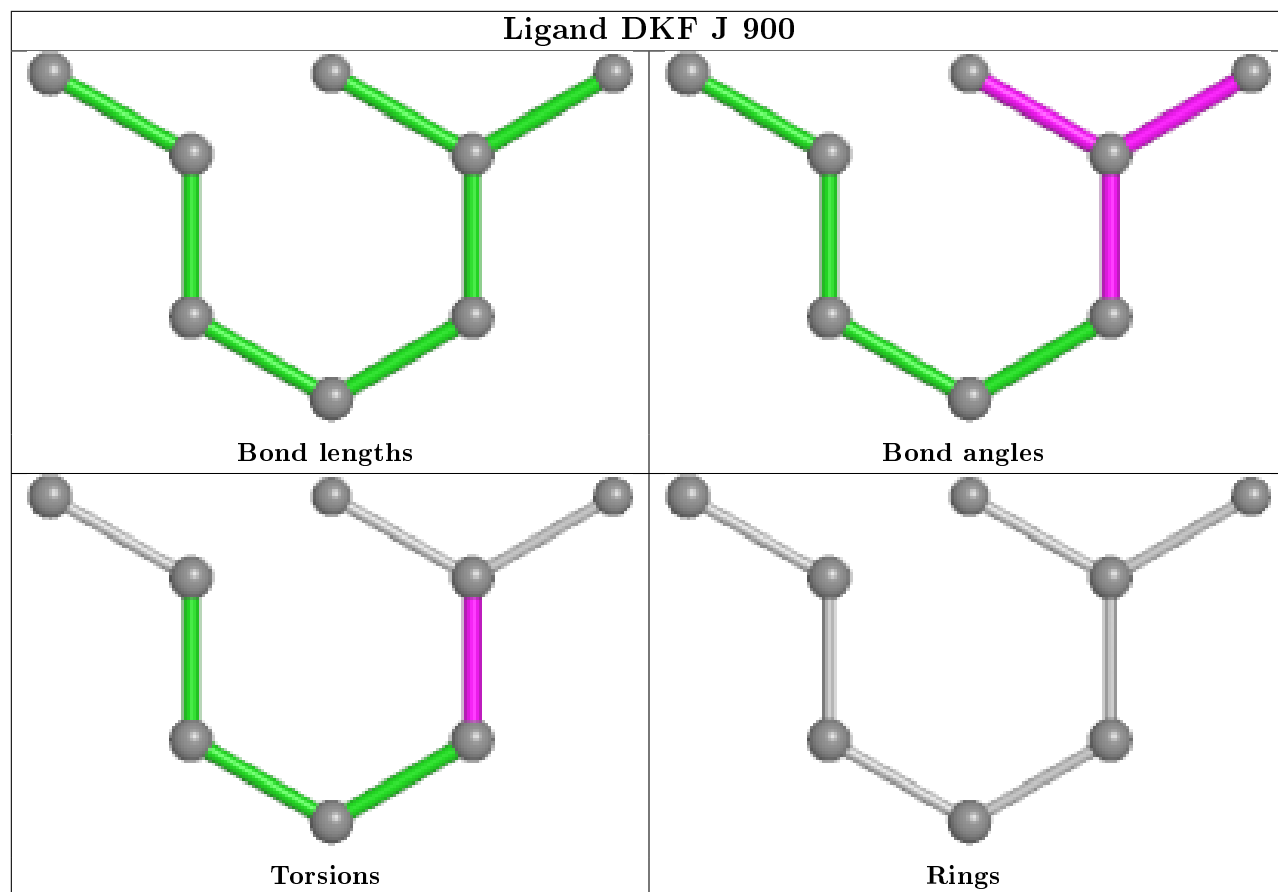


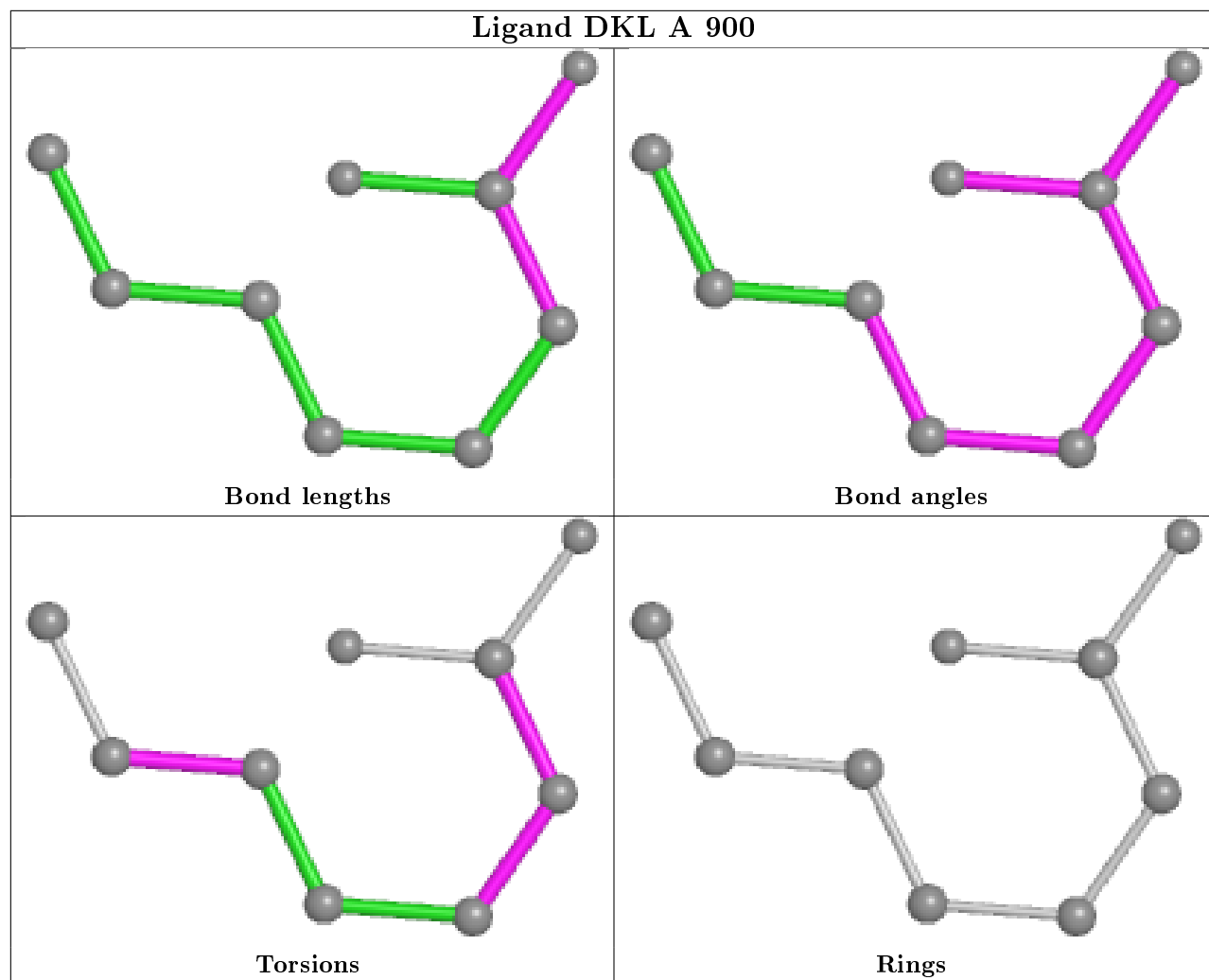


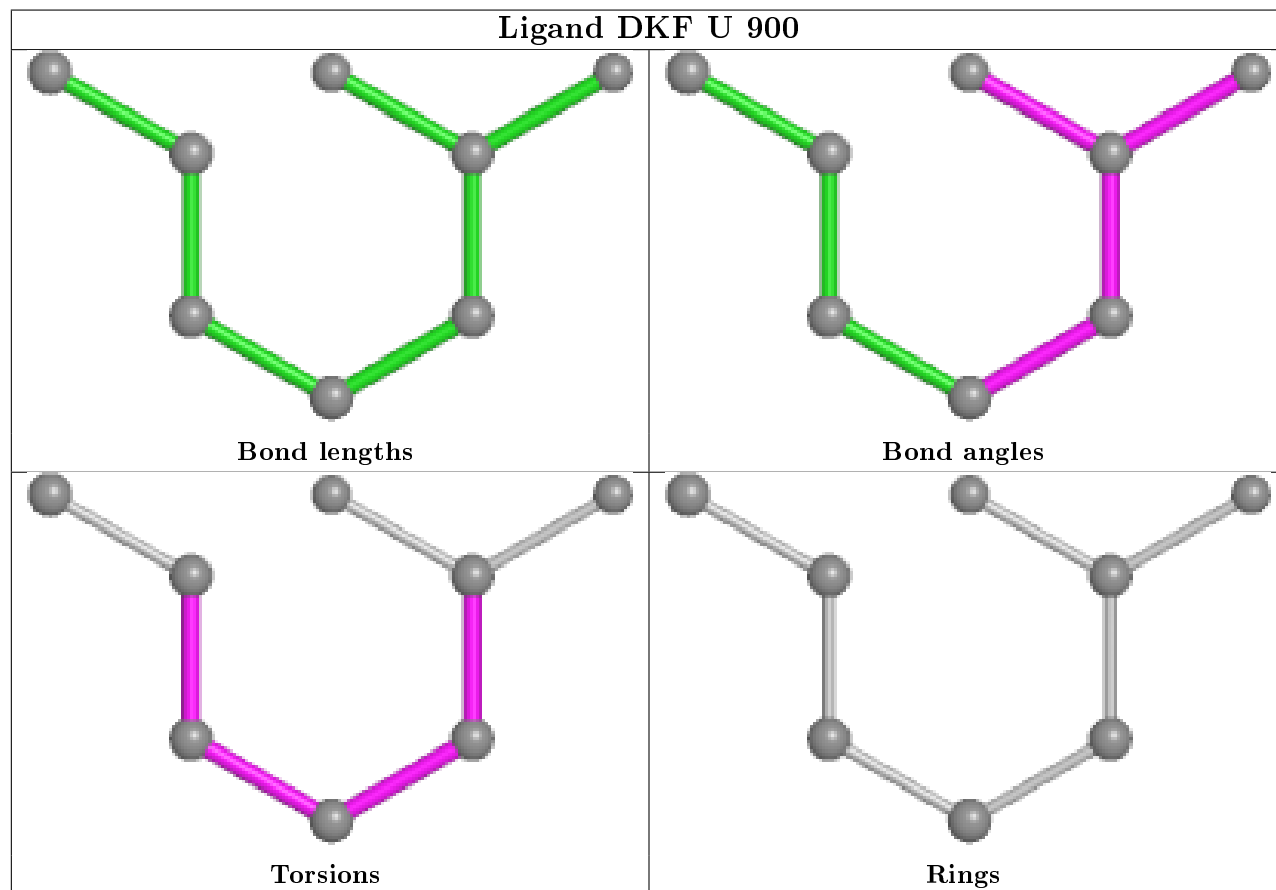
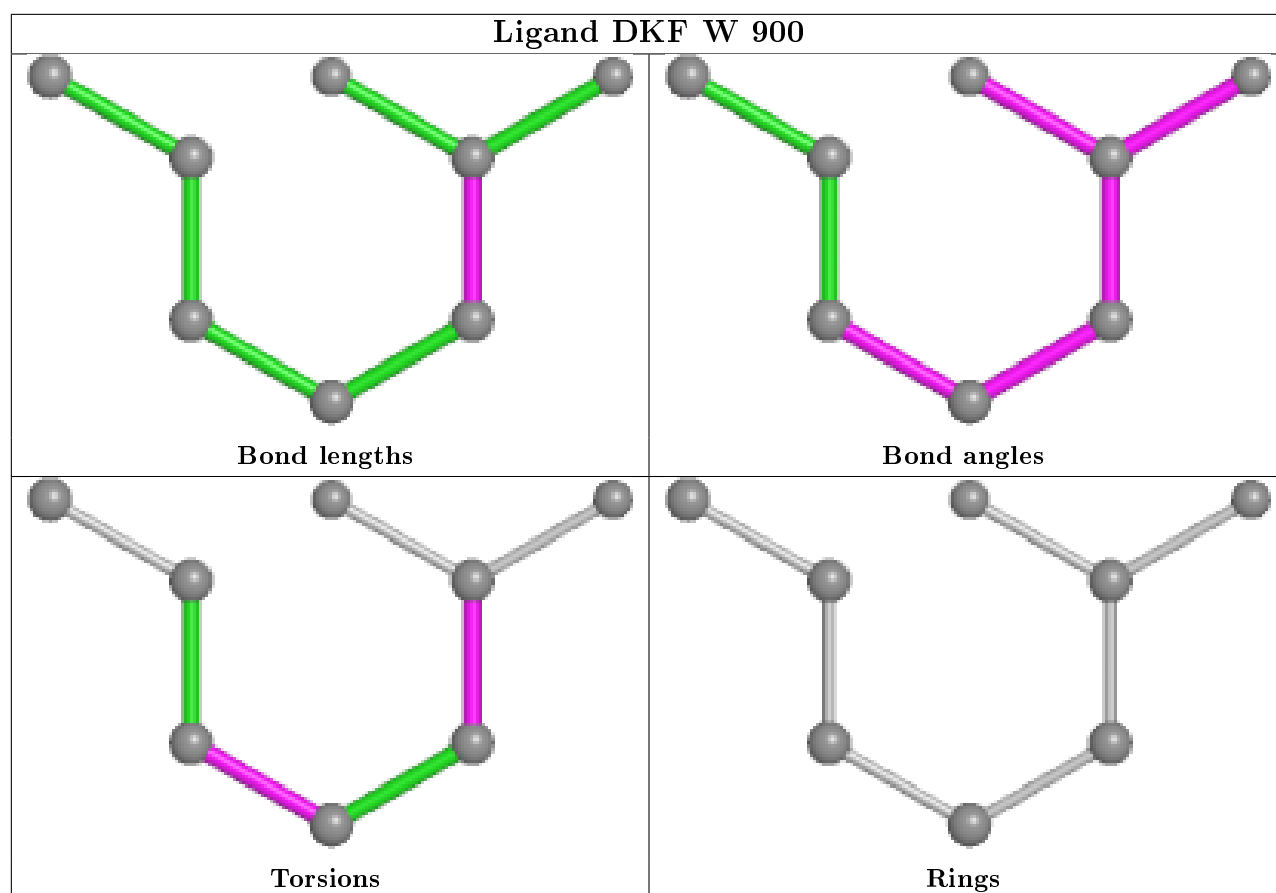


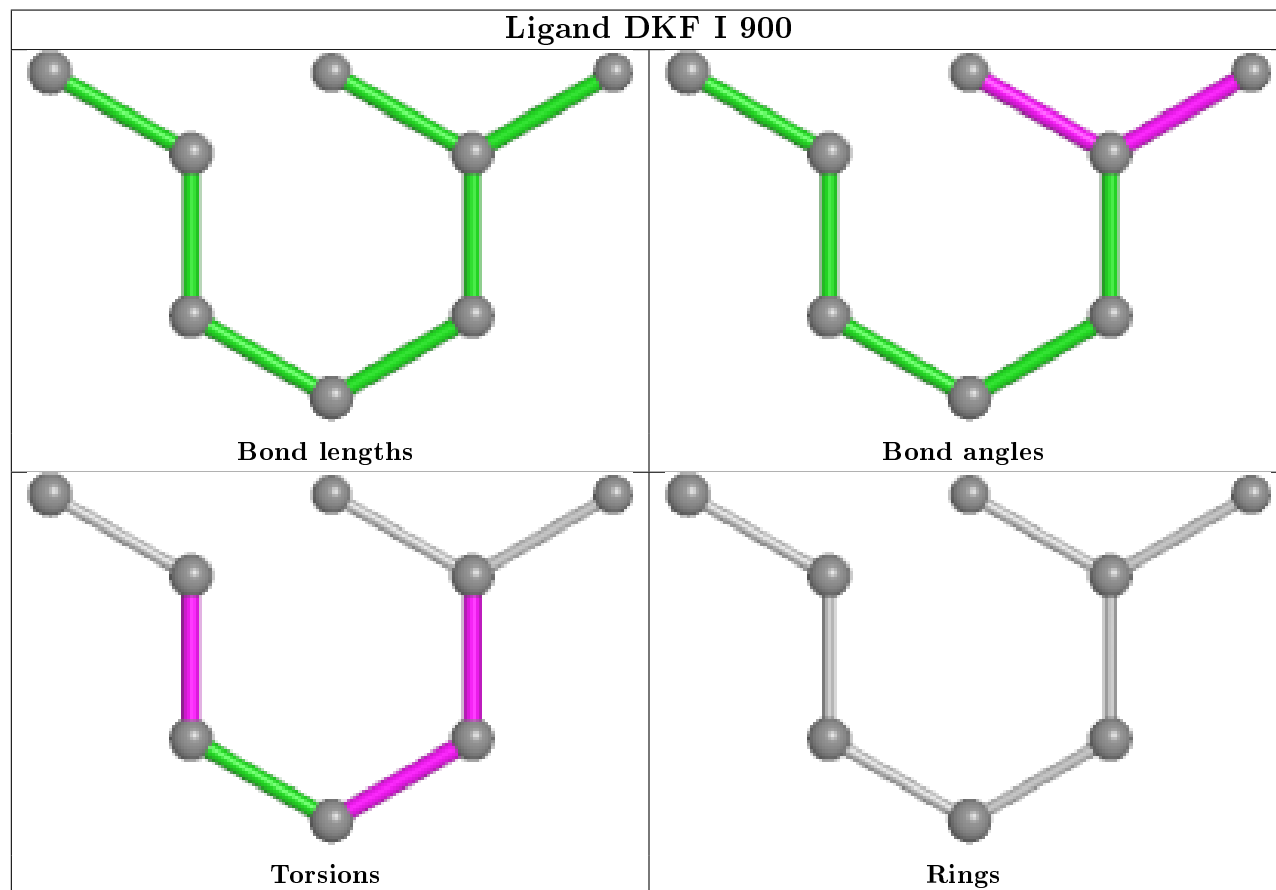
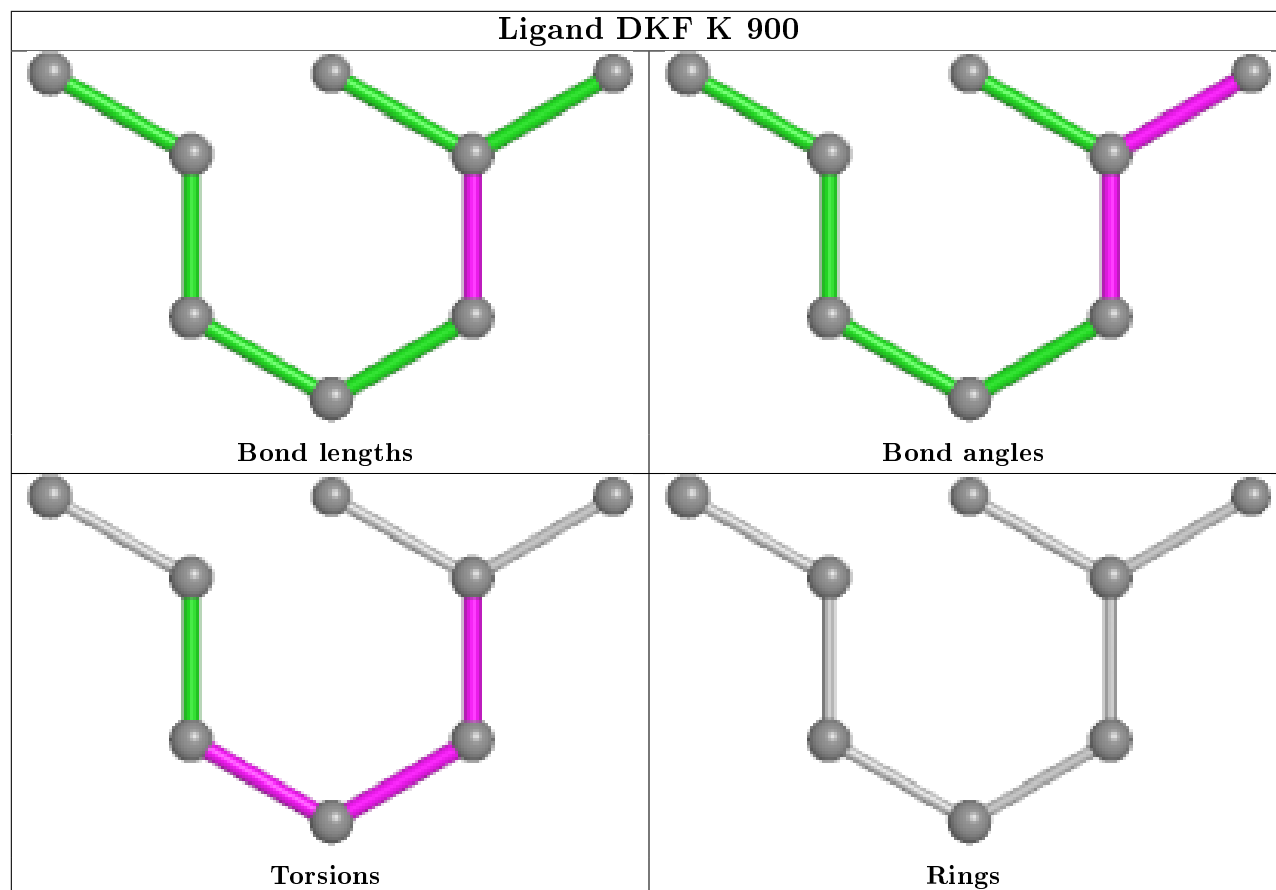


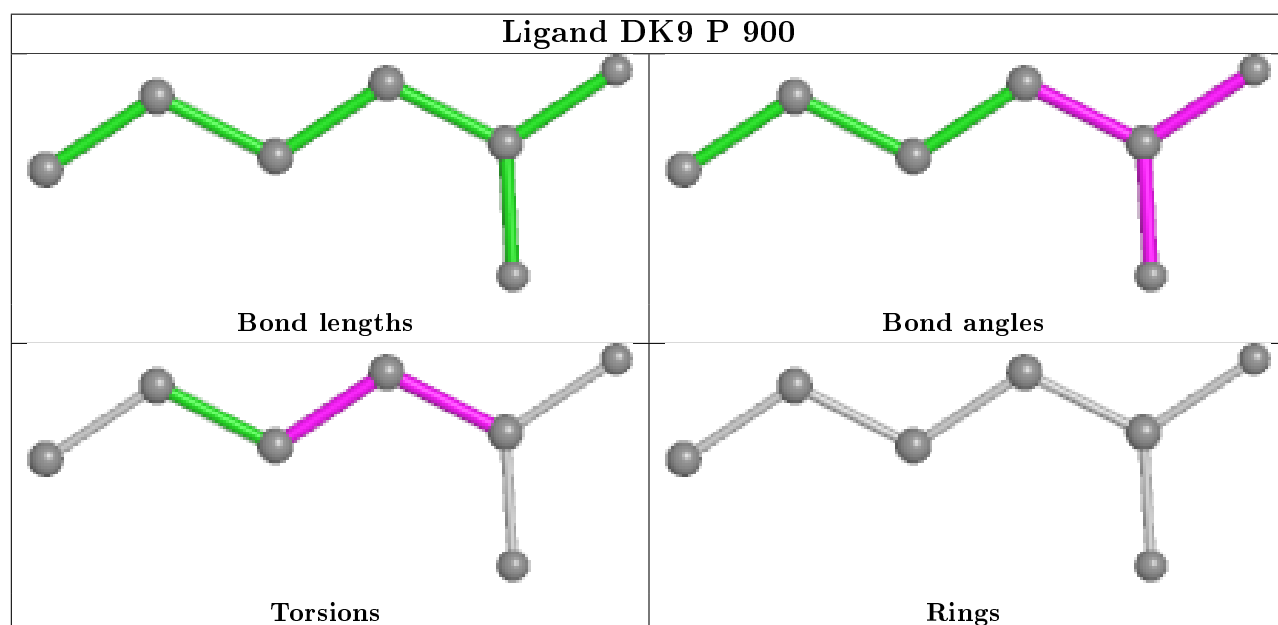
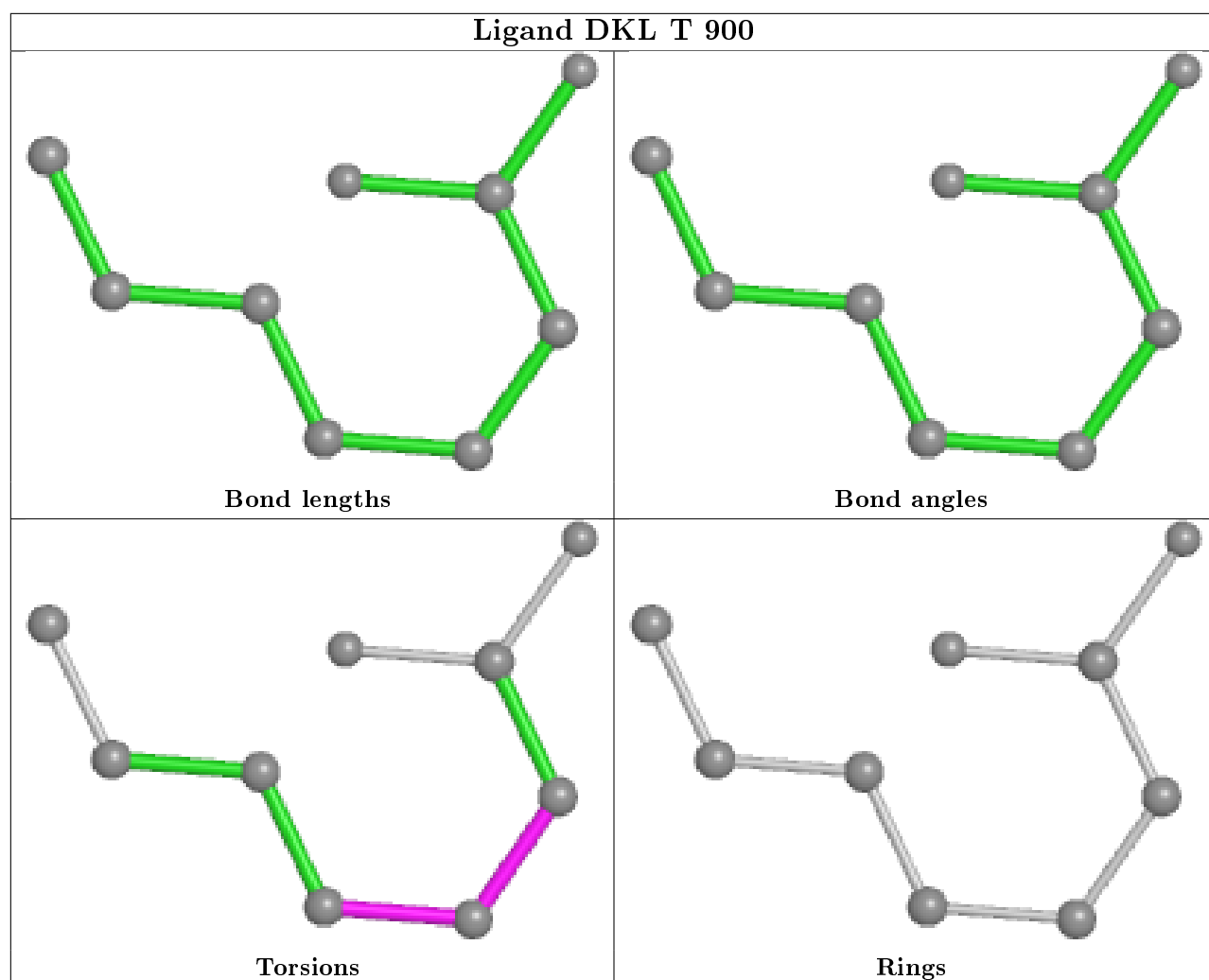


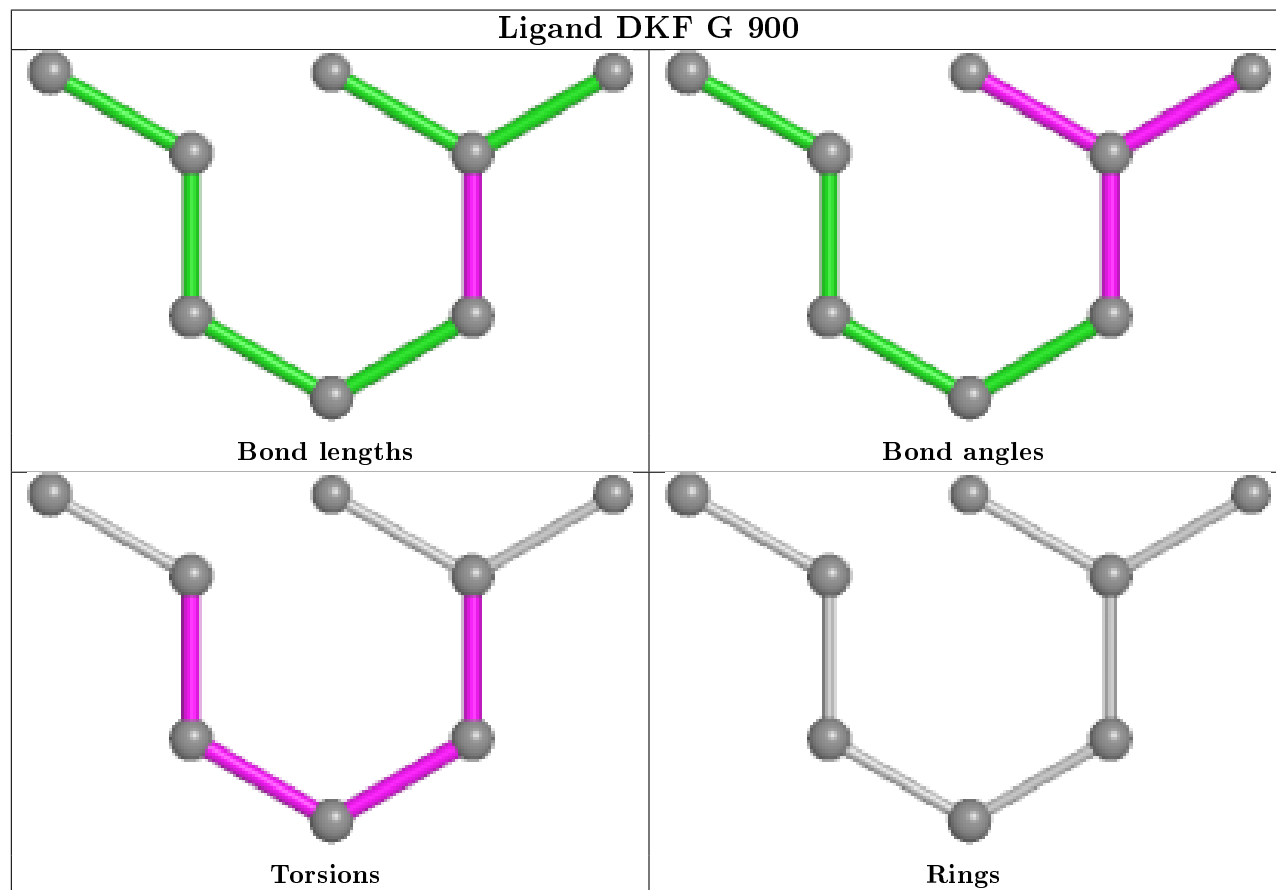
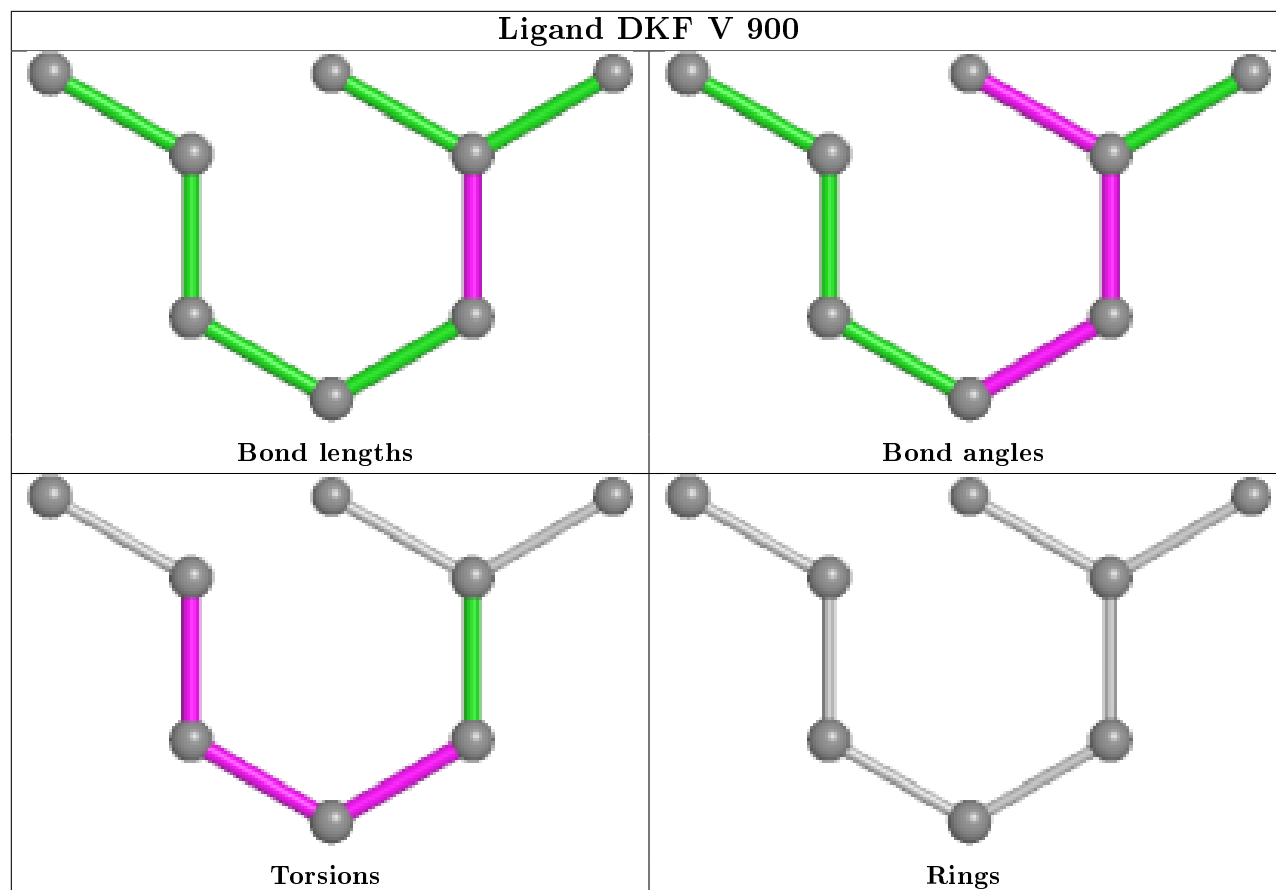


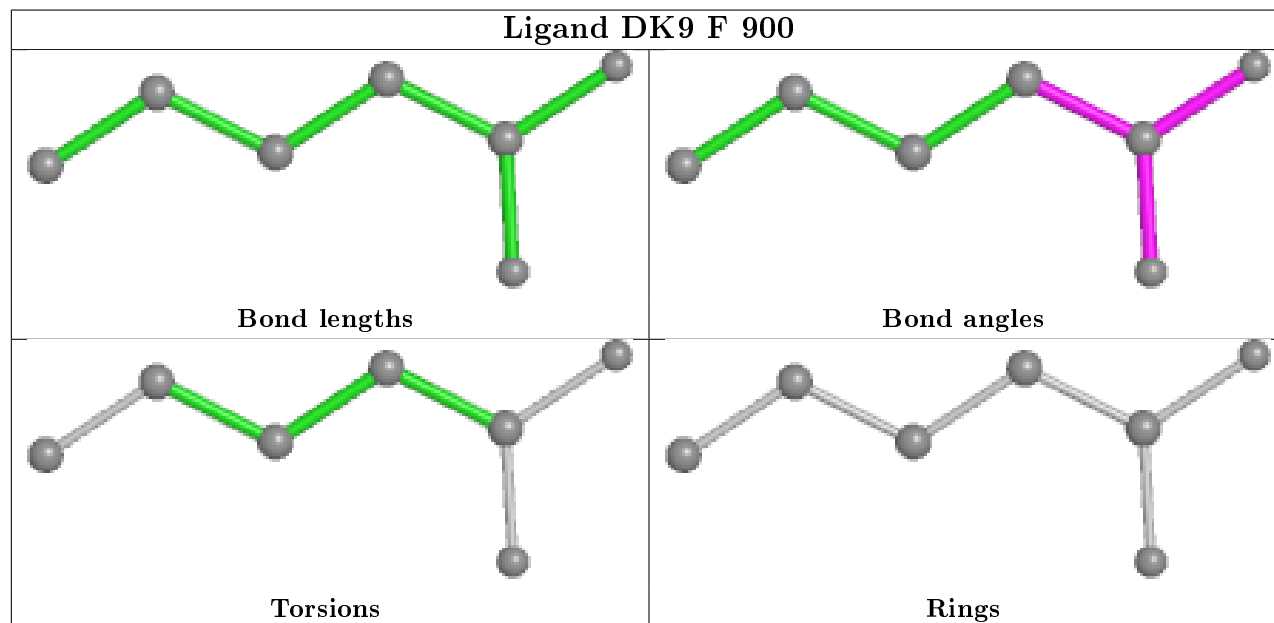
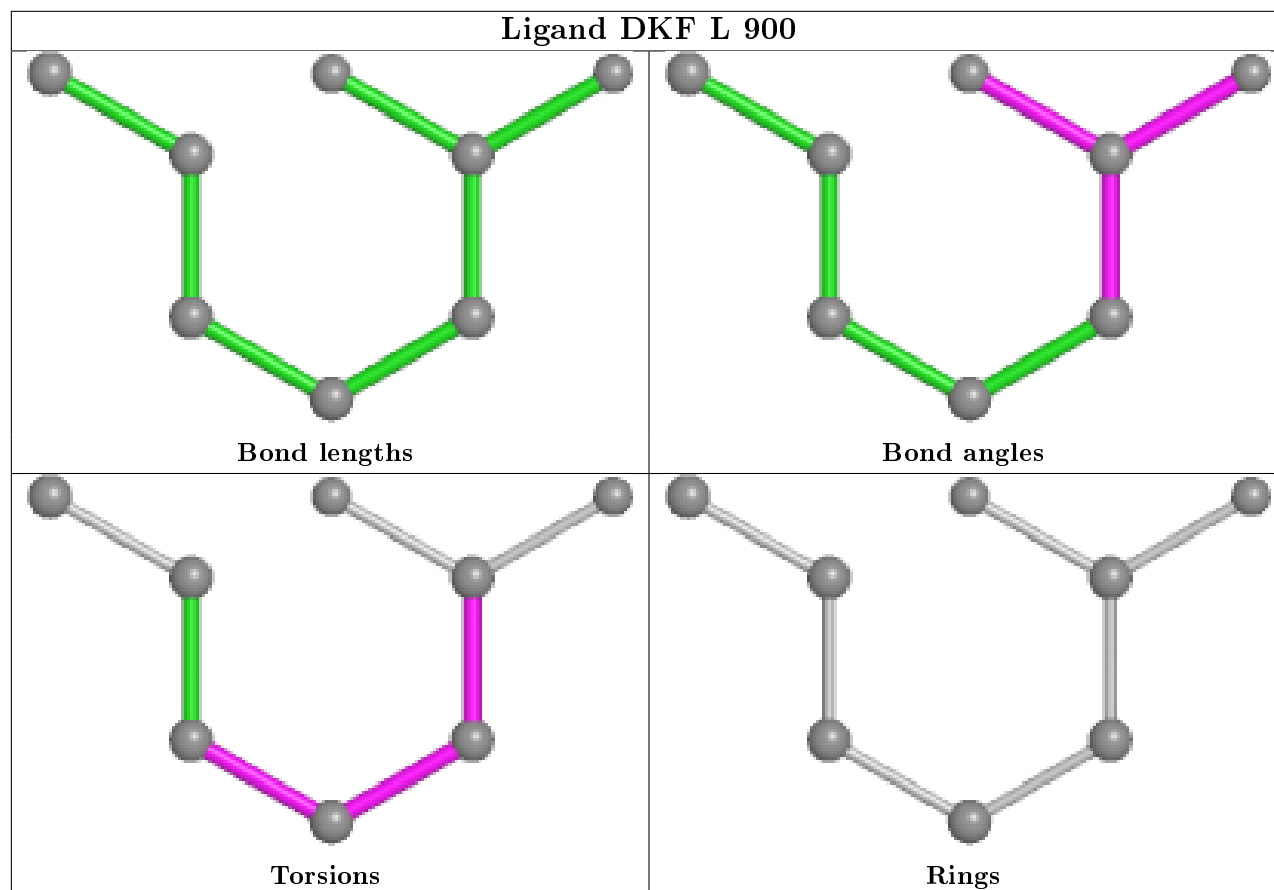


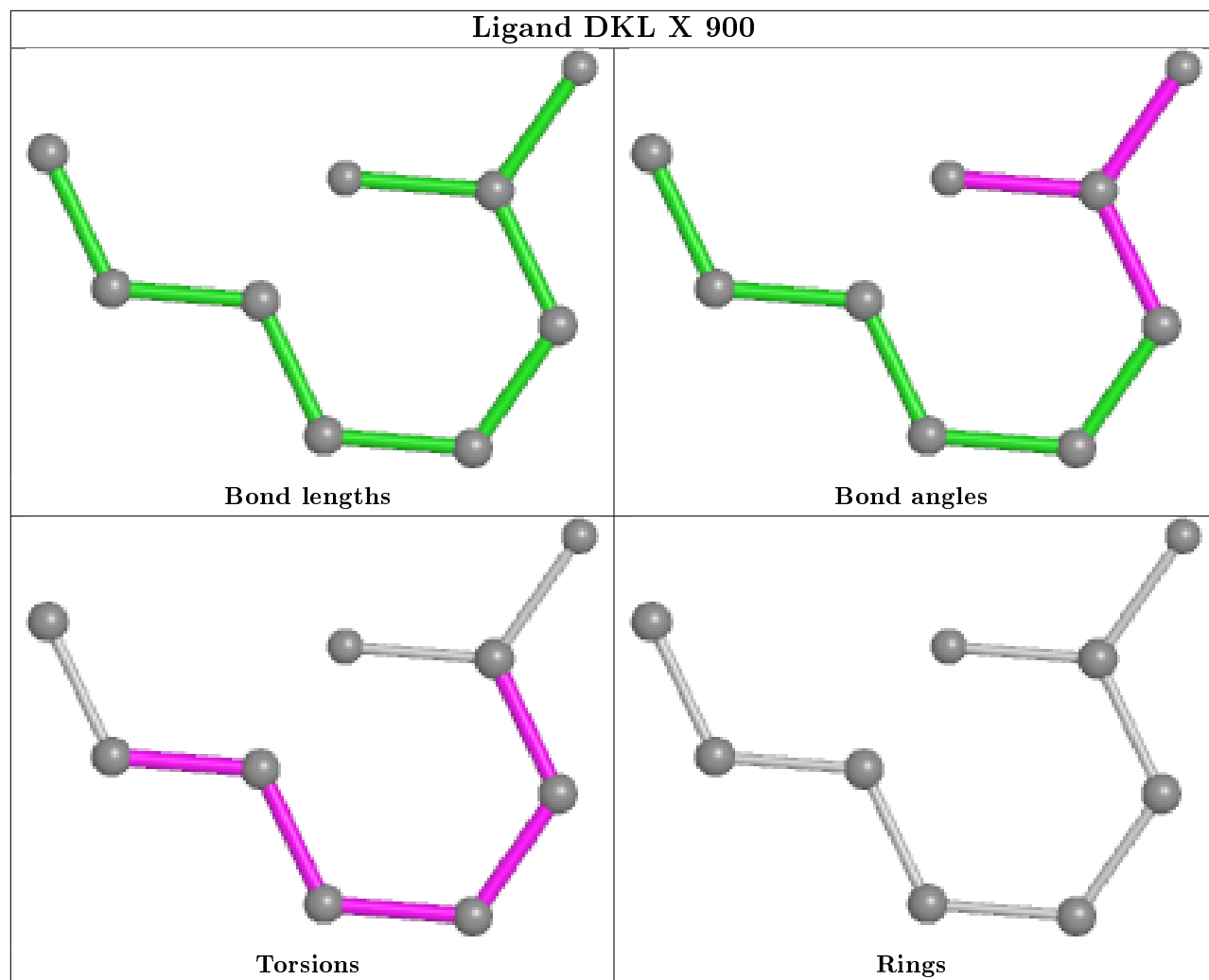


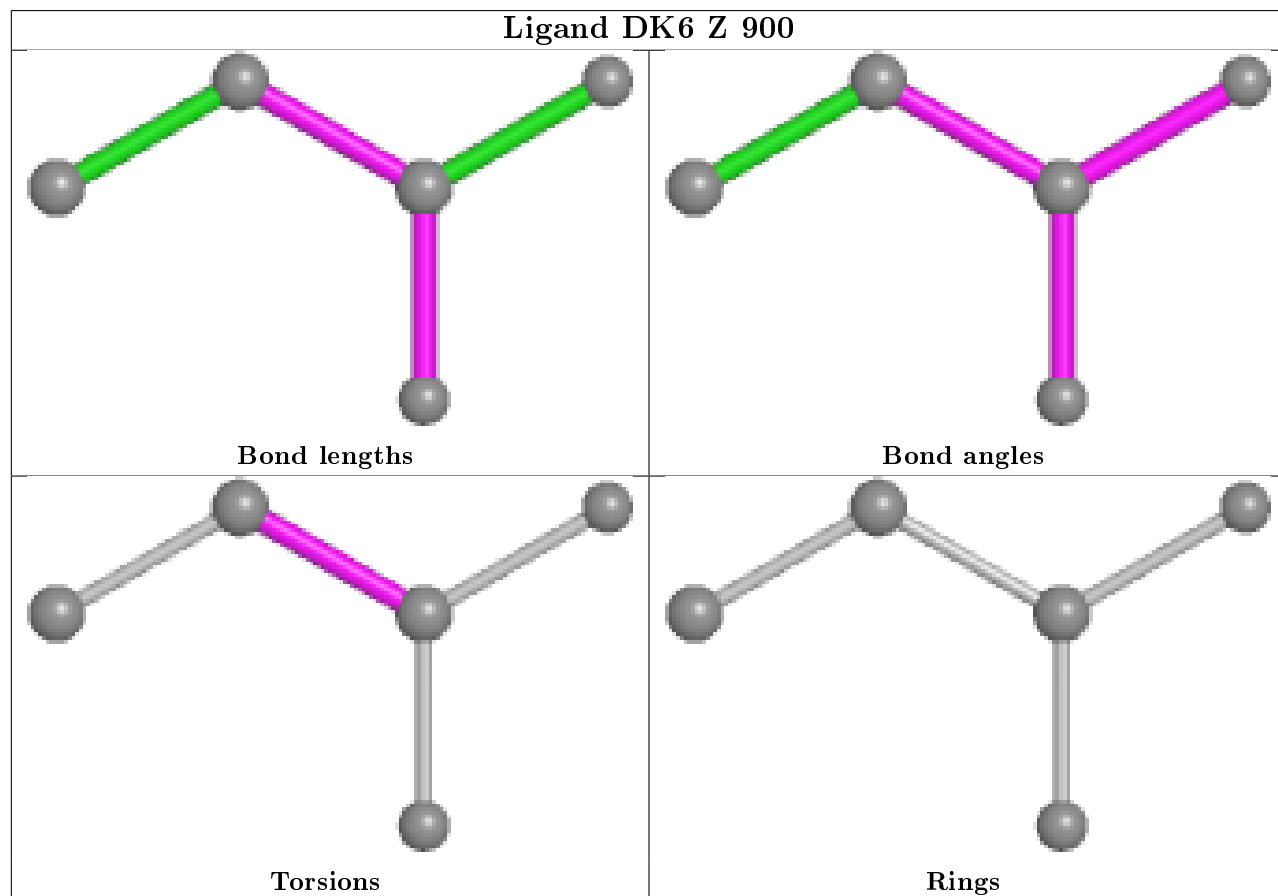
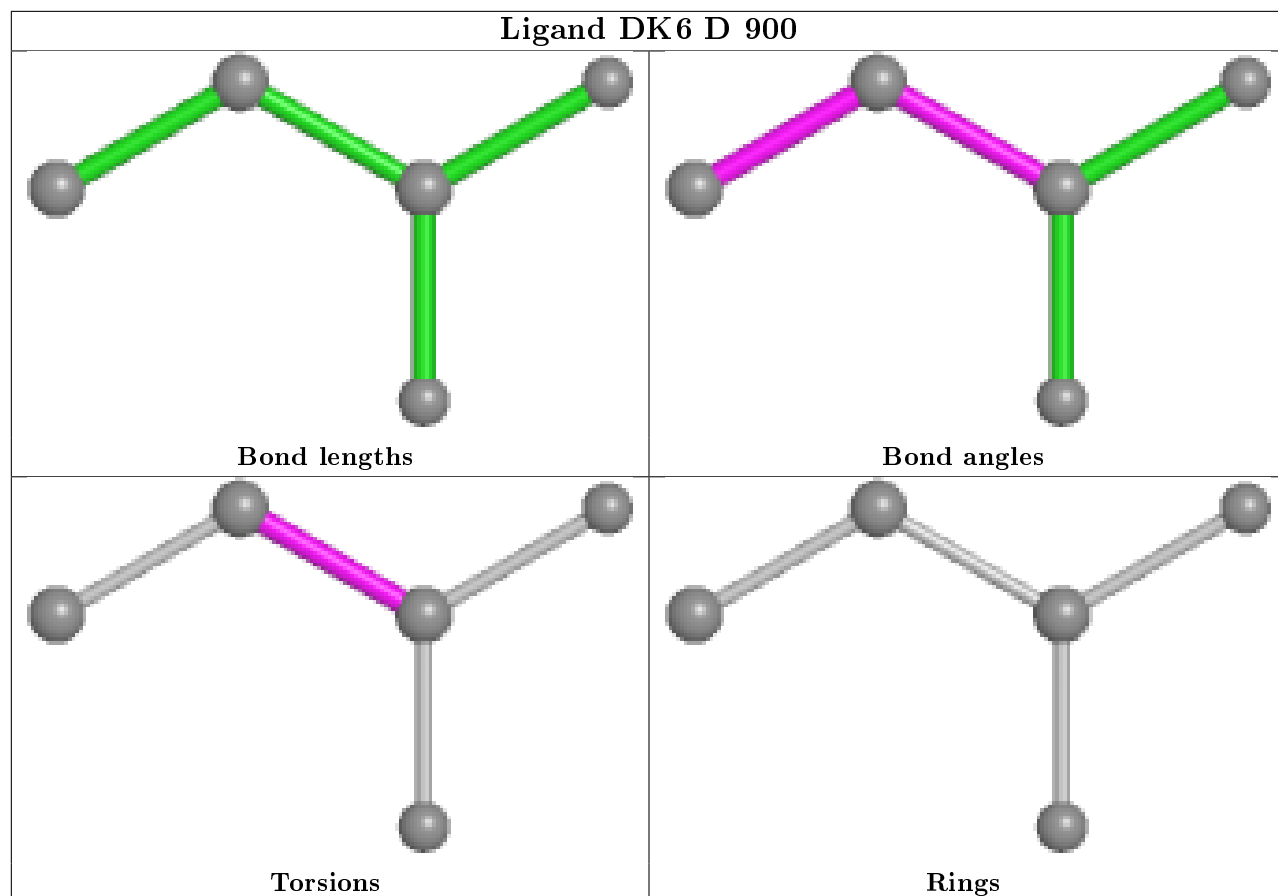


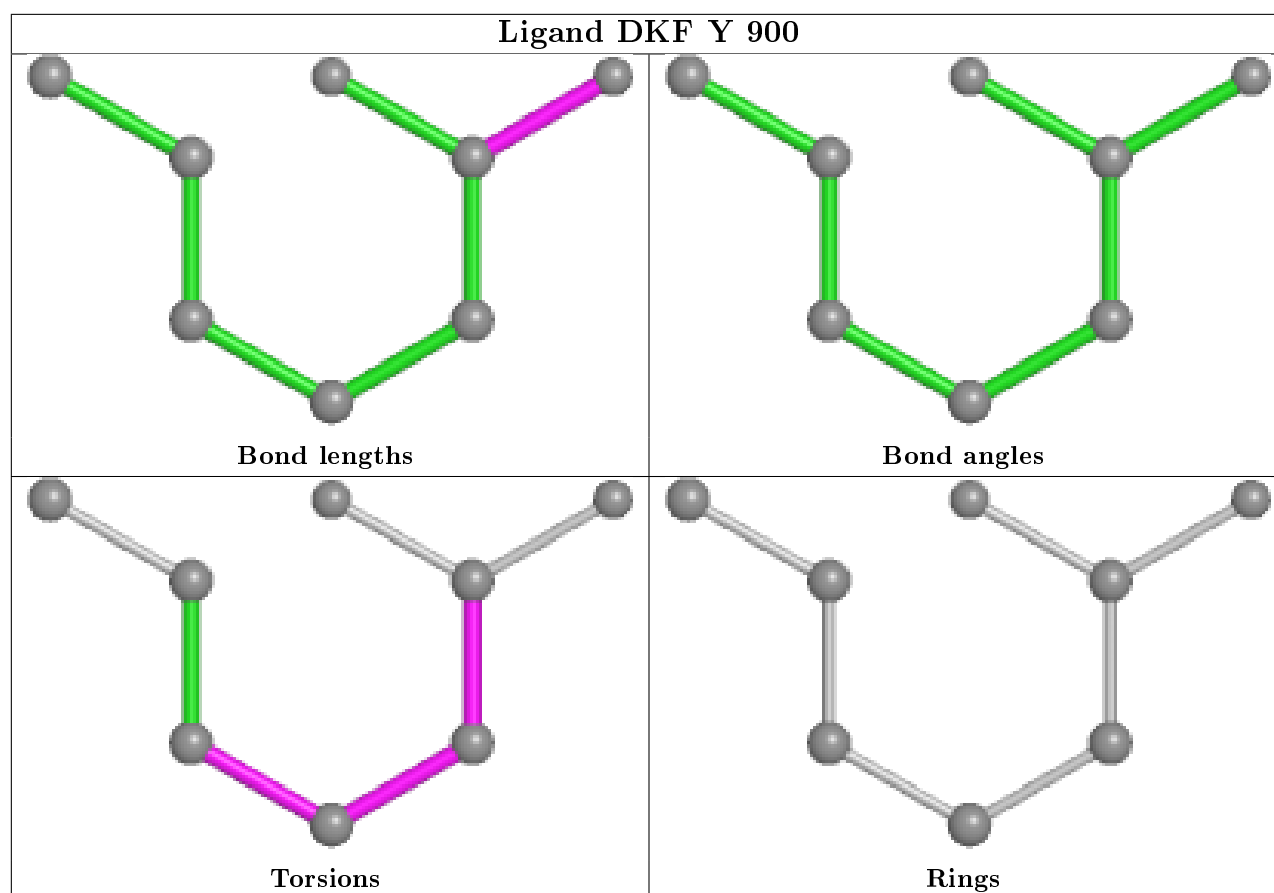












5.7 Other polymers [i](#)

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 ⓘ

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, 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	310/317 (97%)	-0.20	8 (2%) 56 54	19, 28, 49, 94	0
1	B	309/317 (97%)	-0.33	4 (1%) 77 75	19, 27, 44, 81	0
1	C	309/317 (97%)	-0.31	6 (1%) 66 64	18, 27, 46, 77	0
1	D	308/317 (97%)	-0.26	8 (2%) 56 54	18, 27, 45, 77	0
1	E	311/317 (98%)	-0.28	6 (1%) 66 64	20, 28, 46, 89	0
1	F	308/317 (97%)	-0.38	1 (0%) 94 93	18, 26, 46, 74	0
1	G	310/317 (97%)	-0.31	2 (0%) 89 88	18, 28, 45, 88	0
1	H	309/317 (97%)	-0.35	4 (1%) 77 75	19, 27, 46, 78	0
1	I	311/317 (98%)	-0.24	9 (2%) 51 50	19, 31, 50, 97	0
1	J	310/317 (97%)	-0.22	6 (1%) 66 64	19, 31, 51, 77	0
1	K	312/317 (98%)	-0.28	7 (2%) 62 60	17, 27, 48, 80	0
1	L	312/317 (98%)	-0.26	9 (2%) 51 50	17, 26, 47, 90	0
1	M	309/317 (97%)	0.03	13 (4%) 36 35	23, 36, 57, 102	0
1	N	310/317 (97%)	-0.25	4 (1%) 77 75	20, 30, 46, 104	0
1	O	310/317 (97%)	-0.24	8 (2%) 56 54	19, 29, 48, 86	0
1	P	310/317 (97%)	-0.30	6 (1%) 66 64	19, 28, 49, 93	0
1	Q	311/317 (98%)	-0.21	8 (2%) 56 54	21, 31, 53, 92	0
1	R	309/317 (97%)	-0.06	10 (3%) 47 46	22, 34, 58, 105	0
1	S	310/317 (97%)	-0.32	5 (1%) 72 70	16, 27, 45, 84	0
1	T	309/317 (97%)	-0.36	1 (0%) 94 93	15, 26, 41, 84	0
1	U	310/317 (97%)	0.09	12 (3%) 39 38	25, 38, 60, 86	0
1	V	309/317 (97%)	-0.12	7 (2%) 60 58	22, 33, 50, 74	0
1	W	310/317 (97%)	-0.17	6 (1%) 66 64	22, 33, 50, 84	0
1	X	309/317 (97%)	-0.21	6 (1%) 66 64	21, 34, 56, 96	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	Y	309/317 (97%)	-0.22	7 (2%) 60 58	24, 33, 50, 98	0
1	Z	309/317 (97%)	-0.00	12 (3%) 39 38	24, 39, 66, 92	0
All	All	8053/8242 (97%)	-0.22	175 (2%) 62 60	15, 30, 52, 105	0

The worst 5 of 175 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	W	310	ASN	6.4
1	R	310	ASN	5.2
1	U	310	ASN	4.8
1	M	186	ASP	4.6
1	D	211	PHE	4.3

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	DK6	S	900	5/5	0.57	0.53	26,29,34,36	0
5	DKF	W	900	8/8	0.65	0.43	37,41,54,56	0
5	DKF	G	900	8/8	0.68	0.40	29,39,43,43	0
2	DKL	C	900	9/9	0.69	0.59	32,51,84,85	0
5	DKF	Y	900	8/8	0.71	0.37	30,43,54,57	0
5	DKF	M	900	8/8	0.73	0.44	35,49,55,56	0
5	DKF	U	900	8/8	0.74	0.41	40,56,68,68	0
2	DKL	X	900	9/9	0.76	0.42	32,44,66,67	0
2	DKL	A	900	9/9	0.77	0.34	27,39,47,49	0
4	DK6	Z	900	5/5	0.77	0.40	34,39,42,43	0

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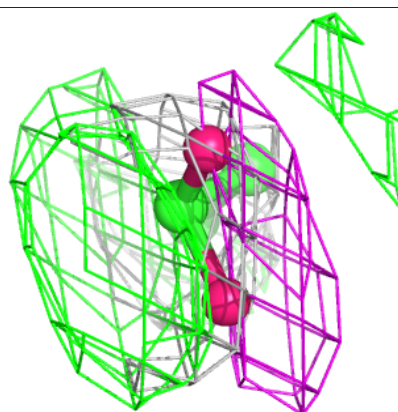
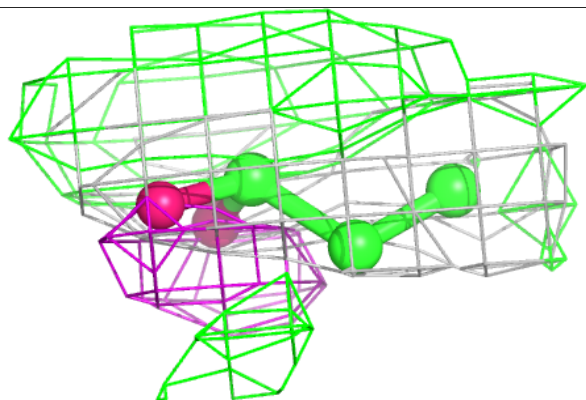
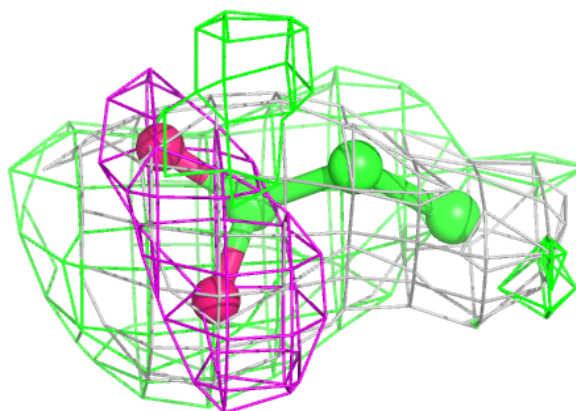
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	DKO	R	900	10/10	0.77	0.38	35,50,68,70	0
3	DKO	B	900	10/10	0.78	0.39	29,48,64,66	0
6	DK9	O	900	7/7	0.80	0.32	27,38,45,45	0
4	DK6	D	900	5/5	0.80	0.43	25,28,34,37	0
5	DKF	I	900	8/8	0.81	0.37	30,48,58,60	0
2	DKL	T	900	9/9	0.81	0.38	28,42,72,78	0
5	DKF	V	900	8/8	0.81	0.34	32,42,52,53	0
5	DKF	K	900	8/8	0.81	0.33	29,39,49,49	0
6	DK9	P	900	7/7	0.82	0.35	23,29,39,41	0
5	DKF	J	900	8/8	0.84	0.33	31,46,53,53	0
2	DKL	Q	900	9/9	0.84	0.35	30,46,54,55	0
4	DK6	H	900	5/5	0.85	0.42	28,31,35,37	0
5	DKF	E	900	8/8	0.87	0.41	27,47,57,59	0
3	DKO	N	900	10/10	0.90	0.34	28,55,82,83	0
6	DK9	F	900	7/7	0.91	0.37	23,29,34,36	0
5	DKF	L	900	8/8	0.92	0.37	30,38,45,46	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.

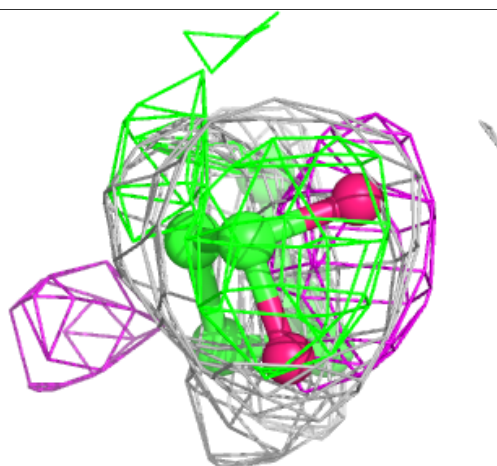
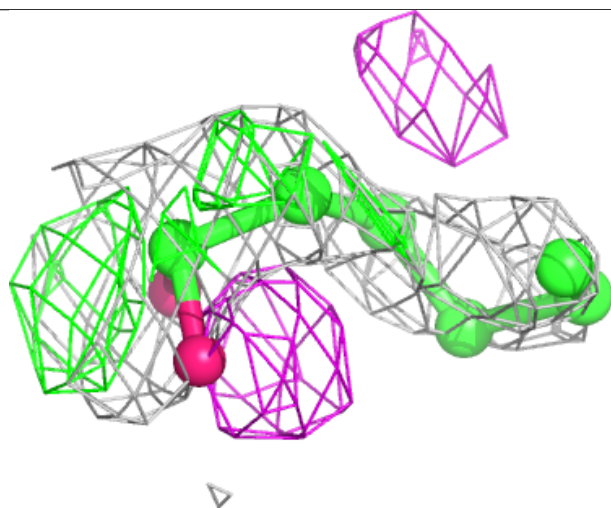
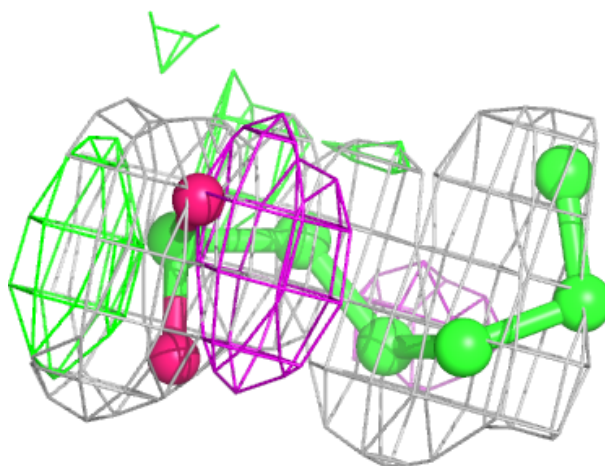
Electron density around DK6 S 900:

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



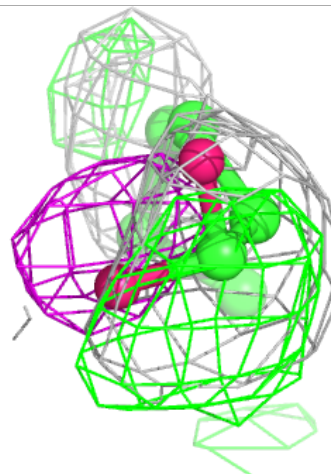
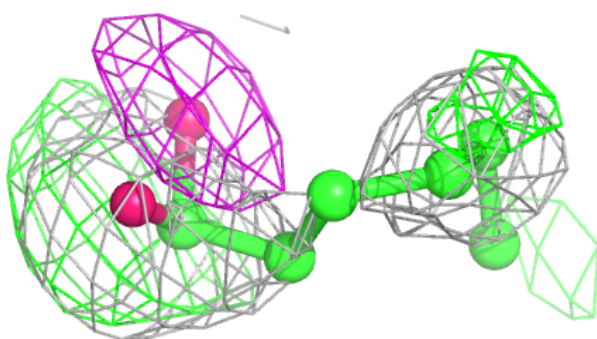
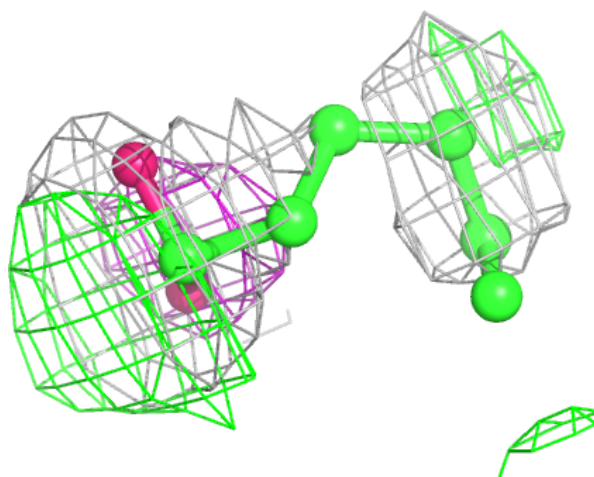
Electron density around DKF W 900:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



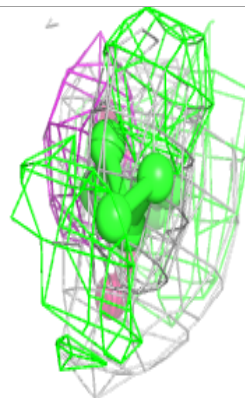
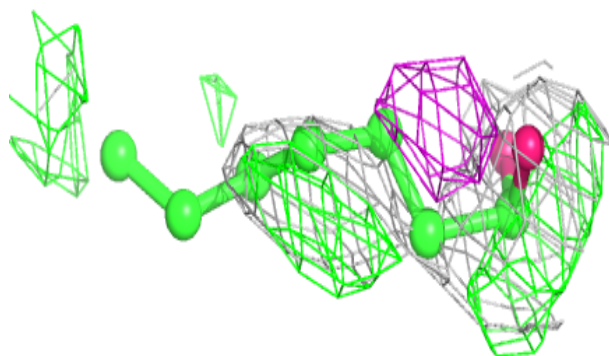
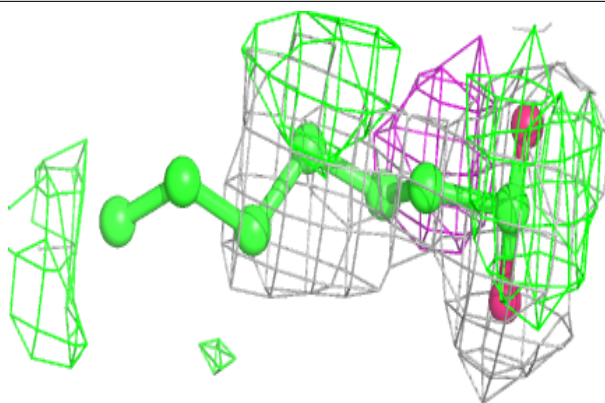
Electron density around DKF G 900:

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and green (positive)

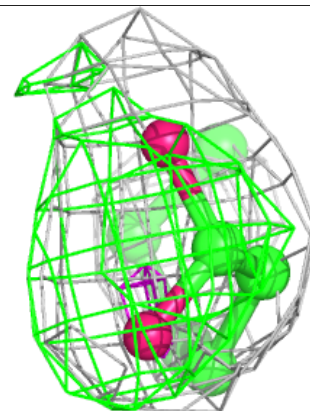
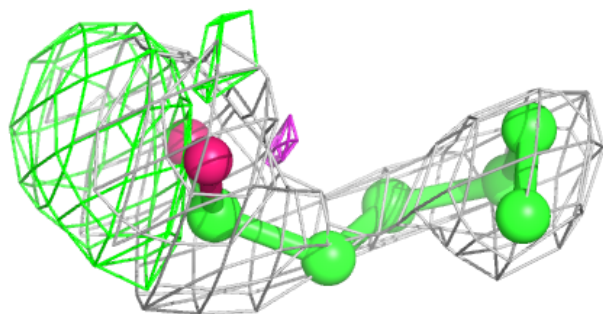
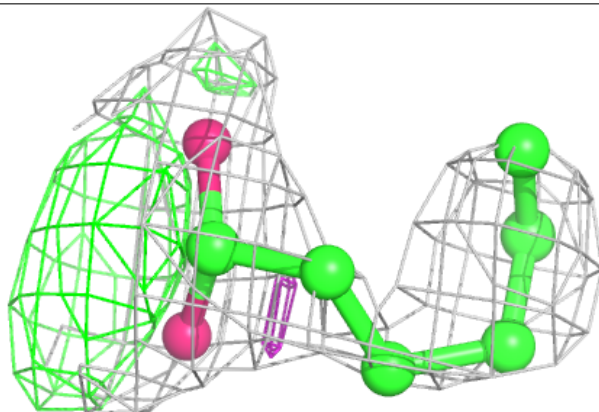


Electron density around DKL C 900:

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and green (positive)

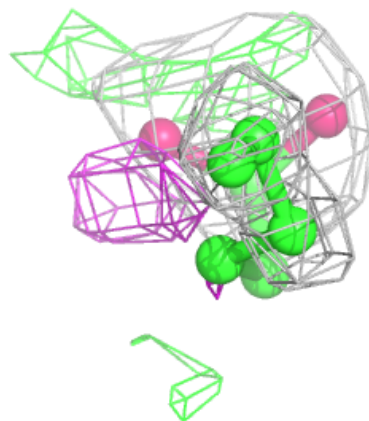
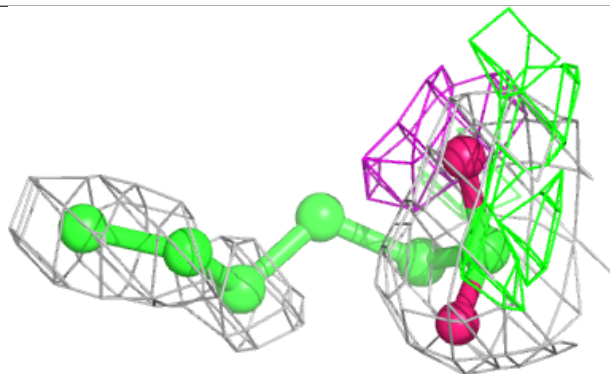
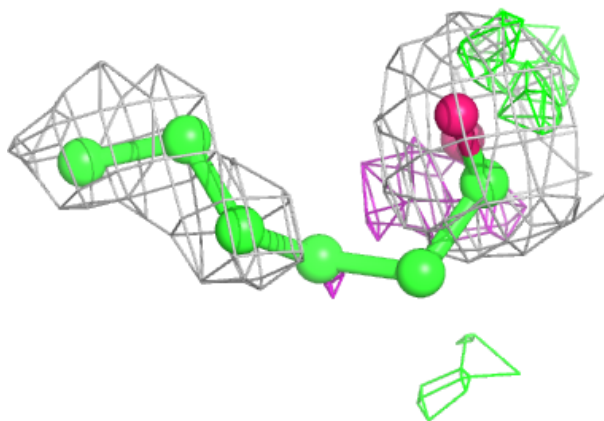
**Electron density around DKF Y 900:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



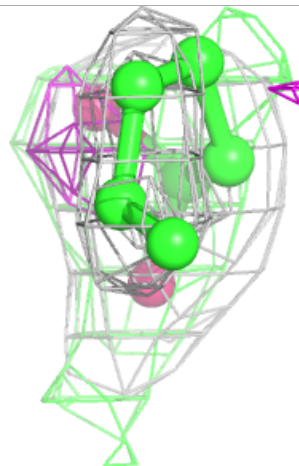
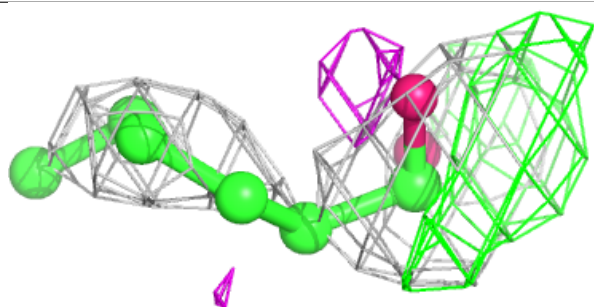
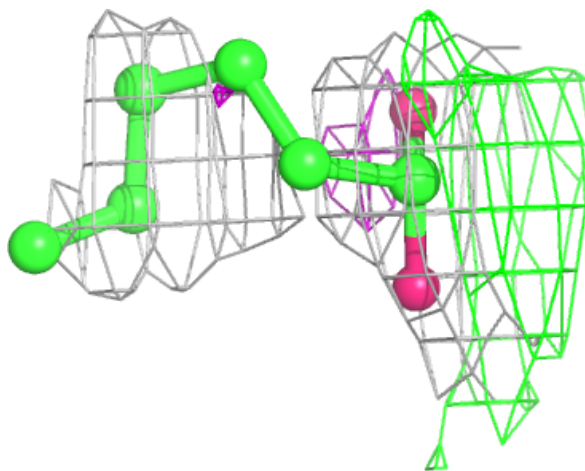
Electron density around DKF M 900:

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



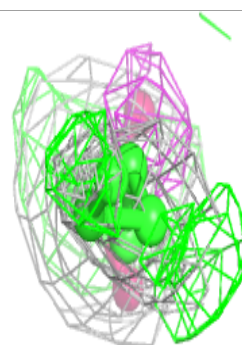
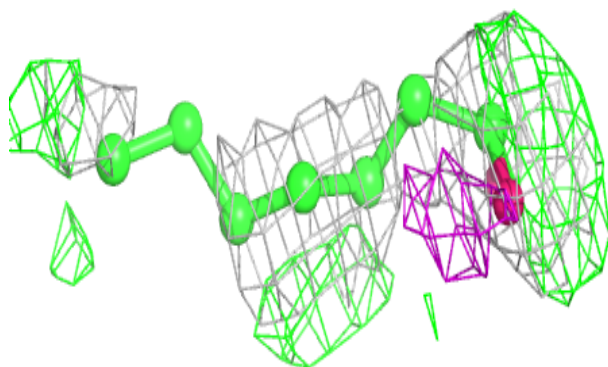
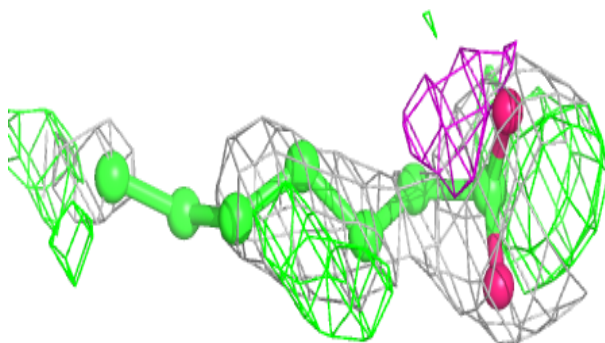
Electron density around DKF U 900:

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



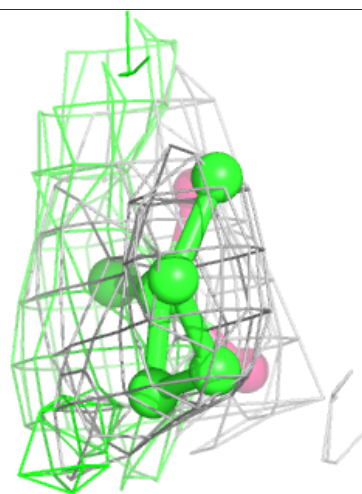
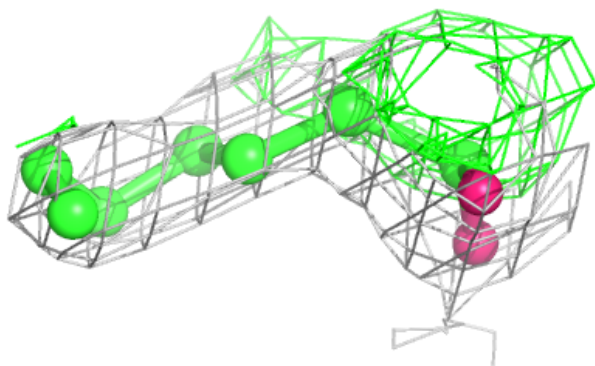
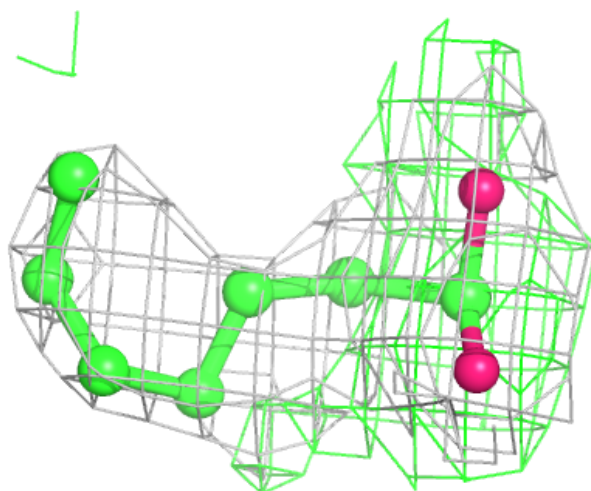
Electron density around DKL X 900:

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



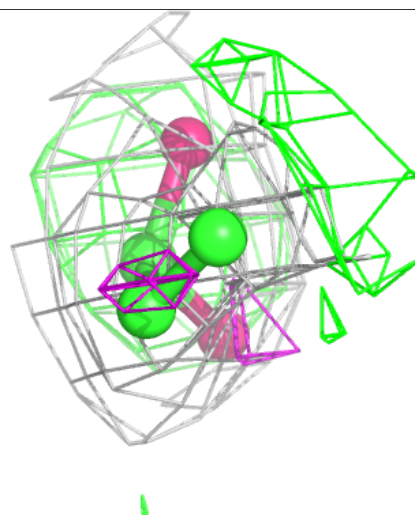
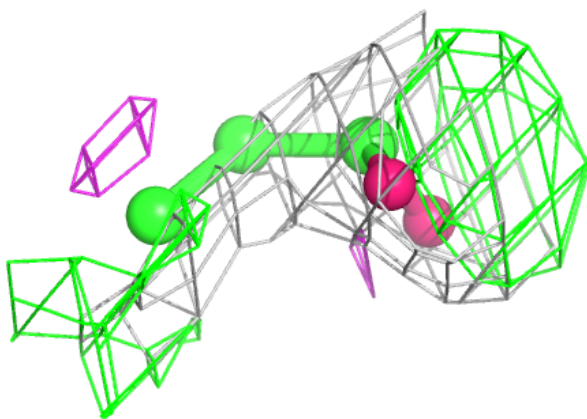
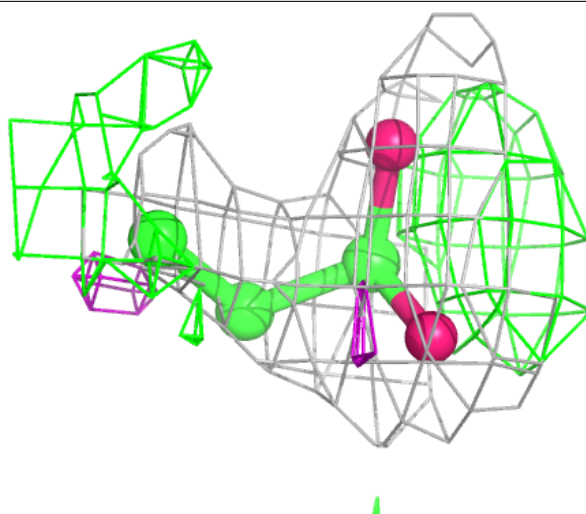
Electron density around DKL A 900:

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



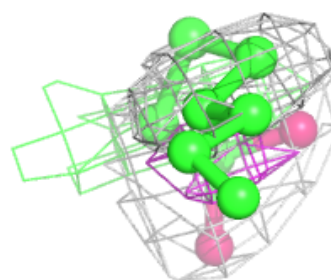
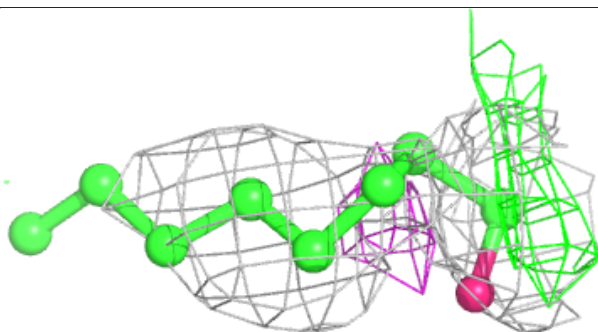
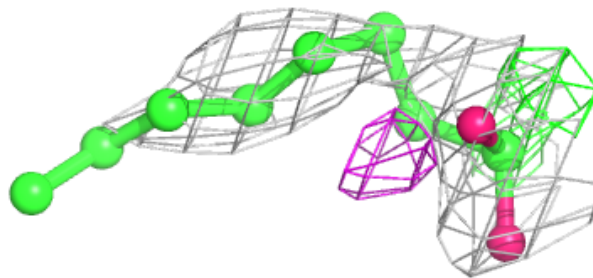
Electron density around DK6 Z 900:

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

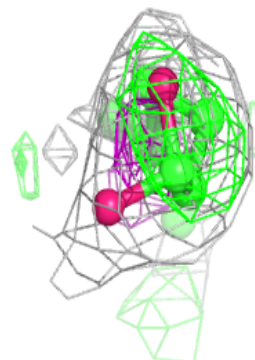
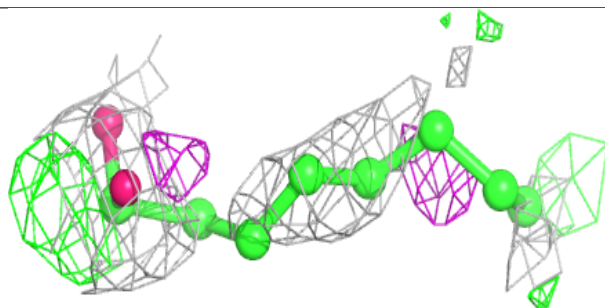
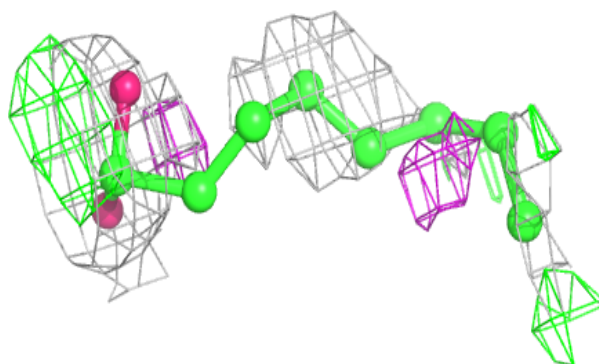


Electron density around DKO R 900:

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

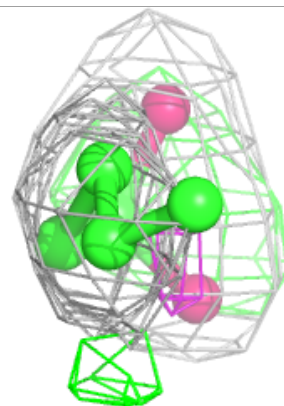
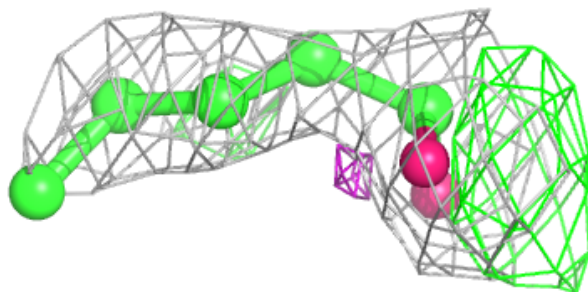
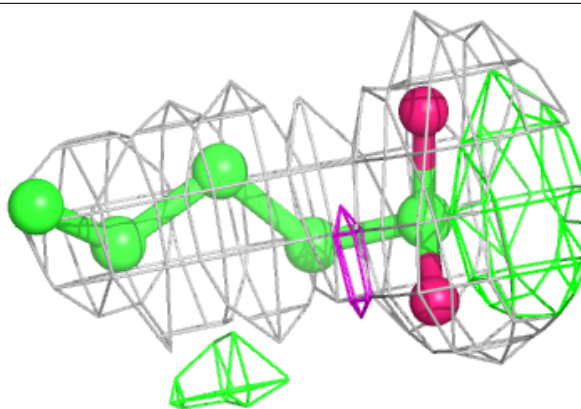
**Electron density around DKO B 900:**

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



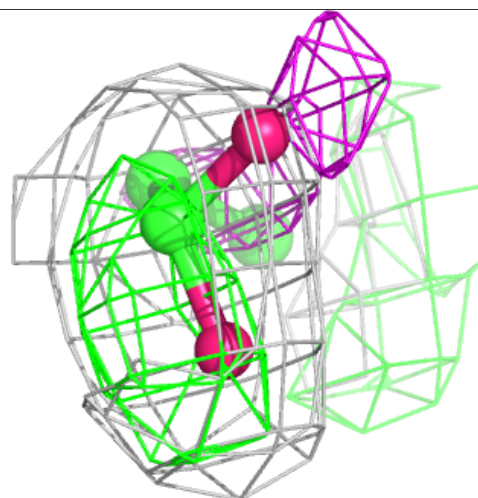
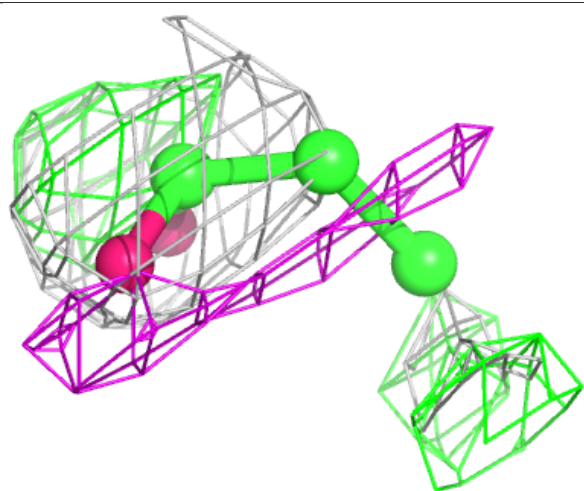
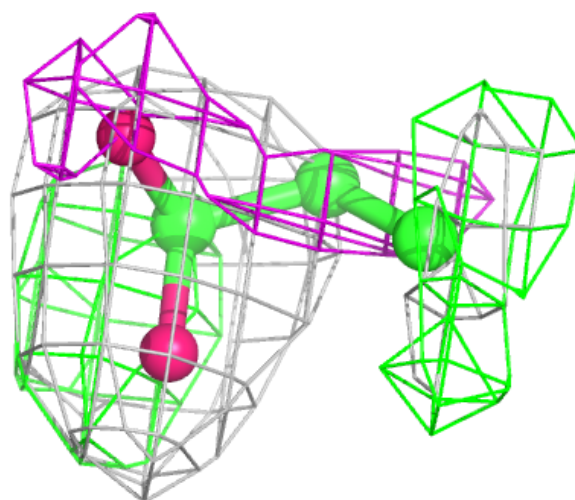
Electron density around DK9 O 900:

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



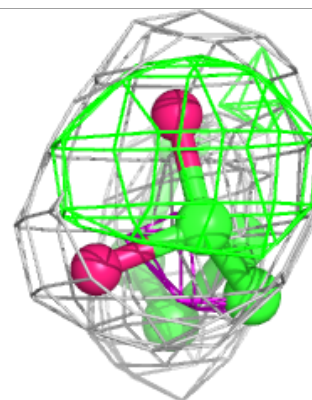
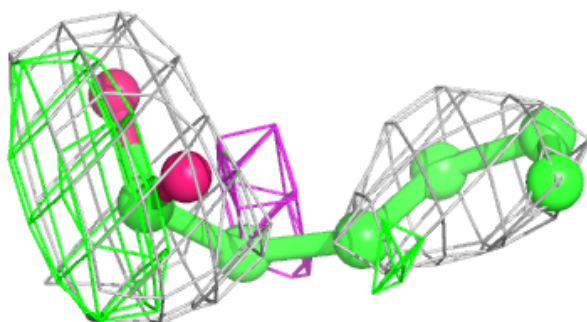
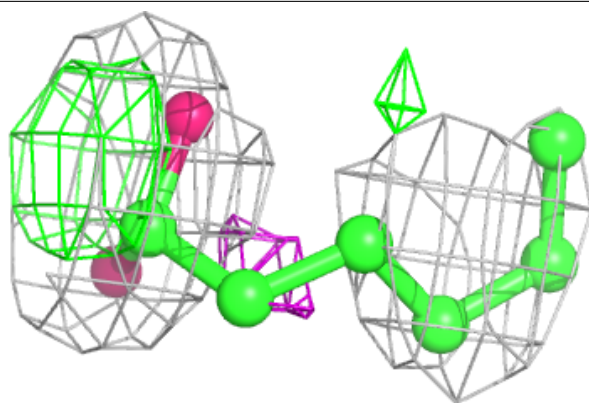
Electron density around DK6 D 900:

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

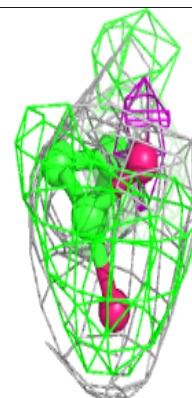
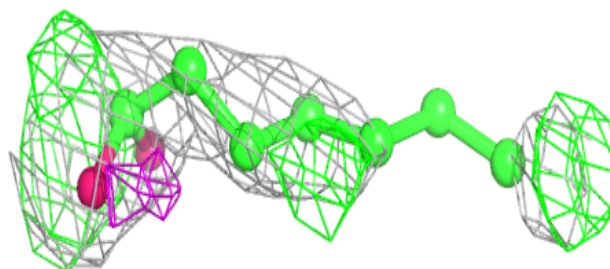
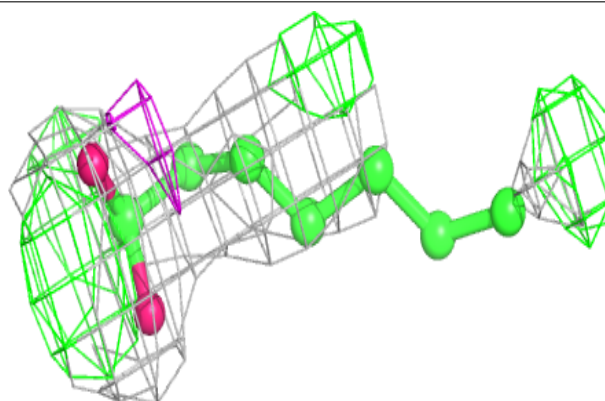


Electron density around DKF I 900:

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

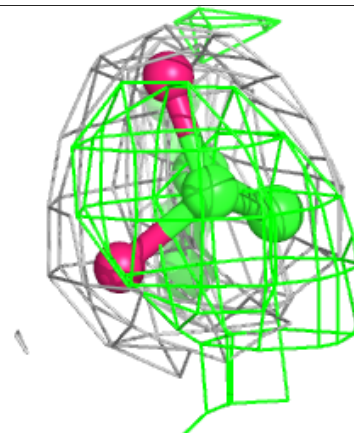
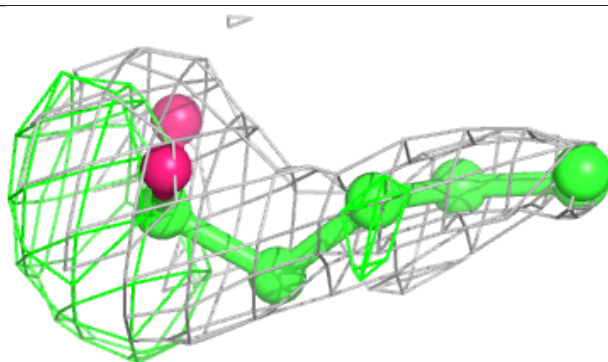
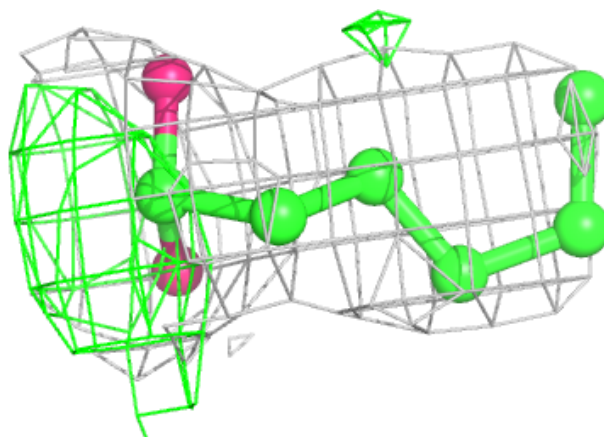
**Electron density around DKL T 900:**

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

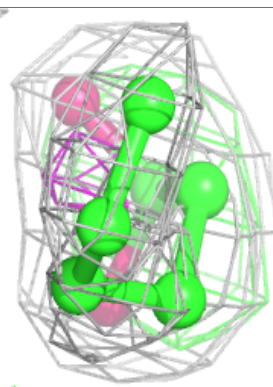
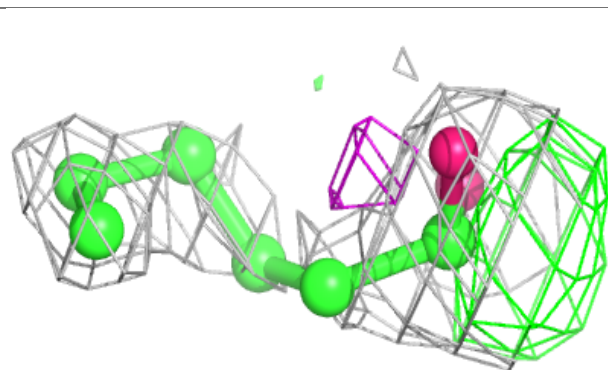
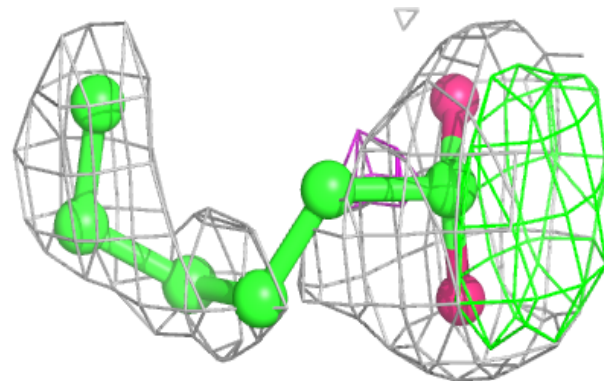


Electron density around DKF V 900:

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

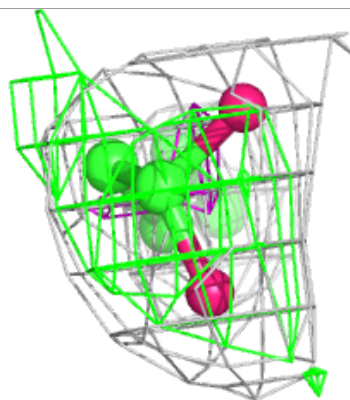
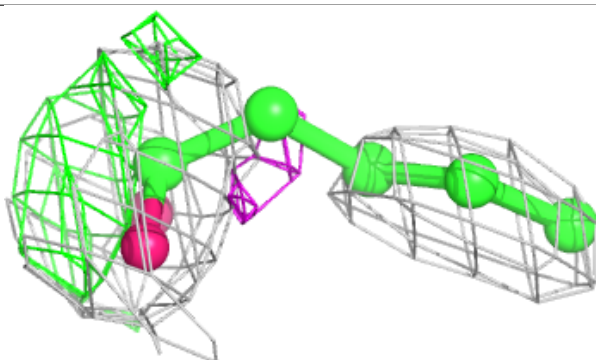
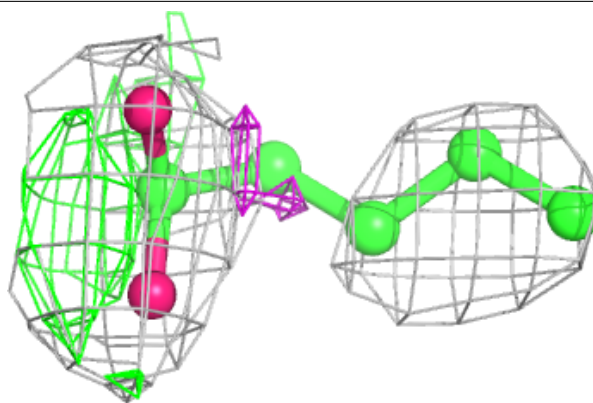
**Electron density around DKF K 900:**

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

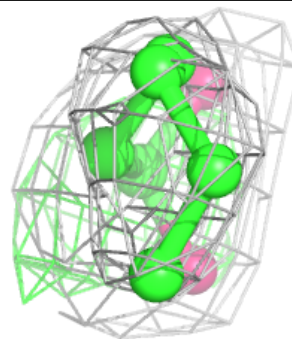
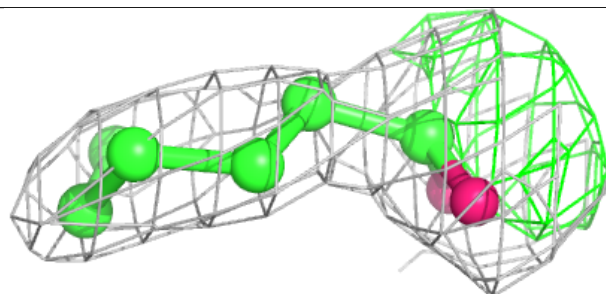
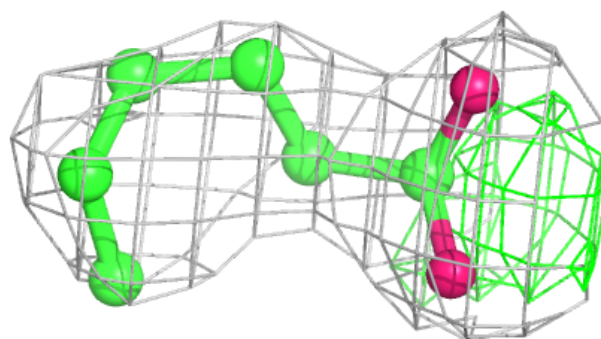


Electron density around DK9 P 900:

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

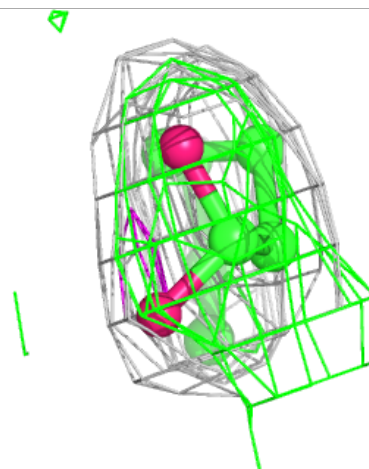
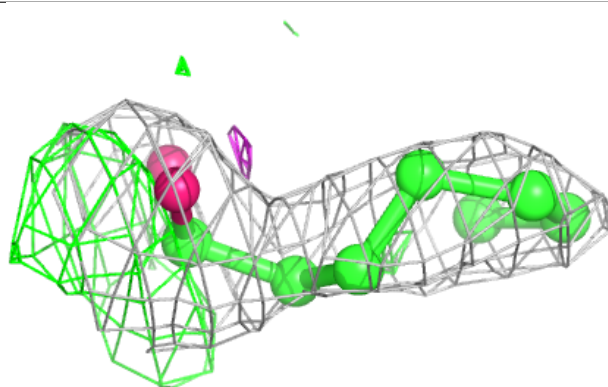
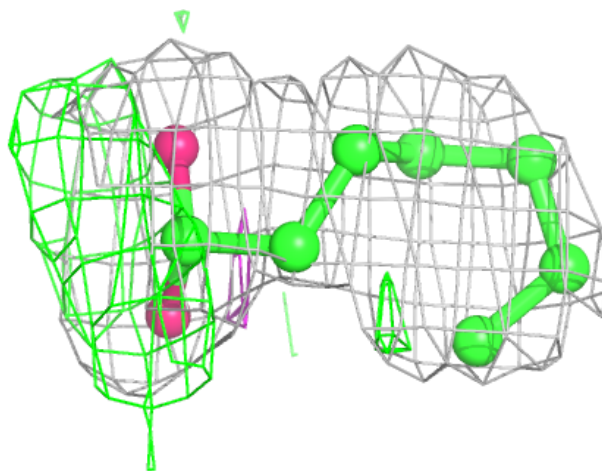
**Electron density around DKF J 900:**

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



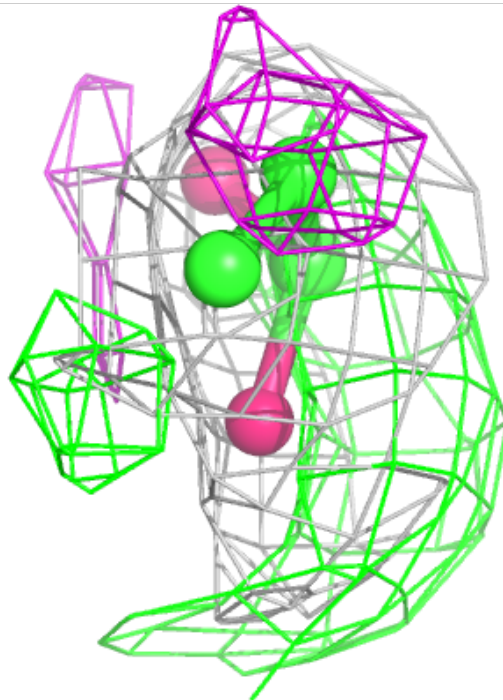
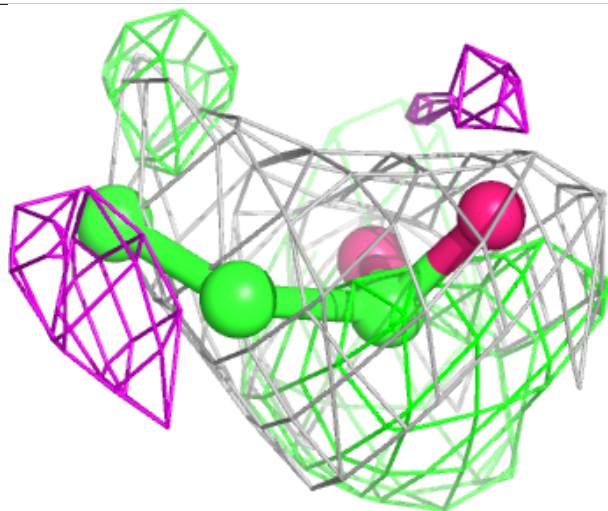
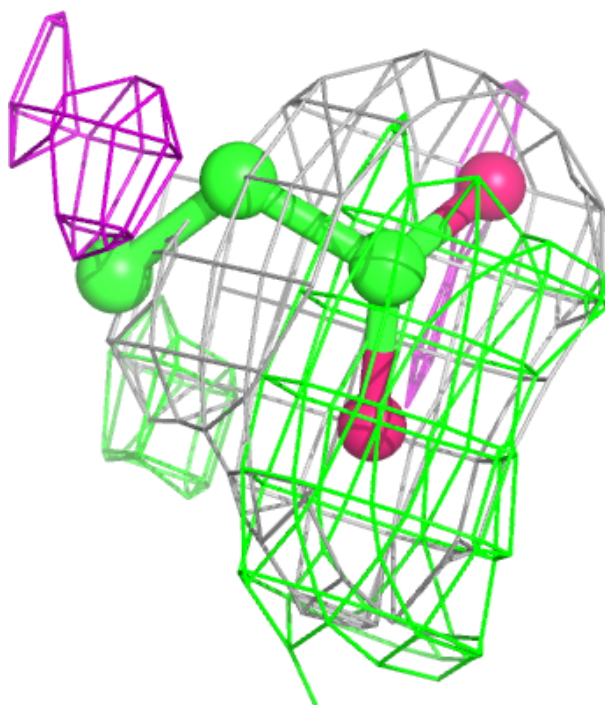
Electron density around DKL Q 900:

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



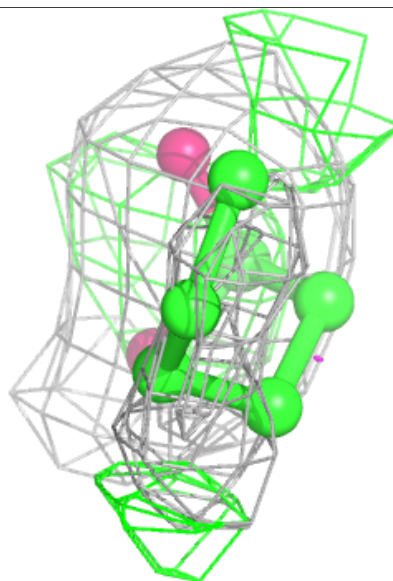
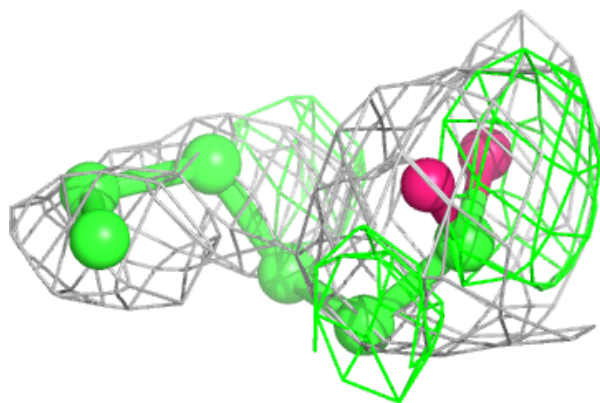
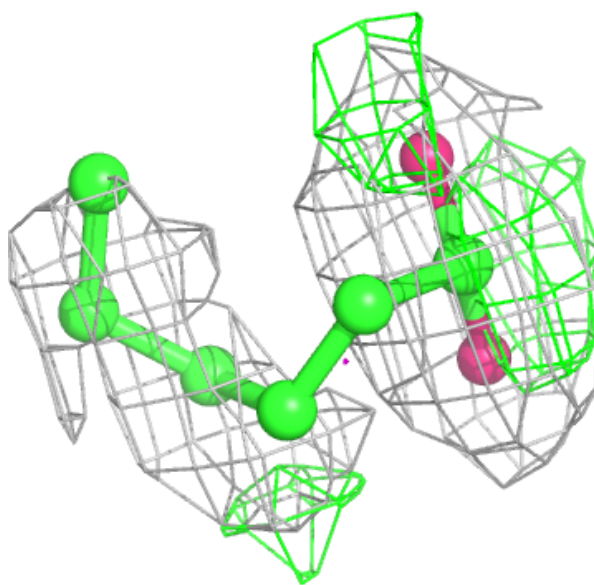
Electron density around DK6 H 900:

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



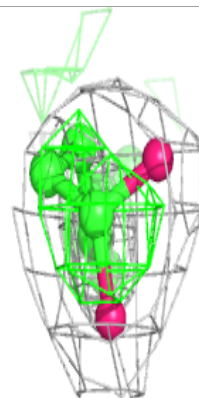
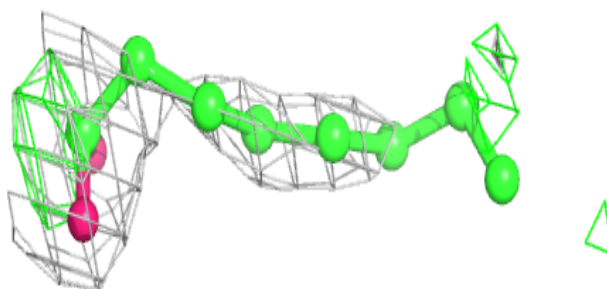
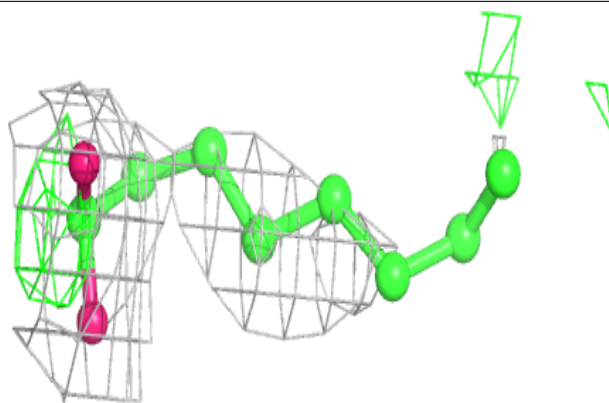
Electron density around DKF E 900:

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

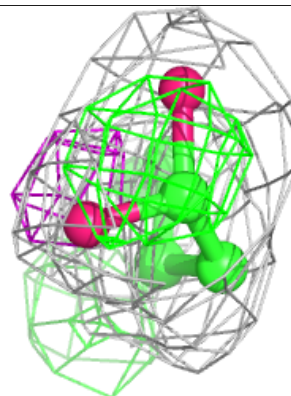
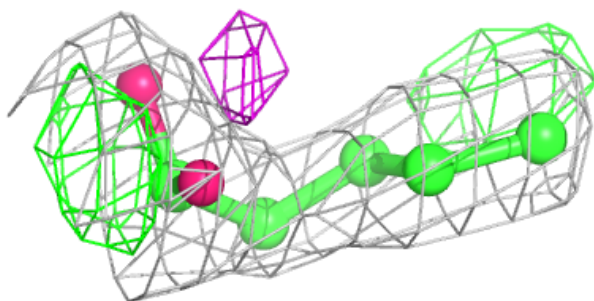
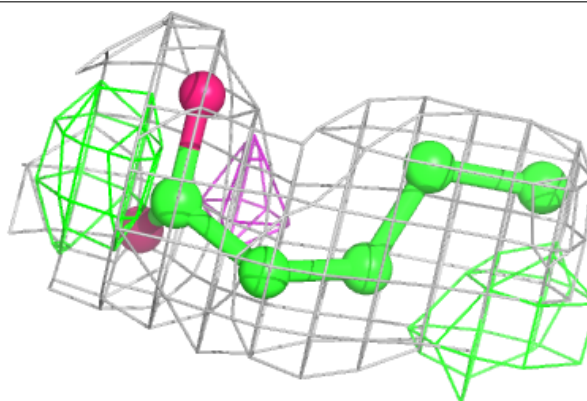


Electron density around DKO N 900:

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

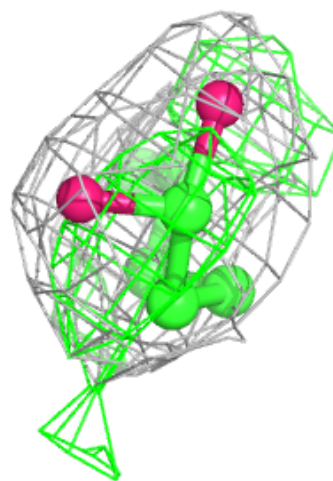
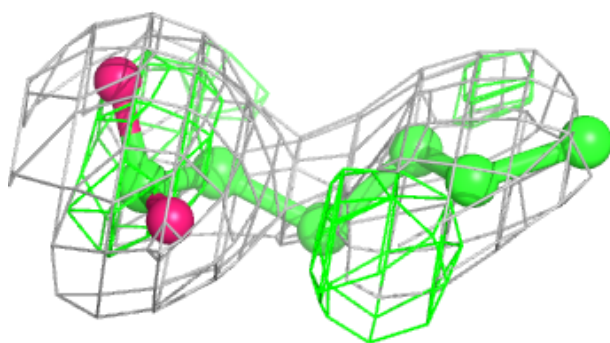
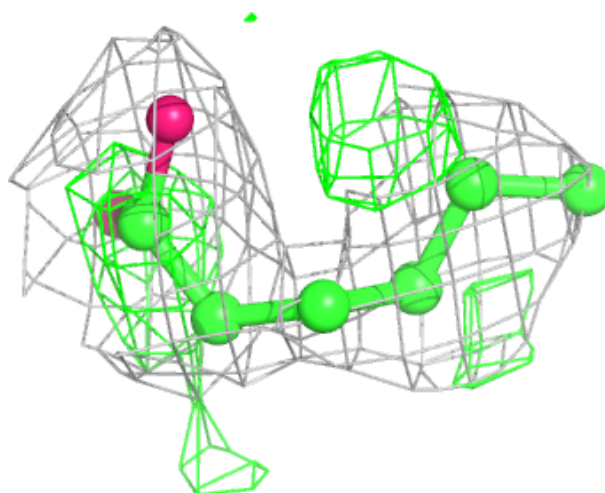
**Electron density around DK9 F 900:**

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



Electron density around DKF L 900:

$2mF_o-DF_c$ (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.