



Full wwPDB X-ray Structure Validation 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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The 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

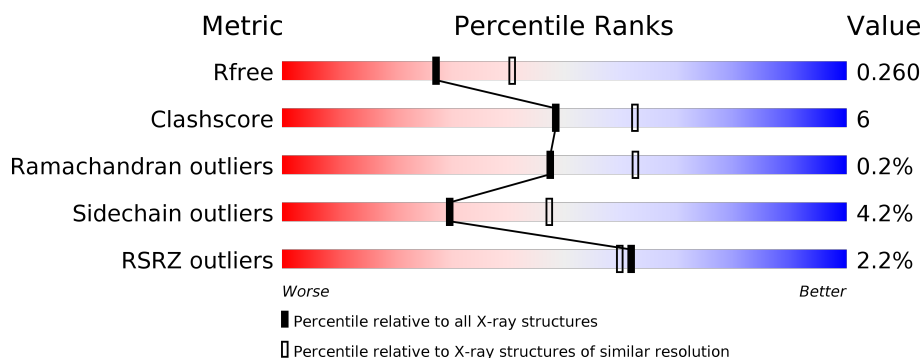
1 Overall quality at a glance

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.







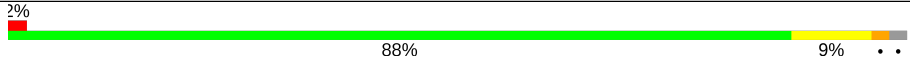
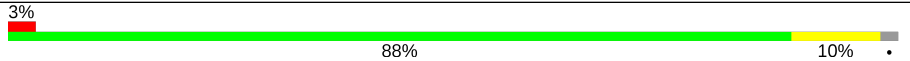
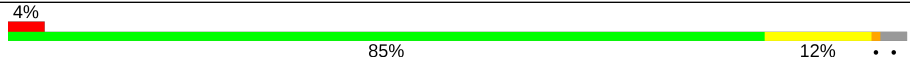
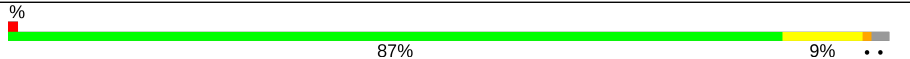
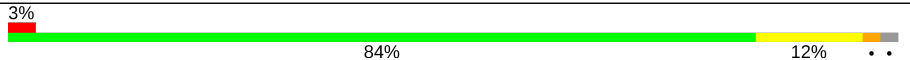
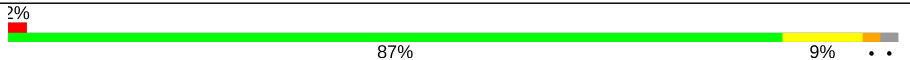
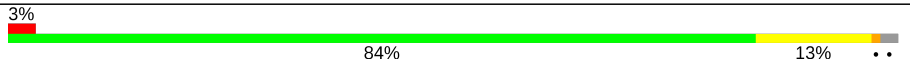
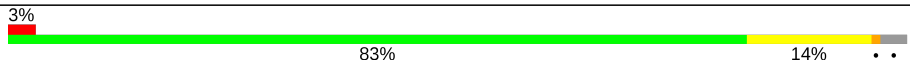
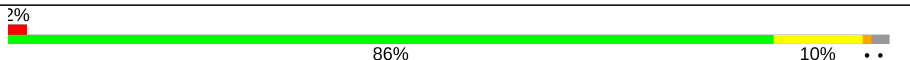



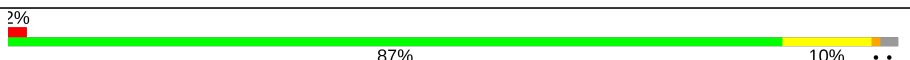
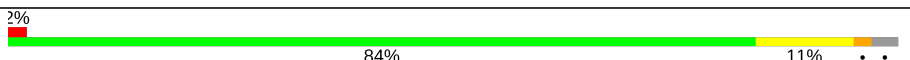
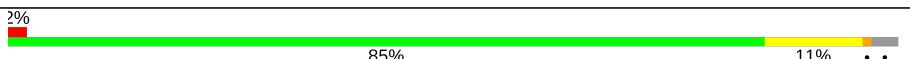
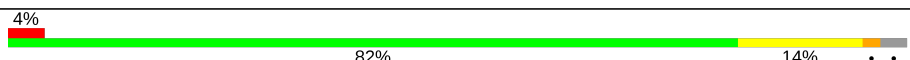
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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.

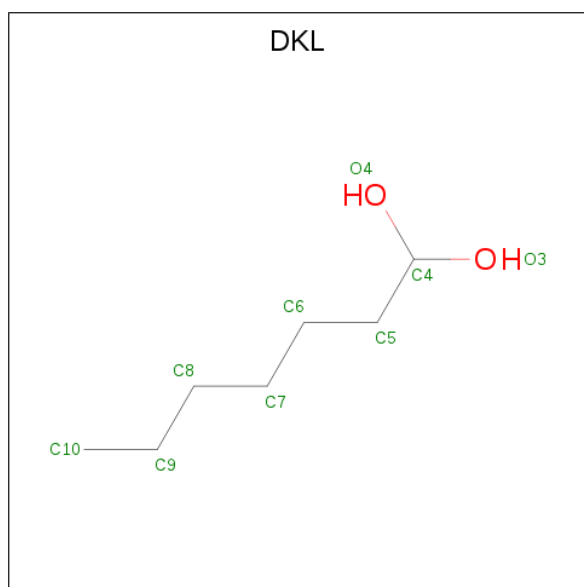
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	310	Total	C	N	O	S	0	0	0
			2360	1476	421	453	10			
1	B	309	Total	C	N	O	S	0	0	0
			2349	1470	417	452	10			
1	C	309	Total	C	N	O	S	0	0	0
			2349	1470	417	452	10			
1	D	308	Total	C	N	O	S	0	0	0
			2341	1466	415	450	10			
1	E	311	Total	C	N	O	S	0	0	0
			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: $C_7H_{16}O_2$) (labeled as "Ligand of Interest" by author).



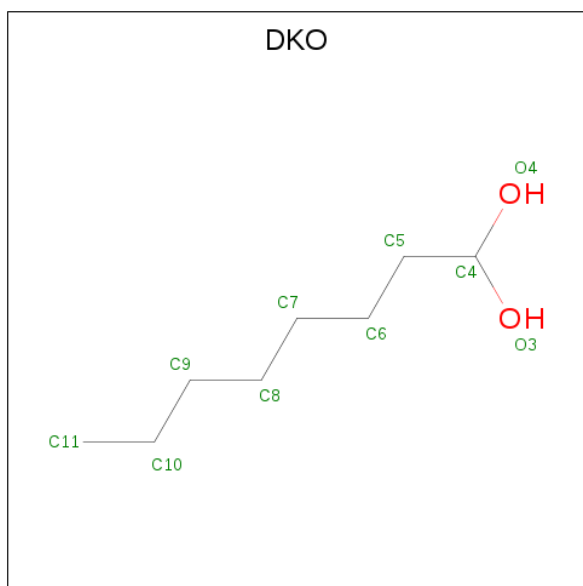
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			9	7	2		

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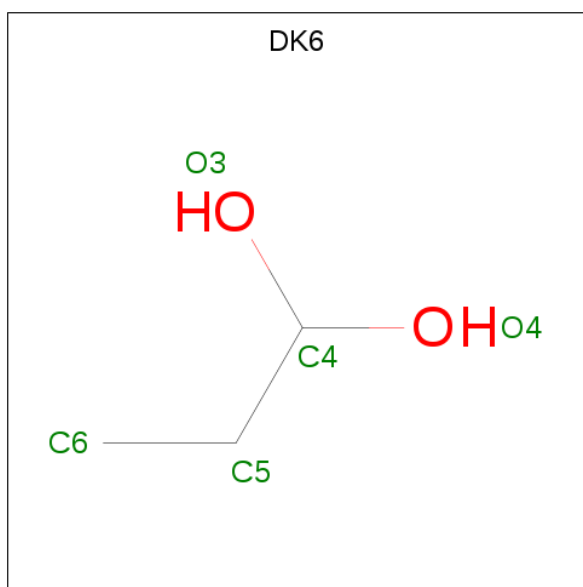
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	C	O	0	0
			9	7	2		
2	Q	1	Total	C	O	0	0
			9	7	2		
2	T	1	Total	C	O	0	0
			9	7	2		
2	X	1	Total	C	O	0	0
			9	7	2		

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



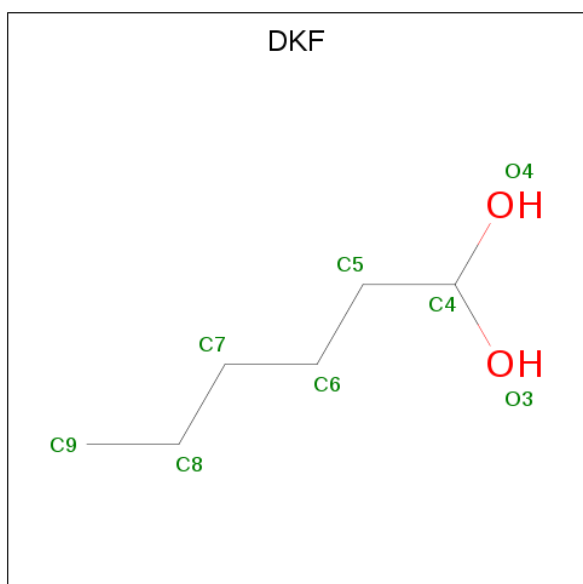
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			10	8	2		
3	N	1	Total	C	O	0	0
			10	8	2		
3	R	1	Total	C	O	0	0
			10	8	2		

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



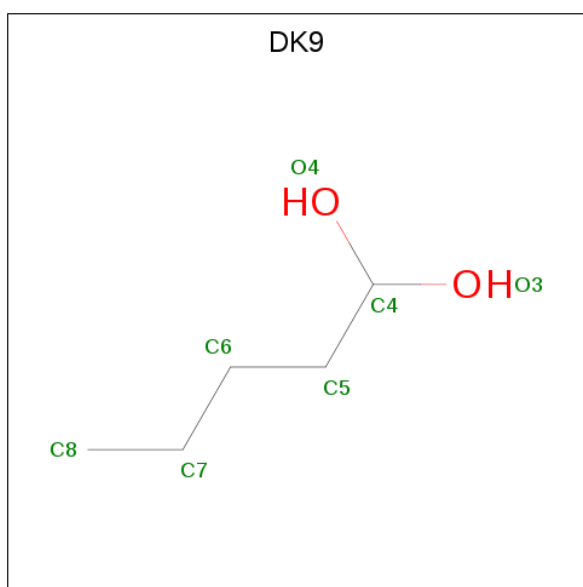
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	C	O	0	0
			5	3	2		
4	H	1	Total	C	O	0	0
			5	3	2		
4	S	1	Total	C	O	0	0
			5	3	2		
4	Z	1	Total	C	O	0	0
			5	3	2		

- Molecule 5 is hexane-1,1-diol (three-letter code: DKF) (formula: C₆H₁₄O₂) (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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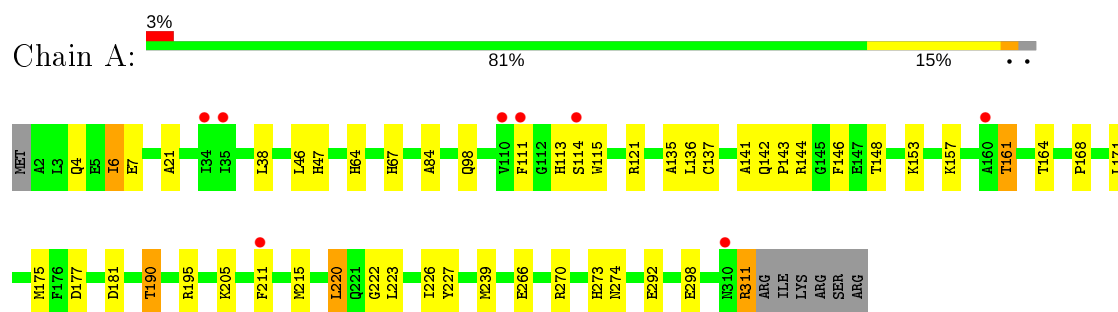
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	R	75	Total 75	O 75	0	0
7	S	128	Total 128	O 128	0	0
7	T	79	Total 79	O 79	0	0
7	U	80	Total 80	O 80	0	0
7	V	83	Total 83	O 83	0	0
7	X	63	Total 63	O 63	0	0
7	Y	82	Total 82	O 82	0	0
7	W	71	Total 71	O 71	0	0
7	Z	47	Total 47	O 47	0	0

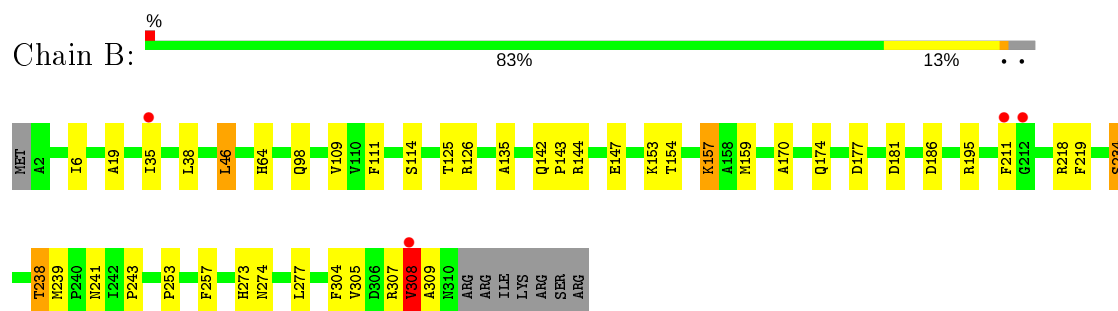
3 Residue-property plots

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.

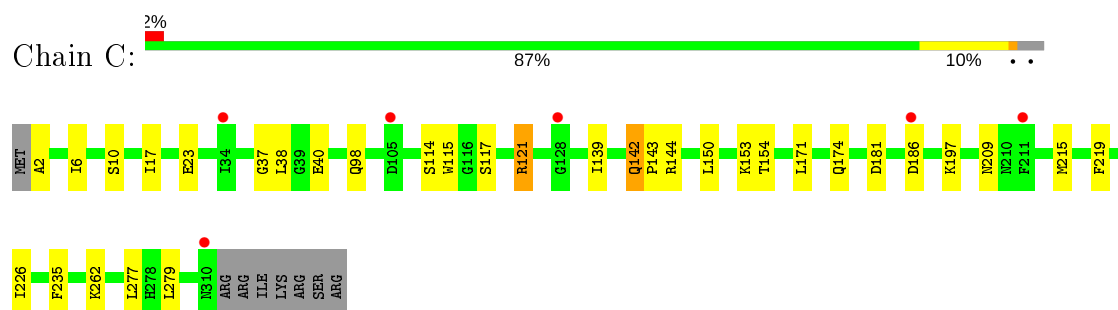
- Molecule 1: Hydrolase, alpha/beta domain protein



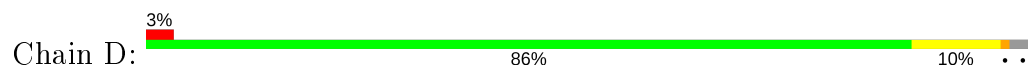
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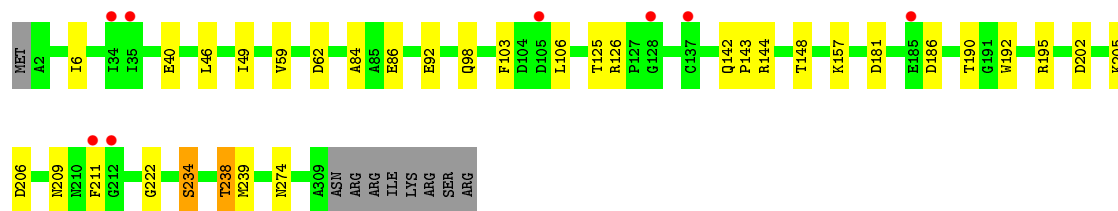


- Molecule 1: Hydrolase, alpha/beta domain protein

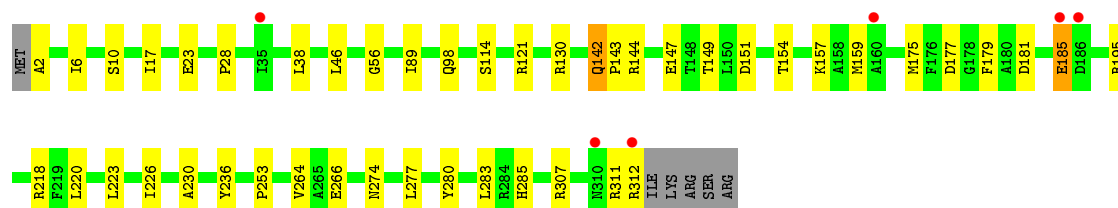
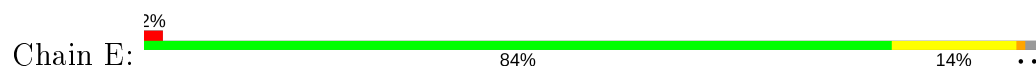


- Molecule 1: Hydrolase, alpha/beta domain protein

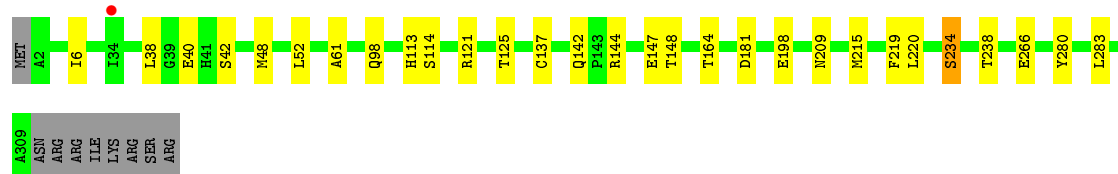
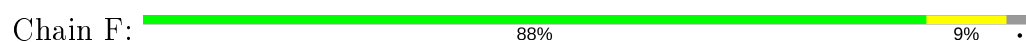




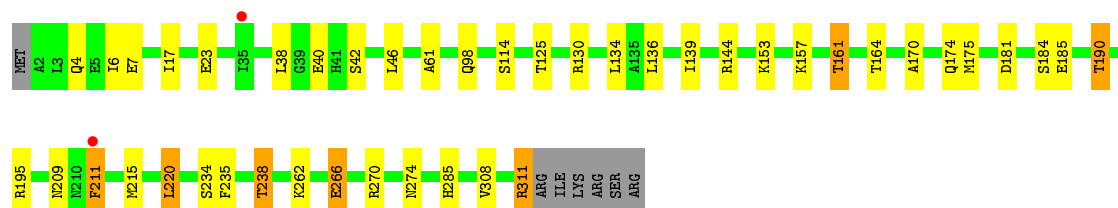
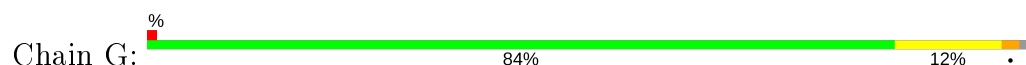
- Molecule 1: Hydrolase, alpha/beta domain protein



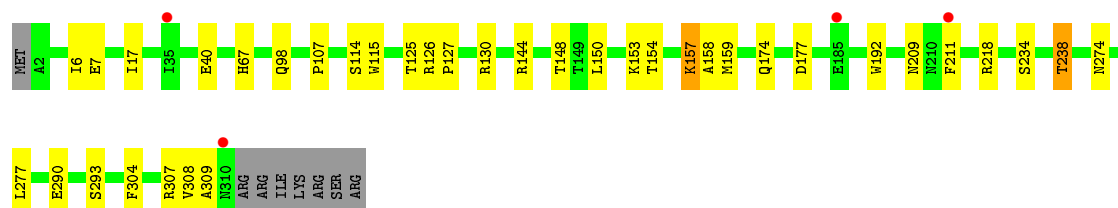
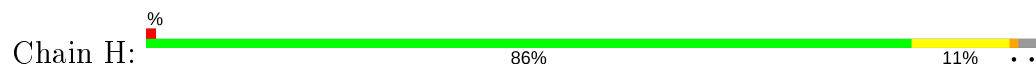
- Molecule 1: Hydrolase, alpha/beta domain protein



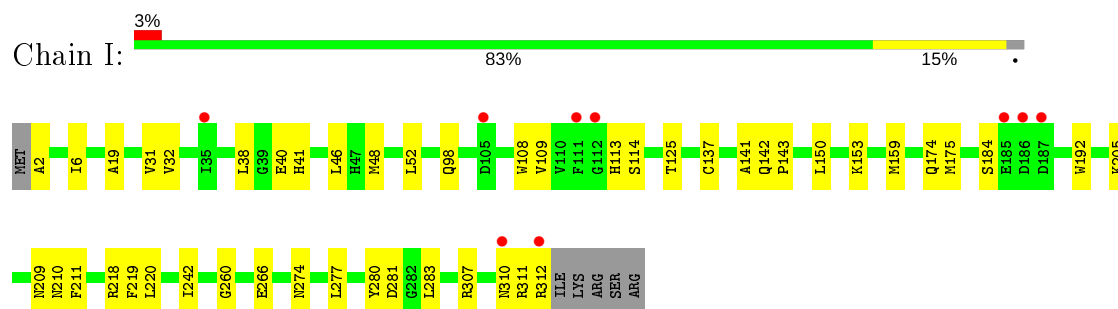
- Molecule 1: Hydrolase, alpha/beta domain protein



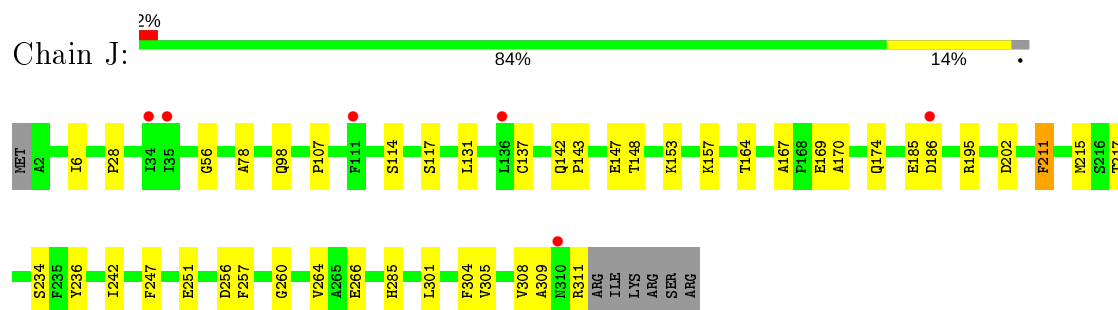
- Molecule 1: Hydrolase, alpha/beta domain protein



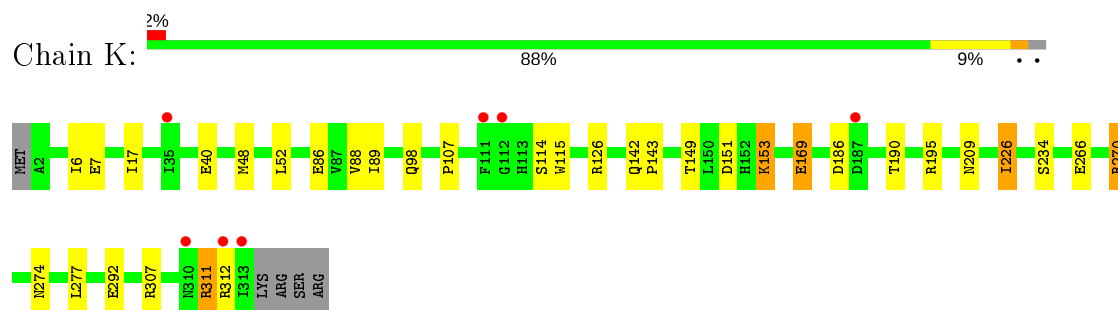
- Molecule 1: Hydrolase, alpha/beta domain protein



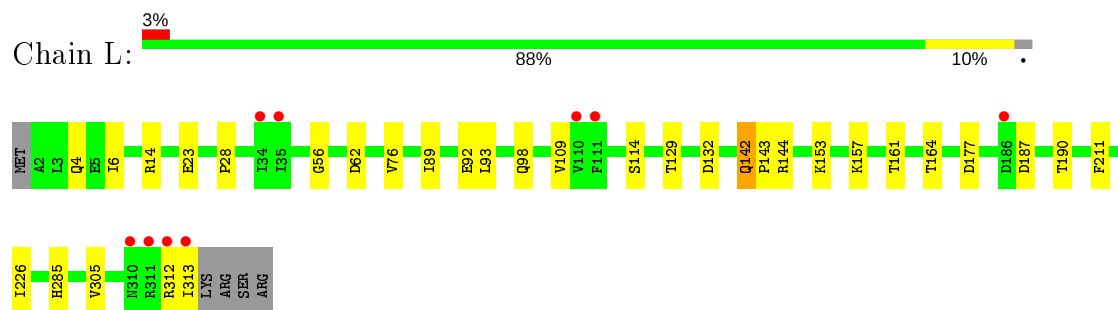
- Molecule 1: Hydrolase, alpha/beta domain protein



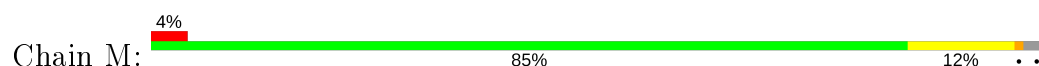
- Molecule 1: Hydrolase, alpha/beta domain protein

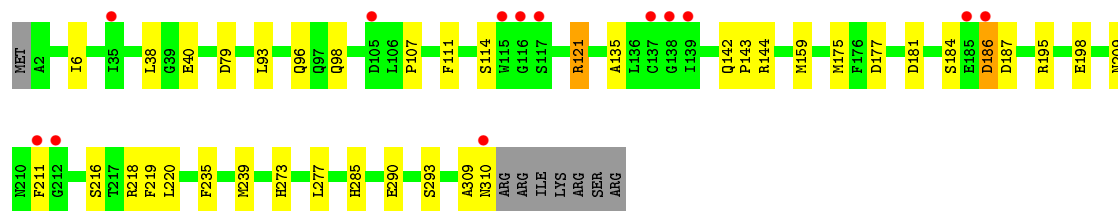


- Molecule 1: Hydrolase, alpha/beta domain protein

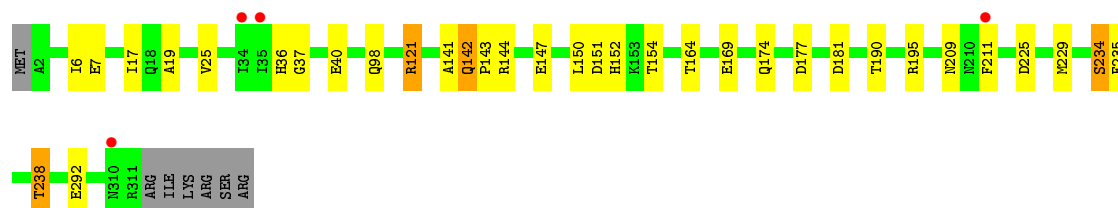
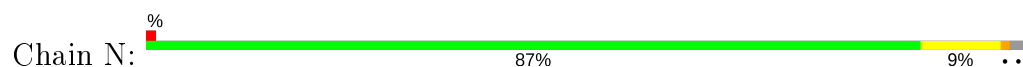


- Molecule 1: Hydrolase, alpha/beta domain protein

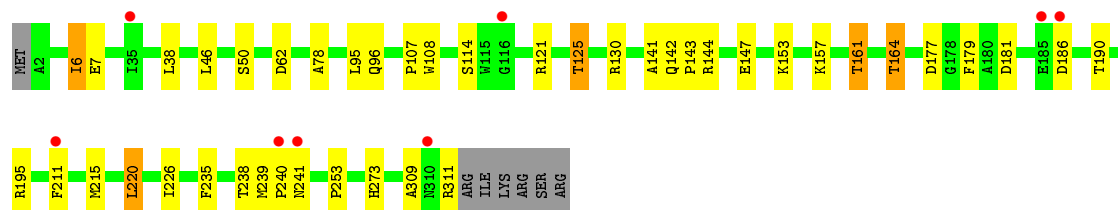
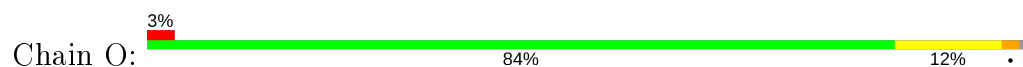




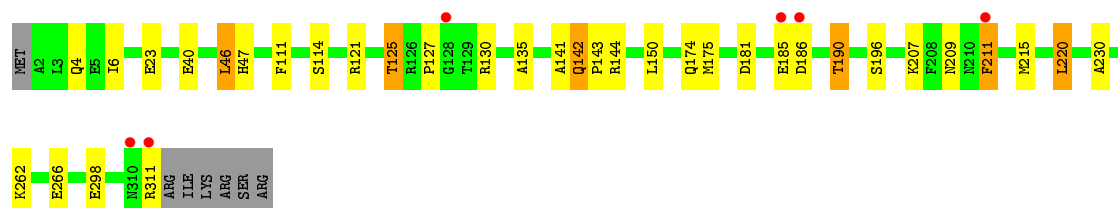
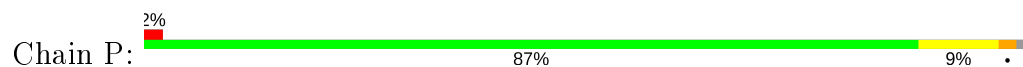
- Molecule 1: Hydrolase, alpha/beta domain protein



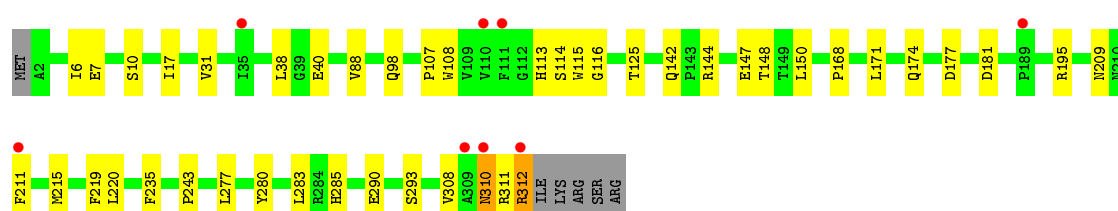
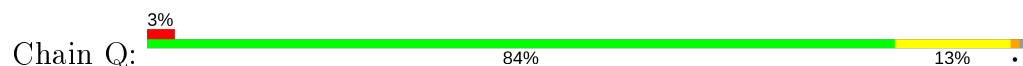
- Molecule 1: Hydrolase, alpha/beta domain protein




- Molecule 1: Hydrolase, alpha/beta domain protein

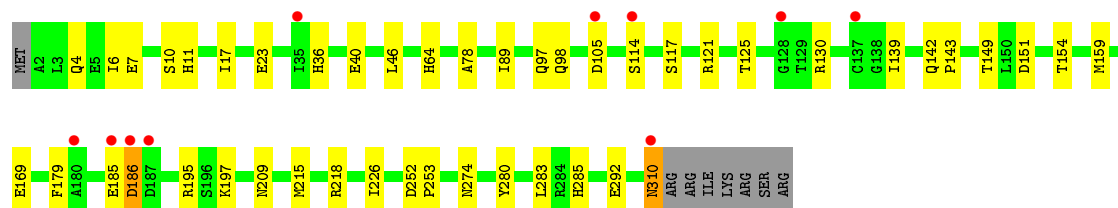


- Molecule 1: Hydrolase, alpha/beta domain protein




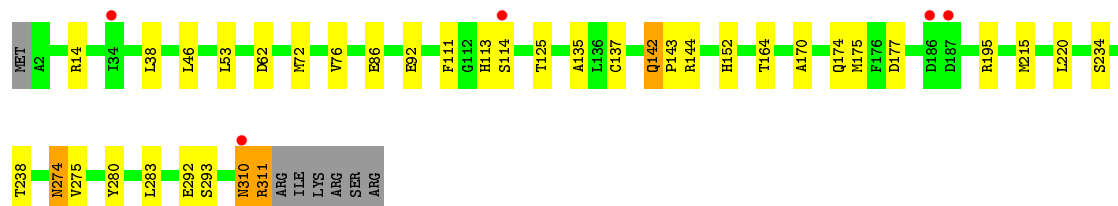
- Molecule 1: Hydrolase, alpha/beta domain protein

Chain R:  3% 83% 14% ..




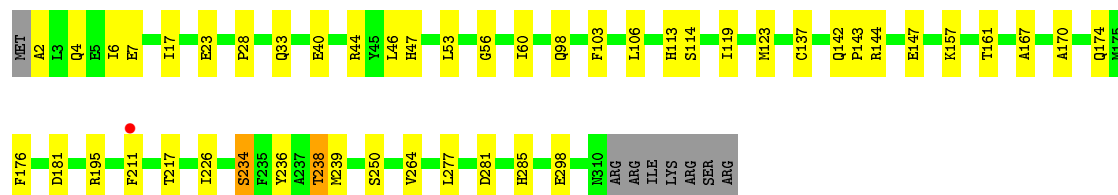
- Molecule 1: Hydrolase, alpha/beta domain protein

Chain S:  2% 86% 10% ..




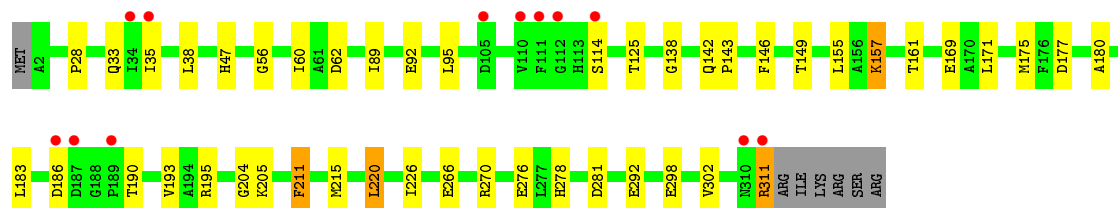
- Molecule 1: Hydrolase, alpha/beta domain protein

Chain T:  82% 15% ..




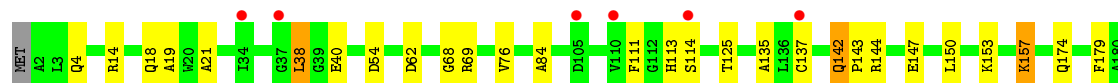
- Molecule 1: Hydrolase, alpha/beta domain protein

Chain U:  4% 83% 13% ..



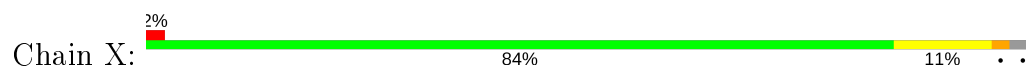
- Molecule 1: Hydrolase, alpha/beta domain protein

Chain V:  2% 83% 14% ..

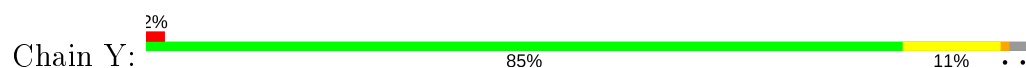




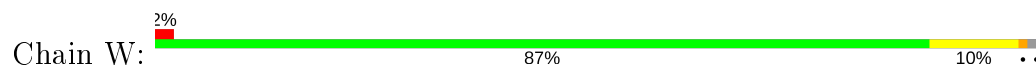
- Molecule 1: Hydrolase, alpha/beta domain protein



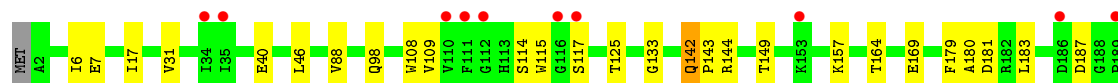
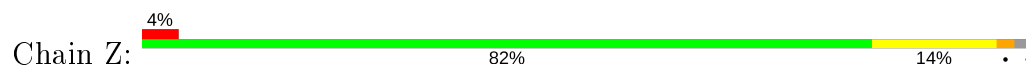
- Molecule 1: Hydrolase, alpha/beta domain protein



- Molecule 1: Hydrolase, alpha/beta domain protein



- Molecule 1: Hydrolase, alpha/beta domain protein



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.*

¹ Intensities estimated from amplitudes.

² Theoretical 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

5.1 Standard geometry

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.

All (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
1:F:114:SER:OG	6:F:900:DK9:C4	1.74	1.35
1:A:114:SER:OG	2:A:900:DKL:C4	1.77	1.32
1:R:114:SER:OG	3:R:900:DKO:C4	1.78	1.31
1:M:114:SER:OG	5:M:900:DKF:C4	1.79	1.29
1:G:114:SER:OG	5:G:900:DKF:C4	1.81	1.29
1:W:114:SER:OG	5:W:900:DKF:C4	1.81	1.28
1:P:114:SER:OG	6:P:900:DK9:C4	1.81	1.27
1:Q:114:SER:OG	2:Q:900:DKL:C4	1.82	1.27
1:X:114:SER:HG	2:X:900:DKL:C4	1.47	1.27
1:O:114:SER:OG	6:O:900:DK9:C4	1.86	1.22
1:V:114:SER:OG	5:V:900:DKF:C4	1.88	1.21
1:I:114:SER:OG	5:I:900:DKF:C4	1.90	1.19
1:T:114:SER:OG	2:T:900:DKL:C4	1.91	1.19
1:F:114:SER:HG	6:F:900:DK9:C4	1.48	1.18
1:X:114:SER:OG	2:X:900:DKL:C4	1.90	1.16
1:C:114:SER:HG	2:C:900:DKL:C4	1.47	1.14
1:U:114:SER:OG	5:U:900:DKF:C4	1.96	1.14
1:O:114:SER:HG	6:O:900:DK9:C4	1.60	1.11
1:Z:114:SER:OG	4:Z:900:DK6:C4	2.01	1.09
1:I:114:SER:HG	5:I:900:DKF:C4	1.66	1.06
1:J:114:SER:OG	5:J:900:DKF:C4	2.03	1.06
1:Y:114:SER:OG	5:Y:900:DKF:C4	2.03	1.05
1:X:234:SER:O	1:X:238:THR:HG23	1.56	1.05
1:S:114:SER:OG	4:S:900:DK6:C4	2.05	1.04
1:T:114:SER:HG	2:T:900:DKL:C4	1.68	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:307:ARG:HH11	1:I:311:ARG:NH2	1.61	0.98
1:W:114:SER:HG	5:W:900:DKF:C4	1.67	0.95
1:K:107:PRO:HB3	1:K:312:ARG:HD3	1.49	0.95
1:M:114:SER:HG	5:M:900:DKF:C4	1.66	0.94
1:Y:114:SER:HG	5:Y:900:DKF:C4	1.79	0.94
1:Z:114:SER:HG	4:Z:900:DK6:C4	1.76	0.94
1:P:114:SER:HG	6:P:900:DK9:C4	1.65	0.94
1:H:234:SER:O	1:H:238:THR:HG23	1.69	0.92
1:X:107:PRO:HG2	1:X:309:ALA:CB	2.01	0.90
1:C:38:LEU:HD23	2:C:900:DKL:C7	2.04	0.87
1:K:312:ARG:HB3	1:K:312:ARG:NH1	1.88	0.87
1:B:243:PRO:HB2	1:B:308:VAL:HG23	1.54	0.87
1:V:234:SER:O	1:V:238:THR:HG23	1.75	0.86
1:C:121:ARG:HG3	1:C:235:PHE:CE1	2.12	0.85
1:G:234:SER:O	1:G:238:THR:HG23	1.76	0.85
1:O:38:LEU:HD23	6:O:900:DK9:C8	2.05	0.85
1:W:270:ARG:HD2	7:W:1003:HOH:O	1.75	0.84
1:T:234:SER:O	1:T:238:THR:HG22	1.77	0.84
1:Z:192:TRP:HH2	4:Z:900:DK6:C6	1.91	0.83
1:G:6:ILE:HG22	1:G:6:ILE:O	1.80	0.81
1:L:312:ARG:NH1	1:L:312:ARG:HB3	1.94	0.81
1:J:114:SER:HG	5:J:900:DKF:C4	1.90	0.81
1:C:38:LEU:HB3	2:C:900:DKL:C6	2.12	0.80
1:O:6:ILE:O	1:O:6:ILE:CG2	2.29	0.79
1:B:305:VAL:HA	1:B:308:VAL:HG12	1.63	0.79
1:K:312:ARG:HB3	1:K:312:ARG:HH11	1.45	0.79
1:X:107:PRO:HG2	1:X:309:ALA:HB2	1.63	0.79
1:K:307:ARG:HH11	1:K:311:ARG:NH2	1.79	0.79
1:L:312:ARG:HB3	1:L:312:ARG:CZ	2.11	0.79
1:I:307:ARG:HH11	1:I:311:ARG:HH21	1.29	0.79
1:S:175:MET:HE3	1:S:220:LEU:HD11	1.63	0.79
1:R:114:SER:HG	3:R:900:DKO:C4	1.92	0.78
1:A:114:SER:HG	2:A:900:DKL:C4	1.95	0.78
1:O:239:MET:SD	1:O:240:PRO:HD2	2.24	0.78
1:L:132:ASP:HB3	1:L:312:ARG:HD2	1.66	0.77
1:R:310:ASN:HD22	1:R:310:ASN:H	1.31	0.76
1:S:175:MET:HE3	1:S:220:LEU:CD1	2.16	0.76
1:K:311:ARG:HH11	1:K:311:ARG:HG2	1.51	0.76
1:G:6:ILE:CG2	1:G:6:ILE:O	2.33	0.75
1:I:211:PHE:HA	7:I:1079:HOH:O	1.85	0.75
1:H:144:ARG:HD2	1:H:177:ASP:OD2	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:125:THR:HB	1:O:238:THR:CG2	2.18	0.74
1:R:114:SER:CB	3:R:900:DKO:C4	2.67	0.72
1:V:38:LEU:HD21	1:V:223:LEU:HD21	1.70	0.72
1:B:234:SER:O	1:B:238:THR:HG23	1.89	0.72
1:U:62:ASP:OD2	1:U:95:LEU:HD22	1.90	0.72
1:S:280:TYR:HB3	1:S:283:LEU:HD12	1.72	0.72
1:S:170:ALA:O	1:S:174:GLN:HG3	1.91	0.71
1:D:144:ARG:NH2	1:D:181:ASP:OD2	2.24	0.71
1:O:6:ILE:O	1:O:6:ILE:HG23	1.91	0.70
1:B:114:SER:CB	3:B:900:DKO:C4	2.69	0.70
1:E:6:ILE:HG21	1:E:98:GLN:HG3	1.73	0.70
1:Y:190:THR:HG21	1:Y:211:PHE:HZ	1.56	0.70
1:X:6:ILE:HG21	1:X:98:GLN:HB3	1.74	0.70
1:T:234:SER:O	1:T:238:THR:CG2	2.40	0.69
1:Q:125:THR:HG21	1:Q:235:PHE:HA	1.75	0.69
1:B:114:SER:HG	3:B:900:DKO:C4	2.06	0.68
1:Y:105:ASP:HB3	7:Y:1069:HOH:O	1.92	0.68
1:X:144:ARG:NH2	1:X:181:ASP:OD2	2.26	0.68
1:A:7:GLU:HG3	7:A:1049:HOH:O	1.94	0.68
1:E:144:ARG:NH2	1:E:181:ASP:OD2	2.27	0.68
1:W:38:LEU:HD23	5:W:900:DKF:C7	2.24	0.67
1:N:234:SER:O	1:N:238:THR:HG23	1.93	0.67
1:P:185:GLU:HG2	1:P:185:GLU:O	1.93	0.67
1:U:311:ARG:N	1:U:311:ARG:HD3	2.10	0.67
1:K:311:ARG:HH11	1:K:311:ARG:CG	2.07	0.66
1:Y:144:ARG:NH2	1:Y:181:ASP:OD2	2.29	0.66
1:A:157:LYS:O	1:A:161:THR:HG23	1.96	0.66
1:A:211:PHE:HA	7:A:1070:HOH:O	1.95	0.66
1:D:86:GLU:OE2	1:D:126:ARG:NH2	2.27	0.66
1:O:125:THR:HB	1:O:238:THR:HG21	1.77	0.66
1:K:312:ARG:CB	1:K:312:ARG:HH11	2.08	0.66
1:E:185:GLU:OE2	1:E:185:GLU:HA	1.94	0.65
1:H:6:ILE:HG21	1:H:98:GLN:HG3	1.79	0.65
1:I:307:ARG:NH1	1:I:311:ARG:HH21	1.92	0.65
1:L:6:ILE:HG21	1:L:98:GLN:HG3	1.79	0.65
1:F:144:ARG:NH2	1:F:181:ASP:OD2	2.29	0.65
1:T:157:LYS:O	1:T:161:THR:HG23	1.97	0.65
1:A:175:MET:HE3	1:A:220:LEU:CD1	2.27	0.65
1:F:198:GLU:HG3	7:F:1116:HOH:O	1.97	0.65
1:H:274:ASN:HD21	1:H:307:ARG:HH12	1.45	0.64
1:Y:142:GLN:HA	1:Y:147:GLU:HG2	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:170:ALA:O	1:T:174:GLN:HG3	1.97	0.64
1:W:270:ARG:CD	7:W:1003:HOH:O	2.41	0.64
1:Z:180:ALA:HA	1:Z:183:LEU:HD12	1.79	0.64
1:X:7:GLU:CD	1:X:7:GLU:H	2.01	0.64
1:P:215:MET:CE	1:P:220:LEU:HD22	2.28	0.63
1:Z:144:ARG:NH2	1:Z:181:ASP:OD2	2.31	0.63
1:H:114:SER:CB	4:H:900:DK6:C4	2.77	0.63
1:O:235:PHE:CE1	1:O:239:MET:CE	2.82	0.63
1:S:310:ASN:OD1	1:S:310:ASN:N	2.28	0.63
1:V:38:LEU:HB2	5:V:900:DKF:O3	1.98	0.63
1:W:121:ARG:HD2	1:W:136:LEU:HD13	1.81	0.63
1:P:6:ILE:O	1:P:6:ILE:CG2	2.46	0.63
1:G:114:SER:HG	5:G:900:DKF:C4	2.07	0.63
1:I:274:ASN:HD21	1:I:311:ARG:NH2	1.97	0.62
1:V:234:SER:O	1:V:238:THR:CG2	2.46	0.62
1:V:190:THR:HG21	1:V:211:PHE:CE2	2.35	0.62
1:A:190:THR:HG21	1:A:211:PHE:CZ	2.35	0.62
1:G:144:ARG:NH2	1:G:181:ASP:OD2	2.32	0.62
1:W:236:TYR:OH	1:W:264:VAL:HG22	2.00	0.62
1:B:243:PRO:CB	1:B:308:VAL:HG23	2.29	0.61
1:R:78:ALA:HB1	1:R:215:MET:HA	1.80	0.61
1:Z:192:TRP:CH2	4:Z:900:DK6:C6	2.81	0.61
1:M:6:ILE:HG21	1:M:98:GLN:HG3	1.80	0.61
1:Y:190:THR:HG21	1:Y:211:PHE:CZ	2.34	0.61
1:B:308:VAL:O	1:B:308:VAL:HG13	1.99	0.61
1:I:242:ILE:HG22	1:I:312:ARG:HH22	1.64	0.61
1:O:235:PHE:CE1	1:O:239:MET:HE2	2.36	0.61
1:A:6:ILE:O	1:A:6:ILE:HG22	2.00	0.61
1:J:142:GLN:N	1:J:143:PRO:HD3	2.15	0.61
1:X:6:ILE:HG21	1:X:98:GLN:CB	2.31	0.61
1:K:114:SER:HG	5:K:900:DKF:C4	2.09	0.61
1:I:6:ILE:HG21	1:I:98:GLN:HG3	1.82	0.61
1:I:307:ARG:NH1	1:I:311:ARG:NH2	2.41	0.61
1:O:235:PHE:HE1	1:O:239:MET:HE3	1.66	0.61
1:X:6:ILE:HG22	1:X:6:ILE:O	2.00	0.61
1:A:157:LYS:O	1:A:161:THR:CG2	2.49	0.60
1:Z:109:VAL:HG21	1:Z:305:VAL:HG22	1.82	0.60
1:G:190:THR:HG21	1:G:211:PHE:CZ	2.36	0.60
1:F:280:TYR:HB3	1:F:283:LEU:HD12	1.84	0.60
1:S:234:SER:O	1:S:238:THR:HG23	2.00	0.60
1:U:311:ARG:HG2	1:U:311:ARG:HH11	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:38:LEU:HB3	5:W:900:DKF:O3	2.00	0.60
1:M:144:ARG:HD2	1:M:177:ASP:OD2	2.02	0.60
1:R:280:TYR:HB3	1:R:283:LEU:HD12	1.84	0.60
1:F:142:GLN:HA	1:F:147:GLU:HG3	1.83	0.60
1:F:6:ILE:HG21	1:F:98:GLN:HG3	1.84	0.60
1:O:107:PRO:HG3	1:O:309:ALA:HA	1.84	0.60
1:O:157:LYS:O	1:O:161:THR:HG23	2.02	0.59
1:C:121:ARG:HG3	1:C:235:PHE:CZ	2.37	0.59
1:W:23:GLU:OE2	1:Z:205:LYS:NZ	2.35	0.59
1:W:234:SER:O	1:W:238:THR:HG23	2.03	0.59
1:Q:6:ILE:HG21	1:Q:98:GLN:HG3	1.85	0.59
1:W:270:ARG:CG	7:W:1003:HOH:O	2.51	0.59
1:E:274:ASN:HD21	1:E:307:ARG:HH12	1.51	0.59
1:J:170:ALA:O	1:J:174:GLN:HG3	2.03	0.59
1:A:175:MET:HE3	1:A:220:LEU:HD11	1.85	0.58
1:R:186:ASP:O	1:R:197:LYS:NZ	2.36	0.58
1:B:6:ILE:HG21	1:B:98:GLN:HG3	1.83	0.58
1:I:40:GLU:HA	1:I:209:ASN:ND2	2.18	0.58
1:L:144:ARG:HD2	1:L:177:ASP:OD2	2.03	0.58
1:N:144:ARG:HD2	1:N:177:ASP:OD2	2.04	0.58
1:Z:304:PHE:O	1:Z:308:VAL:HG13	2.03	0.58
1:G:262:LYS:O	1:G:266:GLU:HG2	2.04	0.57
1:R:10:SER:HB2	1:R:17:ILE:HD11	1.85	0.57
1:J:114:SER:OG	5:J:900:DKF:O4	2.22	0.57
1:B:234:SER:O	1:B:238:THR:CG2	2.52	0.57
1:C:121:ARG:CG	1:C:235:PHE:CE1	2.87	0.57
1:C:142:GLN:N	1:C:143:PRO:CD	2.68	0.57
1:L:132:ASP:CB	1:L:312:ARG:HD2	2.35	0.57
1:J:114:SER:HB2	1:J:285:HIS:NE2	2.20	0.57
1:Z:290:GLU:HB2	1:Z:293:SER:OG	2.05	0.57
1:Q:144:ARG:HD2	1:Q:177:ASP:OD2	2.04	0.57
1:P:215:MET:HE1	1:P:220:LEU:HD22	1.86	0.56
1:P:220:LEU:C	1:P:220:LEU:HD12	2.25	0.56
1:S:280:TYR:CB	1:S:283:LEU:HD12	2.35	0.56
1:M:114:SER:OG	5:M:900:DKF:O3	2.22	0.56
1:Z:6:ILE:HG21	1:Z:98:GLN:HG3	1.88	0.56
1:B:154:THR:O	1:B:157:LYS:HE3	2.06	0.56
1:J:142:GLN:HE21	1:J:260:GLY:HA2	1.70	0.56
1:K:86:GLU:OE1	1:K:126:ARG:NH2	2.38	0.56
1:L:142:GLN:N	1:L:143:PRO:CD	2.68	0.56
1:L:164:THR:HB	7:L:1130:HOH:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:40:GLU:HA	1:M:209:ASN:OD1	2.05	0.56
1:Q:215:MET:CE	1:Q:220:LEU:HD13	2.35	0.56
1:N:6:ILE:HG21	1:N:98:GLN:HG3	1.88	0.56
1:A:175:MET:CE	1:A:220:LEU:CD1	2.84	0.56
1:Y:234:SER:O	1:Y:238:THR:HG23	2.06	0.56
1:E:114:SER:OG	5:E:900:DKF:O3	2.22	0.56
1:P:142:GLN:N	1:P:143:PRO:CD	2.69	0.56
1:S:274:ASN:HD22	1:S:274:ASN:C	2.09	0.56
1:T:114:SER:OG	2:T:900:DKL:O4	2.23	0.56
1:O:142:GLN:N	1:O:143:PRO:CD	2.69	0.56
1:X:107:PRO:HG2	1:X:309:ALA:HB1	1.87	0.56
1:E:142:GLN:HA	1:E:147:GLU:HG2	1.87	0.56
1:K:40:GLU:HA	1:K:209:ASN:OD1	2.06	0.55
1:X:121:ARG:HD2	1:X:136:LEU:HD13	1.87	0.55
2:A:900:DKL:C6	2:A:900:DKL:C10	2.83	0.55
1:E:114:SER:CB	5:E:900:DKF:C4	2.81	0.55
5:J:900:DKF:C5	5:J:900:DKF:C9	2.85	0.55
1:O:144:ARG:NH2	1:O:181:ASP:OD2	2.39	0.55
1:O:239:MET:SD	1:O:240:PRO:CD	2.95	0.55
1:A:144:ARG:NH2	1:A:181:ASP:OD2	2.40	0.55
1:A:121:ARG:HD2	1:A:136:LEU:HD13	1.88	0.55
1:B:274:ASN:HB2	1:K:169:GLU:OE2	2.07	0.55
1:G:38:LEU:HB3	5:G:900:DKF:O4	2.05	0.55
1:R:4:GLN:NE2	1:R:23:GLU:OE1	2.32	0.55
1:R:6:ILE:HG21	1:R:98:GLN:HG3	1.88	0.55
1:V:142:GLN:HA	1:V:147:GLU:HG2	1.88	0.55
1:W:62:ASP:OD2	1:W:92:GLU:OE2	2.24	0.55
1:X:175:MET:HE1	1:X:220:LEU:HD12	1.89	0.55
1:K:6:ILE:HG21	1:K:98:GLN:HG3	1.88	0.55
1:N:142:GLN:N	1:N:143:PRO:CD	2.70	0.55
1:E:151:ASP:OD1	1:E:154:THR:OG1	2.24	0.55
5:G:900:DKF:C5	5:G:900:DKF:C9	2.85	0.55
1:P:220:LEU:HD12	1:P:220:LEU:O	2.07	0.54
1:H:154:THR:O	1:H:157:LYS:CE	2.55	0.54
1:I:38:LEU:HD11	1:I:219:PHE:CE2	2.42	0.54
1:C:10:SER:HB2	1:C:17:ILE:HD11	1.89	0.54
1:F:38:LEU:HD11	1:F:219:PHE:CE1	2.42	0.54
1:K:274:ASN:HD21	1:K:307:ARG:HH12	1.54	0.54
2:Q:900:DKL:C5	2:Q:900:DKL:C10	2.85	0.54
1:R:142:GLN:N	1:R:143:PRO:CD	2.71	0.54
1:O:190:THR:HG21	1:O:211:PHE:CE2	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:170:ALA:O	1:B:174:GLN:HG3	2.08	0.54
1:A:190:THR:HG21	1:A:211:PHE:CE2	2.42	0.54
1:Q:243:PRO:HG2	1:Q:308:VAL:HG22	1.88	0.54
1:R:89:ILE:HD11	1:R:226:ILE:CD1	2.38	0.54
1:T:176:PHE:CD1	2:T:900:DKL:C9	2.90	0.54
1:B:142:GLN:N	1:B:143:PRO:CD	2.71	0.54
1:J:78:ALA:HB1	1:J:215:MET:HA	1.90	0.54
1:Q:142:GLN:HA	1:Q:147:GLU:HG2	1.90	0.54
1:X:142:GLN:N	1:X:143:PRO:CD	2.70	0.54
1:P:262:LYS:O	1:P:266:GLU:HG3	2.09	0.53
1:C:150:LEU:HA	1:C:174:GLN:HB3	1.90	0.53
1:D:62:ASP:OD2	1:D:92:GLU:OE2	2.26	0.53
5:Y:900:DKF:C9	5:Y:900:DKF:C5	2.86	0.53
1:B:38:LEU:HD11	1:B:219:PHE:HE2	1.73	0.53
1:G:175:MET:CE	1:G:220:LEU:HD13	2.39	0.53
1:P:114:SER:OG	6:P:900:DK9:O3	2.25	0.53
1:X:4:GLN:NE2	1:X:23:GLU:OE1	2.41	0.53
1:E:114:SER:OG	5:E:900:DKF:O4	2.23	0.53
1:J:142:GLN:O	1:J:256:ASP:HB2	2.09	0.53
1:N:121:ARG:HG3	1:N:235:PHE:CE1	2.43	0.53
1:U:276:GLU:OE2	1:U:278:HIS:NE2	2.27	0.53
1:H:40:GLU:HA	1:H:209:ASN:OD1	2.09	0.53
1:Y:114:SER:OG	5:Y:900:DKF:O4	2.27	0.53
1:O:239:MET:CE	1:O:239:MET:HA	2.39	0.53
1:E:175:MET:HE3	1:E:220:LEU:HD12	1.90	0.53
1:V:190:THR:HG21	1:V:211:PHE:HE2	1.74	0.53
1:G:125:THR:HG22	1:G:235:PHE:HA	1.90	0.52
1:U:311:ARG:H	1:U:311:ARG:HD3	1.73	0.52
1:V:274:ASN:HD21	1:V:307:ARG:HH12	1.58	0.52
1:Y:234:SER:O	1:Y:238:THR:CG2	2.57	0.52
1:T:144:ARG:NH2	1:T:181:ASP:OD2	2.42	0.52
1:Q:144:ARG:NH2	1:Q:181:ASP:OD2	2.41	0.52
1:S:311:ARG:CD	1:S:311:ARG:N	2.72	0.52
1:O:215:MET:HE1	1:O:220:LEU:HD22	1.91	0.52
1:W:48:MET:O	1:W:52:LEU:HG	2.10	0.52
1:U:180:ALA:HA	1:U:183:LEU:HD12	1.90	0.52
1:K:292:GLU:OE2	1:K:292:GLU:N	2.38	0.52
1:S:152:HIS:HE1	7:S:1066:HOH:O	1.92	0.52
1:H:304:PHE:O	1:H:308:VAL:HG13	2.09	0.52
1:C:38:LEU:HD11	1:C:219:PHE:HE2	1.73	0.51
1:A:142:GLN:N	1:A:143:PRO:CD	2.73	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:ILE:CG2	1:A:98:GLN:HB3	2.40	0.51
1:W:190:THR:HG21	1:W:211:PHE:HZ	1.75	0.51
1:C:38:LEU:CB	2:C:900:DKL:C6	2.86	0.51
1:M:144:ARG:NH2	1:M:181:ASP:OD2	2.43	0.51
1:O:239:MET:O	1:O:273:HIS:HE1	1.93	0.51
1:X:215:MET:HE1	1:X:220:LEU:HD13	1.93	0.51
1:E:10:SER:HB2	1:E:17:ILE:HD11	1.93	0.51
1:I:6:ILE:O	1:I:19:ALA:HB3	2.10	0.51
1:P:190:THR:HG21	1:P:211:PHE:CE2	2.45	0.51
1:R:310:ASN:N	1:R:310:ASN:HD22	1.94	0.51
1:D:6:ILE:HG21	1:D:98:GLN:HG3	1.92	0.51
1:K:311:ARG:NH1	1:K:311:ARG:CG	2.71	0.51
1:S:142:GLN:N	1:S:143:PRO:CD	2.74	0.51
1:K:270:ARG:HD2	1:K:270:ARG:C	2.31	0.51
1:O:235:PHE:CE1	1:O:239:MET:HE3	2.43	0.51
1:N:164:THR:HB	7:N:1050:HOH:O	2.11	0.51
1:P:6:ILE:O	1:P:6:ILE:HG22	2.10	0.51
1:Q:215:MET:HE1	1:Q:220:LEU:CD1	2.40	0.51
1:A:113:HIS:HA	1:A:137:CYS:O	2.11	0.51
1:E:175:MET:HE3	1:E:220:LEU:CD1	2.40	0.51
1:G:134:LEU:HD11	1:G:136:LEU:HD21	1.93	0.51
1:G:308:VAL:O	1:G:311:ARG:HD2	2.11	0.51
1:O:142:GLN:HA	1:O:147:GLU:HG2	1.93	0.51
1:Q:6:ILE:HG21	1:Q:98:GLN:CG	2.41	0.51
1:W:190:THR:HG21	1:W:211:PHE:CZ	2.46	0.51
1:D:234:SER:O	1:D:238:THR:HG23	2.11	0.50
1:W:311:ARG:HG3	1:W:311:ARG:HH11	1.76	0.50
1:Y:89:ILE:HD11	1:Y:226:ILE:CD1	2.41	0.50
1:G:190:THR:HG21	1:G:211:PHE:CE2	2.47	0.50
1:U:215:MET:HE1	1:U:220:LEU:HD22	1.94	0.50
1:E:159:MET:SD	1:E:218:ARG:HA	2.52	0.50
1:L:4:GLN:NE2	1:L:23:GLU:OE1	2.41	0.50
1:S:62:ASP:OD2	1:S:92:GLU:OE2	2.29	0.50
1:D:40:GLU:HA	1:D:209:ASN:OD1	2.12	0.50
1:H:192:TRP:CH2	4:H:900:DK6:C6	2.94	0.50
1:L:28:PRO:HA	1:L:56:GLY:O	2.12	0.50
1:T:114:SER:HB2	1:T:285:HIS:NE2	2.26	0.50
1:T:6:ILE:HG21	1:T:98:GLN:HG3	1.93	0.50
1:X:211:PHE:C	1:X:211:PHE:CD2	2.85	0.50
1:G:40:GLU:HA	1:G:209:ASN:OD1	2.12	0.50
1:Q:38:LEU:HD11	1:Q:219:PHE:HE2	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:121:ARG:O	1:F:125:THR:HG23	2.12	0.49
1:Q:38:LEU:HD11	1:Q:219:PHE:CE2	2.47	0.49
1:V:144:ARG:NH2	1:V:181:ASP:OD2	2.45	0.49
1:A:223:LEU:O	1:A:226:ILE:HG22	2.11	0.49
1:B:38:LEU:HD11	1:B:219:PHE:CE2	2.47	0.49
1:F:40:GLU:HA	1:F:209:ASN:OD1	2.12	0.49
1:G:38:LEU:CB	5:G:900:DKF:O4	2.60	0.49
1:I:38:LEU:HD11	1:I:219:PHE:HE2	1.76	0.49
1:O:50:SER:HB2	1:P:46:LEU:HD23	1.94	0.49
1:E:121:ARG:HD3	1:E:230:ALA:HB1	1.94	0.49
1:O:7:GLU:H	1:O:7:GLU:CD	2.15	0.49
1:R:36:HIS:CE1	1:R:64:HIS:CD2	3.00	0.49
1:V:4:GLN:HB2	1:V:21:ALA:HB3	1.94	0.49
1:L:312:ARG:NH1	1:L:312:ARG:CB	2.72	0.49
1:M:114:SER:HB2	1:M:285:HIS:NE2	2.28	0.49
1:Z:109:VAL:HA	1:Z:133:GLY:O	2.12	0.49
1:A:168:PRO:HD2	1:A:171:LEU:HD12	1.94	0.49
1:G:139:ILE:H	1:G:139:ILE:HD12	1.77	0.49
1:N:144:ARG:HH11	1:N:177:ASP:CG	2.16	0.49
1:S:38:LEU:HB3	4:S:900:DK6:O3	2.12	0.49
1:U:190:THR:O	1:U:193:VAL:HG23	2.12	0.49
1:F:144:ARG:HH22	1:F:181:ASP:CG	2.16	0.49
1:W:179:PHE:HA	1:W:253:PRO:CB	2.42	0.49
1:Z:40:GLU:HA	1:Z:209:ASN:OD1	2.13	0.49
1:A:144:ARG:HD2	1:A:177:ASP:OD2	2.12	0.49
1:F:142:GLN:HA	1:F:147:GLU:CG	2.42	0.49
1:E:142:GLN:N	1:E:143:PRO:CD	2.75	0.49
1:I:114:SER:OG	5:I:900:DKF:O4	2.30	0.49
1:K:114:SER:OG	5:K:900:DKF:O4	2.29	0.49
1:P:40:GLU:HA	1:P:209:ASN:OD1	2.12	0.49
1:Q:107:PRO:HB3	1:Q:312:ARG:HG3	1.94	0.49
1:I:41:HIS:HD2	1:I:209:ASN:ND2	2.11	0.49
1:T:28:PRO:HA	1:T:56:GLY:O	2.13	0.49
1:U:89:ILE:HD11	1:U:226:ILE:HD12	1.95	0.49
1:W:6:ILE:HG21	1:W:98:GLN:HG3	1.94	0.49
1:C:38:LEU:HD23	2:C:900:DKL:C6	2.42	0.48
1:P:47:HIS:CE1	1:P:298:GLU:OE1	2.66	0.48
1:A:146:PHE:CE1	1:A:175:MET:HE2	2.47	0.48
1:F:48:MET:O	1:F:52:LEU:HG	2.12	0.48
1:G:157:LYS:O	1:G:161:THR:CG2	2.61	0.48
1:R:40:GLU:HA	1:R:209:ASN:OD1	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:311:ARG:HG2	1:U:311:ARG:NH1	2.28	0.48
1:X:142:GLN:HA	1:X:147:GLU:HG2	1.96	0.48
1:R:97:GLN:HA	1:R:97:GLN:NE2	2.28	0.48
1:K:307:ARG:HH11	1:K:311:ARG:HH22	1.59	0.48
1:N:6:ILE:O	1:N:19:ALA:HB3	2.14	0.48
1:P:4:GLN:NE2	1:P:23:GLU:OE1	2.35	0.48
1:G:6:ILE:HG23	1:G:98:GLN:HG3	1.94	0.48
1:R:252:ASP:CG	1:R:285:HIS:HA	2.34	0.48
1:U:142:GLN:N	1:U:143:PRO:CD	2.77	0.48
1:C:262:LYS:HE2	1:C:279:LEU:CD2	2.43	0.48
1:C:37:GLY:HA2	1:C:115:TRP:HB3	1.94	0.48
1:C:38:LEU:CD2	2:C:900:DKL:C6	2.92	0.48
1:J:142:GLN:NE2	1:J:260:GLY:HA2	2.29	0.48
1:G:4:GLN:NE2	1:G:23:GLU:OE1	2.45	0.48
1:L:89:ILE:HD11	1:L:226:ILE:CD1	2.44	0.48
1:O:211:PHE:HA	7:O:1033:HOH:O	2.14	0.48
1:B:46:LEU:HD12	1:B:46:LEU:C	2.34	0.48
1:O:125:THR:OG1	1:O:125:THR:O	2.24	0.48
1:M:142:GLN:N	1:M:143:PRO:CD	2.77	0.48
1:M:93:LEU:O	1:M:96:GLN:HB2	2.14	0.48
1:O:6:ILE:O	1:O:6:ILE:HG22	2.12	0.48
1:R:159:MET:SD	1:R:218:ARG:HA	2.54	0.48
1:X:114:SER:OG	2:X:900:DKL:O3	2.28	0.48
1:I:113:HIS:HA	1:I:137:CYS:O	2.14	0.48
1:B:144:ARG:HD2	1:B:177:ASP:OD2	2.14	0.47
1:L:109:VAL:HG21	1:L:305:VAL:HG22	1.95	0.47
1:M:107:PRO:HG3	1:M:309:ALA:CB	2.44	0.47
1:O:62:ASP:OD2	1:O:95:LEU:HD22	2.14	0.47
1:U:38:LEU:HB3	5:U:900:DKF:O4	2.14	0.47
1:C:142:GLN:N	1:C:143:PRO:HD2	2.30	0.47
1:M:211:PHE:CZ	5:M:900:DKF:C9	2.97	0.47
1:O:241:ASN:HA	7:O:1061:HOH:O	2.14	0.47
1:S:53:LEU:CD1	1:T:46:LEU:HD23	2.45	0.47
1:T:119:ILE:O	1:T:123:MET:HG3	2.15	0.47
1:T:142:GLN:HA	1:T:147:GLU:CG	2.45	0.47
1:U:89:ILE:HD11	1:U:226:ILE:CD1	2.45	0.47
1:G:220:LEU:C	1:G:220:LEU:HD12	2.35	0.47
1:G:4:GLN:HA	7:G:1085:HOH:O	2.15	0.47
1:G:7:GLU:HA	1:G:17:ILE:O	2.15	0.47
1:J:211:PHE:C	1:J:211:PHE:CD2	2.87	0.47
1:U:175:MET:CE	1:U:220:LEU:HD13	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:28:PRO:HA	1:U:56:GLY:O	2.15	0.47
1:U:114:SER:HG	5:U:900:DKF:C4	2.19	0.47
1:Y:7:GLU:HA	1:Y:17:ILE:O	2.15	0.47
1:Z:142:GLN:N	1:Z:143:PRO:CD	2.78	0.47
1:A:121:ARG:NH1	7:A:1002:HOH:O	2.33	0.47
1:K:107:PRO:HB3	1:K:312:ARG:CD	2.32	0.47
1:K:151:ASP:OD1	1:K:153:LYS:HB2	2.14	0.47
1:L:14:ARG:NH1	1:L:76:VAL:HG11	2.30	0.47
1:S:46:LEU:HD13	1:T:53:LEU:CD1	2.45	0.47
1:M:79:ASP:OD1	1:M:216:SER:OG	2.21	0.47
1:I:307:ARG:HH11	1:I:311:ARG:HH22	1.55	0.47
1:Q:114:SER:HB2	1:Q:285:HIS:NE2	2.29	0.47
1:R:151:ASP:OD2	1:R:154:THR:OG1	2.32	0.47
1:U:175:MET:HE1	1:U:220:LEU:HD13	1.96	0.47
1:U:47:HIS:HD2	1:V:54:ASP:OD1	1.98	0.47
1:A:215:MET:HE2	1:A:220:LEU:HD22	1.95	0.47
1:C:40:GLU:HA	1:C:209:ASN:OD1	2.15	0.47
1:H:154:THR:O	1:H:157:LYS:HE3	2.15	0.47
1:H:192:TRP:CZ3	4:H:900:DK6:C6	2.97	0.47
1:N:142:GLN:HA	1:N:147:GLU:HG3	1.96	0.47
1:N:152:HIS:HE1	7:N:1033:HOH:O	1.98	0.47
1:D:192:TRP:HH2	4:D:900:DK6:C6	2.28	0.47
1:Z:274:ASN:OD1	1:Z:274:ASN:C	2.53	0.47
1:I:31:VAL:HG11	1:I:108:TRP:CZ3	2.51	0.46
1:S:215:MET:CE	1:S:220:LEU:HB2	2.45	0.46
1:Z:7:GLU:HA	1:Z:17:ILE:O	2.15	0.46
1:B:243:PRO:HB2	1:B:308:VAL:CG2	2.36	0.46
1:K:89:ILE:HD11	1:K:226:ILE:HD12	1.96	0.46
1:Z:239:MET:SD	1:Z:240:PRO:HD2	2.55	0.46
1:H:7:GLU:HA	1:H:17:ILE:O	2.15	0.46
1:N:7:GLU:HA	1:N:17:ILE:O	2.15	0.46
1:S:215:MET:HE1	1:S:220:LEU:HD13	1.96	0.46
1:R:185:GLU:HG3	1:R:185:GLU:O	2.15	0.46
1:G:114:SER:HB2	1:G:285:HIS:HE2	1.81	0.46
1:J:142:GLN:HA	1:J:147:GLU:HG2	1.97	0.46
1:N:36:HIS:ND1	1:N:37:GLY:O	2.45	0.46
1:Z:142:GLN:NE2	7:Z:1002:HOH:O	2.47	0.46
1:F:42:SER:HB2	1:F:61:ALA:HB1	1.97	0.46
1:I:159:MET:SD	1:I:218:ARG:HA	2.56	0.46
1:L:114:SER:HB2	1:L:285:HIS:NE2	2.30	0.46
1:T:2:ALA:HB3	1:T:23:GLU:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:142:GLN:HA	1:B:147:GLU:HG2	1.97	0.46
1:M:121:ARG:HG3	1:M:235:PHE:CE1	2.49	0.46
1:N:142:GLN:HA	1:N:147:GLU:CG	2.46	0.46
1:N:150:LEU:HA	1:N:174:GLN:HB3	1.97	0.46
1:S:14:ARG:NH1	1:S:76:VAL:HG11	2.31	0.46
1:W:311:ARG:NH1	1:W:311:ARG:HG3	2.31	0.46
1:J:6:ILE:HG21	1:J:98:GLN:HG3	1.98	0.46
1:K:142:GLN:N	1:K:143:PRO:CD	2.79	0.46
1:F:38:LEU:HD11	1:F:219:PHE:HE1	1.81	0.46
1:T:114:SER:HB2	1:T:285:HIS:CE1	2.50	0.46
1:Y:176:PHE:O	1:Y:179:PHE:HB2	2.15	0.46
1:Z:241:ASN:HD22	1:Z:241:ASN:C	2.19	0.46
1:C:6:ILE:HG21	1:C:98:GLN:HG3	1.98	0.46
1:F:234:SER:O	1:F:238:THR:HG23	2.15	0.46
1:K:307:ARG:NH1	1:K:311:ARG:NH2	2.56	0.46
1:H:67:HIS:CE1	1:H:115:TRP:CZ3	3.04	0.45
1:I:280:TYR:HB3	1:I:283:LEU:HD12	1.97	0.45
1:J:236:TYR:OH	1:J:264:VAL:HG22	2.16	0.45
1:O:114:SER:OG	6:O:900:DK9:O3	2.32	0.45
1:R:179:PHE:HA	1:R:253:PRO:CB	2.46	0.45
1:A:190:THR:CG2	1:A:211:PHE:HZ	2.30	0.45
1:J:211:PHE:O	1:J:211:PHE:CD2	2.70	0.45
1:J:137:CYS:HA	1:J:247:PHE:O	2.17	0.45
1:P:121:ARG:HD3	1:P:230:ALA:HB1	1.99	0.45
1:T:236:TYR:OH	1:T:264:VAL:HG22	2.16	0.45
1:U:35:ILE:HD13	1:U:92:GLU:HG3	1.97	0.45
1:Y:78:ALA:HB1	1:Y:215:MET:HA	1.97	0.45
1:B:46:LEU:O	1:B:46:LEU:HD12	2.16	0.45
1:C:215:MET:HG3	1:C:219:PHE:CD2	2.51	0.45
1:E:144:ARG:HD2	1:E:177:ASP:OD2	2.17	0.45
1:I:150:LEU:HA	1:I:174:GLN:HB3	1.97	0.45
1:K:312:ARG:HB3	1:K:312:ARG:CZ	2.38	0.45
1:O:78:ALA:HB1	1:O:215:MET:HA	1.99	0.45
1:V:142:GLN:N	1:V:143:PRO:CD	2.79	0.45
1:X:270:ARG:NH2	7:X:1002:HOH:O	2.47	0.45
1:Z:114:SER:HB2	1:Z:285:HIS:NE2	2.31	0.45
1:A:111:PHE:HA	1:A:135:ALA:O	2.17	0.45
1:G:234:SER:O	1:G:238:THR:CG2	2.57	0.45
1:R:117:SER:O	1:R:121:ARG:HG3	2.17	0.45
1:U:138:GLY:HA2	7:U:1008:HOH:O	2.15	0.45
1:T:142:GLN:N	1:T:143:PRO:CD	2.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:179:PHE:HA	1:Z:253:PRO:CB	2.46	0.45
1:A:6:ILE:O	1:A:6:ILE:CG2	2.65	0.45
1:B:126:ARG:HD2	7:B:1093:HOH:O	2.16	0.45
1:L:190:THR:HG21	1:L:211:PHE:CE2	2.51	0.45
1:V:179:PHE:HA	1:V:253:PRO:CB	2.47	0.45
1:A:38:LEU:HB3	2:A:900:DKL:C6	2.47	0.45
1:K:48:MET:O	1:K:52:LEU:HG	2.16	0.45
1:K:7:GLU:HA	1:K:17:ILE:O	2.16	0.45
1:N:225:ASP:O	1:N:229:MET:HG3	2.15	0.45
1:P:121:ARG:O	1:P:125:THR:HG23	2.17	0.45
1:P:150:LEU:HA	1:P:174:GLN:HB3	1.98	0.45
1:V:111:PHE:HA	1:V:135:ALA:O	2.16	0.45
1:B:307:ARG:C	1:B:309:ALA:H	2.20	0.45
1:C:121:ARG:CG	1:C:235:PHE:CZ	2.99	0.45
1:E:179:PHE:HA	1:E:253:PRO:CB	2.47	0.45
1:N:144:ARG:NH1	1:N:177:ASP:OD1	2.50	0.45
1:R:7:GLU:N	1:R:7:GLU:CD	2.70	0.45
1:V:84:ALA:HB3	1:V:222:GLY:HA3	1.99	0.45
1:S:144:ARG:HD2	1:S:177:ASP:OD2	2.17	0.45
1:V:113:HIS:HA	1:V:137:CYS:O	2.17	0.45
1:B:305:VAL:HA	1:B:308:VAL:CG1	2.40	0.44
1:G:190:THR:HG21	1:G:211:PHE:HZ	1.81	0.44
1:N:144:ARG:NH2	1:N:181:ASP:OD2	2.50	0.44
1:O:179:PHE:HA	1:O:253:PRO:CB	2.46	0.44
1:X:175:MET:CE	1:X:220:LEU:HD12	2.46	0.44
1:X:236:TYR:OH	1:X:264:VAL:HG22	2.17	0.44
1:C:154:THR:HB	1:C:171:LEU:HD21	1.98	0.44
1:F:114:SER:OG	6:F:900:DK9:O3	2.28	0.44
1:O:239:MET:HB2	1:O:239:MET:HE2	1.80	0.44
1:B:239:MET:O	1:B:273:HIS:HE1	2.00	0.44
1:S:274:ASN:C	1:S:274:ASN:ND2	2.70	0.44
1:Z:277:LEU:HD22	1:Z:278:HIS:N	2.33	0.44
1:X:190:THR:HG21	1:X:211:PHE:CZ	2.53	0.44
1:Y:283:LEU:CD1	1:Y:293:SER:HB3	2.48	0.44
1:H:107:PRO:HG3	1:H:309:ALA:HA	2.00	0.44
1:J:301:LEU:O	1:J:305:VAL:HG23	2.18	0.44
1:L:93:LEU:HD21	1:L:129:THR:OG1	2.17	0.44
1:O:141:ALA:C	1:O:143:PRO:HD3	2.38	0.44
1:N:141:ALA:C	1:N:143:PRO:HD3	2.38	0.44
1:O:121:ARG:O	1:O:125:THR:CG2	2.66	0.44
1:W:136:LEU:HD12	1:W:246:LEU:CD2	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:38:LEU:HB3	2:C:900:DKL:C7	2.47	0.44
1:I:114:SER:CB	5:I:900:DKF:C4	2.89	0.44
1:M:175:MET:HE3	1:M:220:LEU:HD11	1.98	0.44
1:Q:215:MET:CE	1:Q:220:LEU:CD1	2.96	0.44
1:S:311:ARG:CD	1:S:311:ARG:H	2.31	0.44
1:D:142:GLN:N	1:D:143:PRO:CD	2.81	0.44
1:E:236:TYR:OH	1:E:264:VAL:HG22	2.18	0.44
1:E:28:PRO:HA	1:E:56:GLY:O	2.18	0.44
1:M:186:ASP:OD2	1:M:186:ASP:N	2.42	0.44
1:R:195:ARG:NH2	1:R:292:GLU:OE2	2.51	0.44
1:S:175:MET:CE	1:S:220:LEU:HD12	2.48	0.44
1:X:175:MET:CE	1:X:220:LEU:CD1	2.96	0.44
1:K:88:VAL:HG11	1:K:115:TRP:CZ2	2.53	0.44
1:X:211:PHE:C	1:X:211:PHE:HD2	2.20	0.44
1:D:238:THR:O	1:D:239:MET:C	2.55	0.43
1:E:38:LEU:O	5:E:900:DKF:C9	2.66	0.43
1:F:215:MET:HE2	1:F:220:LEU:HD12	1.99	0.43
1:M:121:ARG:HG3	1:M:235:PHE:CZ	2.53	0.43
1:Q:168:PRO:HG2	1:Q:171:LEU:HD12	2.00	0.43
1:D:190:THR:HG21	1:D:211:PHE:CE1	2.53	0.43
1:G:170:ALA:O	1:G:174:GLN:HG3	2.18	0.43
1:J:153:LYS:HA	1:J:153:LYS:HD3	1.82	0.43
1:O:220:LEU:C	1:O:220:LEU:CD1	2.87	0.43
1:R:226:ILE:HA	1:R:226:ILE:HD12	1.93	0.43
1:U:298:GLU:O	1:U:302:VAL:HG23	2.19	0.43
1:I:175:MET:SD	1:I:220:LEU:CD1	3.06	0.43
1:Z:114:SER:OG	4:Z:900:DK6:O4	2.35	0.43
1:A:227:TYR:CD2	1:A:227:TYR:C	2.92	0.43
1:O:121:ARG:O	1:O:125:THR:HG23	2.18	0.43
1:T:238:THR:O	1:T:239:MET:C	2.55	0.43
1:U:149:THR:HG21	1:U:177:ASP:OD2	2.18	0.43
1:V:68:GLY:HA2	1:V:208:PHE:O	2.18	0.43
1:A:84:ALA:HB3	1:A:222:GLY:HA3	2.01	0.43
1:A:7:GLU:CD	1:A:7:GLU:H	2.22	0.43
1:C:2:ALA:N	1:D:202:ASP:OD1	2.52	0.43
1:J:131:LEU:HG	1:J:242:ILE:CD1	2.48	0.43
1:L:142:GLN:N	1:L:143:PRO:HD2	2.33	0.43
1:O:144:ARG:HD2	1:O:177:ASP:OD2	2.19	0.43
1:O:144:ARG:HH11	1:O:177:ASP:CG	2.22	0.43
1:P:175:MET:HE3	1:P:220:LEU:HD11	2.00	0.43
1:T:103:PHE:HB3	1:T:106:LEU:HD12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:137:CYS:HA	1:V:247:PHE:O	2.19	0.43
1:V:157:LYS:HB3	1:V:157:LYS:HE3	1.66	0.43
1:E:280:TYR:HB3	1:E:283:LEU:HD12	2.00	0.43
1:L:62:ASP:OD2	1:L:92:GLU:OE2	2.35	0.43
1:O:239:MET:O	1:O:273:HIS:CE1	2.69	0.43
1:Q:280:TYR:HB3	1:Q:283:LEU:HD12	2.01	0.43
1:T:113:HIS:HA	1:T:137:CYS:O	2.18	0.43
1:X:53:LEU:HD12	1:Y:46:LEU:HD23	1.99	0.43
1:A:215:MET:CE	1:A:220:LEU:HD22	2.49	0.43
1:I:48:MET:O	1:I:52:LEU:HG	2.18	0.43
1:T:250:SER:OG	1:T:281:ASP:HA	2.18	0.43
1:X:142:GLN:HA	1:X:147:GLU:CG	2.49	0.43
1:Y:27:THR:HA	1:Y:28:PRO:HD2	1.95	0.43
1:A:190:THR:CG2	1:A:211:PHE:CZ	3.00	0.43
1:A:239:MET:O	1:A:273:HIS:HE1	2.02	0.43
1:E:2:ALA:HB3	1:E:23:GLU:HB2	2.00	0.43
1:S:175:MET:CE	1:S:220:LEU:CD1	2.91	0.43
1:S:283:LEU:CD1	1:S:293:SER:HB3	2.49	0.43
1:D:192:TRP:CH2	4:D:900:DK6:C6	3.02	0.43
1:H:157:LYS:HE3	1:H:158:ALA:N	2.34	0.43
1:V:40:GLU:HA	1:V:209:ASN:OD1	2.19	0.43
1:B:304:PHE:O	1:B:308:VAL:HB	2.19	0.42
1:D:206:ASP:HB3	1:D:209:ASN:ND2	2.34	0.42
1:I:2:ALA:N	1:J:202:ASP:OD1	2.52	0.42
1:Q:114:SER:OG	2:Q:900:DKL:O4	2.32	0.42
1:Q:88:VAL:HG11	1:Q:115:TRP:CZ2	2.54	0.42
1:Q:310:ASN:HA	1:Q:310:ASN:HD22	1.66	0.42
1:V:19:ALA:HA	1:V:62:ASP:HA	2.00	0.42
1:W:280:TYR:HB3	1:W:283:LEU:HD12	2.01	0.42
1:I:175:MET:SD	1:I:220:LEU:HD12	2.59	0.42
1:M:159:MET:SD	1:M:218:ARG:HA	2.58	0.42
1:U:190:THR:HG21	1:U:211:PHE:CZ	2.54	0.42
1:L:312:ARG:HH11	1:L:312:ARG:CB	2.32	0.42
1:M:107:PRO:HG3	1:M:309:ALA:HB2	2.01	0.42
1:P:141:ALA:C	1:P:143:PRO:HD3	2.40	0.42
1:B:159:MET:SD	1:B:218:ARG:HA	2.59	0.42
1:H:159:MET:SD	1:H:218:ARG:HA	2.59	0.42
1:L:157:LYS:O	1:L:161:THR:HG23	2.20	0.42
1:M:198:GLU:HB3	1:N:25:VAL:HG13	2.01	0.42
1:V:38:LEU:HD11	1:V:219:PHE:HE2	1.85	0.42
1:X:145:GLY:HA3	1:X:175:MET:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:239:MET:O	1:Y:273:HIS:HE1	2.02	0.42
1:A:6:ILE:HG23	1:A:98:GLN:HB3	2.02	0.42
1:G:220:LEU:C	1:G:220:LEU:CD1	2.88	0.42
1:O:164:THR:HB	7:O:1040:HOH:O	2.19	0.42
1:T:47:HIS:CE1	1:T:298:GLU:OE1	2.72	0.42
1:I:141:ALA:O	1:I:260:GLY:HA3	2.20	0.42
1:J:304:PHE:O	1:J:308:VAL:HG23	2.19	0.42
1:N:151:ASP:OD2	1:N:154:THR:OG1	2.34	0.42
1:P:144:ARG:NH2	1:P:181:ASP:OD2	2.53	0.42
1:V:18:GLN:HG3	1:V:69:ARG:HG2	2.01	0.42
1:J:215:MET:HB2	1:J:215:MET:HE2	1.79	0.42
1:B:154:THR:O	1:B:157:LYS:CE	2.68	0.42
1:G:215:MET:CE	1:G:220:LEU:HB2	2.49	0.42
1:Q:290:GLU:HB2	1:Q:293:SER:OG	2.19	0.42
1:B:253:PRO:HB3	1:B:257:PHE:CZ	2.55	0.42
1:Q:150:LEU:HA	1:Q:174:GLN:HB3	2.01	0.42
1:Q:10:SER:HB2	1:Q:17:ILE:HD11	2.02	0.42
1:R:139:ILE:HD12	1:R:139:ILE:H	1.84	0.42
1:V:293:SER:O	1:V:294:ARG:C	2.58	0.42
1:J:251:GLU:HA	1:J:257:PHE:HD1	1.84	0.42
1:W:270:ARG:HG3	7:W:1003:HOH:O	2.18	0.42
1:A:67:HIS:CE1	1:A:115:TRP:CZ3	3.07	0.41
1:B:6:ILE:O	1:B:19:ALA:HB3	2.20	0.41
1:I:142:GLN:N	1:I:143:PRO:HD3	2.35	0.41
1:Z:31:VAL:HG11	1:Z:108:TRP:CZ3	2.55	0.41
1:B:111:PHE:HA	1:B:135:ALA:O	2.20	0.41
1:B:305:VAL:CA	1:B:308:VAL:HG12	2.44	0.41
1:C:215:MET:HG3	1:C:219:PHE:HD2	1.83	0.41
1:D:103:PHE:HB3	1:D:106:LEU:HD12	2.01	0.41
1:N:6:ILE:HG21	1:N:98:GLN:CG	2.50	0.41
1:T:167:ALA:HA	1:T:217:THR:OG1	2.20	0.41
1:A:141:ALA:C	1:A:143:PRO:HD3	2.41	0.41
1:G:46:LEU:HD23	1:G:46:LEU:C	2.40	0.41
1:J:28:PRO:HA	1:J:56:GLY:O	2.21	0.41
1:V:150:LEU:HA	1:V:174:GLN:HB3	2.02	0.41
1:X:93:LEU:O	1:X:96:GLN:HB2	2.20	0.41
1:Y:144:ARG:HH22	1:Y:181:ASP:CG	2.24	0.41
1:B:109:VAL:HG21	1:B:308:VAL:HG11	2.02	0.41
1:B:109:VAL:HG21	1:B:308:VAL:CG1	2.51	0.41
1:C:23:GLU:OE1	1:D:205:LYS:CE	2.68	0.41
1:E:38:LEU:HB3	5:E:900:DKF:C9	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:274:ASN:HD21	1:H:307:ARG:NH1	2.16	0.41
1:A:4:GLN:HB2	1:A:21:ALA:HB3	2.02	0.41
1:B:304:PHE:CZ	1:B:308:VAL:HG21	2.55	0.41
1:C:262:LYS:HE2	1:C:279:LEU:HD22	2.02	0.41
1:N:40:GLU:HA	1:N:209:ASN:OD1	2.21	0.41
1:U:33:GLN:HA	1:U:60:ILE:O	2.20	0.41
1:V:142:GLN:HA	1:V:147:GLU:CG	2.48	0.41
1:V:14:ARG:NH1	1:V:76:VAL:HG11	2.36	0.41
1:B:109:VAL:CG2	1:B:308:VAL:CG1	2.98	0.41
1:M:290:GLU:HB2	1:M:293:SER:OG	2.20	0.41
1:T:176:PHE:CD2	2:T:900:DKL:C10	3.04	0.41
1:Z:183:LEU:HA	1:Z:187:ASP:OD2	2.20	0.41
1:K:274:ASN:ND2	7:K:1007:HOH:O	2.52	0.41
1:M:38:LEU:HD11	1:M:219:PHE:CE2	2.55	0.41
1:P:175:MET:CE	1:P:220:LEU:CD1	2.99	0.41
1:S:152:HIS:CE1	7:S:1066:HOH:O	2.70	0.41
1:S:311:ARG:HD2	1:S:311:ARG:N	2.36	0.41
1:Y:28:PRO:HA	1:Y:56:GLY:O	2.21	0.41
1:B:35:ILE:HG23	1:B:64:HIS:CE1	2.56	0.41
1:G:42:SER:HB2	1:G:61:ALA:HB1	2.03	0.41
1:Q:31:VAL:HG11	1:Q:108:TRP:CZ3	2.56	0.41
1:U:146:PHE:CE1	1:U:175:MET:HE2	2.56	0.41
1:E:223:LEU:HA	1:E:226:ILE:HG22	2.03	0.41
1:F:113:HIS:HA	1:F:137:CYS:O	2.21	0.41
1:G:157:LYS:O	1:G:161:THR:HG23	2.21	0.41
1:G:175:MET:CE	1:G:220:LEU:CD1	2.98	0.41
1:M:239:MET:O	1:M:273:HIS:CE1	2.74	0.41
1:T:4:GLN:NE2	1:T:23:GLU:OE2	2.44	0.41
1:U:155:LEU:HD12	1:U:171:LEU:HD13	2.03	0.41
1:E:114:SER:HB2	1:E:285:HIS:NE2	2.36	0.41
1:H:126:ARG:HA	1:H:127:PRO:HD3	1.88	0.41
1:O:96:GLN:HG2	1:O:108:TRP:CZ2	2.56	0.41
1:Q:113:HIS:O	1:Q:116:GLY:N	2.54	0.41
1:Q:215:MET:HE2	1:Q:215:MET:HB2	1.77	0.41
1:S:113:HIS:HA	1:S:137:CYS:O	2.21	0.41
1:T:33:GLN:HA	1:T:60:ILE:O	2.21	0.41
1:C:144:ARG:NH2	1:C:181:ASP:OD2	2.54	0.41
1:G:157:LYS:O	1:G:161:THR:HG22	2.20	0.41
1:Z:88:VAL:HG11	1:Z:115:TRP:CZ2	2.56	0.41
1:A:47:HIS:CE1	1:A:298:GLU:OE1	2.74	0.40
1:A:311:ARG:C	1:A:311:ARG:HD3	2.41	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:84:ALA:HB3	1:D:222:GLY:HA3	2.02	0.40
1:M:111:PHE:HA	1:M:135:ALA:O	2.21	0.40
1:O:190:THR:HG21	1:O:211:PHE:HE2	1.85	0.40
1:S:111:PHE:HA	1:S:135:ALA:O	2.21	0.40
1:U:171:LEU:HD23	1:U:171:LEU:HA	1.92	0.40
1:Z:239:MET:HA	1:Z:240:PRO:HD3	1.95	0.40
1:H:290:GLU:HB2	1:H:293:SER:OG	2.22	0.40
1:I:32:VAL:HA	1:I:109:VAL:O	2.20	0.40
1:J:167:ALA:HA	1:J:217:THR:OG1	2.21	0.40
1:J:107:PRO:HG3	1:J:309:ALA:HA	2.03	0.40
1:Q:40:GLU:HA	1:Q:209:ASN:OD1	2.21	0.40
1:S:274:ASN:HD22	1:S:275:VAL:N	2.19	0.40
1:T:7:GLU:HA	1:T:17:ILE:O	2.21	0.40
1:X:301:LEU:O	1:X:304:PHE:HB3	2.22	0.40
1:Y:192:TRP:HH2	5:Y:900:DKF:C5	2.34	0.40
1:Z:206:ASP:HB3	1:Z:209:ASN:ND2	2.36	0.40
1:I:192:TRP:HH2	5:I:900:DKF:C6	2.34	0.40
1:X:144:ARG:HH22	1:X:181:ASP:CG	2.22	0.40
1:X:215:MET:HB2	1:X:215:MET:HE2	1.90	0.40
1:X:280:TYR:HB3	1:X:283:LEU:HD12	2.04	0.40
1:H:150:LEU:HA	1:H:174:GLN:HB3	2.03	0.40
1:P:111:PHE:HA	1:P:135:ALA:O	2.21	0.40
1:T:40:GLU:OE1	1:T:44:ARG:HD3	2.21	0.40
1:U:157:LYS:O	1:U:161:THR:HG23	2.21	0.40
1:W:215:MET:HE2	1:W:215:MET:HB2	1.89	0.40
1:X:6:ILE:CG2	1:X:98:GLN:HB3	2.47	0.40
1:B:144:ARG:NH2	1:B:181:ASP:OD2	2.54	0.40
1:D:49:ILE:HG12	1:D:59:VAL:HG11	2.04	0.40
1:E:89:ILE:HD11	1:E:226:ILE:CD1	2.52	0.40
1:M:239:MET:O	1:M:273:HIS:HE1	2.04	0.40
1:Q:114:SER:OG	2:Q:900:DKL:O3	2.32	0.40
1:S:175:MET:HE3	1:S:220:LEU:HD12	1.95	0.40
1:U:204:GLY:HA2	1:U:211:PHE:CD2	2.56	0.40
1:U:215:MET:CE	1:U:220:LEU:HD22	2.52	0.40

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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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

All (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
1	X	211	PHE
1	Z	169	GLU
1	P	142	GLN
1	R	11	HIS
1	L	142	GLN
1	S	142	GLN
1	Y	186	ASP
1	Z	142	GLN
1	V	142	GLN
1	W	142	GLN
1	B	308	VAL
1	X	142	GLN
1	E	142	GLN

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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

All (260) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ILE
1	A	46	LEU
1	A	64	HIS
1	A	148	THR
1	A	153	LYS
1	A	161	THR
1	A	164	THR
1	A	190	THR
1	A	195	ARG

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Mol	Chain	Res	Type
1	A	205	LYS
1	A	220	LEU
1	A	266	GLU
1	A	270	ARG
1	A	274	ASN
1	A	292	GLU
1	A	311	ARG
1	B	46	LEU
1	B	125	THR
1	B	153	LYS
1	B	157	LYS
1	B	186	ASP
1	B	195	ARG
1	B	211	PHE
1	B	234	SER
1	B	238	THR
1	B	241	ASN
1	B	277	LEU
1	B	308	VAL
1	C	117	SER
1	C	121	ARG
1	C	139	ILE
1	C	153	LYS
1	C	186	ASP
1	C	197	LYS
1	C	226	ILE
1	C	277	LEU
1	D	46	LEU
1	D	125	THR
1	D	148	THR
1	D	157	LYS
1	D	186	ASP
1	D	195	ARG
1	D	234	SER
1	D	238	THR
1	D	274	ASN
1	E	46	LEU
1	E	130	ARG
1	E	149	THR
1	E	157	LYS
1	E	185	GLU
1	E	195	ARG

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Mol	Chain	Res	Type
1	E	266	GLU
1	E	277	LEU
1	E	311	ARG
1	E	312	ARG
1	F	148	THR
1	F	164	THR
1	F	234	SER
1	F	266	GLU
1	G	130	ARG
1	G	153	LYS
1	G	161	THR
1	G	164	THR
1	G	184	SER
1	G	185	GLU
1	G	190	THR
1	G	195	ARG
1	G	220	LEU
1	G	238	THR
1	G	266	GLU
1	G	270	ARG
1	G	274	ASN
1	G	311	ARG
1	H	125	THR
1	H	130	ARG
1	H	148	THR
1	H	153	LYS
1	H	157	LYS
1	H	211	PHE
1	H	238	THR
1	H	277	LEU
1	I	46	LEU
1	I	125	THR
1	I	153	LYS
1	I	184	SER
1	I	205	LYS
1	I	210	ASN
1	I	266	GLU
1	I	277	LEU
1	I	281	ASP
1	I	310	ASN
1	J	117	SER
1	J	148	THR

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Mol	Chain	Res	Type
1	J	157	LYS
1	J	164	THR
1	J	169	GLU
1	J	185	GLU
1	J	186	ASP
1	J	195	ARG
1	J	211	PHE
1	J	234	SER
1	J	266	GLU
1	J	311	ARG
1	K	149	THR
1	K	153	LYS
1	K	169	GLU
1	K	186	ASP
1	K	190	THR
1	K	195	ARG
1	K	226	ILE
1	K	234	SER
1	K	266	GLU
1	K	270	ARG
1	K	277	LEU
1	K	311	ARG
1	L	153	LYS
1	L	187	ASP
1	L	313	ILE
1	M	121	ARG
1	M	184	SER
1	M	186	ASP
1	M	187	ASP
1	M	195	ARG
1	M	277	LEU
1	M	310	ASN
1	N	121	ARG
1	N	169	GLU
1	N	190	THR
1	N	195	ARG
1	N	211	PHE
1	N	234	SER
1	N	238	THR
1	N	292	GLU
1	O	6	ILE
1	O	46	LEU

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Mol	Chain	Res	Type
1	O	125	THR
1	O	130	ARG
1	O	153	LYS
1	O	161	THR
1	O	164	THR
1	O	186	ASP
1	O	195	ARG
1	O	220	LEU
1	O	226	ILE
1	O	311	ARG
1	P	46	LEU
1	P	125	THR
1	P	127	PRO
1	P	130	ARG
1	P	186	ASP
1	P	190	THR
1	P	196	SER
1	P	207	LYS
1	P	220	LEU
1	P	311	ARG
1	Q	7	GLU
1	Q	148	THR
1	Q	195	ARG
1	Q	211	PHE
1	Q	277	LEU
1	Q	310	ASN
1	Q	311	ARG
1	Q	312	ARG
1	R	46	LEU
1	R	105	ASP
1	R	125	THR
1	R	130	ARG
1	R	149	THR
1	R	169	GLU
1	R	186	ASP
1	R	274	ASN
1	R	310	ASN
1	S	72	MET
1	S	86	GLU
1	S	125	THR
1	S	164	THR
1	S	195	ARG

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Mol	Chain	Res	Type
1	S	274	ASN
1	S	292	GLU
1	S	310	ASN
1	S	311	ARG
1	T	195	ARG
1	T	211	PHE
1	T	226	ILE
1	T	234	SER
1	T	238	THR
1	T	277	LEU
1	U	125	THR
1	U	157	LYS
1	U	169	GLU
1	U	186	ASP
1	U	195	ARG
1	U	205	LYS
1	U	220	LEU
1	U	266	GLU
1	U	270	ARG
1	U	281	ASP
1	U	292	GLU
1	U	311	ARG
1	V	38	LEU
1	V	125	THR
1	V	153	LYS
1	V	157	LYS
1	V	195	ARG
1	V	238	THR
1	V	277	LEU
1	V	310	ASN
1	X	4	GLN
1	X	6	ILE
1	X	121	ARG
1	X	148	THR
1	X	153	LYS
1	X	169	GLU
1	X	184	SER
1	X	195	ARG
1	X	205	LYS
1	X	211	PHE
1	X	238	THR
1	X	266	GLU

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Mol	Chain	Res	Type
1	X	281	ASP
1	X	307	ARG
1	Y	25	VAL
1	Y	149	THR
1	Y	157	LYS
1	Y	185	GLU
1	Y	186	ASP
1	Y	195	ARG
1	Y	210	ASN
1	Y	211	PHE
1	Y	238	THR
1	Y	241	ASN
1	Y	277	LEU
1	Y	307	ARG
1	Y	308	VAL
1	W	148	THR
1	W	186	ASP
1	W	195	ARG
1	W	205	LYS
1	W	210	ASN
1	W	220	LEU
1	W	266	GLU
1	W	270	ARG
1	W	281	ASP
1	W	311	ARG
1	Z	46	LEU
1	Z	117	SER
1	Z	125	THR
1	Z	149	THR
1	Z	157	LYS
1	Z	164	THR
1	Z	190	THR
1	Z	195	ARG
1	Z	226	ILE
1	Z	241	ASN
1	Z	242	ILE
1	Z	270	ARG
1	Z	274	ASN
1	Z	277	LEU
1	Z	300	SER
1	Z	308	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (55) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	273	HIS
1	A	274	ASN
1	B	203	HIS
1	B	241	ASN
1	B	273	HIS
1	B	274	ASN
1	C	83	ASN
1	C	98	GLN
1	C	274	ASN
1	D	274	ASN
1	E	152	HIS
1	E	273	HIS
1	E	274	ASN
1	F	273	HIS
1	G	310	ASN
1	H	152	HIS
1	H	241	ASN
1	H	274	ASN
1	I	209	ASN
1	I	210	ASN
1	I	274	ASN
1	I	310	ASN
1	J	142	GLN
1	K	83	ASN
1	K	274	ASN
1	M	152	HIS
1	M	273	HIS
1	M	274	ASN
1	N	152	HIS
1	O	273	HIS
1	Q	152	HIS
1	Q	310	ASN
1	R	97	GLN
1	R	203	HIS
1	R	310	ASN
1	S	152	HIS
1	S	273	HIS
1	S	274	ASN
1	T	241	ASN
1	T	274	ASN
1	U	273	HIS
1	V	241	ASN

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Mol	Chain	Res	Type
1	V	273	HIS
1	V	274	ASN
1	X	11	HIS
1	X	142	GLN
1	X	273	HIS
1	Y	83	ASN
1	Y	210	ASN
1	Y	241	ASN
1	Y	273	HIS
1	Y	274	ASN
1	W	142	GLN
1	W	210	ASN
1	Z	241	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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	-
3	DKO	B	900	-	-	5/7/7/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-

All (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
5	K	900	DKF	C5-C4	4.13	1.59	1.50
5	V	900	DKF	C5-C4	2.87	1.56	1.50
2	A	900	DKL	O4-C4	2.80	1.46	1.40
5	W	900	DKF	C5-C4	2.43	1.55	1.50
5	Y	900	DKF	O4-C4	2.16	1.45	1.40
5	G	900	DKF	C5-C4	2.15	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	Z	900	DK6	O4-C4	2.14	1.45	1.40
4	H	900	DK6	O3-C4	2.12	1.45	1.40
2	C	900	DKL	O4-C4	2.04	1.45	1.40
4	Z	900	DK6	C5-C4	2.02	1.54	1.50

All (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
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
2	A	900	DKL	C6-C5-C4	6.48	128.37	113.38
5	L	900	DKF	O3-C4-C5	-5.75	96.58	109.17
2	A	900	DKL	O4-C4-C5	-5.68	96.74	109.17
4	Z	900	DK6	O4-C4-C5	5.21	119.24	109.43
5	I	900	DKF	O3-C4-O4	-4.91	102.33	111.36
2	C	900	DKL	O4-C4-C5	-4.85	98.55	109.17
3	R	900	DKO	O3-C4-C5	-4.78	98.70	109.17
5	W	900	DKF	O4-C4-C5	-4.50	99.32	109.17
3	B	900	DKO	C6-C5-C4	4.32	123.36	113.38
2	C	900	DKL	O3-C4-C5	-4.29	99.78	109.17
5	V	900	DKF	O3-C4-C5	-4.27	99.83	109.17
2	A	900	DKL	O3-C4-C5	4.18	118.33	109.17
4	S	900	DK6	C6-C5-C4	-4.16	106.10	113.57
3	B	900	DKO	O3-C4-O4	-4.11	103.80	111.36
2	X	900	DKL	O3-C4-O4	-3.93	104.12	111.36
2	Q	900	DKL	O3-C4-O4	-3.90	104.19	111.36
3	B	900	DKO	O4-C4-C5	-3.71	101.06	109.17
5	G	900	DKF	O3-C4-C5	-3.66	101.16	109.17
5	W	900	DKF	O3-C4-C5	-3.66	101.17	109.17
5	U	900	DKF	O4-C4-C5	-3.62	101.24	109.17
2	A	900	DKL	O3-C4-O4	3.36	117.53	111.36
5	L	900	DKF	O3-C4-O4	-3.35	105.19	111.36
5	J	900	DKF	O3-C4-C5	3.28	116.36	109.17
2	A	900	DKL	C8-C7-C6	-3.17	98.35	114.42
5	U	900	DKF	C6-C5-C4	3.01	120.34	113.38
5	J	900	DKF	O4-C4-C5	2.92	115.58	109.17
5	K	900	DKF	O4-C4-C5	-2.71	103.24	109.17
4	Z	900	DK6	O3-C4-C5	-2.70	104.33	109.43
6	O	900	DK9	O4-C4-C5	-2.66	103.34	109.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	900	DKF	O3-C4-O4	-2.60	106.57	111.36
3	R	900	DKO	C8-C7-C6	-2.48	101.86	114.42
5	W	900	DKF	C7-C6-C5	2.36	121.99	113.62
5	J	900	DKF	O3-C4-O4	-2.35	107.03	111.36
3	R	900	DKO	O3-C4-O4	-2.34	107.05	111.36
3	B	900	DKO	C7-C6-C5	2.33	121.88	113.62
4	D	900	DK6	C6-C5-C4	2.29	117.68	113.57
2	X	900	DKL	O3-C4-C5	-2.27	104.20	109.17
5	W	900	DKF	C6-C5-C4	2.27	118.62	113.38
6	P	900	DK9	O3-C4-C5	2.18	113.96	109.17
4	Z	900	DK6	O4-C4-O3	-2.18	107.34	111.36
3	R	900	DKO	C7-C6-C5	-2.17	105.93	113.62
6	F	900	DK9	O3-C4-O4	-2.17	107.37	111.36
5	V	900	DKF	C6-C5-C4	-2.12	108.47	113.38
5	U	900	DKF	O3-C4-C5	-2.08	104.61	109.17
6	F	900	DK9	O3-C4-C5	2.07	113.72	109.17
4	H	900	DK6	O4-C4-C5	-2.06	105.55	109.43
6	P	900	DK9	O3-C4-O4	-2.04	107.60	111.36
3	N	900	DKO	O3-C4-C5	2.02	113.61	109.17

There are no chirality outliers.

All (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
4	H	900	DK6	O4-C4-C5-C6
2	Q	900	DKL	O4-C4-C5-C6
5	M	900	DKF	O4-C4-C5-C6
5	J	900	DKF	O4-C4-C5-C6
2	A	900	DKL	O3-C4-C5-C6
5	W	900	DKF	O4-C4-C5-C6
5	U	900	DKF	O4-C4-C5-C6
5	K	900	DKF	O4-C4-C5-C6
5	I	900	DKF	O4-C4-C5-C6
6	P	900	DK9	O3-C4-C5-C6
5	L	900	DKF	O4-C4-C5-C6
2	X	900	DKL	O3-C4-C5-C6
4	Z	900	DK6	O3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
4	Z	900	DK6	O4-C4-C5-C6
5	Y	900	DKF	O3-C4-C5-C6
5	U	900	DKF	C5-C6-C7-C8
5	U	900	DKF	O3-C4-C5-C6
5	G	900	DKF	O3-C4-C5-C6
5	L	900	DKF	O3-C4-C5-C6
2	Q	900	DKL	C7-C8-C9-C10
5	I	900	DKF	C6-C7-C8-C9
2	Q	900	DKL	C5-C6-C7-C8
2	X	900	DKL	C6-C7-C8-C9
5	G	900	DKF	C5-C6-C7-C8
5	L	900	DKF	C5-C6-C7-C8
3	B	900	DKO	O4-C4-C5-C6
2	Q	900	DKL	O3-C4-C5-C6
5	J	900	DKF	O3-C4-C5-C6
5	K	900	DKF	O3-C4-C5-C6
5	Y	900	DKF	O4-C4-C5-C6
5	M	900	DKF	C5-C6-C7-C8
3	B	900	DKO	C7-C8-C9-C10
5	V	900	DKF	C6-C7-C8-C9
5	W	900	DKF	C5-C6-C7-C8
3	R	900	DKO	O3-C4-C5-C6
5	E	900	DKF	O4-C4-C5-C6
6	O	900	DK9	O4-C4-C5-C6
2	A	900	DKL	O4-C4-C5-C6
5	I	900	DKF	O3-C4-C5-C6
2	C	900	DKL	C5-C6-C7-C8
5	U	900	DKF	C6-C7-C8-C9
5	Y	900	DKF	C5-C6-C7-C8
5	M	900	DKF	C6-C7-C8-C9
2	C	900	DKL	C7-C8-C9-C10
4	D	900	DK6	O4-C4-C5-C6
2	T	900	DKL	C5-C6-C7-C8
2	X	900	DKL	C7-C8-C9-C10
5	I	900	DKF	C4-C5-C6-C7
5	V	900	DKF	C5-C6-C7-C8
2	A	900	DKL	C7-C8-C9-C10
5	U	900	DKF	C4-C5-C6-C7
5	V	900	DKF	C4-C5-C6-C7
5	K	900	DKF	C5-C6-C7-C8
2	T	900	DKL	C4-C5-C6-C7
6	P	900	DK9	O4-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
3	B	900	DKO	C5-C6-C7-C8
5	L	900	DKF	C4-C5-C6-C7
2	X	900	DKL	C5-C6-C7-C8
3	B	900	DKO	C4-C5-C6-C7
6	P	900	DK9	C4-C5-C6-C7
2	X	900	DKL	C4-C5-C6-C7
5	Y	900	DKF	C4-C5-C6-C7
2	Q	900	DKL	C6-C7-C8-C9
3	N	900	DKO	C7-C8-C9-C10
5	E	900	DKF	C5-C6-C7-C8
5	G	900	DKF	C4-C5-C6-C7
5	M	900	DKF	C4-C5-C6-C7
3	R	900	DKO	O4-C4-C5-C6
3	R	900	DKO	C4-C5-C6-C7
2	Q	900	DKL	C4-C5-C6-C7
5	K	900	DKF	C4-C5-C6-C7
3	N	900	DKO	C11-C10-C9-C8
6	O	900	DK9	C4-C5-C6-C7
2	A	900	DKL	C4-C5-C6-C7
3	N	900	DKO	O4-C4-C5-C6
4	D	900	DK6	O3-C4-C5-C6
5	G	900	DKF	C6-C7-C8-C9

There are no ring outliers.

24 monomers are involved in 94 short contacts:

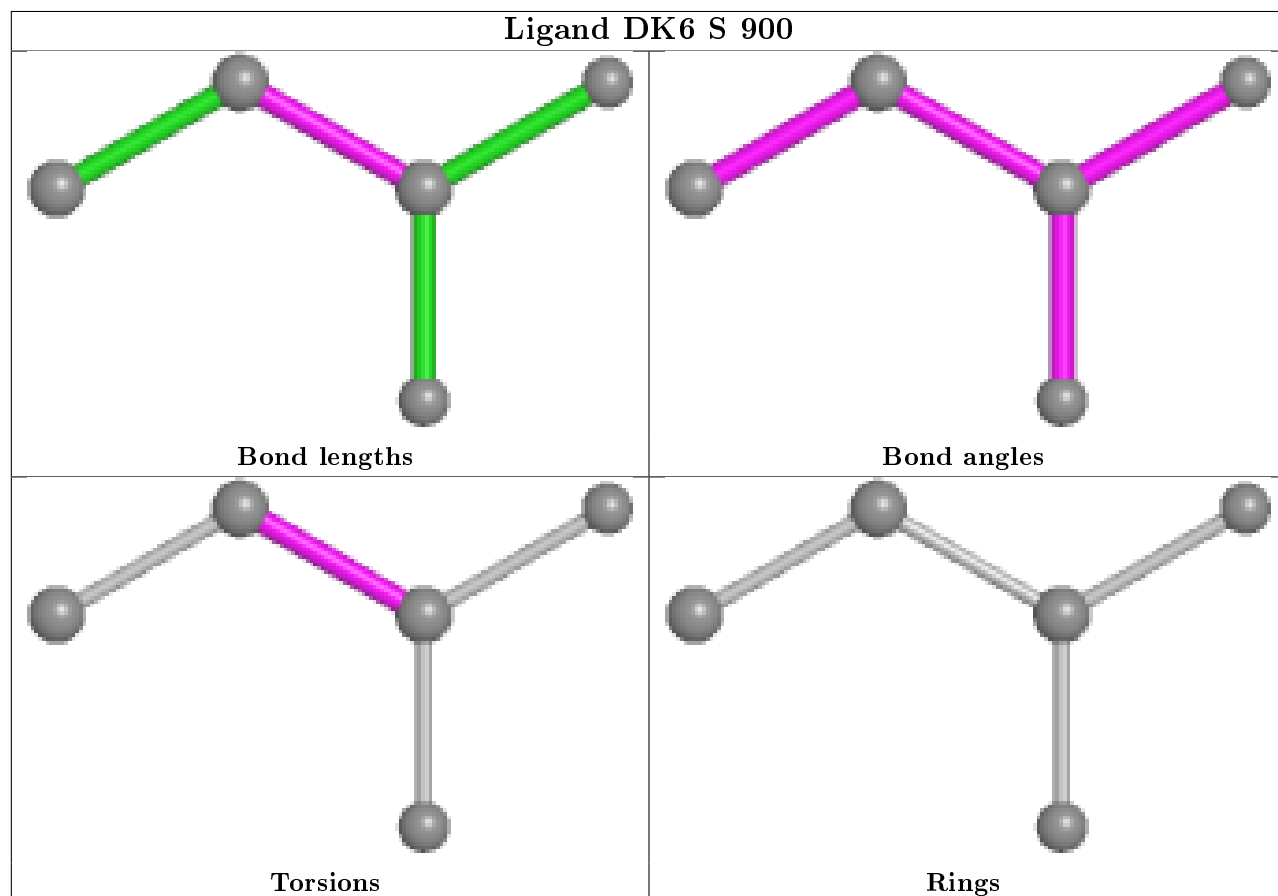
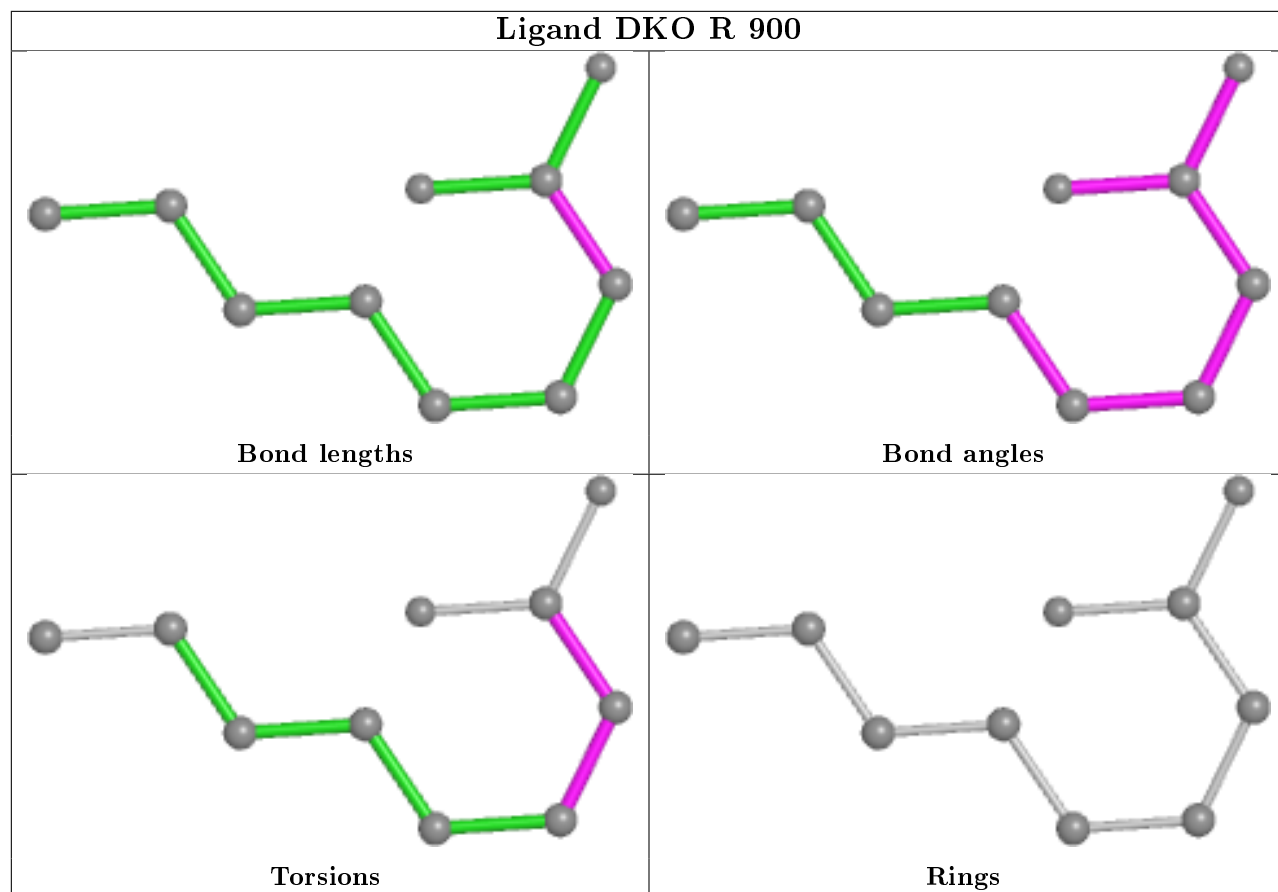
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	R	900	DKO	3	0
4	S	900	DK6	2	0
5	E	900	DKF	6	0
3	B	900	DKO	3	0
6	O	900	DK9	4	0
4	H	900	DK6	4	0
2	Q	900	DKL	4	0
5	M	900	DKF	4	0
2	C	900	DKL	8	0
5	J	900	DKF	4	0
2	A	900	DKL	4	0
5	W	900	DKF	4	0
5	U	900	DKF	3	0
5	K	900	DKF	3	0
5	I	900	DKF	5	0

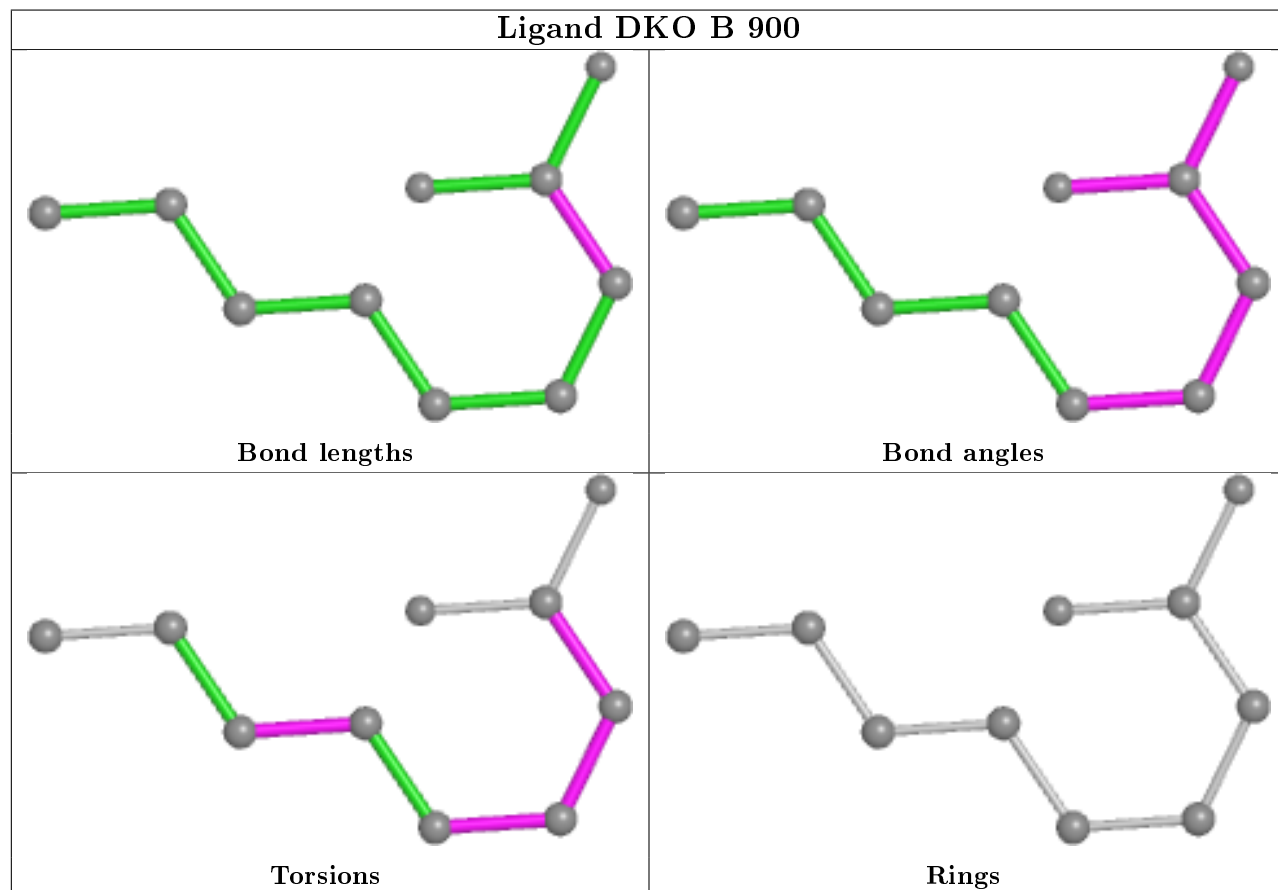
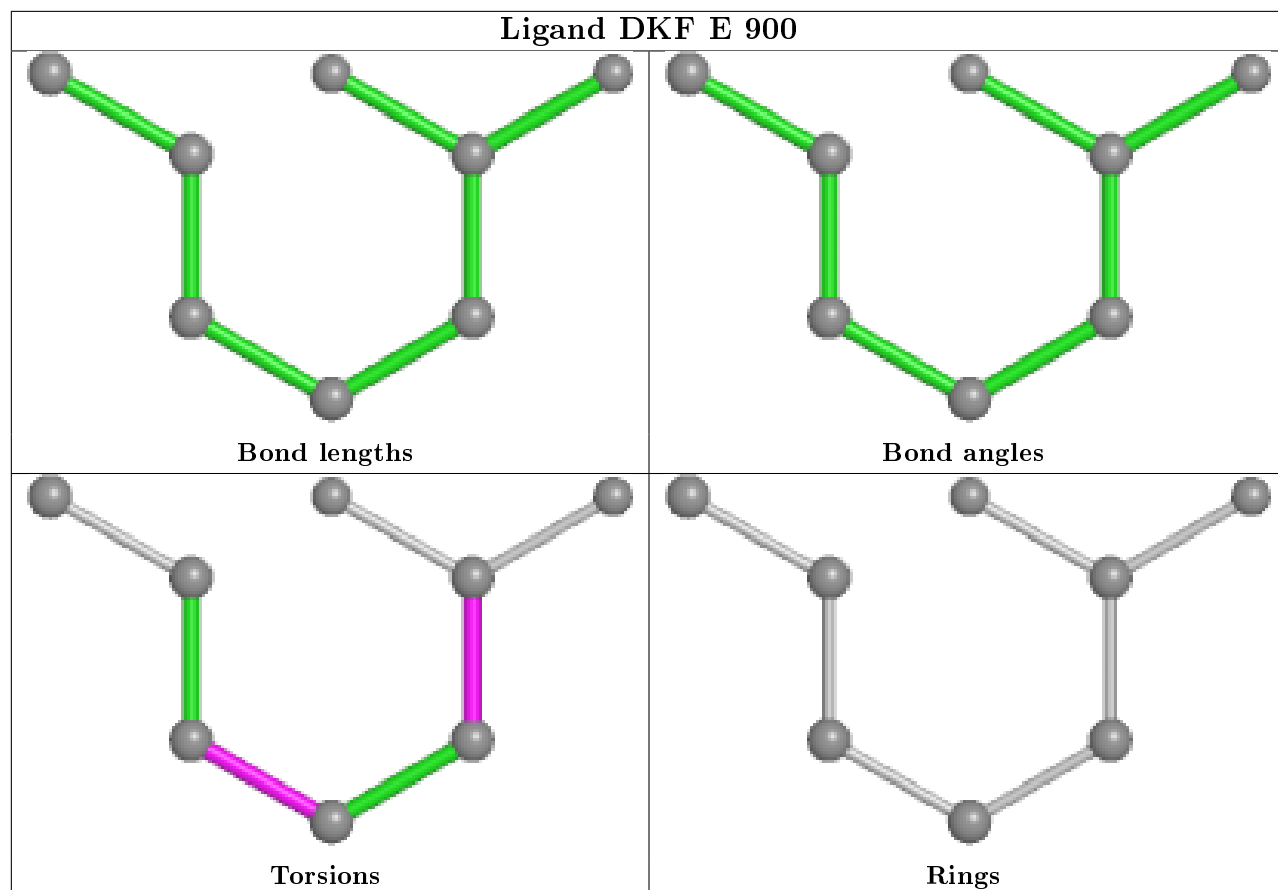
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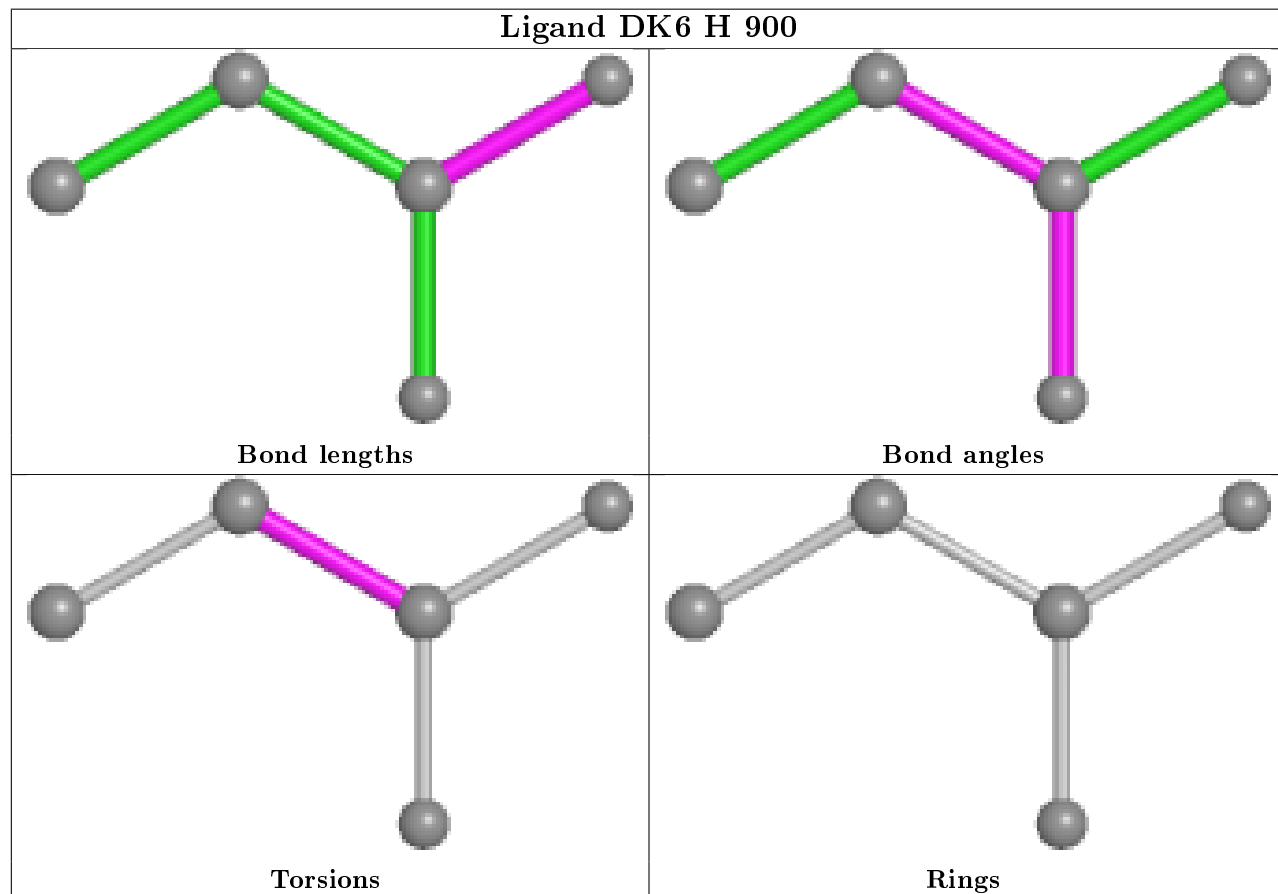
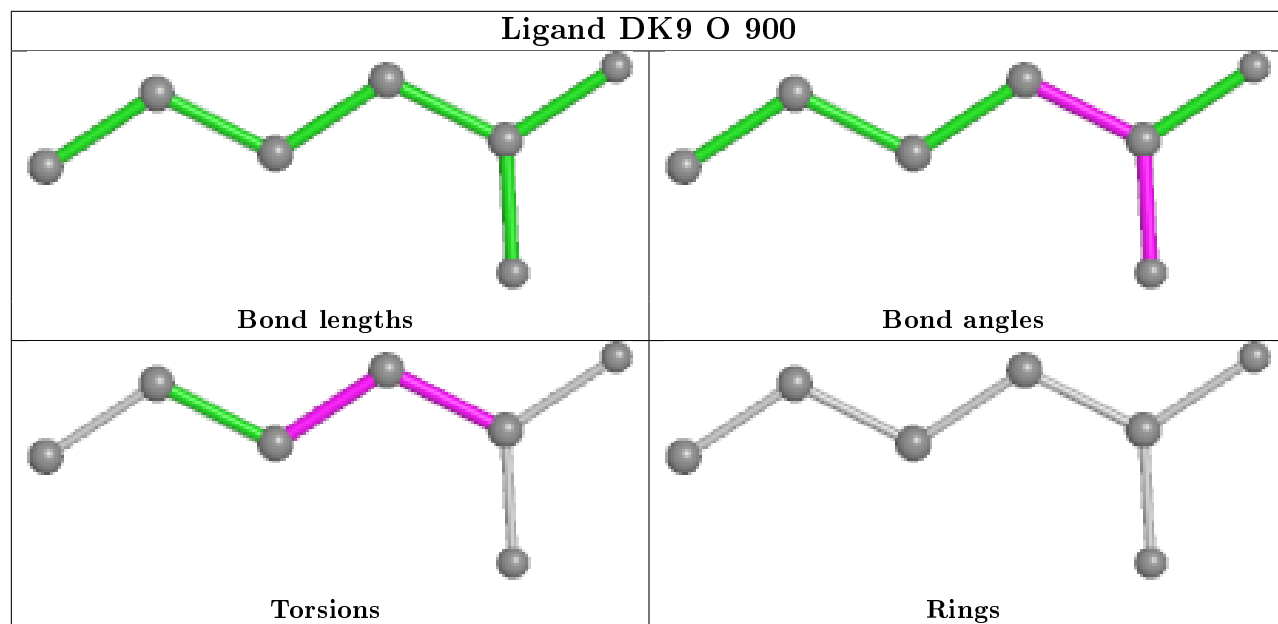
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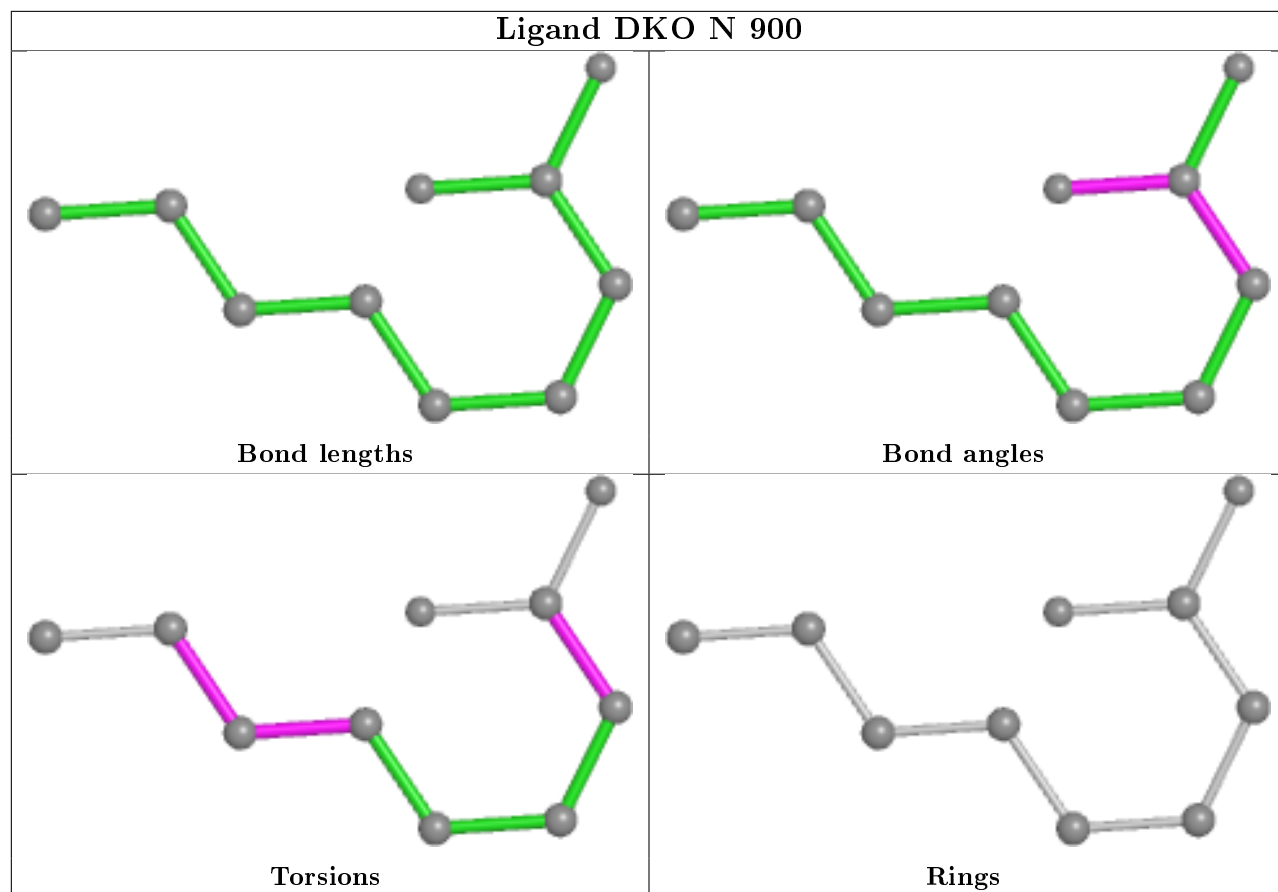
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	T	900	DKL	5	0
6	P	900	DK9	3	0
5	V	900	DKF	2	0
5	G	900	DKF	5	0
6	F	900	DK9	3	0
2	X	900	DKL	3	0
4	D	900	DK6	2	0
4	Z	900	DK6	5	0
5	Y	900	DKF	5	0

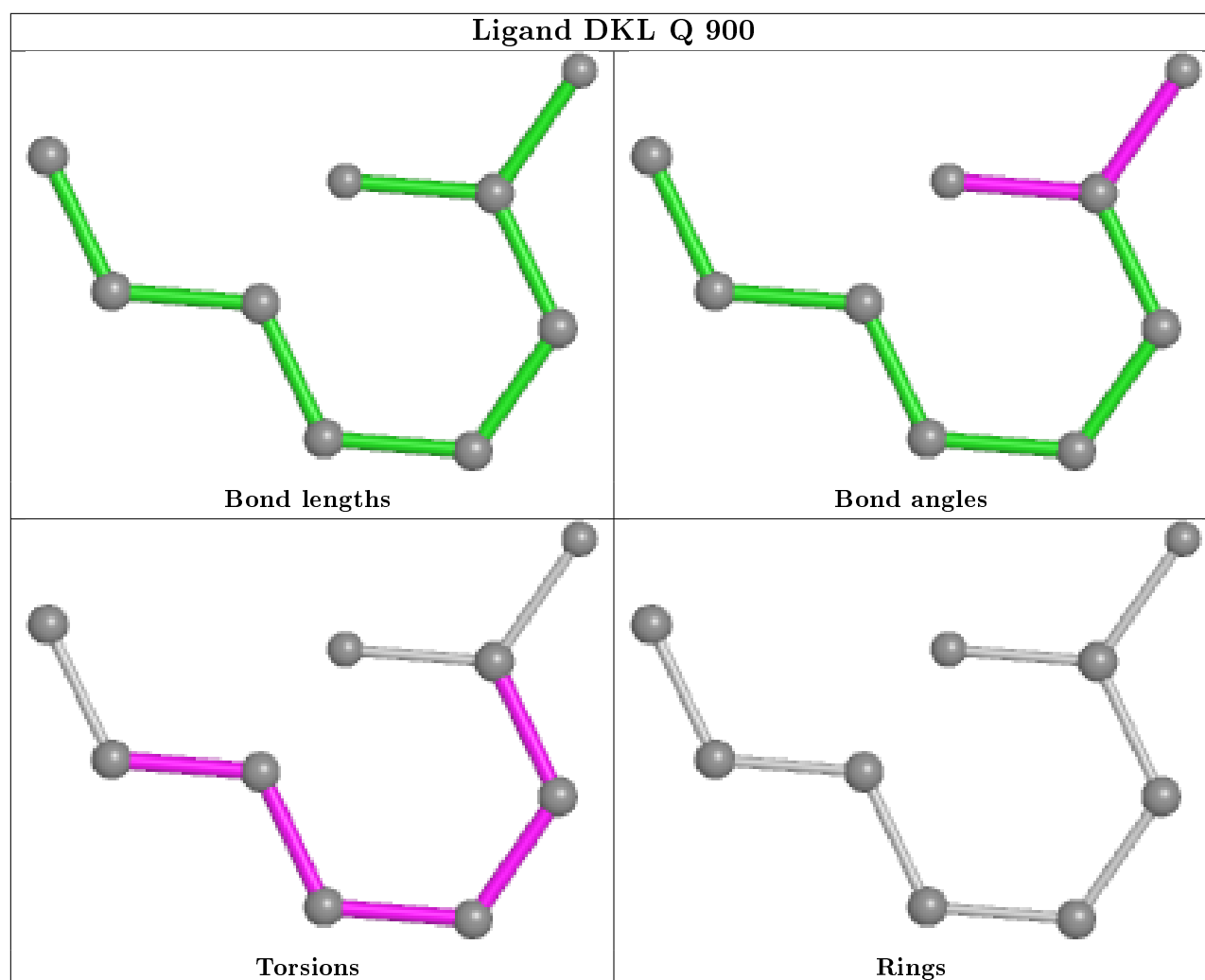
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

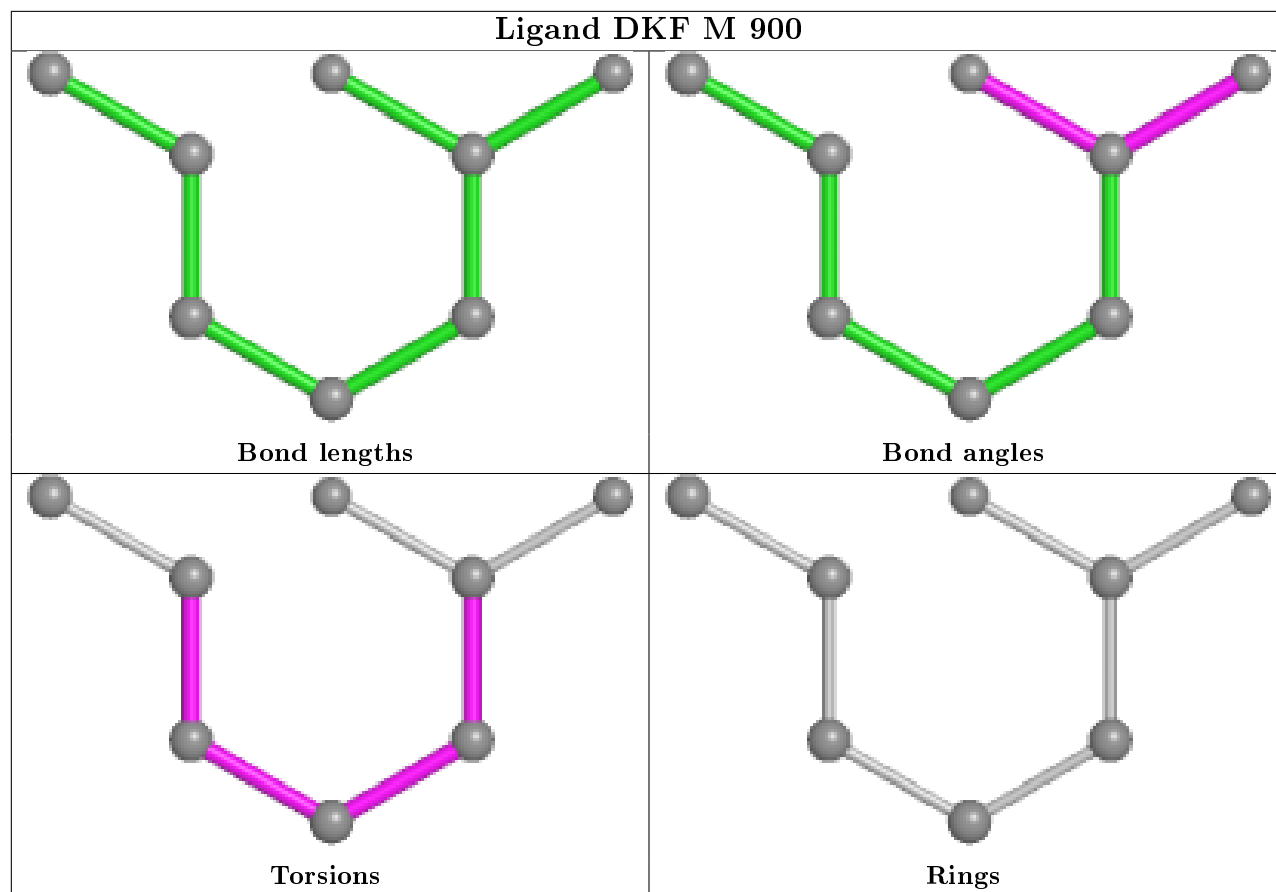


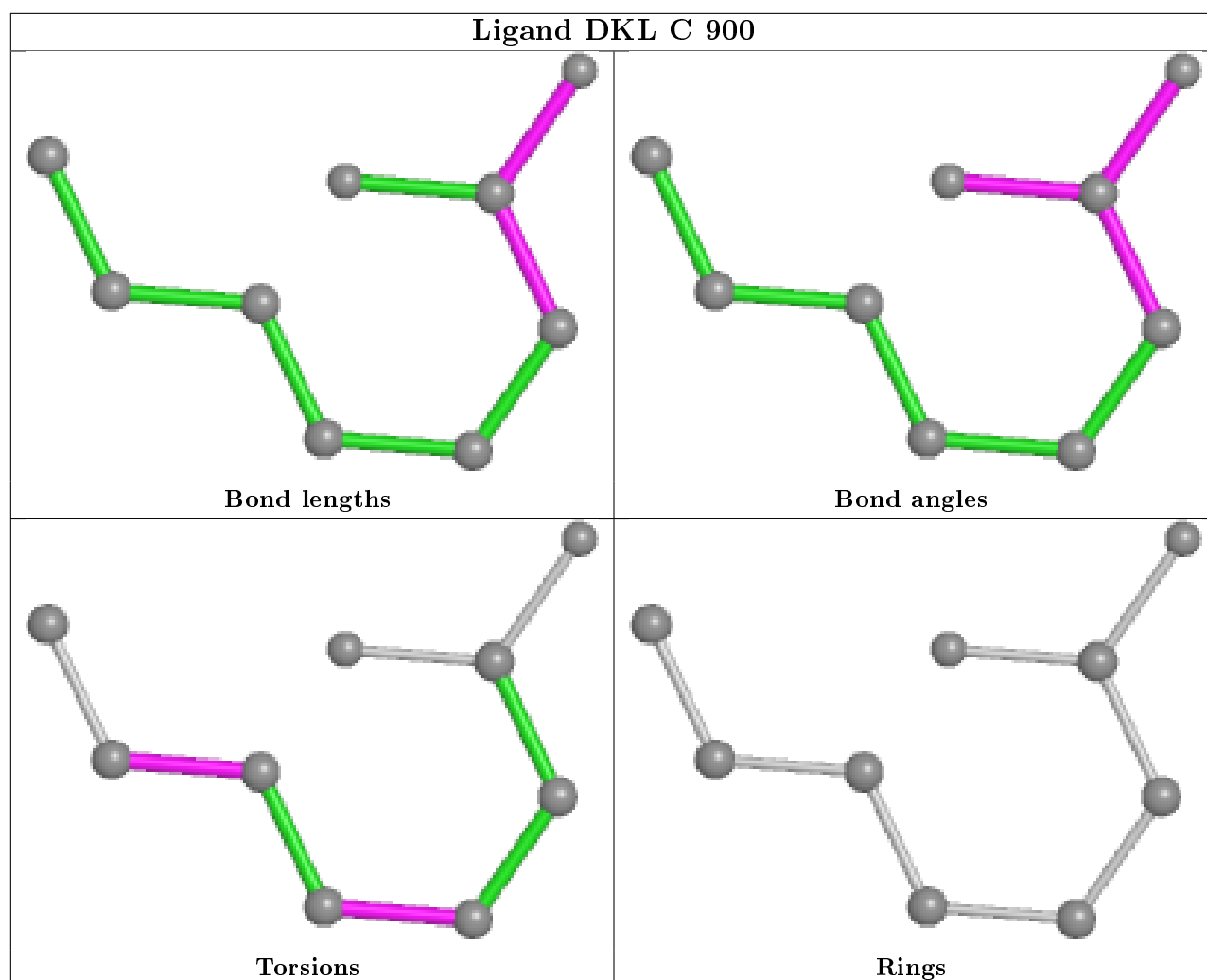


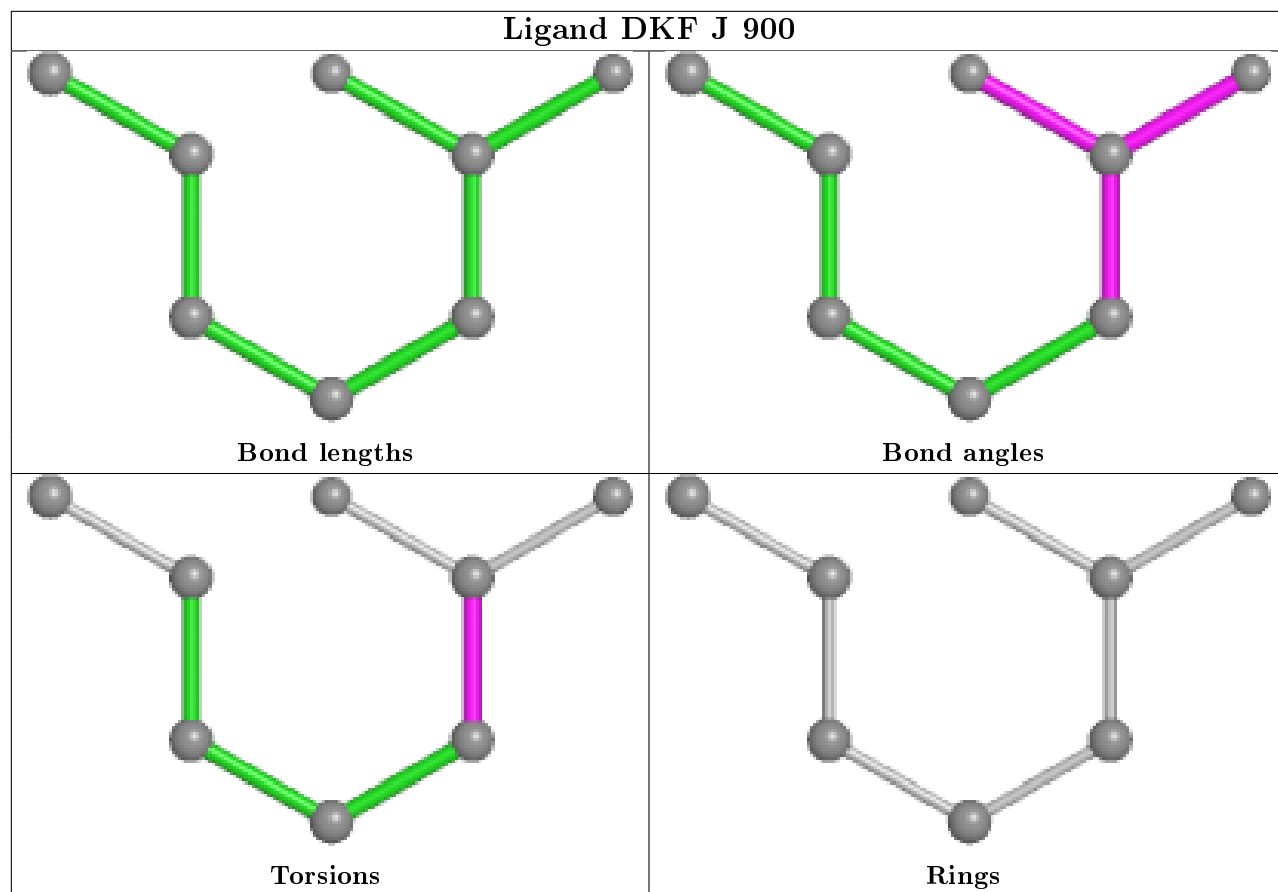


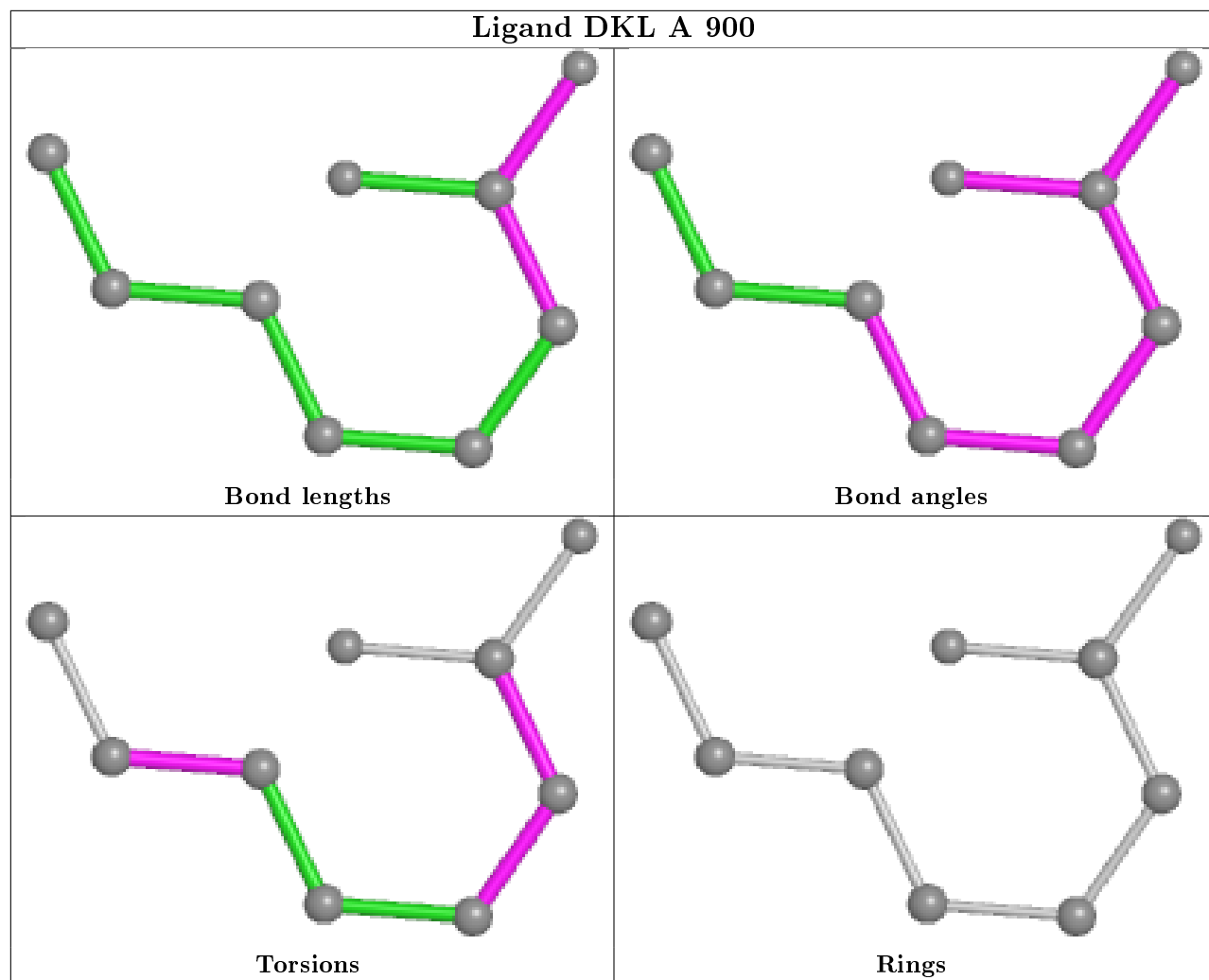


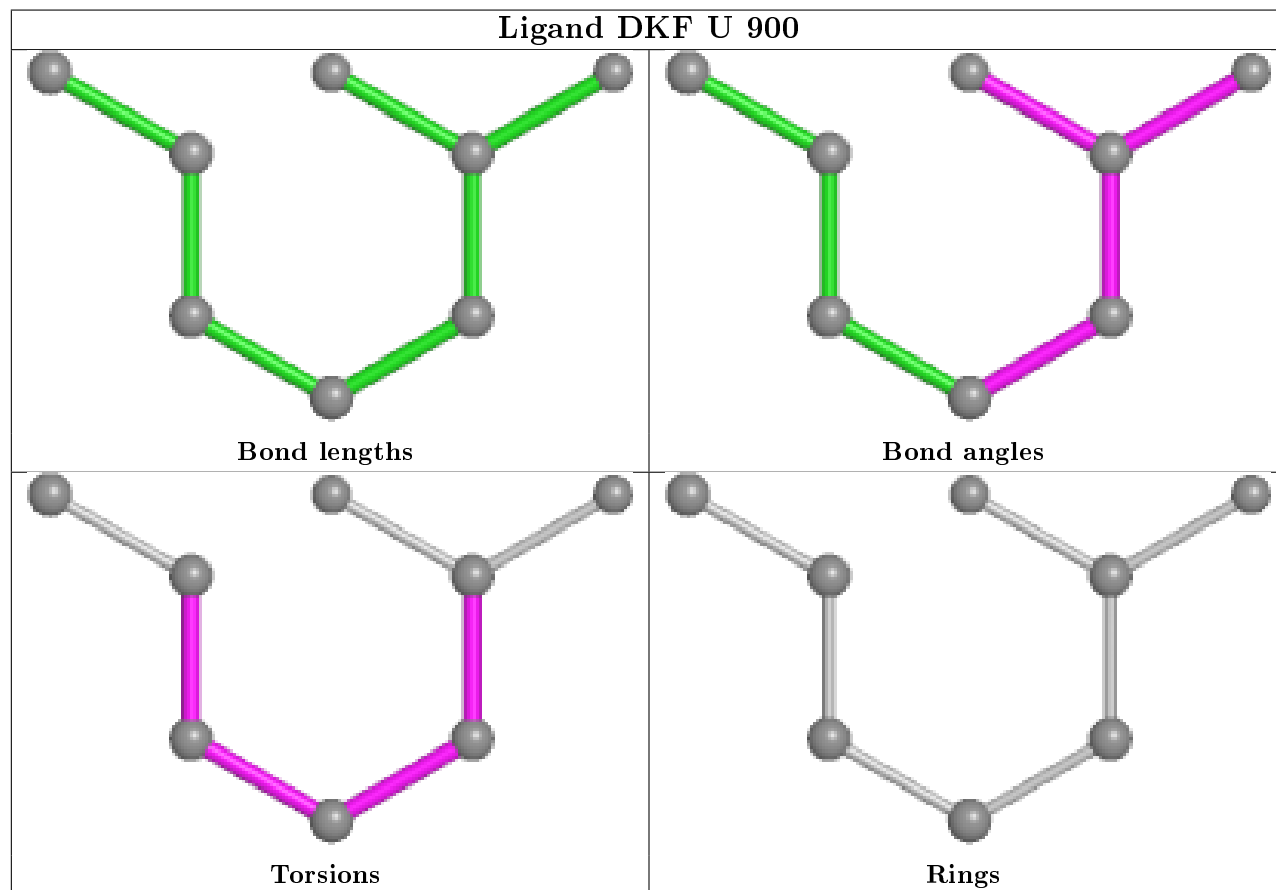
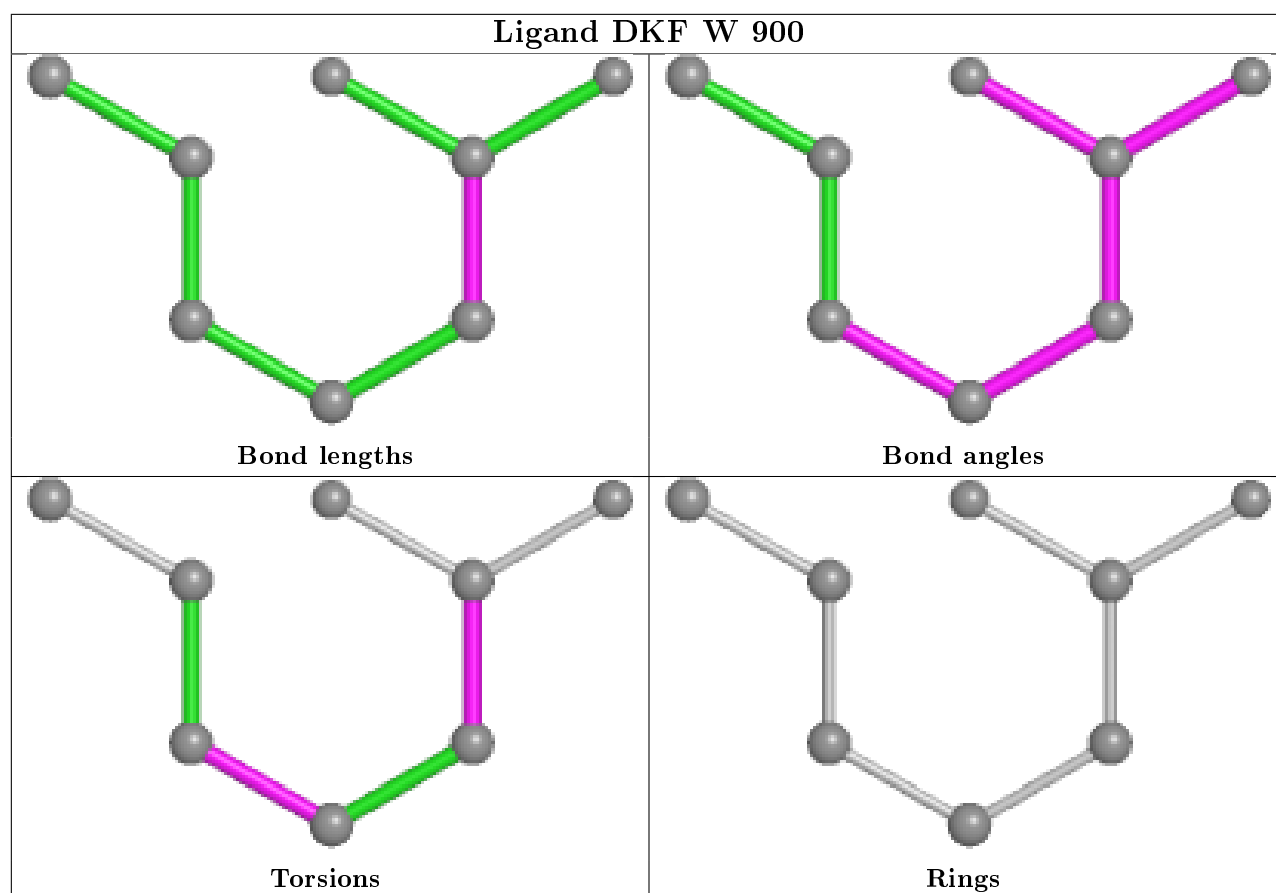


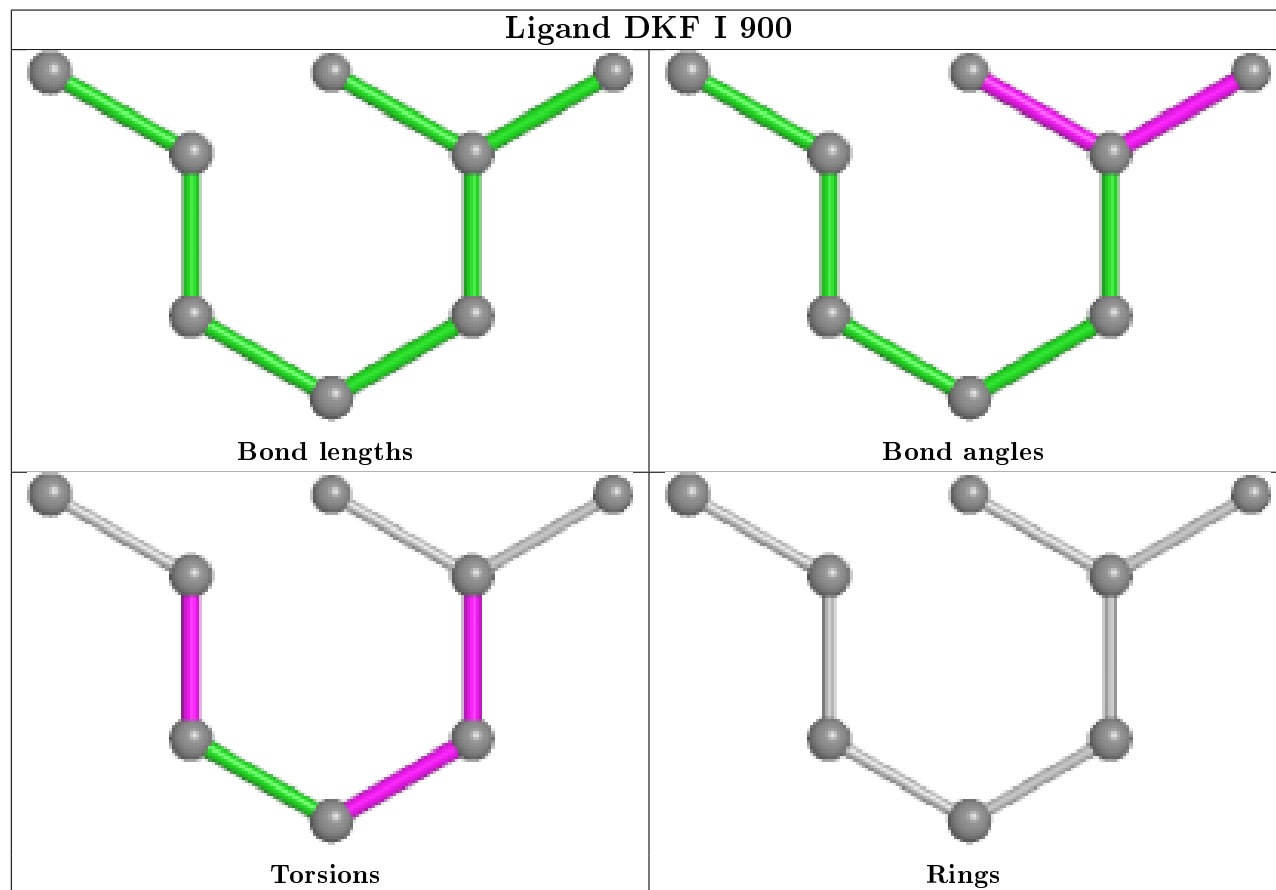
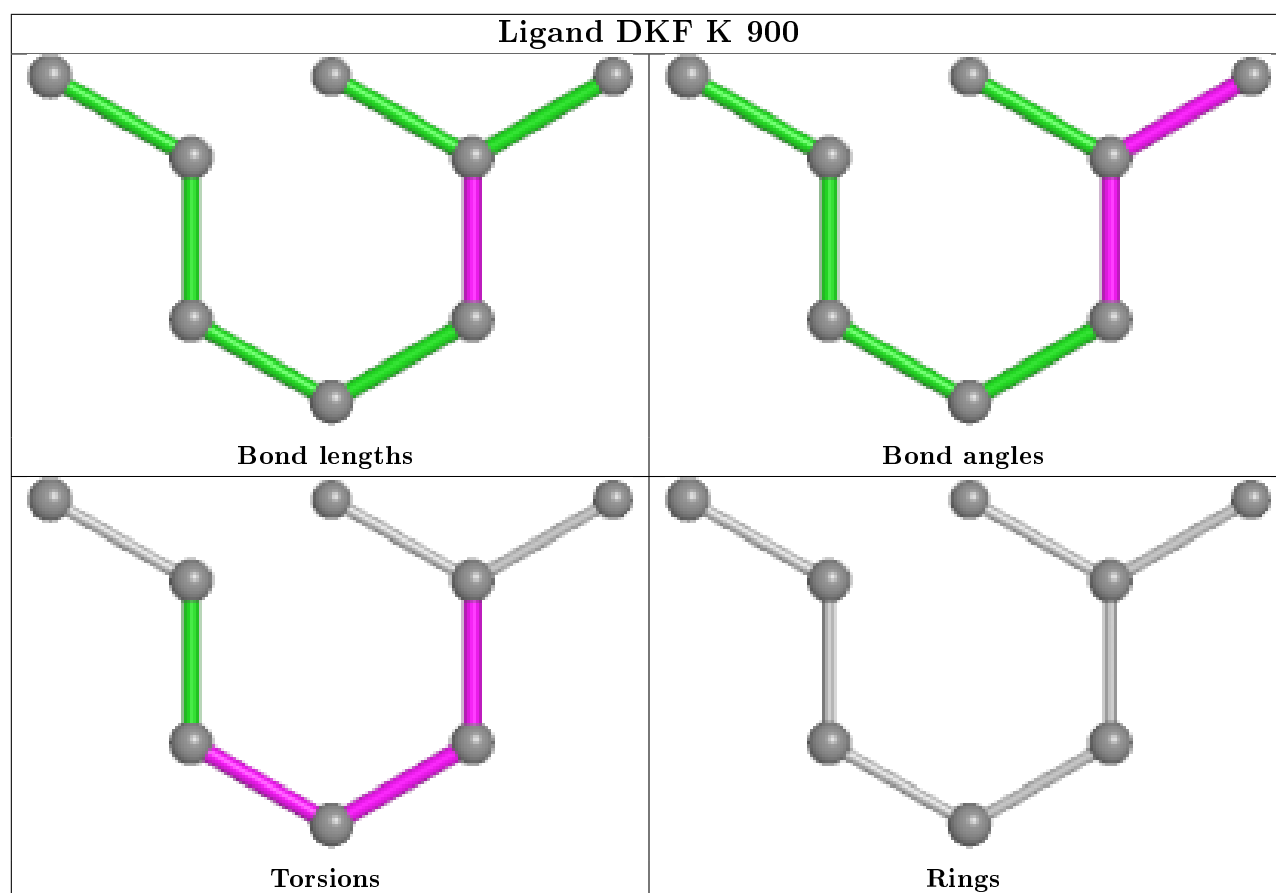


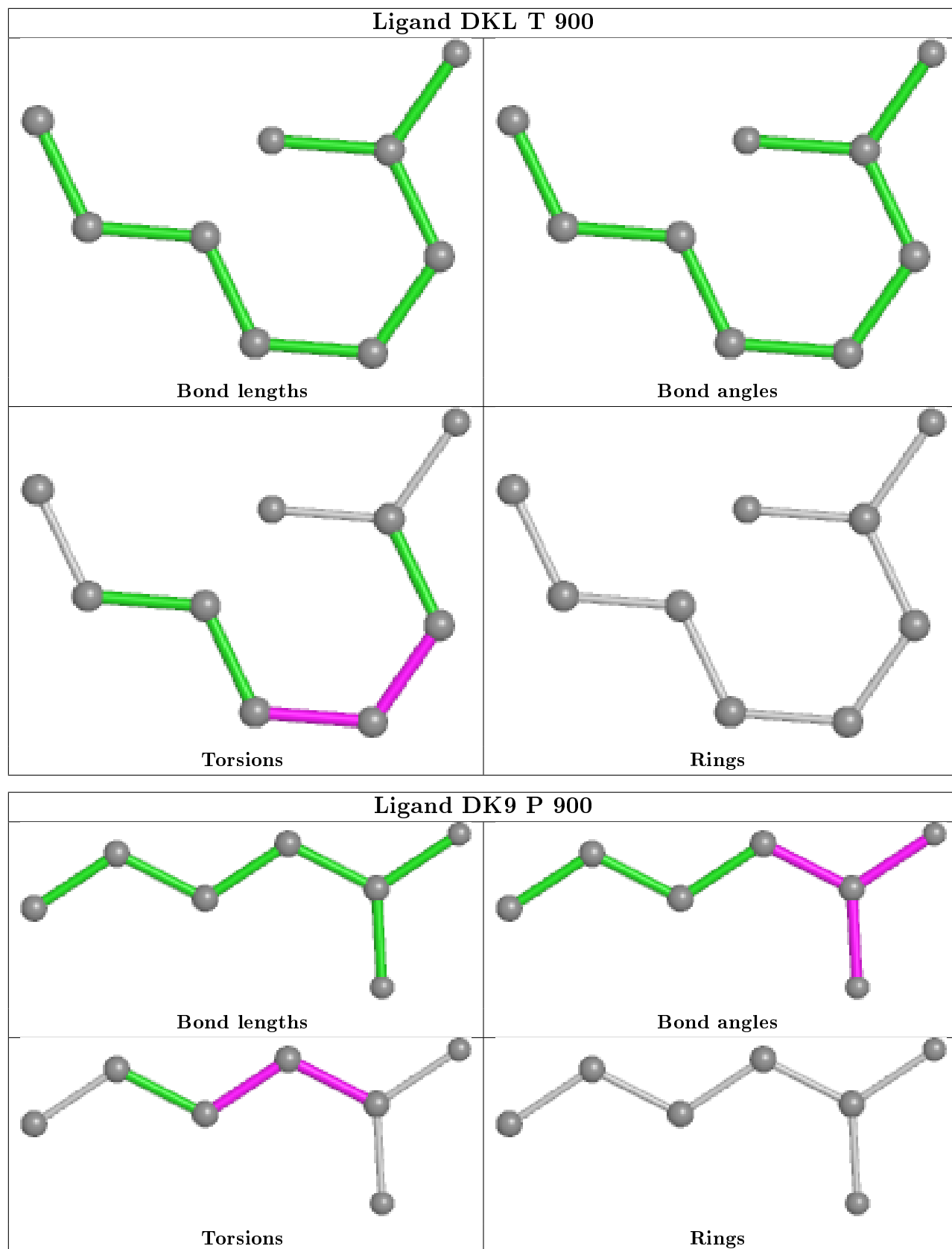


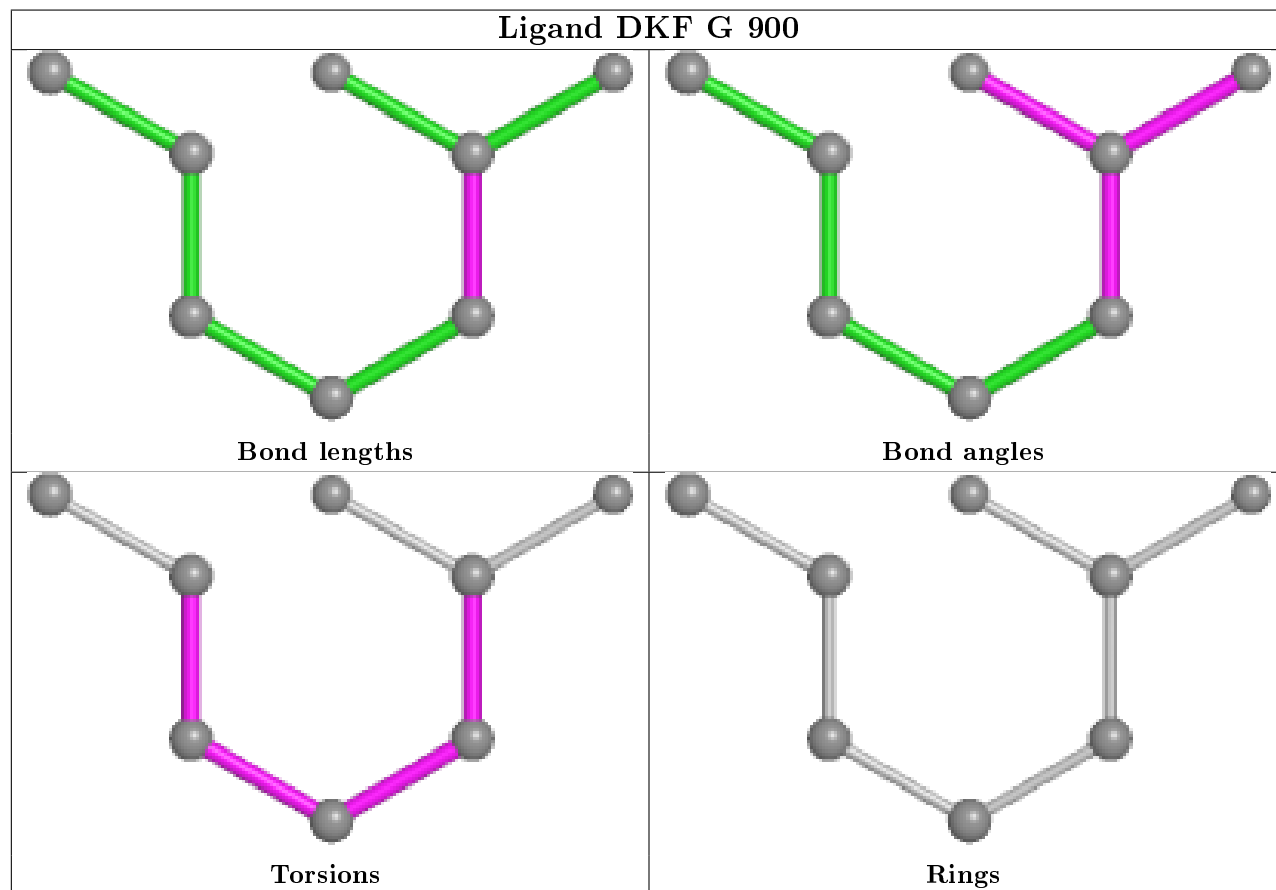
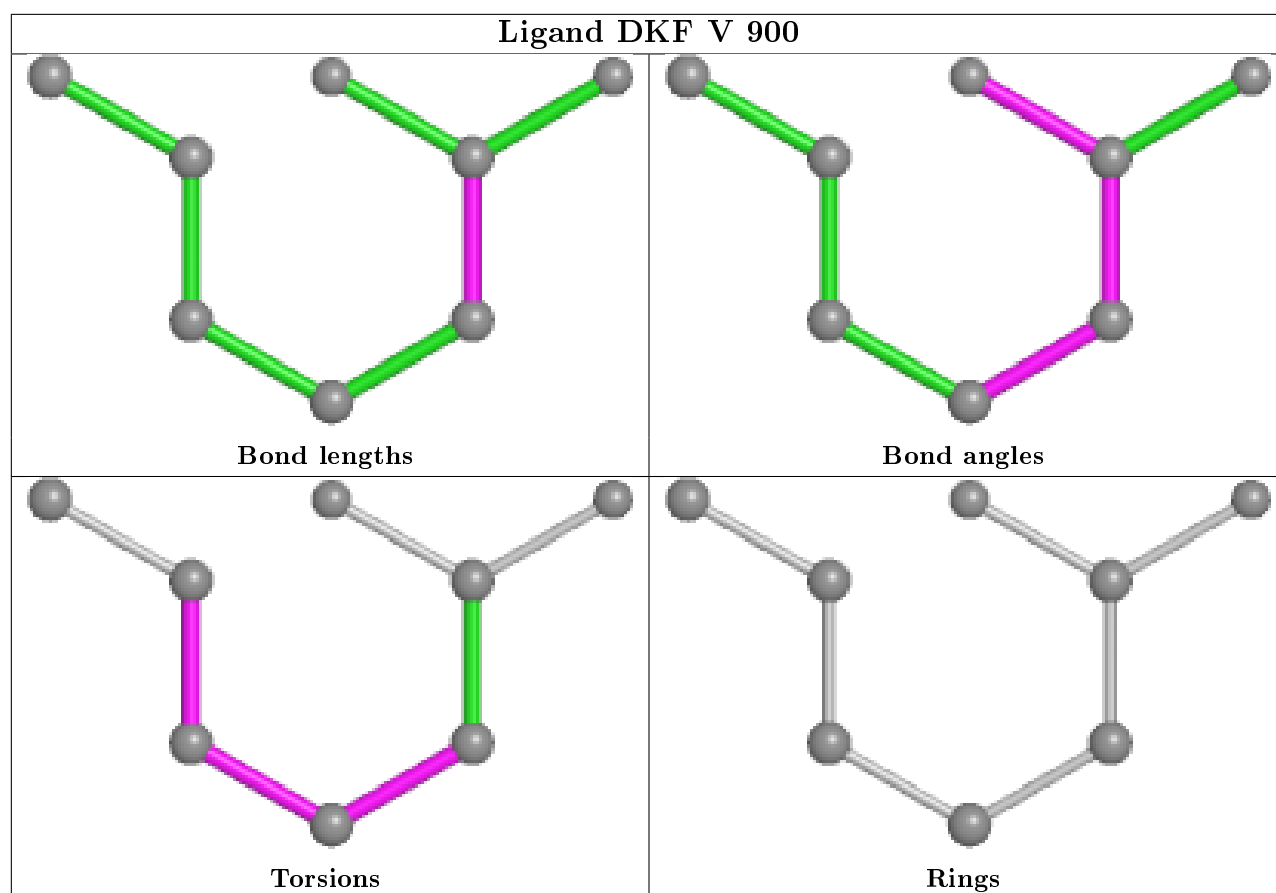


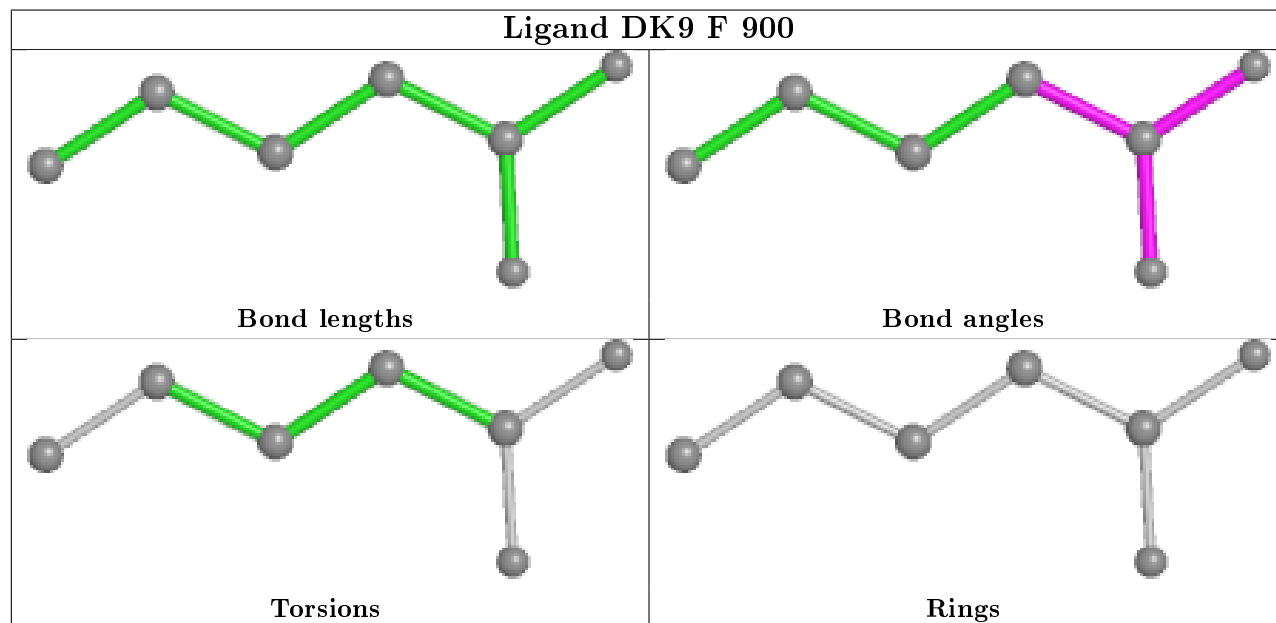
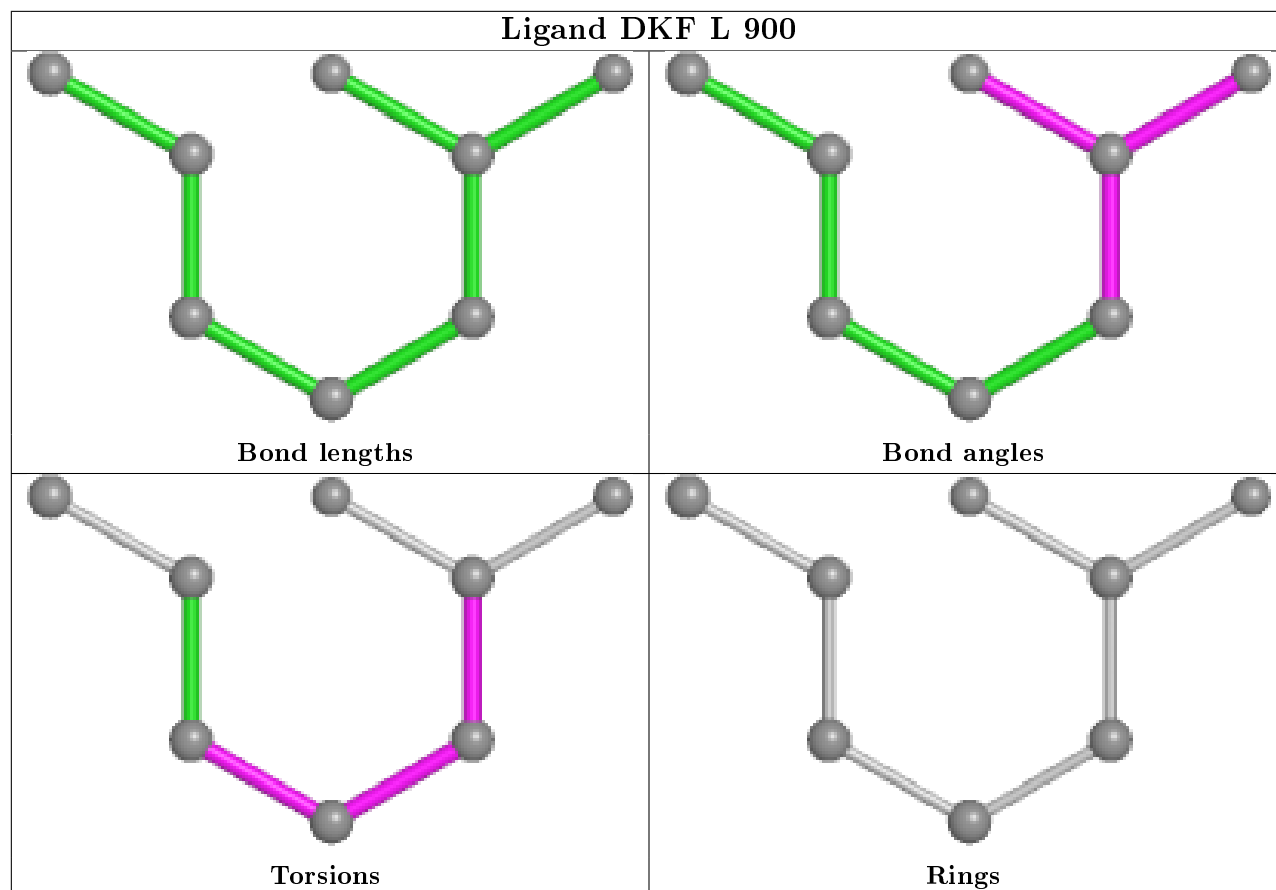


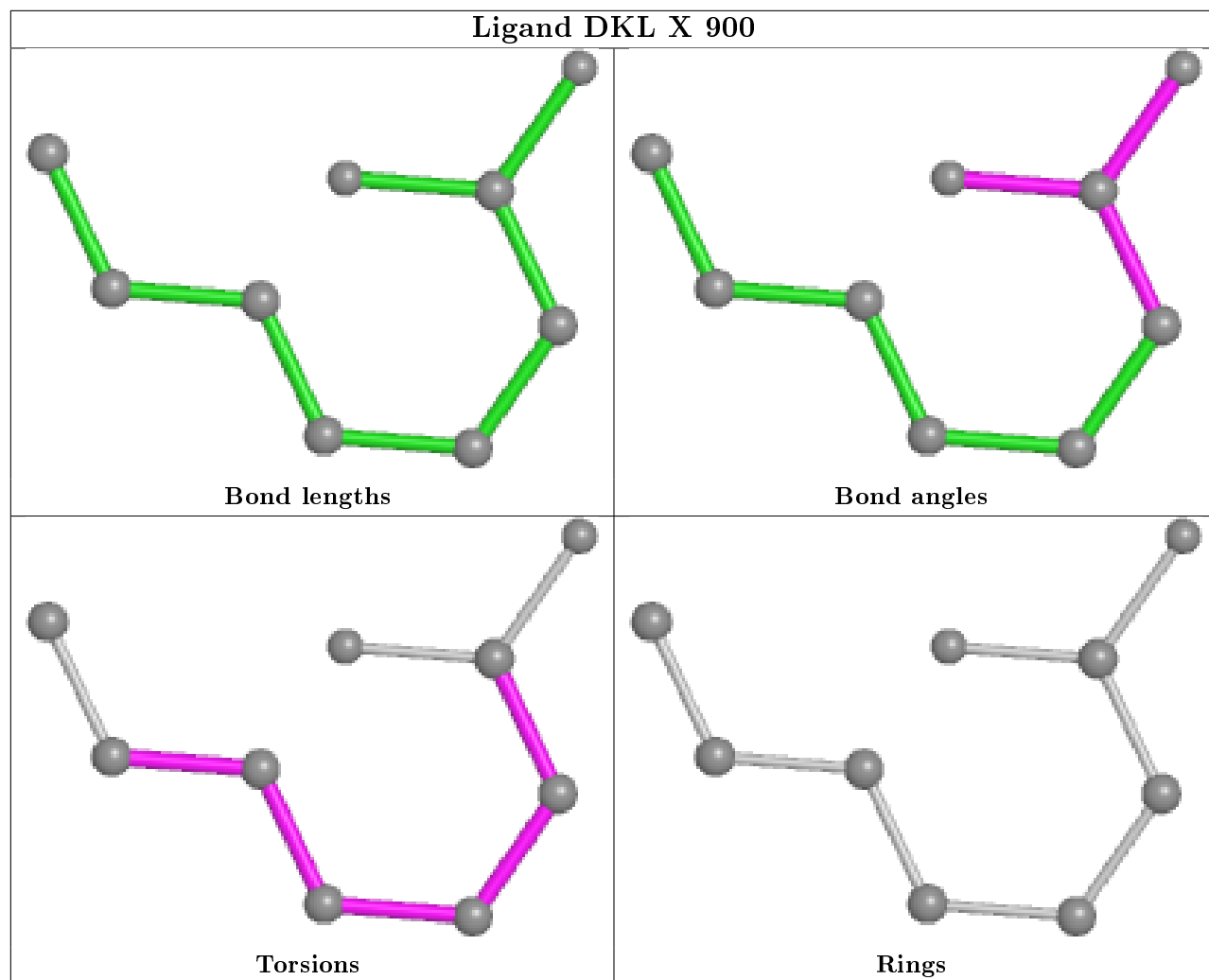


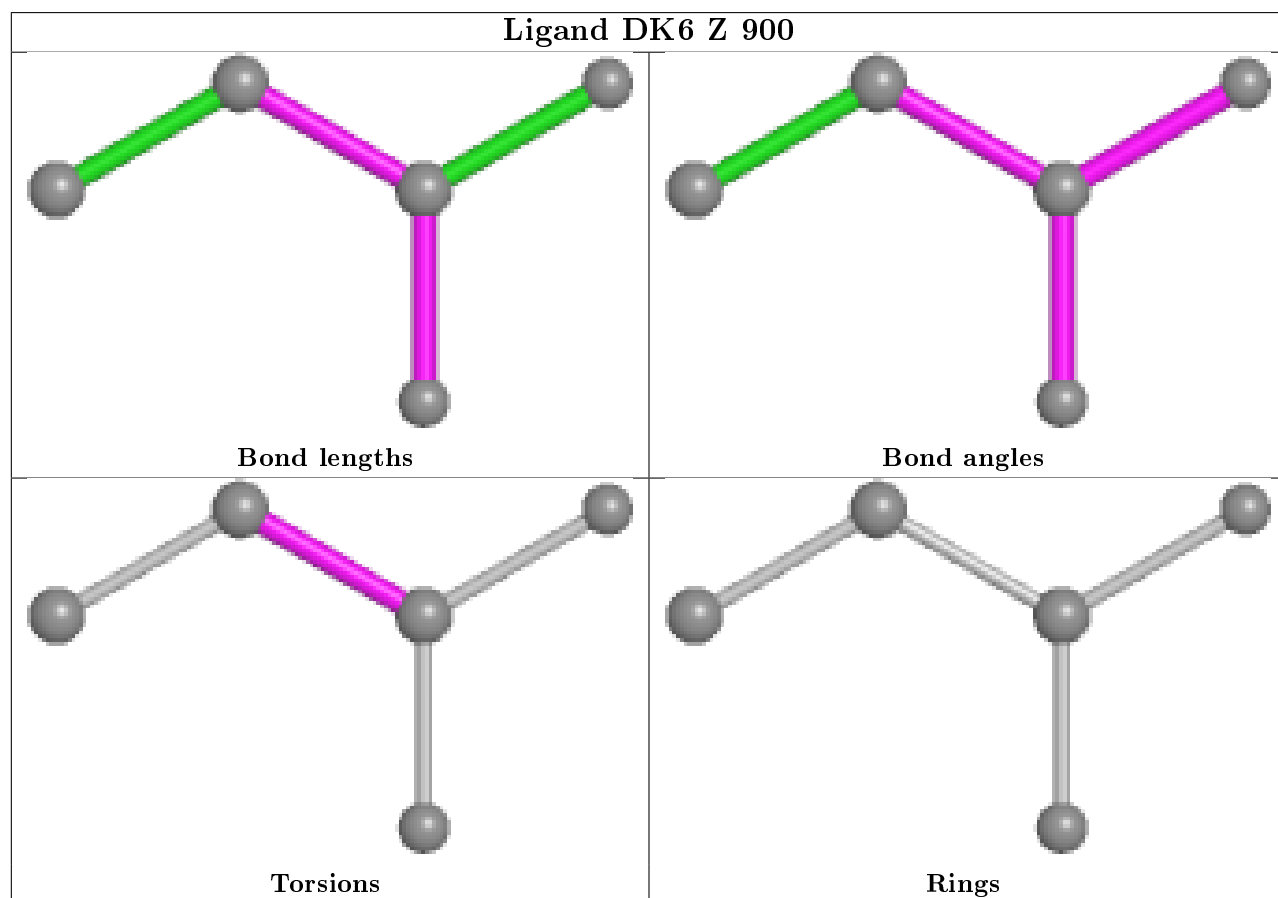
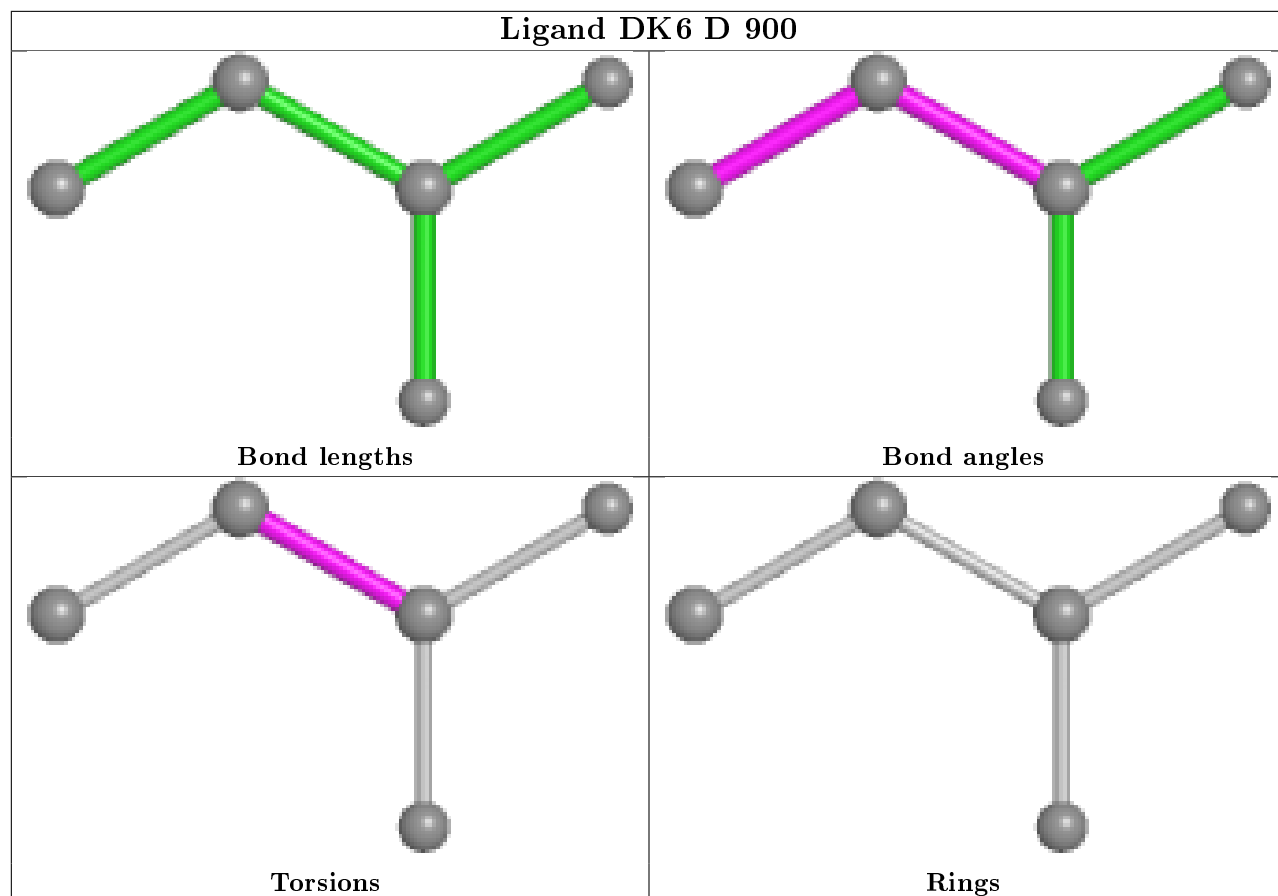


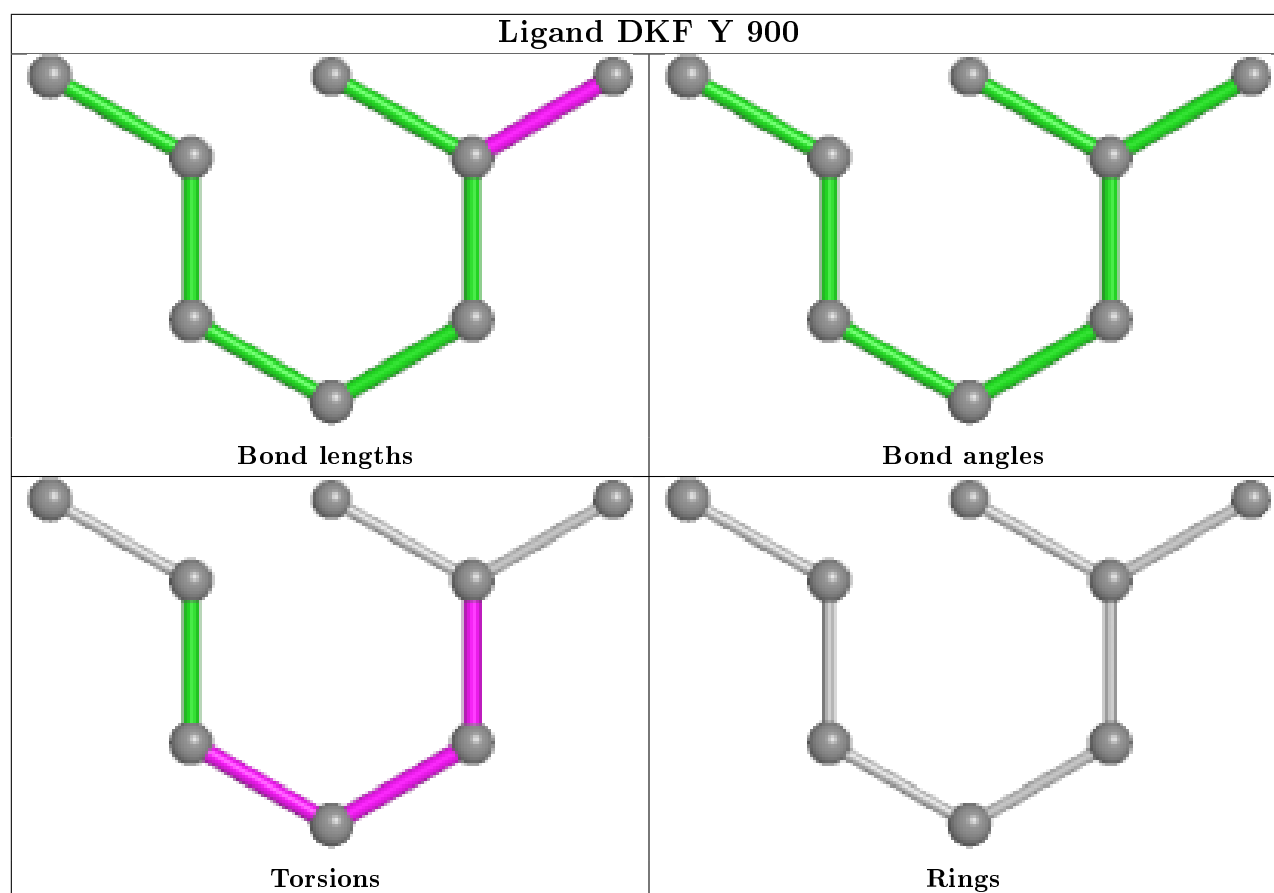












5.7 Other polymers [i](#)

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

All (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
1	Q	310	ASN	4.2
1	O	211	PHE	4.2
1	W	311	ARG	4.1
1	P	310	ASN	4.1
1	E	185	GLU	4.1
1	U	311	ARG	4.1
1	A	211	PHE	3.9
1	P	211	PHE	3.9
1	W	212	GLY	3.9
1	B	308	VAL	3.9
1	Q	211	PHE	3.8
1	U	35	ILE	3.8
1	P	185	GLU	3.7
1	L	313	ILE	3.7
1	X	211	PHE	3.7
1	M	185	GLU	3.6
1	R	187	ASP	3.6
1	U	112	GLY	3.6
1	Q	312	ARG	3.5
1	J	310	ASN	3.5
1	Z	35	ILE	3.4
1	L	311	ARG	3.4
1	K	312	ARG	3.4
1	M	310	ASN	3.3
1	U	111	PHE	3.3
1	N	211	PHE	3.3
1	I	312	ARG	3.3
1	M	211	PHE	3.3
1	S	186	ASP	3.3

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Mol	Chain	Res	Type	RSRZ
1	N	310	ASN	3.3
1	Z	310	ASN	3.3
1	Z	112	GLY	3.2
1	O	310	ASN	3.2
1	E	160	ALA	3.2
1	P	128	GLY	3.1
1	D	105	ASP	3.1
1	C	128	GLY	3.1
1	O	185	GLU	3.1
1	U	189	PRO	3.1
1	A	310	ASN	3.1
1	X	105	ASP	3.0
1	L	186	ASP	3.0
1	C	310	ASN	3.0
1	R	186	ASP	3.0
1	T	211	PHE	3.0
1	M	212	GLY	3.0
1	A	111	PHE	2.9
1	X	310	ASN	2.9
1	R	128	GLY	2.9
1	C	105	ASP	2.9
1	M	137	CYS	2.9
1	O	240	PRO	2.9
1	O	241	ASN	2.8
1	Z	186	ASP	2.8
1	Q	189	PRO	2.8
1	X	186	ASP	2.8
1	B	211	PHE	2.8
1	K	313	ILE	2.8
1	Y	211	PHE	2.8
1	V	37	GLY	2.8
1	O	186	ASP	2.7
1	Z	110	VAL	2.7
1	P	311	ARG	2.7
1	Z	34	ILE	2.7
1	V	105	ASP	2.7
1	K	310	ASN	2.6
1	I	310	ASN	2.6
1	I	186	ASP	2.6
1	W	185	GLU	2.6
1	E	186	ASP	2.6
1	A	35	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	G	211	PHE	2.6
1	H	211	PHE	2.6
1	L	111	PHE	2.6
1	R	185	GLU	2.6
1	C	211	PHE	2.6
1	S	34	ILE	2.6
1	A	34	ILE	2.6
1	R	137	CYS	2.5
1	G	35	ILE	2.5
1	K	112	GLY	2.5
1	L	310	ASN	2.5
1	O	116	GLY	2.5
1	R	114	SER	2.5
1	K	35	ILE	2.5
1	U	105	ASP	2.5
1	E	312	ARG	2.5
1	Q	35	ILE	2.5
1	H	310	ASN	2.5
1	Q	111	PHE	2.5
1	K	187	ASP	2.5
1	U	114	SER	2.5
1	K	111	PHE	2.4
1	D	212	GLY	2.4
1	M	138	GLY	2.4
1	O	35	ILE	2.4
1	W	270	ARG	2.4
1	D	34	ILE	2.4
1	D	128	GLY	2.4
1	X	116	GLY	2.4
1	I	185	GLU	2.4
1	U	110	VAL	2.4
1	M	116	GLY	2.4
1	N	34	ILE	2.4
1	Z	116	GLY	2.3
1	I	35	ILE	2.3
1	S	187	ASP	2.3
1	H	185	GLU	2.3
1	Z	117	SER	2.3
1	A	110	VAL	2.3
1	B	212	GLY	2.3
1	D	35	ILE	2.3
1	M	105	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	I	112	GLY	2.3
1	Z	309	ALA	2.3
1	U	34	ILE	2.3
1	J	186	ASP	2.3
1	R	105	ASP	2.2
1	Y	35	ILE	2.2
1	Z	111	PHE	2.2
1	P	186	ASP	2.2
1	C	34	ILE	2.2
1	Y	34	ILE	2.2
1	L	312	ARG	2.2
1	C	186	ASP	2.2
1	A	114	SER	2.2
1	F	34	ILE	2.2
1	W	35	ILE	2.2
1	Y	185	GLU	2.2
1	B	35	ILE	2.2
1	L	35	ILE	2.2
1	I	187	ASP	2.2
1	Q	110	VAL	2.2
1	N	35	ILE	2.2
1	J	111	PHE	2.2
1	V	110	VAL	2.1
1	Y	310	ASN	2.1
1	J	35	ILE	2.1
1	V	34	ILE	2.1
1	E	310	ASN	2.1
1	A	160	ALA	2.1
1	M	35	ILE	2.1
1	M	139	ILE	2.1
1	I	111	PHE	2.1
1	D	185	GLU	2.1
1	S	310	ASN	2.1
1	L	110	VAL	2.1
1	E	35	ILE	2.1
1	R	35	ILE	2.1
1	Q	309	ALA	2.1
1	U	187	ASP	2.1
1	V	137	CYS	2.1
1	Y	9	THR	2.1
1	J	34	ILE	2.1
1	J	136	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	M	117	SER	2.1
1	R	180	ALA	2.0
1	L	34	ILE	2.0
1	V	310	ASN	2.0
1	X	34	ILE	2.0
1	V	114	SER	2.0
1	U	186	ASP	2.0
1	M	115	TRP	2.0
1	Z	189	PRO	2.0
1	D	137	CYS	2.0
1	S	114	SER	2.0
1	Y	110	VAL	2.0
1	H	35	ILE	2.0
1	I	105	ASP	2.0
1	Z	153	LYS	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
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

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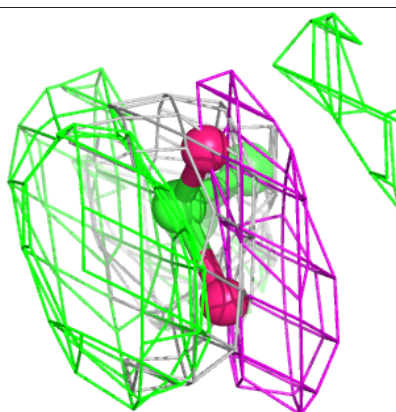
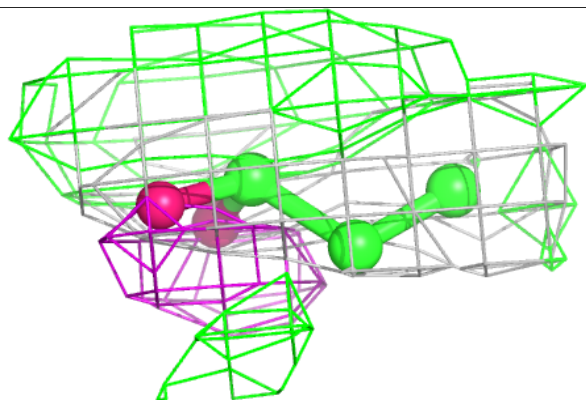
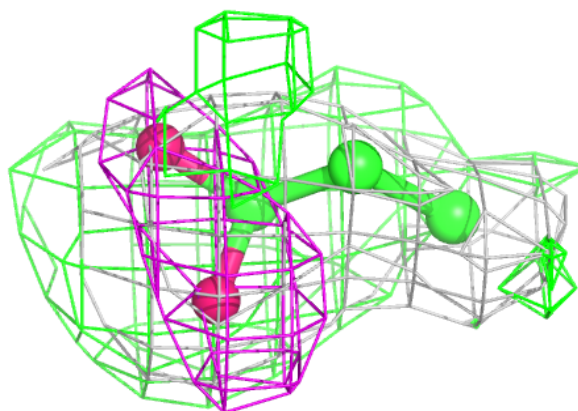
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	DKL	A	900	9/9	0.77	0.34	27,39,47,49	0
4	DK6	Z	900	5/5	0.77	0.40	34,39,42,43	0
3	DKO	R	900	10/10	0.77	0.38	35,50,68,70	0
3	DKO	B	900	10/10	0.78	0.39	29,48,64,66	0
6	DK9	O	900	7/7	0.80	0.32	27,38,45,45	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.

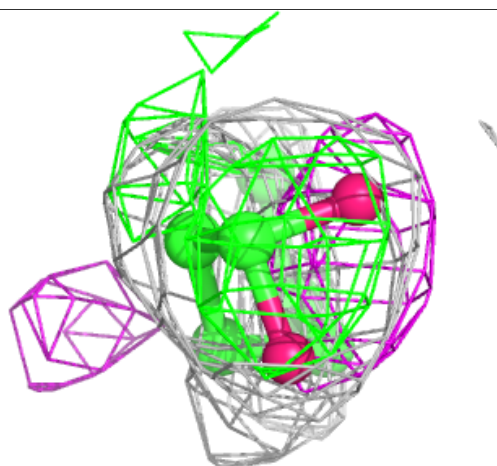
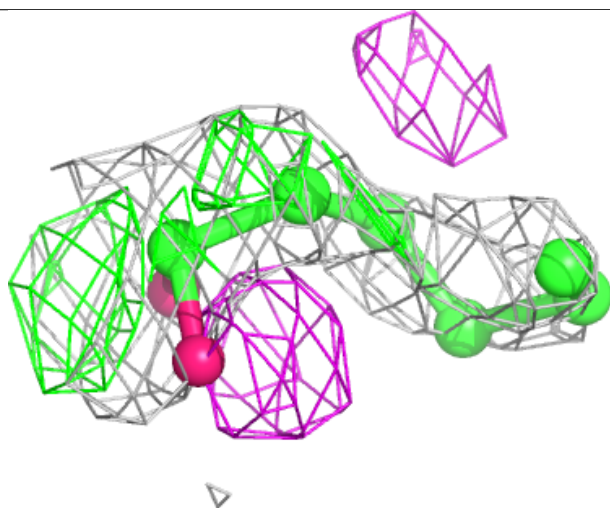
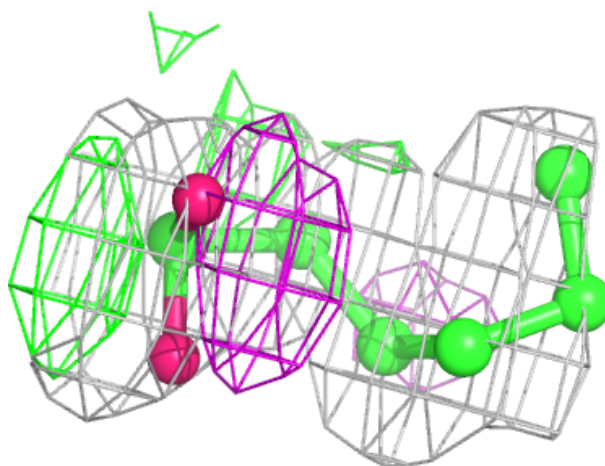
Electron density around DK6 S 900:

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



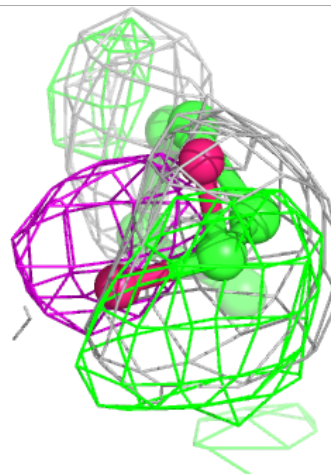
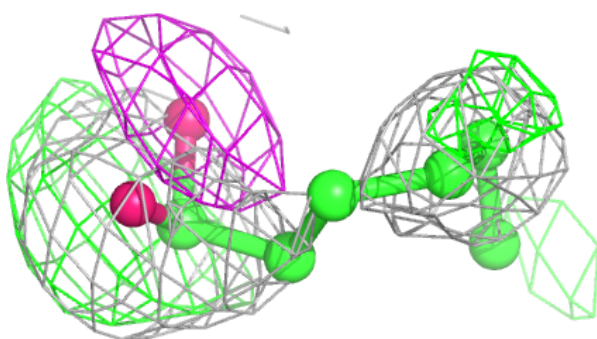
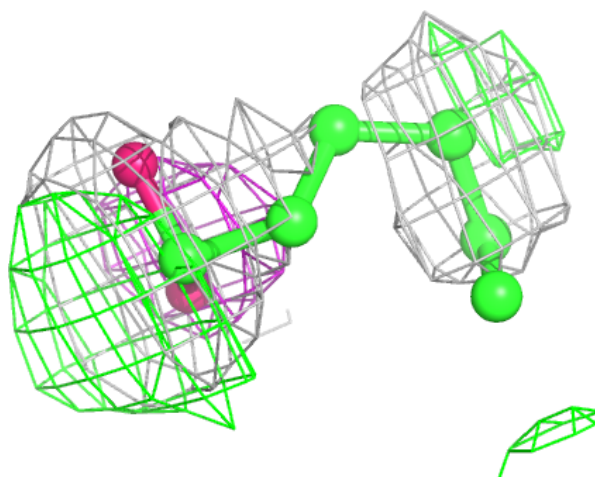
Electron density around DKF W 900:

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



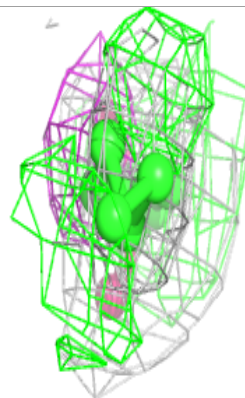
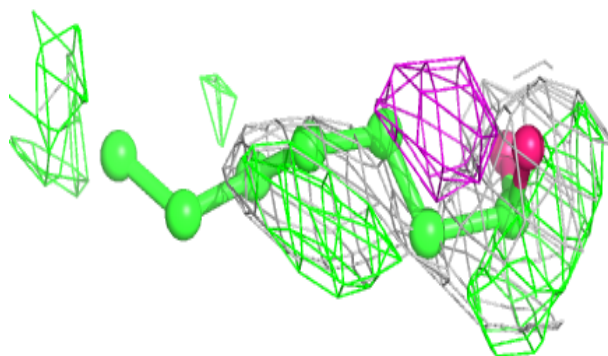
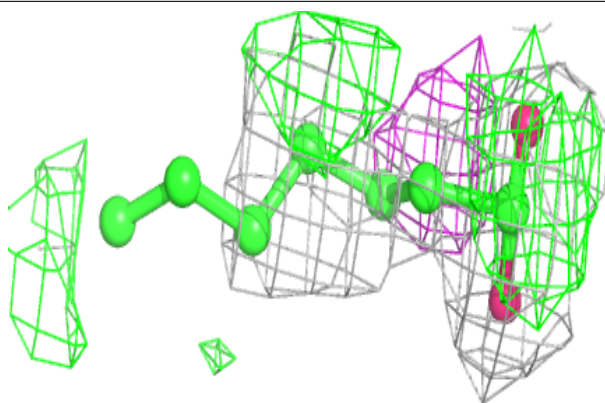
Electron density around DKF G 900:

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

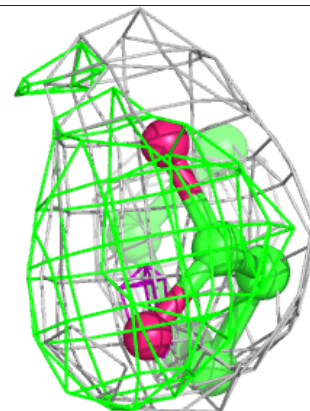
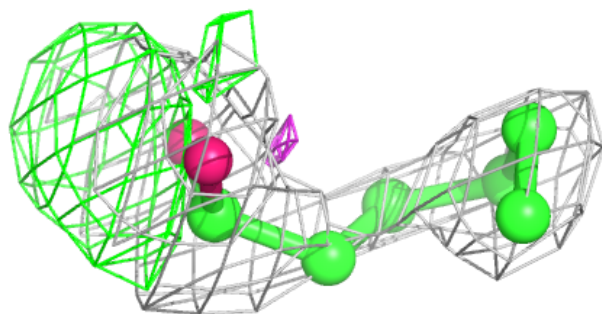
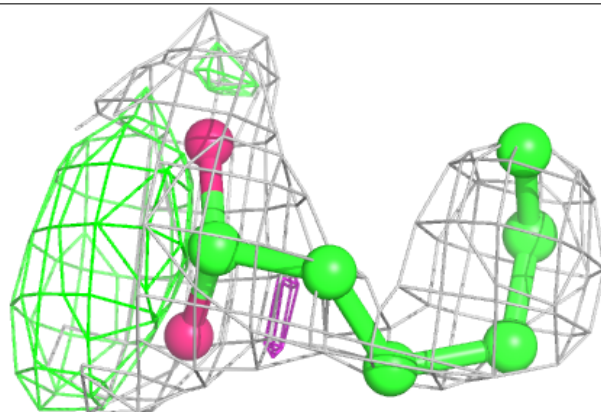


Electron density around DKL C 900:

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

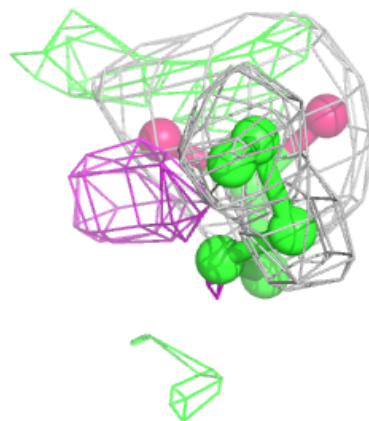
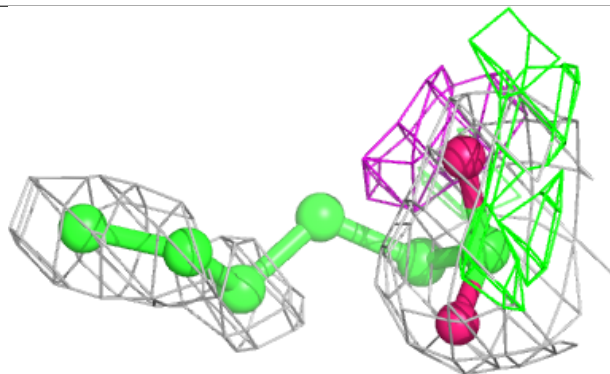
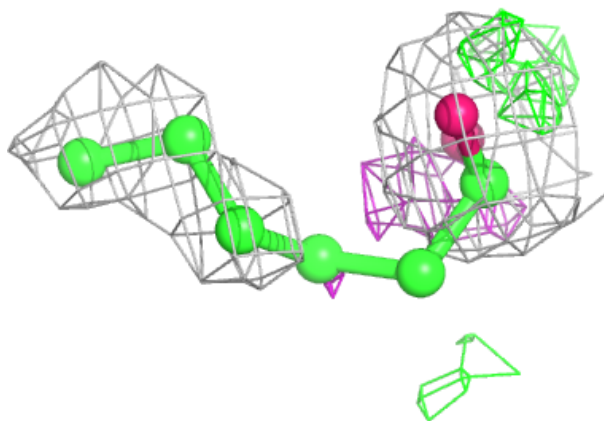
**Electron density around DKF Y 900:**

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



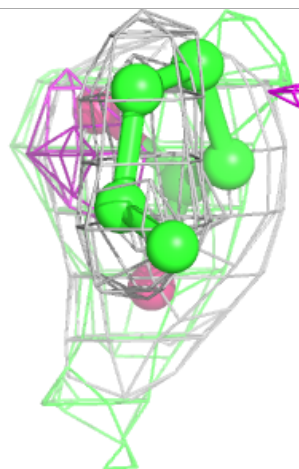
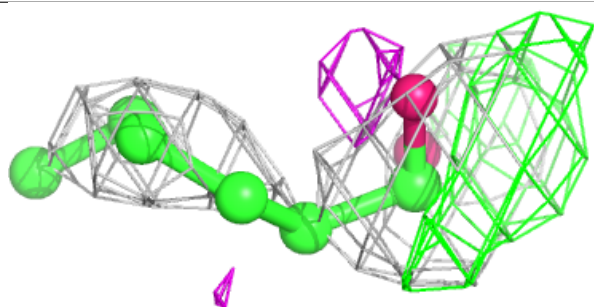
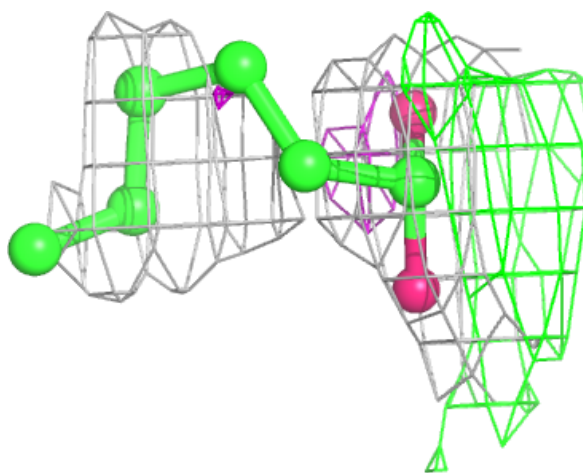
Electron density around DKF M 900:

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



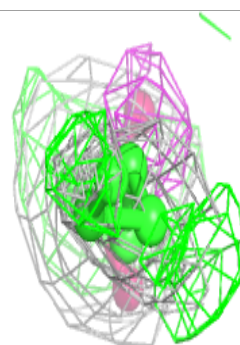
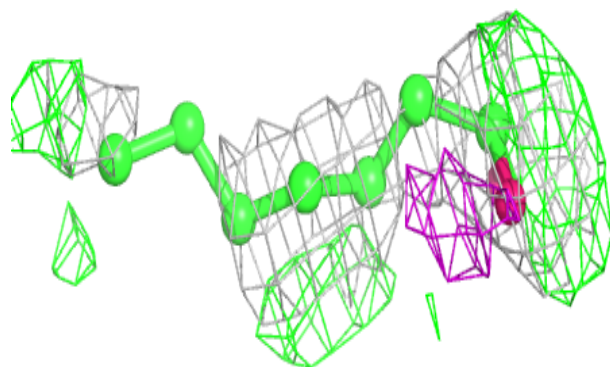
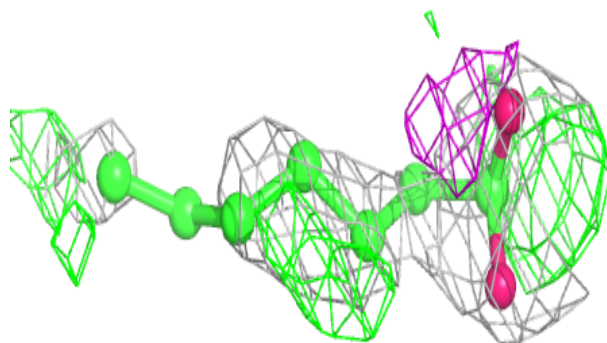
Electron density around DKF U 900:

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



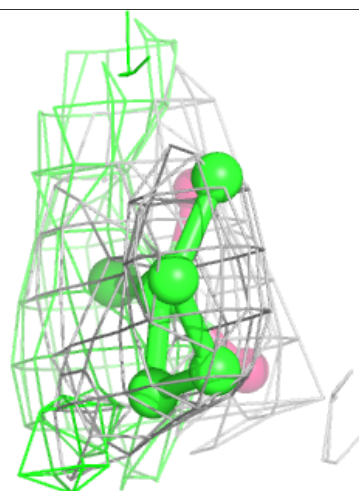
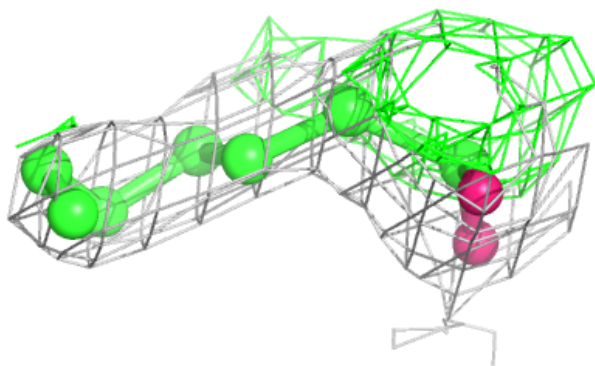
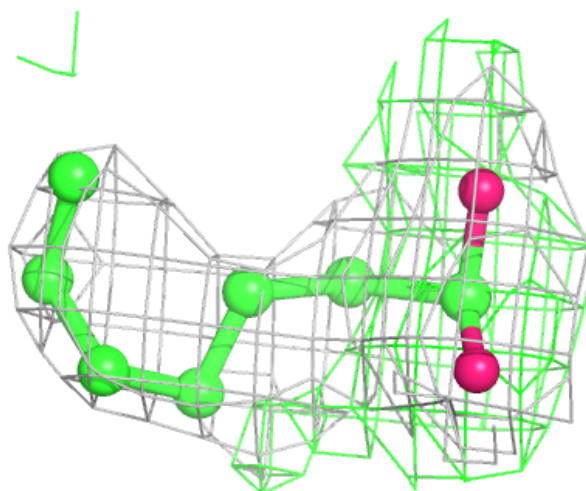
Electron density around DKL X 900:

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



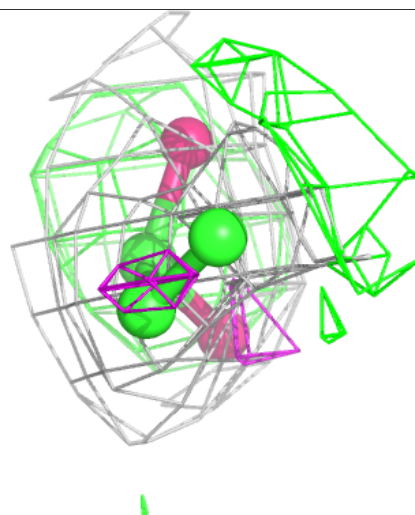
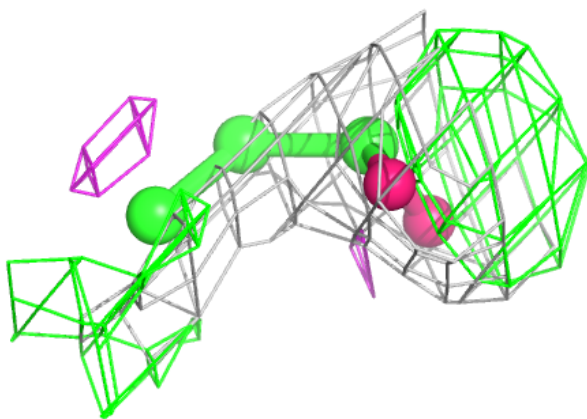
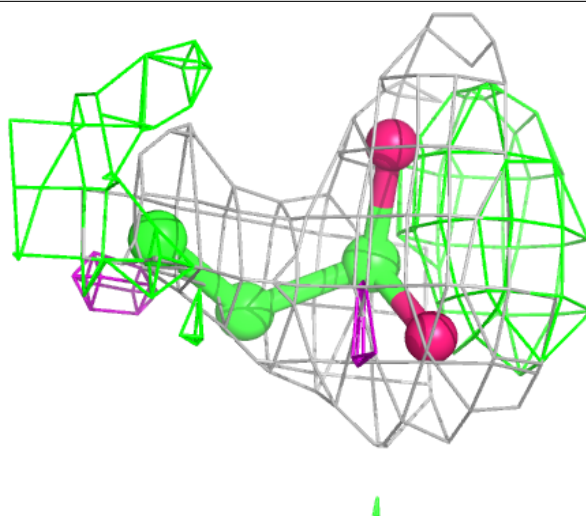
Electron density around DKL A 900:

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



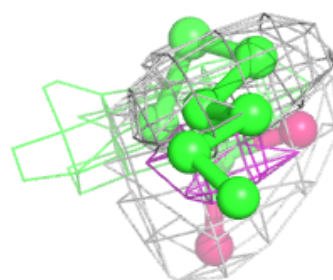
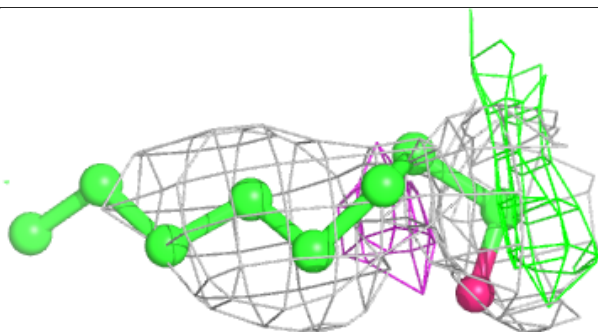
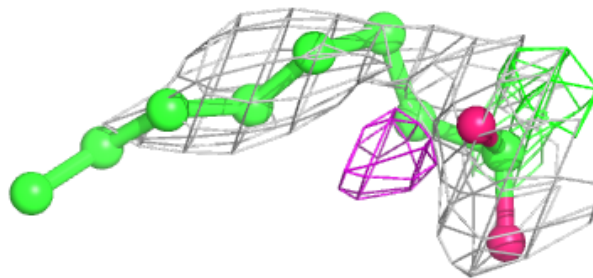
Electron density around DK6 Z 900:

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

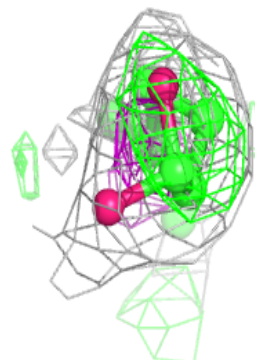
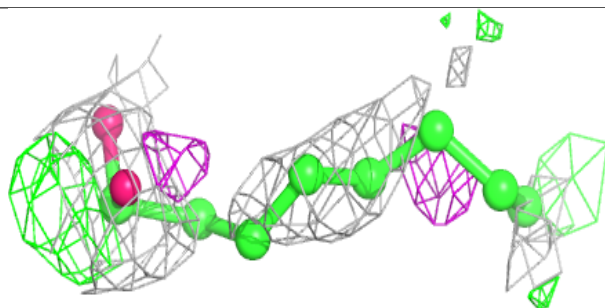
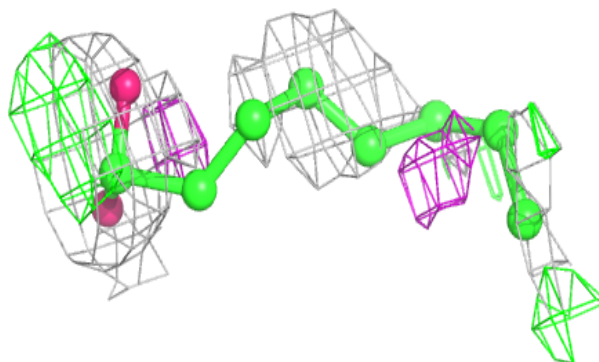


Electron density around DKO R 900:

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

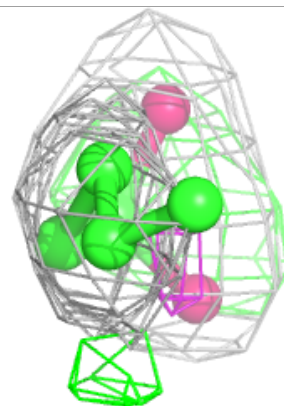
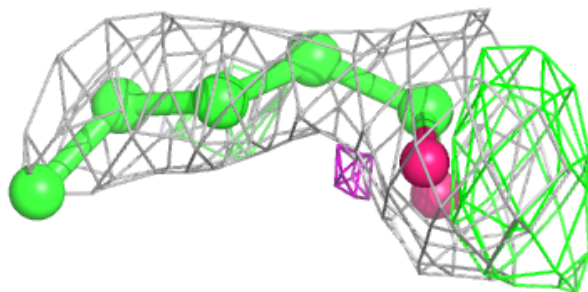
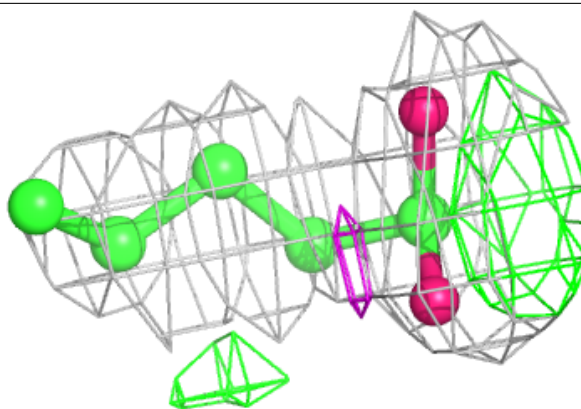
**Electron density around DKO B 900:**

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



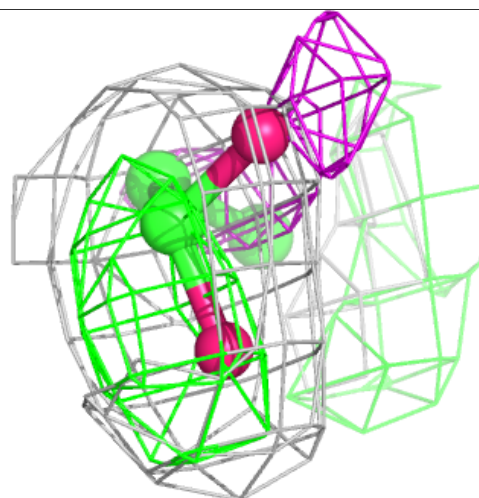
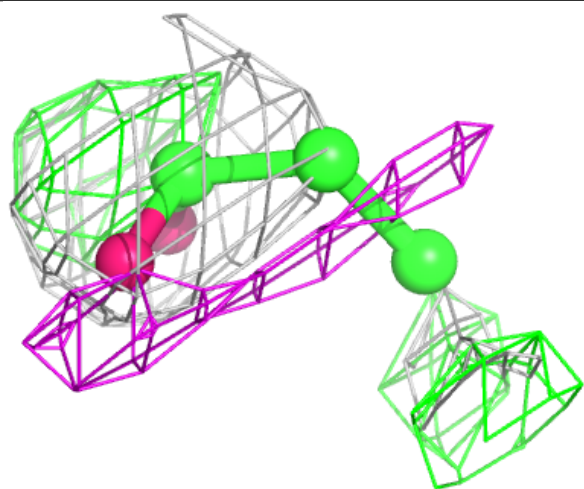
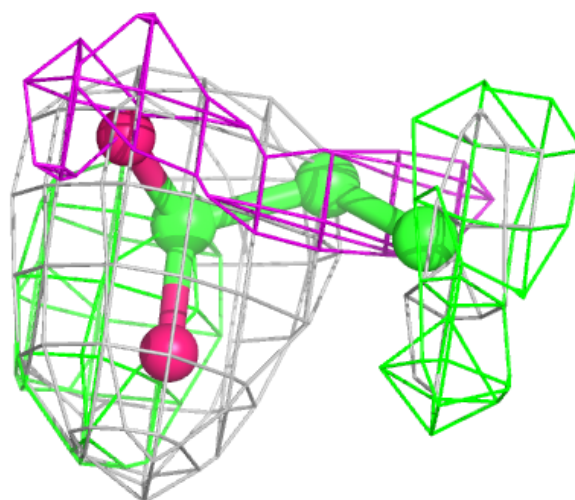
Electron density around DK9 O 900:

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



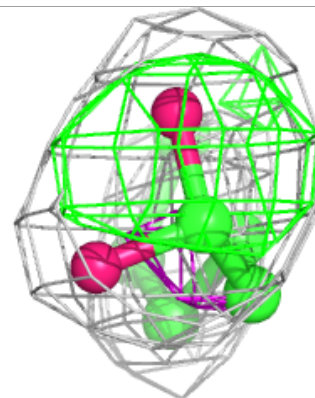
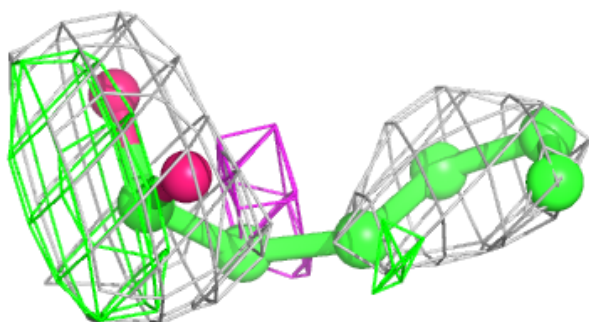
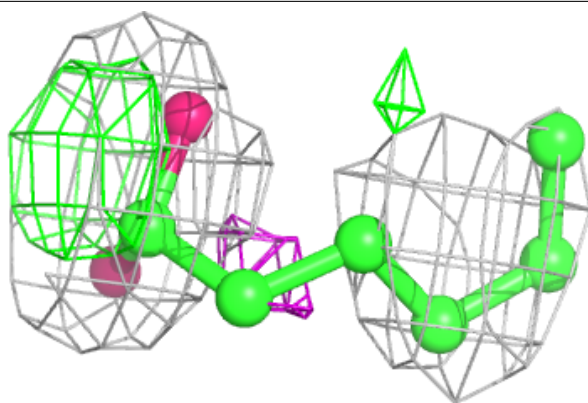
Electron density around DK6 D 900:

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

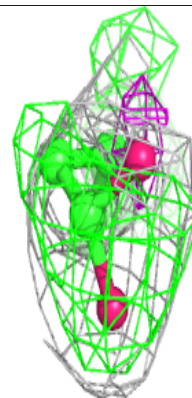
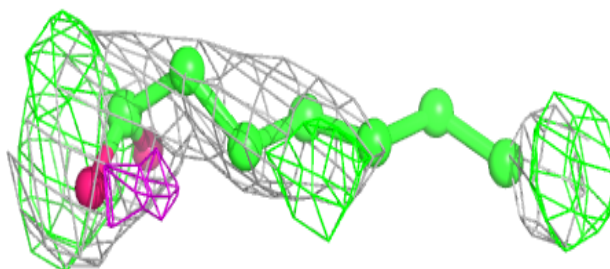
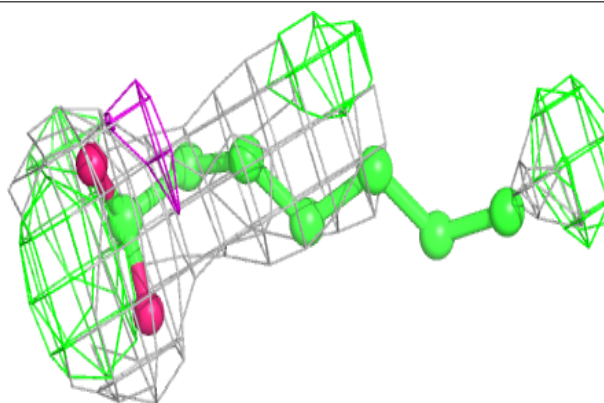


Electron density around DKF I 900:

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

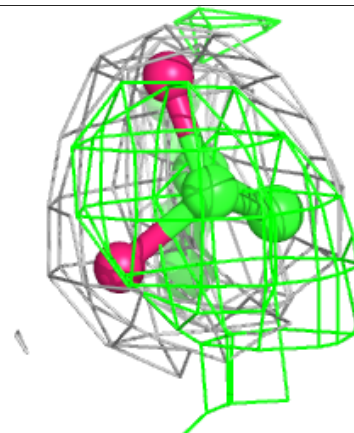
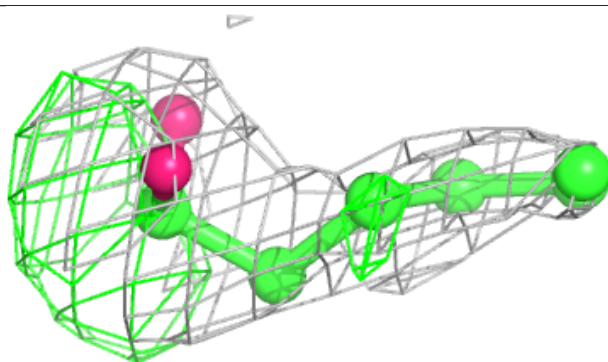
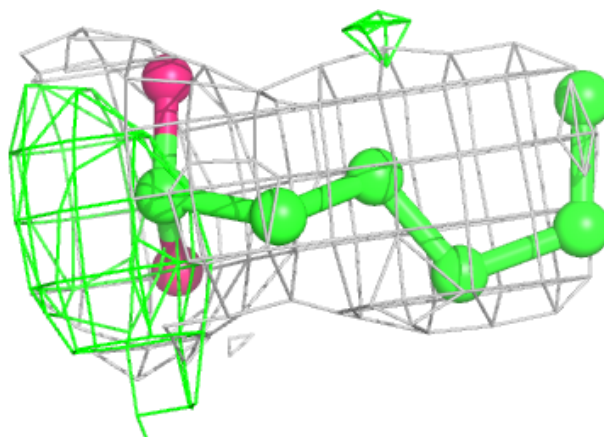
**Electron density around DKL T 900:**

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

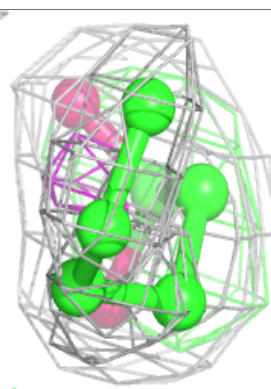
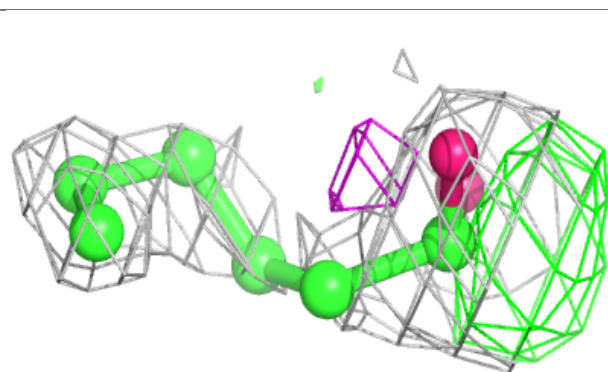
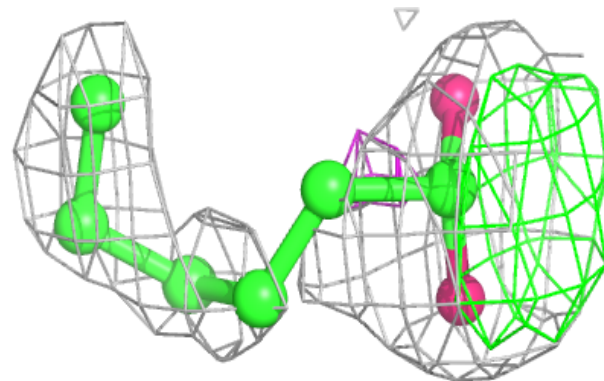


Electron density around DKF V 900:

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

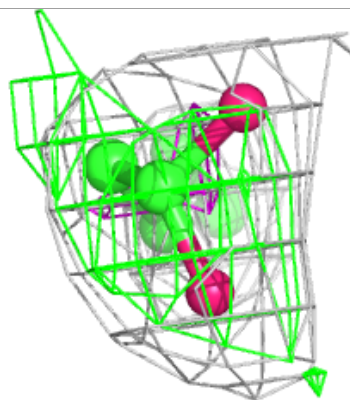
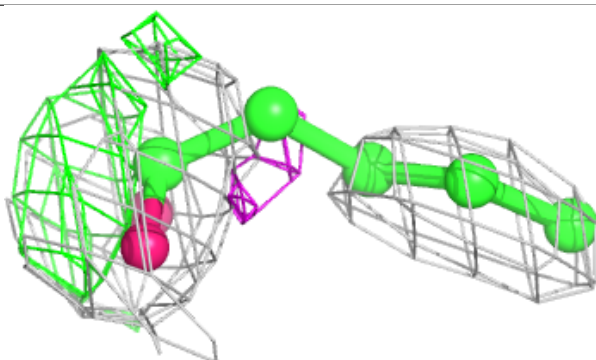
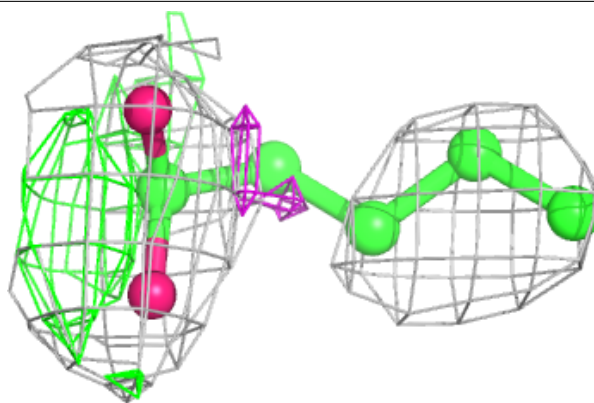
**Electron density around DKF K 900:**

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

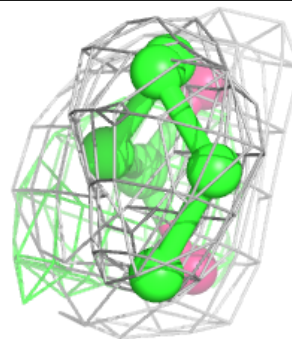
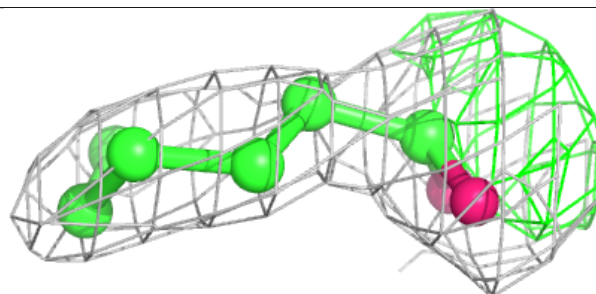
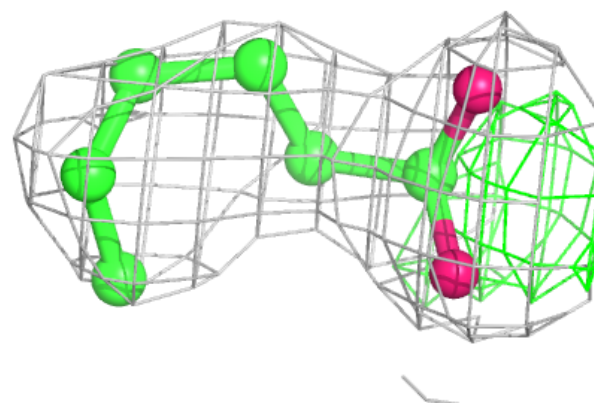


Electron density around DK9 P 900:

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

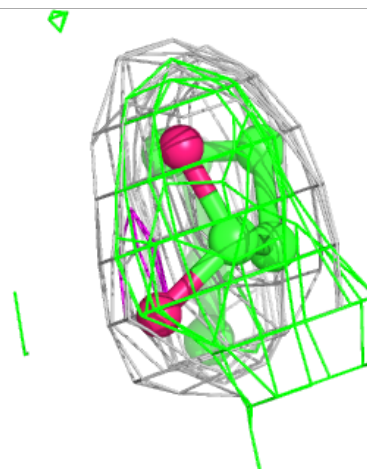
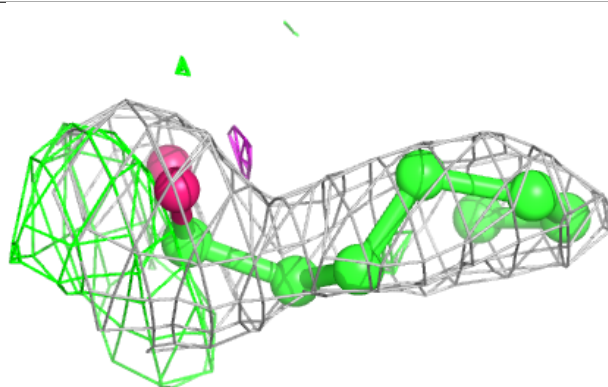
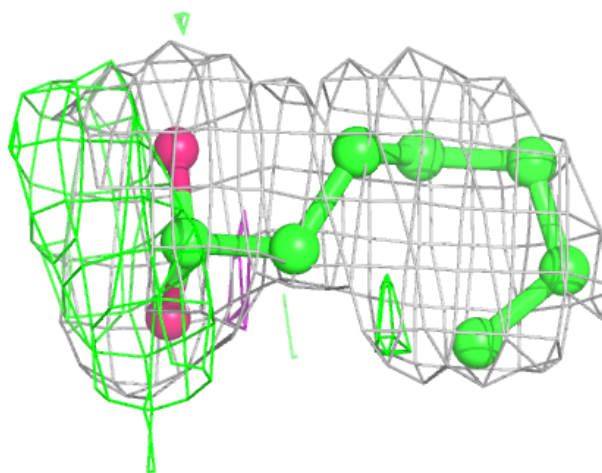
**Electron density around DKF J 900:**

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



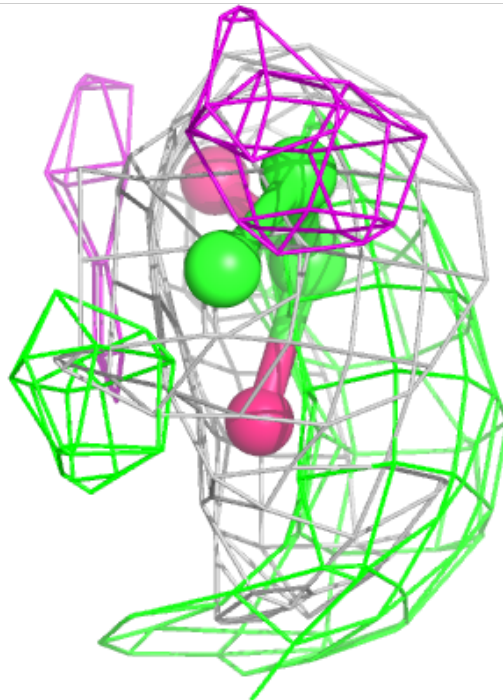
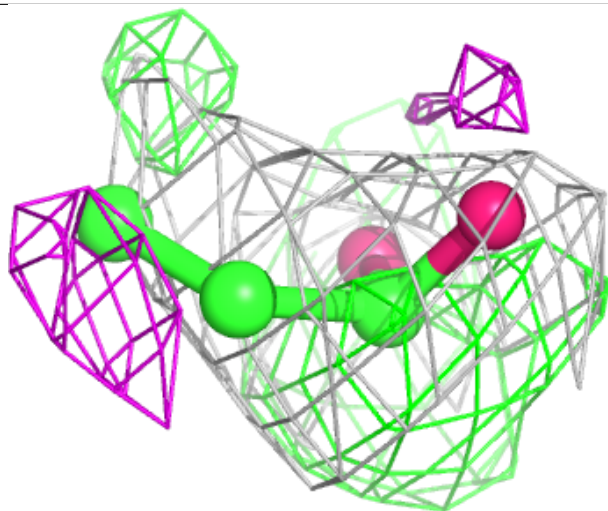
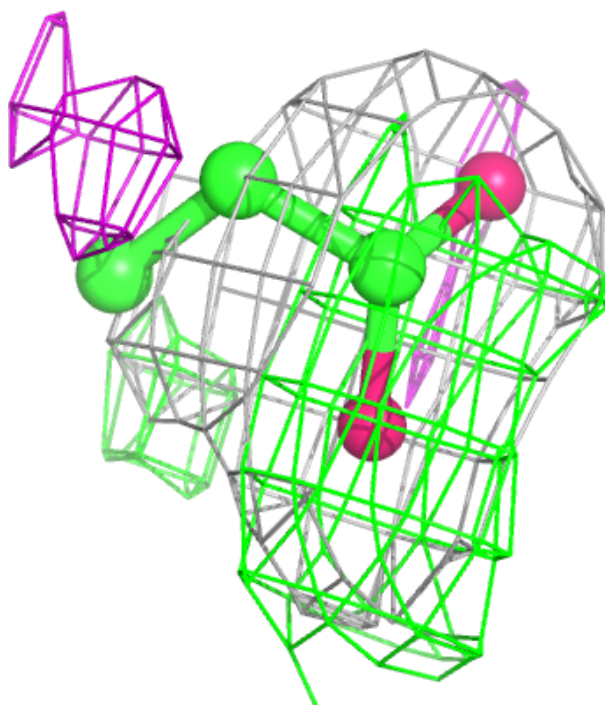
Electron density around DKL Q 900:

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



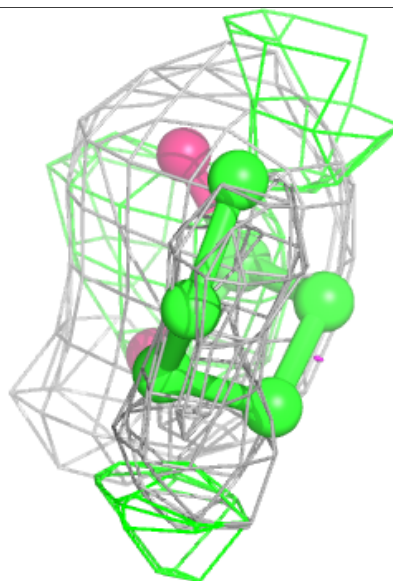
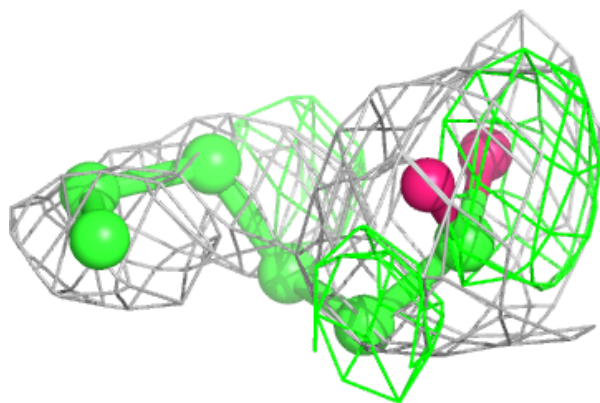
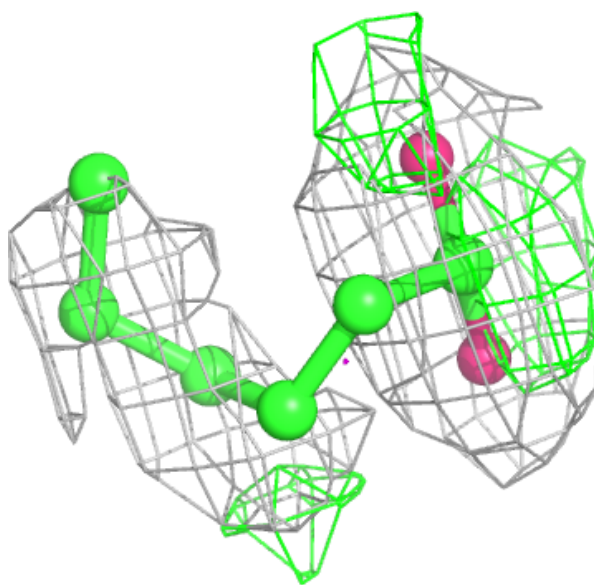
Electron density around DK6 H 900:

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



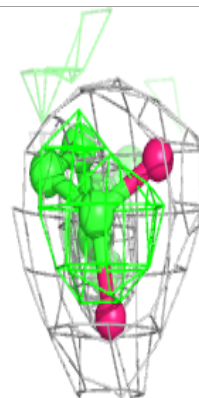
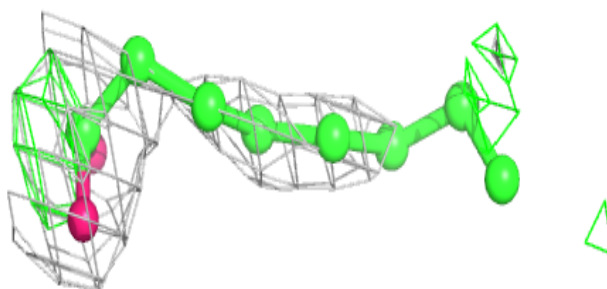
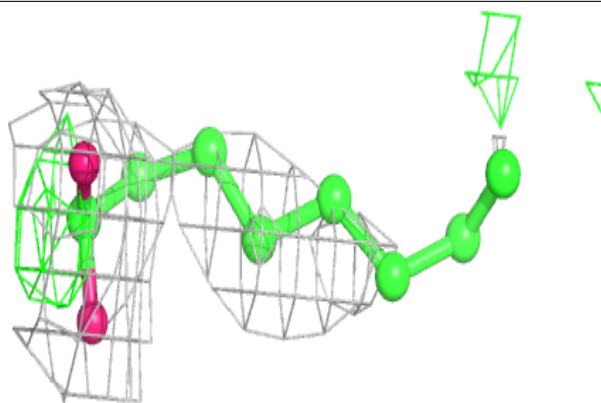
Electron density around DKF E 900:

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

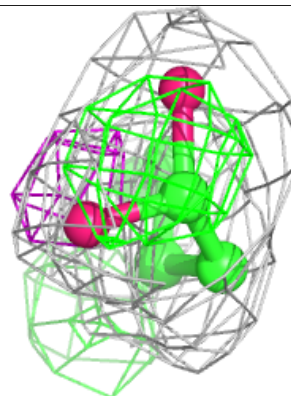
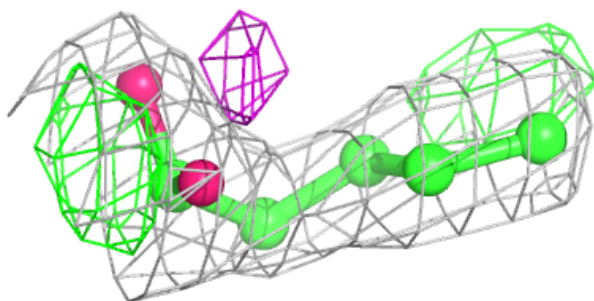
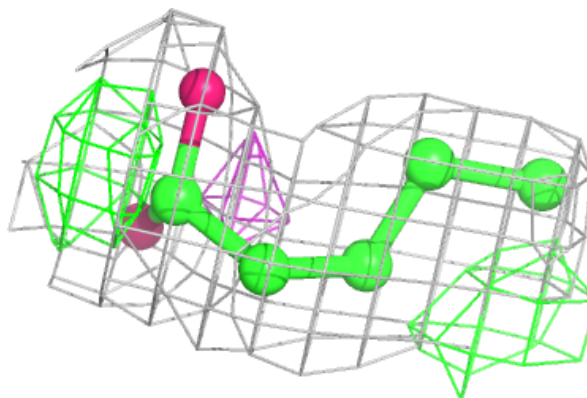


Electron density around DKO N 900:

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

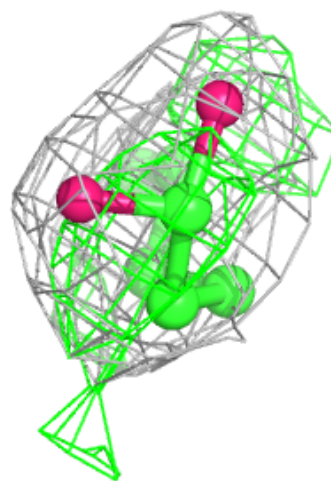
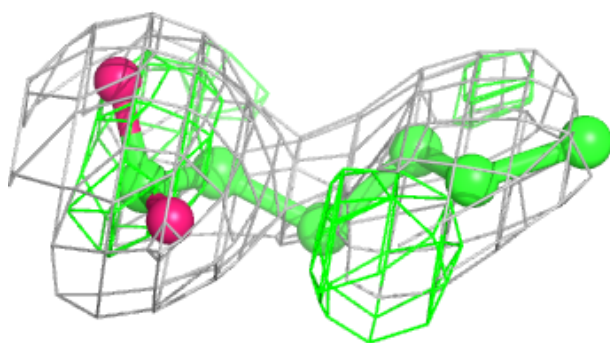
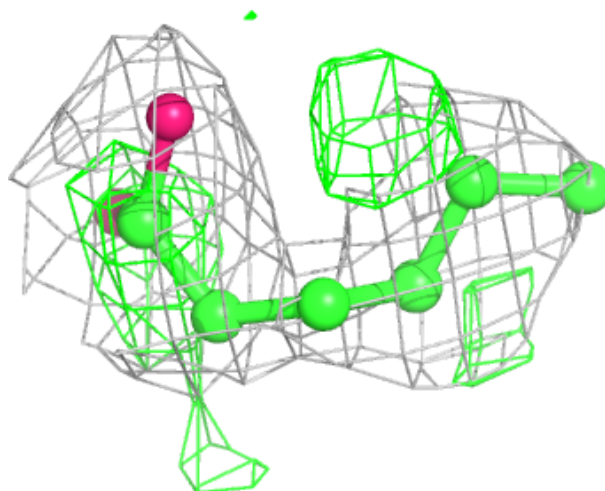
**Electron density around DK9 F 900:**

$2mF_o-DF_c$ (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.