



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 06:19 AM UTC

PDB ID : 7ALQ / pdb_00007alq
Title : human GCH-GFRP inhibitory complex 7-deaza-GTP bound
Authors : Ebenhoch, R.; Nar, H.
Deposited on : 2020-10-07
Resolution : 2.21 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

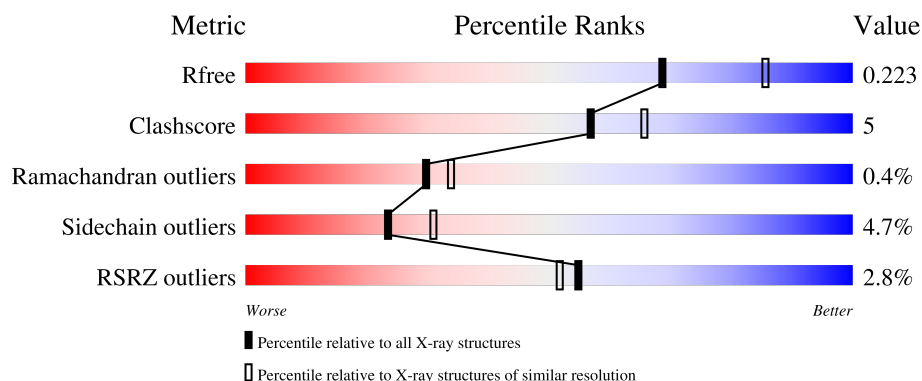
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.21 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}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	209	0% 80% 11% 8%
1	B	209	2% 79% 11% 8%
1	C	209	2% 80% 10% 8%
1	D	209	2% 78% 11% 8%
1	E	209	3% 73% 16% 8%

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Mol	Chain	Length	Quality of chain
1	F	209	
1	G	209	
1	H	209	
1	I	209	
1	J	209	
1	K	209	
1	L	209	
1	M	209	
1	N	209	
1	O	209	
1	P	209	
1	Q	209	
1	R	209	
1	S	209	
1	T	209	
2	a	87	
2	b	87	
2	c	87	
2	d	87	
2	e	87	
2	f	87	
2	g	87	
2	h	87	
2	i	87	
2	j	87	

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Mol	Chain	Length	Quality of chain
2	k	87	80% 14% ..
2	l	87	2% 82% 14% ..
2	m	87	5% 80% 15% ..
2	n	87	% 80% 14% ..
2	o	87	2% 78% 17% ..
2	p	87	6% 79% 16% ..
2	q	87	3% 79% 15% ..
2	r	87	% 77% 18% ..
2	s	87	% 83% 11% ..
2	t	87	5% 75% 18% ..

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 47586 atoms, of which 600 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 GTP cyclohydrolase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	192	Total	C	N	O	S	0	0	0
			1515	956	265	283	11			
1	B	192	Total	C	N	O	S	0	0	0
			1515	956	265	283	11			
1	C	192	Total	C	N	O	S	0	0	0
			1515	956	265	283	11			
1	D	192	Total	C	N	O	S	0	0	0
			1515	956	265	283	11			
1	E	192	Total	C	N	O	S	0	0	0
			1515	956	265	283	11			
1	F	192	Total	C	N	O	S	0	0	0
			1515	956	265	283	11			
1	G	192	Total	C	N	O	S	0	0	0
			1515	956	265	283	11			
1	H	192	Total	C	N	O	S	0	0	0
			1515	956	265	283	11			
1	I	192	Total	C	N	O	S	0	0	0
			1515	956	265	283	11			
1	J	192	Total	C	N	O	S	0	0	0
			1515	956	265	283	11			
1	K	192	Total	C	N	O	S	0	0	0
			1515	956	265	283	11			
1	L	192	Total	C	N	O	S	0	0	0
			1515	956	265	283	11			
1	M	192	Total	C	N	O	S	0	0	0
			1515	956	265	283	11			
1	N	192	Total	C	N	O	S	0	0	0
			1515	956	265	283	11			
1	O	192	Total	C	N	O	S	0	0	0
			1515	956	265	283	11			
1	P	192	Total	C	N	O	S	0	0	0
			1515	956	265	283	11			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	192	Total	C	N	O	S	0	0	0
			1515	956	265	283	11			
1	R	192	Total	C	N	O	S	0	0	0
			1515	956	265	283	11			
1	S	192	Total	C	N	O	S	0	0	0
			1515	956	265	283	11			
1	T	192	Total	C	N	O	S	0	0	0
			1515	956	265	283	11			

- Molecule 2 is a protein called GTP cyclohydrolase 1 feedback regulatory protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	a	84	Total	C	N	O	S	0	0	0
			678	429	119	124	6			
2	b	84	Total	C	N	O	S	0	0	0
			678	429	119	124	6			
2	c	84	Total	C	N	O	S	0	0	0
			678	429	119	124	6			
2	d	84	Total	C	N	O	S	0	0	0
			678	429	119	124	6			
2	e	84	Total	C	N	O	S	0	0	0
			678	429	119	124	6			
2	f	83	Total	C	N	O	S	0	0	0
			669	424	118	121	6			
2	g	84	Total	C	N	O	S	0	0	0
			678	429	119	124	6			
2	h	84	Total	C	N	O	S	0	0	0
			678	429	119	124	6			
2	i	84	Total	C	N	O	S	0	0	0
			678	429	119	124	6			
2	j	84	Total	C	N	O	S	0	0	0
			678	429	119	124	6			
2	k	84	Total	C	N	O	S	0	0	0
			678	429	119	124	6			
2	l	84	Total	C	N	O	S	0	0	0
			678	429	119	124	6			
2	m	84	Total	C	N	O	S	0	0	0
			678	429	119	124	6			
2	n	84	Total	C	N	O	S	0	0	0
			678	429	119	124	6			
2	o	84	Total	C	N	O	S	0	0	0
			678	429	119	124	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	p	84	Total 678	C 429	N 119	O 124	S 6	0	0	0
2	q	84	Total 678	C 429	N 119	O 124	S 6	0	0	0
2	r	84	Total 678	C 429	N 119	O 124	S 6	0	0	0
2	s	84	Total 678	C 429	N 119	O 124	S 6	0	0	0
2	t	84	Total 678	C 429	N 119	O 124	S 6	0	0	0

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	-2	GLY	-	expression tag	UNP P30047
a	-1	SER	-	expression tag	UNP P30047
a	0	HIS	-	expression tag	UNP P30047
b	-2	GLY	-	expression tag	UNP P30047
b	-1	SER	-	expression tag	UNP P30047
b	0	HIS	-	expression tag	UNP P30047
c	-2	GLY	-	expression tag	UNP P30047
c	-1	SER	-	expression tag	UNP P30047
c	0	HIS	-	expression tag	UNP P30047
d	-2	GLY	-	expression tag	UNP P30047
d	-1	SER	-	expression tag	UNP P30047
d	0	HIS	-	expression tag	UNP P30047
e	-2	GLY	-	expression tag	UNP P30047
e	-1	SER	-	expression tag	UNP P30047
e	0	HIS	-	expression tag	UNP P30047
f	-2	GLY	-	expression tag	UNP P30047
f	-1	SER	-	expression tag	UNP P30047
f	0	HIS	-	expression tag	UNP P30047
g	-2	GLY	-	expression tag	UNP P30047
g	-1	SER	-	expression tag	UNP P30047
g	0	HIS	-	expression tag	UNP P30047
h	-2	GLY	-	expression tag	UNP P30047
h	-1	SER	-	expression tag	UNP P30047
h	0	HIS	-	expression tag	UNP P30047
i	-2	GLY	-	expression tag	UNP P30047
i	-1	SER	-	expression tag	UNP P30047
i	0	HIS	-	expression tag	UNP P30047
j	-2	GLY	-	expression tag	UNP P30047
j	-1	SER	-	expression tag	UNP P30047

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Chain	Residue	Modelled	Actual	Comment	Reference
j	0	HIS	-	expression tag	UNP P30047
k	-2	GLY	-	expression tag	UNP P30047
k	-1	SER	-	expression tag	UNP P30047
k	0	HIS	-	expression tag	UNP P30047
l	-2	GLY	-	expression tag	UNP P30047
l	-1	SER	-	expression tag	UNP P30047
l	0	HIS	-	expression tag	UNP P30047
m	-2	GLY	-	expression tag	UNP P30047
m	-1	SER	-	expression tag	UNP P30047
m	0	HIS	-	expression tag	UNP P30047
n	-2	GLY	-	expression tag	UNP P30047
n	-1	SER	-	expression tag	UNP P30047
n	0	HIS	-	expression tag	UNP P30047
o	-2	GLY	-	expression tag	UNP P30047
o	-1	SER	-	expression tag	UNP P30047
o	0	HIS	-	expression tag	UNP P30047
p	-2	GLY	-	expression tag	UNP P30047
p	-1	SER	-	expression tag	UNP P30047
p	0	HIS	-	expression tag	UNP P30047
q	-2	GLY	-	expression tag	UNP P30047
q	-1	SER	-	expression tag	UNP P30047
q	0	HIS	-	expression tag	UNP P30047
r	-2	GLY	-	expression tag	UNP P30047
r	-1	SER	-	expression tag	UNP P30047
r	0	HIS	-	expression tag	UNP P30047
s	-2	GLY	-	expression tag	UNP P30047
s	-1	SER	-	expression tag	UNP P30047
s	0	HIS	-	expression tag	UNP P30047
t	-2	GLY	-	expression tag	UNP P30047
t	-1	SER	-	expression tag	UNP P30047
t	0	HIS	-	expression tag	UNP P30047

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

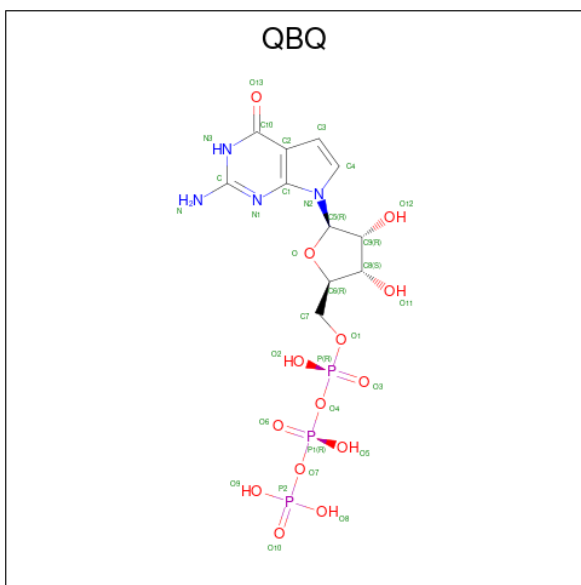
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Zn 1 1	0	0
3	B	1	Total Zn 1 1	0	0
3	C	1	Total Zn 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	1	Total	Zn	0	0
			1	1		
3	E	1	Total	Zn	0	0
			1	1		
3	F	1	Total	Zn	0	0
			1	1		
3	G	1	Total	Zn	0	0
			1	1		
3	H	1	Total	Zn	0	0
			1	1		
3	I	1	Total	Zn	0	0
			1	1		
3	J	1	Total	Zn	0	0
			1	1		
3	K	1	Total	Zn	0	0
			1	1		
3	L	1	Total	Zn	0	0
			1	1		
3	M	1	Total	Zn	0	0
			1	1		
3	N	1	Total	Zn	0	0
			1	1		
3	O	1	Total	Zn	0	0
			1	1		
3	P	1	Total	Zn	0	0
			1	1		
3	Q	1	Total	Zn	0	0
			1	1		
3	R	1	Total	Zn	0	0
			1	1		
3	S	1	Total	Zn	0	0
			1	1		
3	T	1	Total	Zn	0	0
			1	1		

- Molecule 4 is 7-deaza-GTP (CCD ID: QBQ) (formula: $C_{11}H_{17}N_4O_{14}P_3$) (labeled as "Ligand of Interest" by depositor).



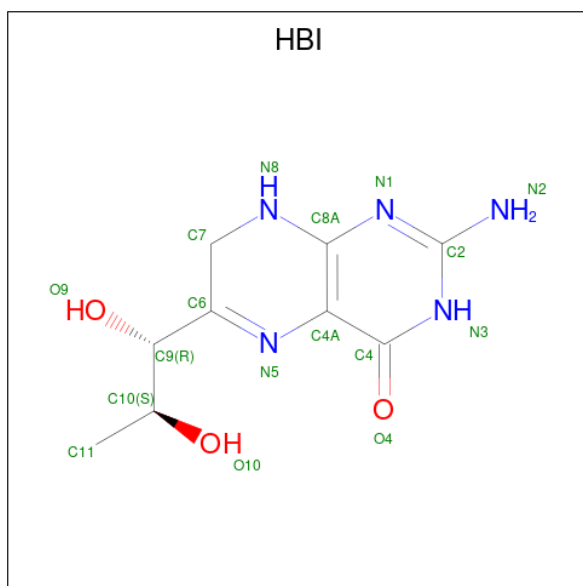
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total 49	C 11	H 17	N 4	O 14	P 3	17	0
4	B	1	Total 49	C 11	H 17	N 4	O 14	P 3	17	0
4	C	1	Total 49	C 11	H 17	N 4	O 14	P 3	17	0
4	D	1	Total 49	C 11	H 17	N 4	O 14	P 3	17	0
4	E	1	Total 49	C 11	H 17	N 4	O 14	P 3	17	0
4	F	1	Total 49	C 11	H 17	N 4	O 14	P 3	17	0
4	G	1	Total 49	C 11	H 17	N 4	O 14	P 3	17	0
4	H	1	Total 49	C 11	H 17	N 4	O 14	P 3	17	0
4	I	1	Total 49	C 11	H 17	N 4	O 14	P 3	17	0
4	J	1	Total 49	C 11	H 17	N 4	O 14	P 3	17	0
4	K	1	Total 49	C 11	H 17	N 4	O 14	P 3	17	0
4	L	1	Total 49	C 11	H 17	N 4	O 14	P 3	17	0
4	M	1	Total 49	C 11	H 17	N 4	O 14	P 3	17	0
4	N	1	Total 49	C 11	H 17	N 4	O 14	P 3	17	0

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	O	1	Total	C	H	N	O	P	17	0
			49	11	17	4	14	3		
4	P	1	Total	C	H	N	O	P	17	0
			49	11	17	4	14	3		
4	Q	1	Total	C	H	N	O	P	17	0
			49	11	17	4	14	3		
4	R	1	Total	C	H	N	O	P	17	0
			49	11	17	4	14	3		
4	S	1	Total	C	H	N	O	P	17	0
			49	11	17	4	14	3		
4	T	1	Total	C	H	N	O	P	17	0
			49	11	17	4	14	3		

- Molecule 5 is 7,8-DIHYDROBIOPTERIN (CCD ID: HBI) (formula: $C_9H_{13}N_5O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total	C	H	N	O		13	0
			30	9	13	5	3			
5	A	1	Total	C	H	N	O		13	0
			30	9	13	5	3			
5	B	1	Total	C	H	N	O		13	0
			30	9	13	5	3			
5	D	1	Total	C	H	N	O		13	0
			30	9	13	5	3			
5	E	1	Total	C	H	N	O		13	0
			30	9	13	5	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	F	1	Total	C	H	N	O	13	0
			30	9	13	5	3		
5	G	1	Total	C	H	N	O	13	0
			30	9	13	5	3		
5	H	1	Total	C	H	N	O	13	0
			30	9	13	5	3		
5	I	1	Total	C	H	N	O	13	0
			30	9	13	5	3		
5	I	1	Total	C	H	N	O	13	0
			30	9	13	5	3		
5	K	1	Total	C	H	N	O	13	0
			30	9	13	5	3		
5	L	1	Total	C	H	N	O	13	0
			30	9	13	5	3		
5	L	1	Total	C	H	N	O	13	0
			30	9	13	5	3		
5	M	1	Total	C	H	N	O	13	0
			30	9	13	5	3		
5	O	1	Total	C	H	N	O	13	0
			30	9	13	5	3		
5	P	1	Total	C	H	N	O	13	0
			30	9	13	5	3		
5	Q	1	Total	C	H	N	O	13	0
			30	9	13	5	3		
5	R	1	Total	C	H	N	O	13	0
			30	9	13	5	3		
5	S	1	Total	C	H	N	O	13	0
			30	9	13	5	3		
5	T	1	Total	C	H	N	O	13	0
			30	9	13	5	3		

- Molecule 6 is POTASSIUM ION (CCD ID: K) (formula: K) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	a	1	Total	K	0	0
			1	1		
6	b	1	Total	K	0	0
			1	1		
6	c	1	Total	K	0	0
			1	1		
6	d	1	Total	K	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	e	1	Total K 1 1	0	0
6	f	1	Total K 1 1	0	0
6	g	1	Total K 1 1	0	0
6	h	1	Total K 1 1	0	0
6	i	1	Total K 1 1	0	0
6	j	1	Total K 1 1	0	0
6	k	1	Total K 1 1	0	0
6	l	1	Total K 1 1	0	0
6	m	1	Total K 1 1	0	0
6	n	1	Total K 1 1	0	0
6	o	1	Total K 1 1	0	0
6	p	1	Total K 1 1	0	0
6	q	1	Total K 1 1	0	0
6	r	1	Total K 1 1	0	0
6	s	1	Total K 1 1	0	0
6	t	1	Total K 1 1	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	80	Total O 80 80	0	0
7	B	67	Total O 67 67	0	0
7	C	83	Total O 83 83	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	D	61	Total O 61 61	0	0
7	E	66	Total O 66 66	0	0
7	F	91	Total O 91 91	0	0
7	G	57	Total O 57 57	0	0
7	H	83	Total O 83 83	0	0
7	I	67	Total O 67 67	0	0
7	J	96	Total O 96 96	0	0
7	K	70	Total O 70 70	0	0
7	L	61	Total O 61 61	0	0
7	M	72	Total O 72 72	0	0
7	N	73	Total O 73 73	0	0
7	O	73	Total O 73 73	0	0
7	P	66	Total O 66 66	0	0
7	Q	82	Total O 82 82	0	0
7	R	72	Total O 72 72	0	0
7	S	68	Total O 68 68	0	0
7	T	76	Total O 76 76	0	0
7	a	39	Total O 39 39	0	0
7	b	24	Total O 24 24	0	0
7	c	15	Total O 15 15	0	0
7	d	27	Total O 27 27	0	0

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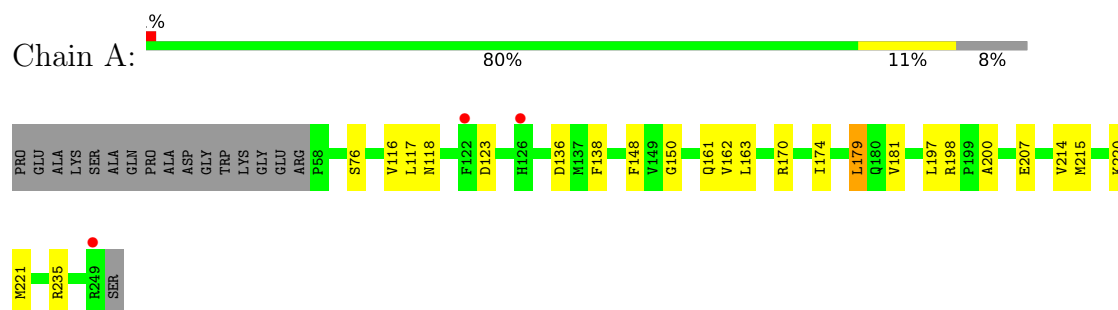
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	e	24	Total 24	O 24	0	0
7	f	33	Total 33	O 33	0	0
7	g	35	Total 35	O 35	0	0
7	h	24	Total 24	O 24	0	0
7	i	35	Total 35	O 35	0	0
7	j	34	Total 34	O 34	0	0
7	k	45	Total 45	O 45	0	0
7	l	31	Total 31	O 31	0	0
7	m	37	Total 37	O 37	0	0
7	n	42	Total 42	O 42	0	0
7	o	55	Total 55	O 55	0	0
7	p	24	Total 24	O 24	0	0
7	q	32	Total 32	O 32	0	0
7	r	42	Total 42	O 42	0	0
7	s	29	Total 29	O 29	0	0
7	t	24	Total 24	O 24	0	0

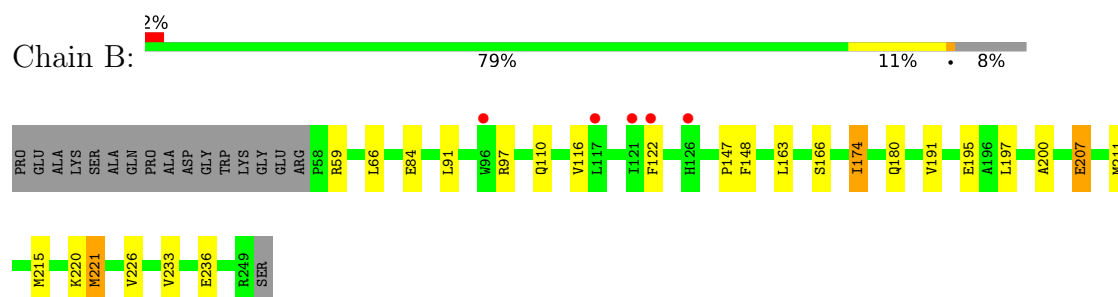
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

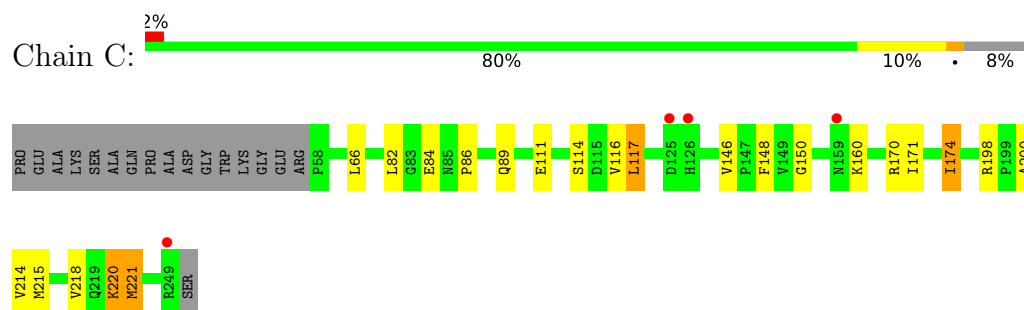
- Molecule 1: GTP cyclohydrolase 1



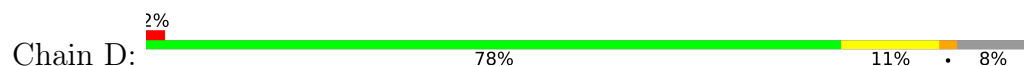
- Molecule 1: GTP cyclohydrolase 1

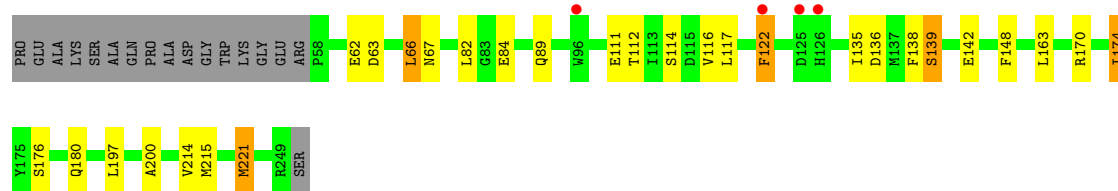


- Molecule 1: GTP cyclohydrolase 1

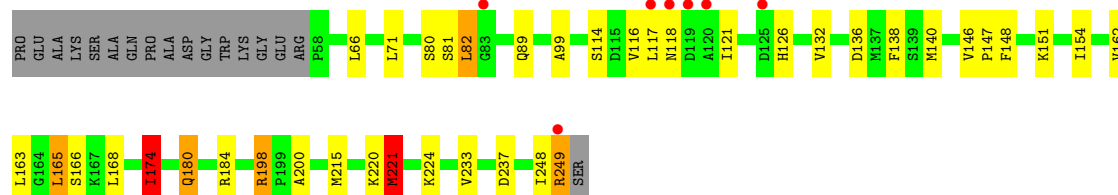
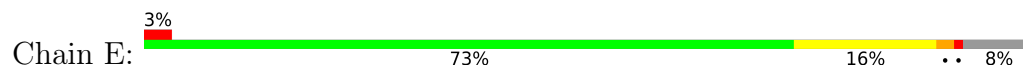


- Molecule 1: GTP cyclohydrolase 1

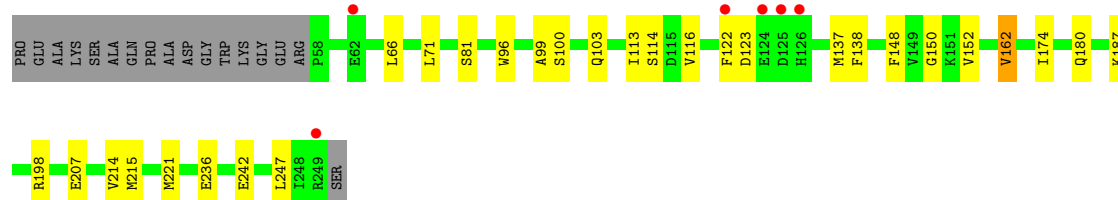
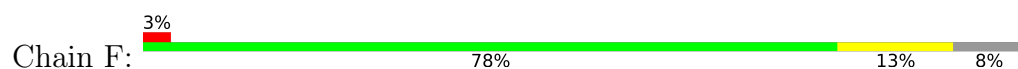




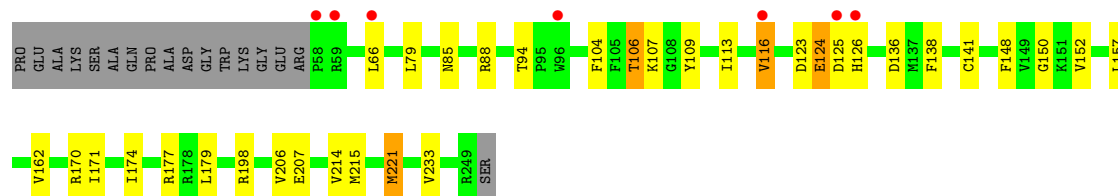
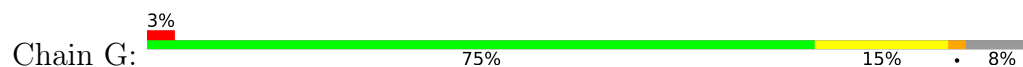
- Molecule 1: GTP cyclohydrolase 1



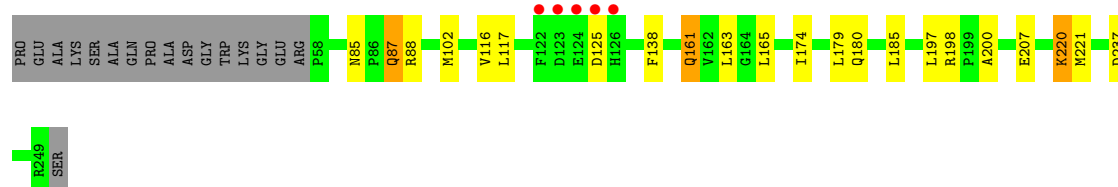
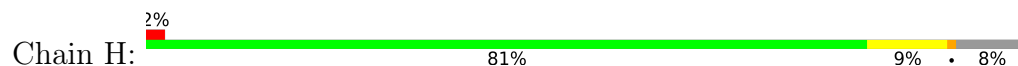
- Molecule 1: GTP cyclohydrolase 1



- Molecule 1: GTP cyclohydrolase 1

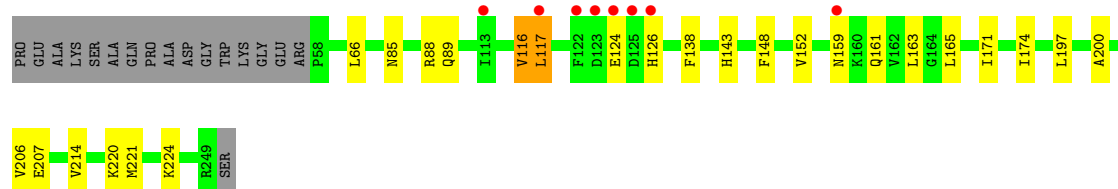


- Molecule 1: GTP cyclohydrolase 1



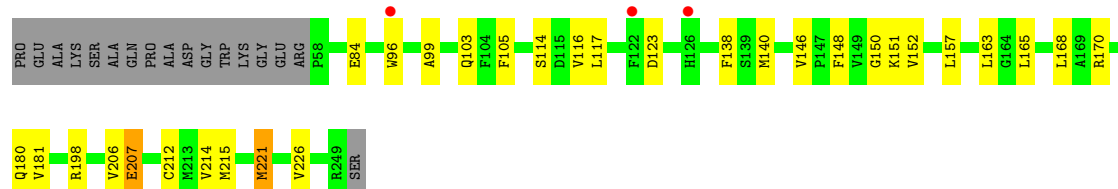
- Molecule 1: GTP cyclohydrolase 1

Chain I: 



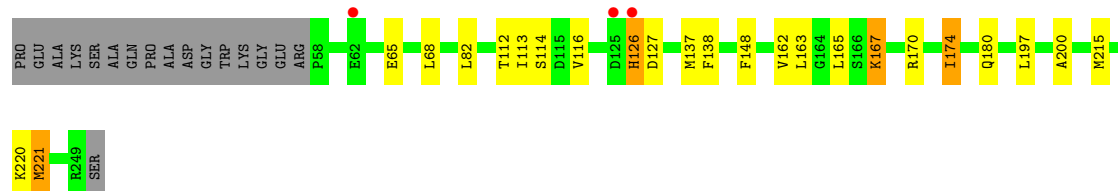
- Molecule 1: GTP cyclohydrolase 1

Chain J: 



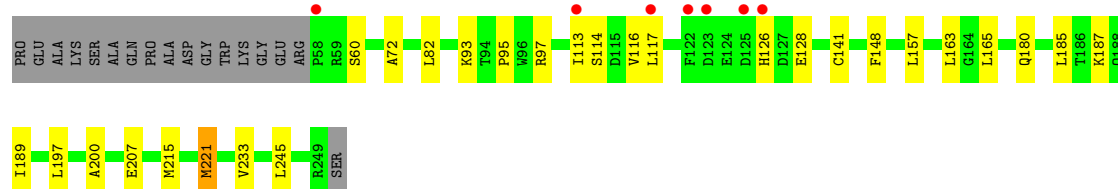
- Molecule 1: GTP cyclohydrolase 1

Chain K: 



- Molecule 1: GTP cyclohydrolase 1

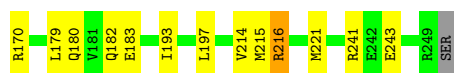
Chain L: 



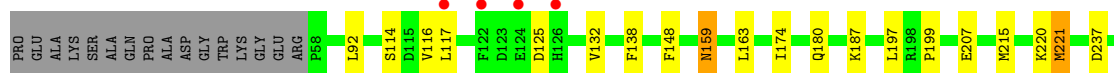
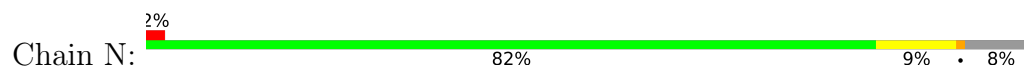
- Molecule 1: GTP cyclohydrolase 1

Chain M: 

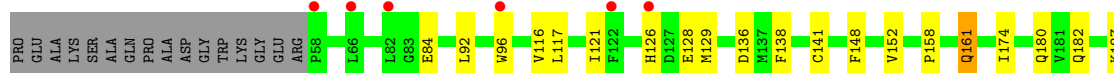
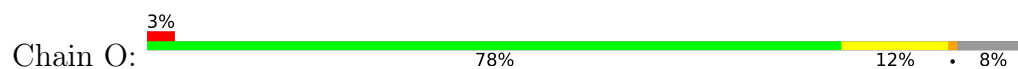




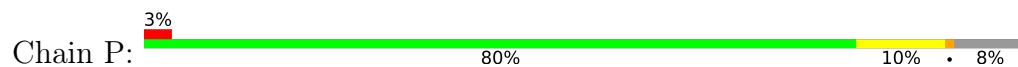
- Molecule 1: GTP cyclohydrolase 1



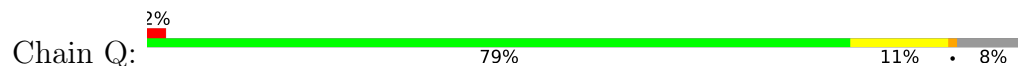
- Molecule 1: GTP cyclohydrolase 1



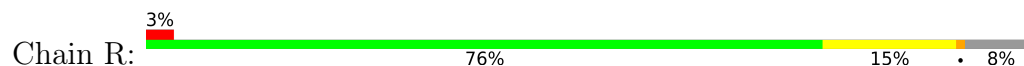
- Molecule 1: GTP cyclohydrolase 1

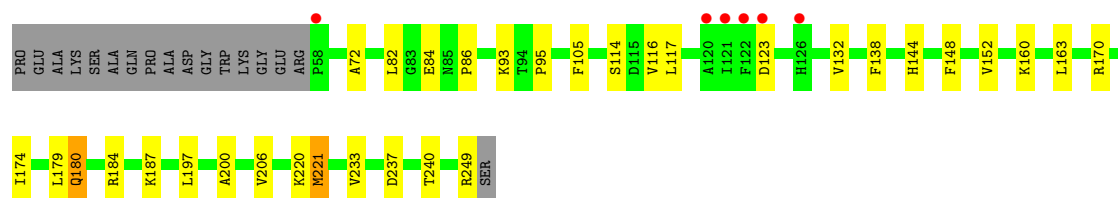


- Molecule 1: GTP cyclohydrolase 1

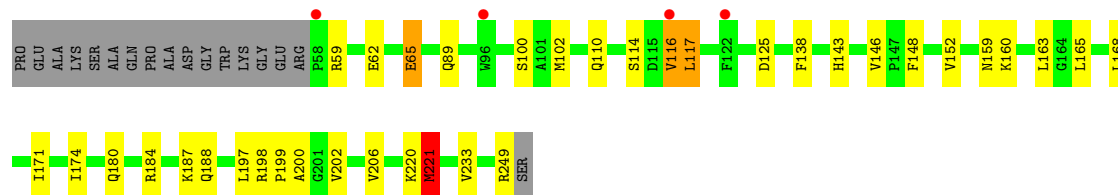
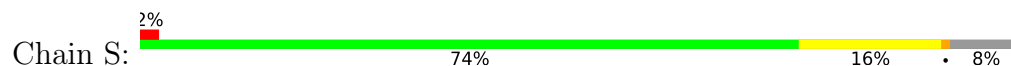


- Molecule 1: GTP cyclohydrolase 1

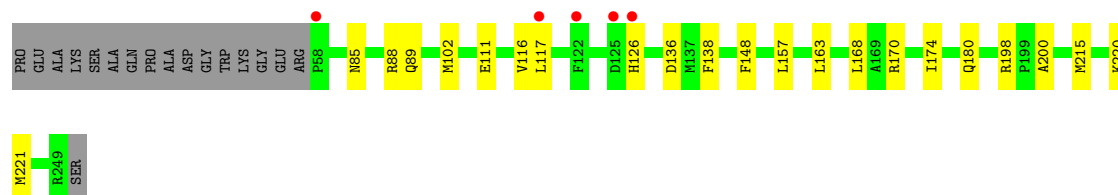
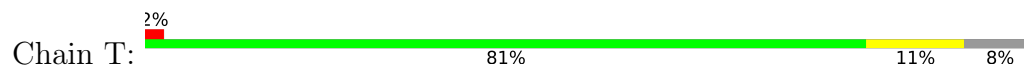




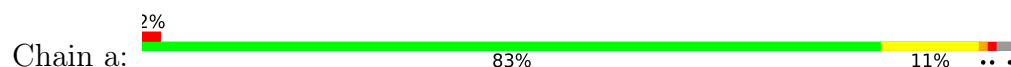
- Molecule 1: GTP cyclohydrolase 1



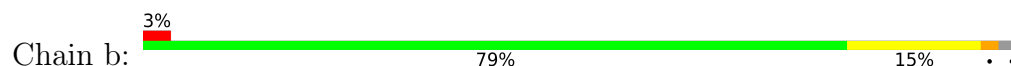
- Molecule 1: GTP cyclohydrolase 1



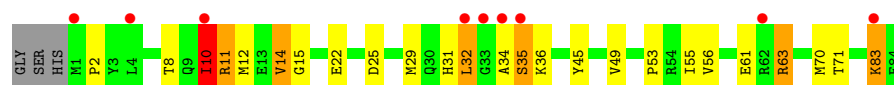
- Molecule 2: GTP cyclohydrolase 1 feedback regulatory protein



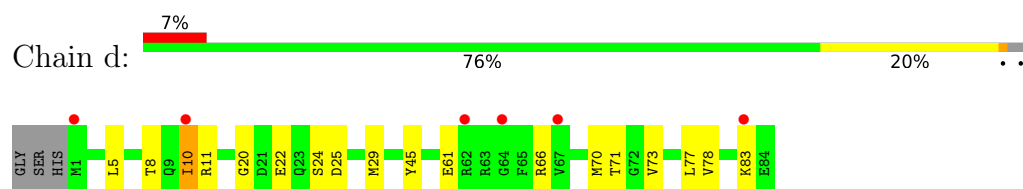
- Molecule 2: GTP cyclohydrolase 1 feedback regulatory protein



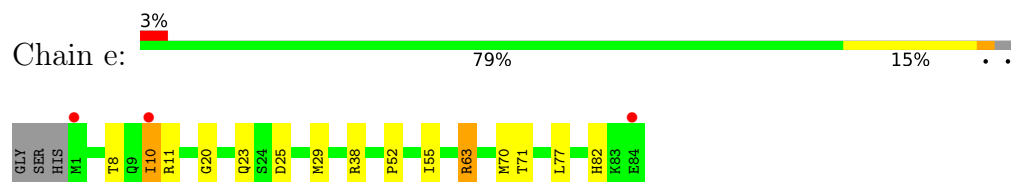
- Molecule 2: GTP cyclohydrolase 1 feedback regulatory protein



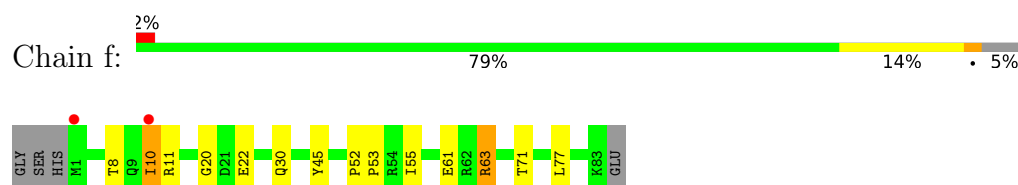
- Molecule 2: GTP cyclohydrolase 1 feedback regulatory protein



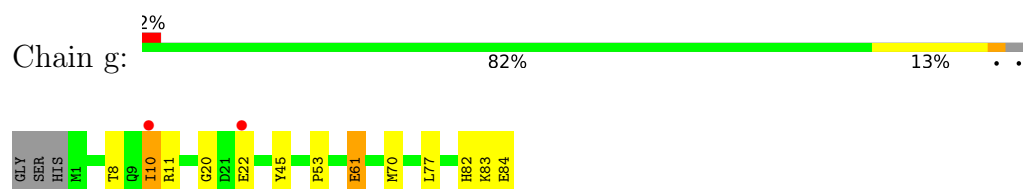
- Molecule 2: GTP cyclohydrolase 1 feedback regulatory protein



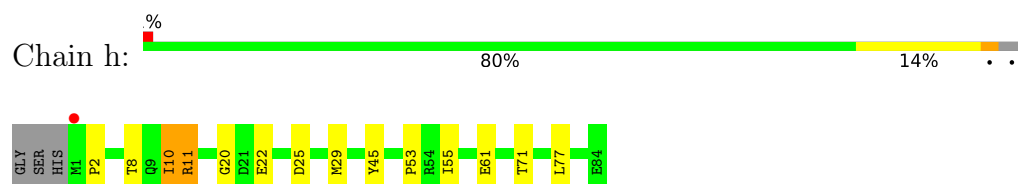
- Molecule 2: GTP cyclohydrolase 1 feedback regulatory protein



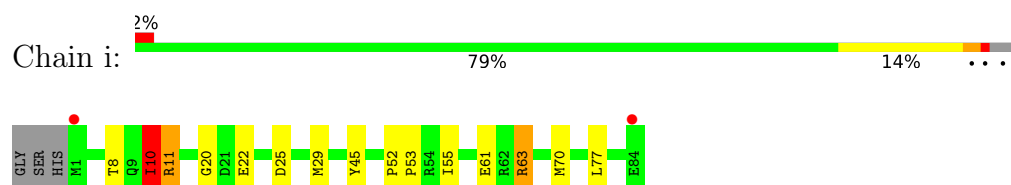
- Molecule 2: GTP cyclohydrolase 1 feedback regulatory protein



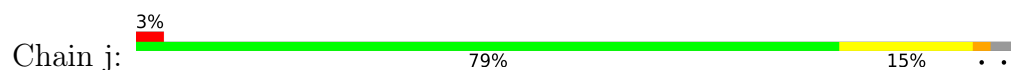
- Molecule 2: GTP cyclohydrolase 1 feedback regulatory protein



- Molecule 2: GTP cyclohydrolase 1 feedback regulatory protein



- Molecule 2: GTP cyclohydrolase 1 feedback regulatory protein

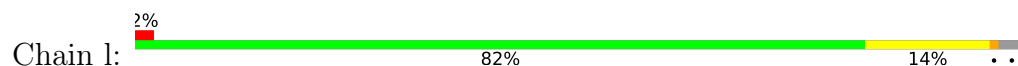




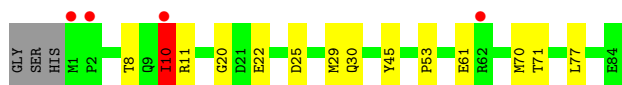
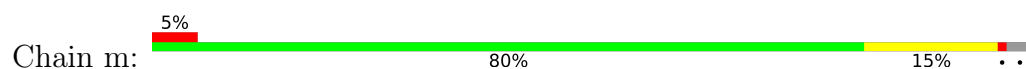
- Molecule 2: GTP cyclohydrolase 1 feedback regulatory protein



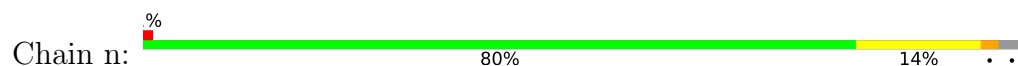
- Molecule 2: GTP cyclohydrolase 1 feedback regulatory protein



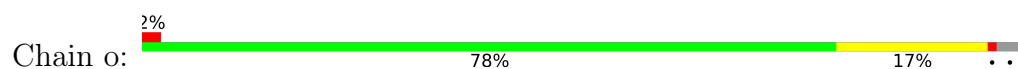
- Molecule 2: GTP cyclohydrolase 1 feedback regulatory protein



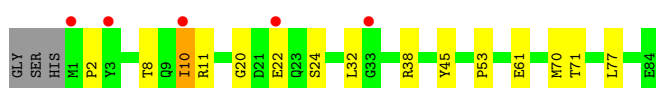
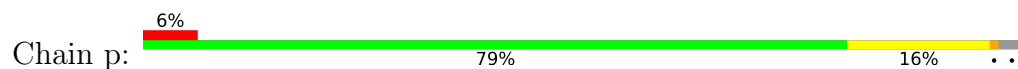
- Molecule 2: GTP cyclohydrolase 1 feedback regulatory protein



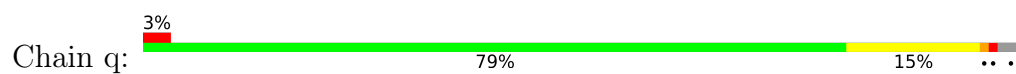
- Molecule 2: GTP cyclohydrolase 1 feedback regulatory protein



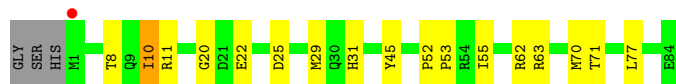
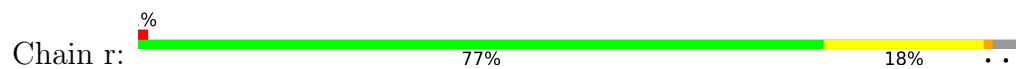
- Molecule 2: GTP cyclohydrolase 1 feedback regulatory protein



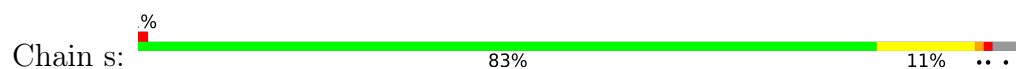
- Molecule 2: GTP cyclohydrolase 1 feedback regulatory protein



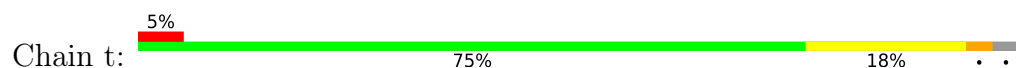
- Molecule 2: GTP cyclohydrolase 1 feedback regulatory protein



- Molecule 2: GTP cyclohydrolase 1 feedback regulatory protein



- Molecule 2: GTP cyclohydrolase 1 feedback regulatory protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	106.10Å 185.42Å 184.23Å 90.00° 97.94° 90.00°	Depositor
Resolution (Å)	182.47 – 2.21 182.47 – 2.21	Depositor EDS
% Data completeness (in resolution range)	63.3 (182.47-2.21) 63.3 (182.47-2.21)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.49 (at 2.20Å)	Xtriage
Refinement program	BUSTER 2.11.7 (18-SEP-2020)	Depositor
R, R_{free}	0.177 , 0.222 0.181 , 0.223	Depositor DCC
R_{free} test set	11261 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	38.0	Xtriage
Anisotropy	0.035	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 52.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	47586	wwPDB-VP
Average B, all atoms (Å ²)	45.0	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 23.96 % 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 4.2081e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: HBI, K, QBQ, ZN

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	0/1540	1.18	8/2079 (0.4%)
1	B	0.78	0/1540	1.17	8/2079 (0.4%)
1	C	0.80	0/1540	1.16	3/2079 (0.1%)
1	D	0.81	0/1540	1.12	5/2079 (0.2%)
1	E	0.85	1/1540 (0.1%)	1.21	11/2079 (0.5%)
1	F	0.80	0/1540	1.14	4/2079 (0.2%)
1	G	0.79	1/1540 (0.1%)	1.21	4/2079 (0.2%)
1	H	0.78	0/1540	1.17	6/2079 (0.3%)
1	I	0.77	0/1540	1.14	5/2079 (0.2%)
1	J	0.80	0/1540	1.14	4/2079 (0.2%)
1	K	0.80	1/1540 (0.1%)	1.17	5/2079 (0.2%)
1	L	0.77	0/1540	1.13	4/2079 (0.2%)
1	M	0.76	0/1540	1.09	4/2079 (0.2%)
1	N	0.83	0/1540	1.12	6/2079 (0.3%)
1	O	0.79	0/1540	1.15	3/2079 (0.1%)
1	P	0.74	0/1540	1.11	6/2079 (0.3%)
1	Q	0.80	0/1540	1.11	3/2079 (0.1%)
1	R	0.82	0/1540	1.17	6/2079 (0.3%)
1	S	0.81	1/1540 (0.1%)	1.16	4/2079 (0.2%)
1	T	0.81	1/1540 (0.1%)	1.18	4/2079 (0.2%)
2	a	0.69	0/692	1.12	4/934 (0.4%)
2	b	0.67	0/692	1.06	3/934 (0.3%)
2	c	0.77	0/692	1.17	2/934 (0.2%)
2	d	0.69	0/692	1.12	3/934 (0.3%)
2	e	0.63	0/692	1.08	3/934 (0.3%)
2	f	0.68	0/683	1.08	3/922 (0.3%)
2	g	0.62	0/692	1.04	3/934 (0.3%)
2	h	0.64	0/692	1.05	3/934 (0.3%)
2	i	0.63	0/692	1.07	4/934 (0.4%)
2	j	0.65	0/692	1.06	4/934 (0.4%)
2	k	0.68	0/692	1.07	4/934 (0.4%)
2	l	0.62	0/692	1.06	4/934 (0.4%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	m	0.64	0/692	1.06	4/934 (0.4%)
2	n	0.68	0/692	1.03	3/934 (0.3%)
2	o	0.71	0/692	1.09	4/934 (0.4%)
2	p	0.66	0/692	1.09	4/934 (0.4%)
2	q	0.71	1/692 (0.1%)	1.09	3/934 (0.3%)
2	r	0.70	0/692	1.08	3/934 (0.3%)
2	s	0.63	0/692	1.06	4/934 (0.4%)
2	t	0.65	0/692	1.06	3/934 (0.3%)
All	All	0.76	6/44631 (0.0%)	1.13	171/60248 (0.3%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	q	11	ARG	CA-C	-5.91	1.44	1.52
1	E	221	MET	SD-CE	-5.14	1.66	1.79
1	K	221	MET	SD-CE	-5.09	1.66	1.79
1	S	221	MET	SD-CE	-5.07	1.66	1.79
1	G	109	TYR	CA-C	5.04	1.59	1.52
1	T	198	ARG	CA-CB	5.02	1.56	1.52

All (171) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	a	10	ILE	CA-C-N	10.05	140.74	121.54
2	a	10	ILE	C-N-CA	10.05	140.74	121.54
2	q	10	ILE	CA-C-N	9.80	140.27	121.54
2	q	10	ILE	C-N-CA	9.80	140.27	121.54
2	o	10	ILE	CA-C-N	9.40	139.49	121.54
2	o	10	ILE	C-N-CA	9.40	139.49	121.54
2	k	10	ILE	CA-C-N	9.07	138.87	121.54
2	k	10	ILE	C-N-CA	9.07	138.87	121.54
2	l	10	ILE	CA-C-N	9.00	138.74	121.54
2	l	10	ILE	C-N-CA	9.00	138.74	121.54
2	e	10	ILE	CA-C-N	8.93	138.59	121.54
2	e	10	ILE	C-N-CA	8.93	138.59	121.54
2	s	10	ILE	CA-C-N	8.79	138.34	121.54
2	s	10	ILE	C-N-CA	8.79	138.34	121.54
2	i	10	ILE	CA-C-N	8.73	138.21	121.54
2	i	10	ILE	C-N-CA	8.73	138.21	121.54
2	d	10	ILE	CA-C-N	8.71	138.18	121.54
2	d	10	ILE	C-N-CA	8.71	138.18	121.54
2	f	10	ILE	CA-C-N	8.70	138.16	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	f	10	ILE	C-N-CA	8.70	138.16	121.54
2	g	10	ILE	CA-C-N	8.61	137.98	121.54
2	g	10	ILE	C-N-CA	8.61	137.98	121.54
2	j	10	ILE	CA-C-N	8.54	137.86	121.54
2	j	10	ILE	C-N-CA	8.54	137.86	121.54
2	h	10	ILE	CA-C-N	8.47	137.71	121.54
2	h	10	ILE	C-N-CA	8.47	137.71	121.54
2	t	10	ILE	CA-C-N	8.43	137.64	121.54
2	t	10	ILE	C-N-CA	8.43	137.64	121.54
1	M	148	PHE	CA-CB-CG	8.31	122.11	113.80
1	E	82	LEU	N-CA-C	-8.30	99.82	110.53
1	B	148	PHE	CA-CB-CG	8.28	122.08	113.80
2	m	10	ILE	CA-C-N	8.23	137.25	121.54
2	m	10	ILE	C-N-CA	8.23	137.25	121.54
2	r	10	ILE	CA-C-N	8.20	137.19	121.54
2	r	10	ILE	C-N-CA	8.20	137.19	121.54
1	E	148	PHE	CA-CB-CG	8.14	121.94	113.80
2	p	10	ILE	CA-C-N	8.08	136.97	121.54
2	p	10	ILE	C-N-CA	8.08	136.97	121.54
2	n	10	ILE	CA-C-N	7.96	136.73	121.54
2	n	10	ILE	C-N-CA	7.96	136.73	121.54
1	L	148	PHE	CA-CB-CG	7.83	121.63	113.80
2	c	10	ILE	CA-C-N	7.71	136.26	121.54
2	c	10	ILE	C-N-CA	7.71	136.26	121.54
1	T	148	PHE	CA-CB-CG	7.67	121.47	113.80
1	F	148	PHE	CA-CB-CG	7.54	121.34	113.80
1	P	148	PHE	CA-CB-CG	7.37	121.17	113.80
1	I	148	PHE	CA-CB-CG	7.27	121.07	113.80
1	F	214	VAL	N-CA-CB	-7.07	103.63	111.41
1	N	148	PHE	CA-CB-CG	7.04	120.84	113.80
1	M	180	GLN	N-CA-C	6.91	118.60	108.86
1	A	148	PHE	CA-CB-CG	6.90	120.70	113.80
1	F	180	GLN	N-CA-C	6.85	119.83	109.41
1	T	220	LYS	CA-C-N	6.69	129.54	120.38
1	T	220	LYS	C-N-CA	6.69	129.54	120.38
1	D	148	PHE	CA-CB-CG	6.64	120.44	113.80
1	K	148	PHE	CA-CB-CG	6.43	120.23	113.80
1	N	220	LYS	CA-C-N	6.42	129.76	120.38
1	N	220	LYS	C-N-CA	6.42	129.76	120.38
1	R	180	GLN	CA-C-N	6.38	131.87	123.06
1	R	180	GLN	C-N-CA	6.38	131.87	123.06
2	b	10	ILE	CA-C-N	6.35	133.66	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	b	10	ILE	C-N-CA	6.35	133.66	121.54
1	G	109	TYR	N-CA-C	-6.32	104.49	111.82
1	H	180	GLN	N-CA-C	6.28	118.49	109.14
1	I	220	LYS	CA-C-N	6.27	128.97	120.38
1	I	220	LYS	C-N-CA	6.27	128.97	120.38
1	J	214	VAL	N-CA-CB	-6.25	104.53	111.41
1	P	127	ASP	CA-CB-CG	6.23	118.83	112.60
1	M	182	GLN	N-CA-C	6.14	118.75	111.33
1	E	237	ASP	CA-CB-CG	6.12	118.72	112.60
2	d	20	GLY	N-CA-C	6.12	119.73	110.18
2	p	32	LEU	N-CA-C	-6.12	102.63	110.53
1	L	180	GLN	N-CA-C	6.08	118.20	109.14
1	K	127	ASP	CA-CB-CG	6.06	118.66	112.60
1	O	180	GLN	N-CA-C	6.06	117.78	109.18
1	R	148	PHE	CA-CB-CG	6.05	119.85	113.80
1	J	180	GLN	N-CA-C	6.03	119.03	109.81
2	f	20	GLY	N-CA-C	6.02	119.58	110.18
1	P	180	GLN	N-CA-C	5.98	118.31	109.69
1	P	159	ASN	CA-CB-CG	5.94	118.54	112.60
1	P	182	GLN	N-CA-C	5.94	118.52	111.33
2	j	20	GLY	N-CA-C	5.93	119.43	110.18
2	a	20	GLY	N-CA-C	5.88	119.36	110.18
1	B	220	LYS	CA-C-N	5.87	128.94	120.38
1	B	220	LYS	C-N-CA	5.87	128.94	120.38
1	R	220	LYS	CA-C-N	5.80	128.85	120.38
1	R	220	LYS	C-N-CA	5.80	128.85	120.38
2	p	20	GLY	N-CA-C	5.79	119.21	110.18
1	E	220	LYS	CA-C-N	5.78	128.81	120.38
1	E	220	LYS	C-N-CA	5.78	128.81	120.38
2	s	10	ILE	N-CA-CB	5.76	117.85	110.13
1	D	180	GLN	N-CA-C	5.73	116.93	108.86
1	J	181	VAL	N-CA-CB	5.73	119.31	111.41
2	o	10	ILE	N-CA-CB	5.72	117.60	110.05
1	N	180	GLN	N-CA-C	5.68	117.25	109.18
1	S	148	PHE	CA-CB-CG	5.68	119.48	113.80
2	q	20	GLY	N-CA-C	5.68	119.04	110.18
1	S	180	GLN	N-CA-C	5.67	118.03	109.41
2	t	20	GLY	N-CA-C	5.66	119.02	110.18
2	r	20	GLY	N-CA-C	5.64	118.72	110.38
1	E	180	GLN	N-CA-C	5.63	117.96	109.41
1	K	180	GLN	N-CA-C	5.62	117.95	109.41
1	F	236	GLU	N-CA-C	5.61	117.48	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	221	MET	N-CA-C	5.61	117.39	111.28
2	e	20	GLY	N-CA-C	5.60	118.74	110.63
2	l	20	GLY	N-CA-C	5.59	118.89	110.18
2	i	10	ILE	N-CA-CB	5.58	117.42	110.05
1	G	124	GLU	CA-C-N	5.58	132.21	121.54
1	G	124	GLU	C-N-CA	5.58	132.21	121.54
2	h	20	GLY	N-CA-C	5.57	118.87	110.18
1	Q	148	PHE	CA-CB-CG	5.57	119.37	113.80
2	i	20	GLY	N-CA-C	5.55	118.84	110.18
1	P	181	VAL	N-CA-C	-5.54	100.09	108.17
1	B	180	GLN	N-CA-C	5.51	117.00	109.18
1	S	220	LYS	CA-C-N	5.50	128.41	120.38
1	S	220	LYS	C-N-CA	5.50	128.41	120.38
2	o	20	GLY	N-CA-C	5.49	118.74	110.18
1	I	159	ASN	CA-CB-CG	5.45	118.05	112.60
2	k	20	GLY	N-CA-C	5.45	118.69	110.18
1	J	148	PHE	CA-CB-CG	5.44	119.24	113.80
1	G	148	PHE	CA-CB-CG	5.44	119.24	113.80
1	D	67	ASN	CA-CB-CG	5.44	118.04	112.60
1	B	180	GLN	CA-C-N	5.43	130.53	122.99
1	B	180	GLN	C-N-CA	5.43	130.53	122.99
1	R	132	VAL	N-CA-CB	5.42	118.73	111.90
1	O	148	PHE	CA-CB-CG	5.42	119.22	113.80
2	m	20	GLY	N-CA-C	5.41	118.63	110.18
2	b	32	LEU	N-CA-C	-5.38	103.29	110.55
2	g	20	GLY	N-CA-C	5.36	118.54	110.18
1	A	220	LYS	CA-C-N	5.36	129.17	120.60
1	A	220	LYS	C-N-CA	5.36	129.17	120.60
1	A	181	VAL	N-CA-C	-5.35	100.42	108.12
1	A	179	LEU	N-CA-C	-5.34	101.08	109.25
1	K	220	LYS	CA-C-N	5.34	127.43	120.28
1	K	220	LYS	C-N-CA	5.34	127.43	120.28
1	E	165	LEU	N-CA-C	5.33	117.51	111.11
1	H	220	LYS	CA-C-N	5.32	127.94	120.28
1	H	220	LYS	C-N-CA	5.32	127.94	120.28
2	s	20	GLY	N-CA-C	5.32	118.47	110.18
1	C	148	PHE	CA-CB-CG	5.30	119.10	113.80
2	n	20	GLY	N-CA-C	5.29	118.44	110.18
1	E	126	HIS	N-CA-C	-5.29	98.68	107.99
1	A	214	VAL	N-CA-CB	-5.29	105.60	111.41
1	C	220	LYS	CA-C-N	5.29	127.89	120.28
1	C	220	LYS	C-N-CA	5.29	127.89	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	m	10	ILE	N-CA-CB	5.23	116.95	110.05
1	E	132	VAL	N-CA-CB	5.21	118.55	112.35
1	N	132	VAL	N-CA-CB	5.21	118.46	111.90
1	H	185	LEU	CA-C-N	5.18	127.53	120.54
1	H	185	LEU	C-N-CA	5.18	127.53	120.54
1	O	182	GLN	N-CA-C	5.17	117.58	111.33
1	M	179	LEU	N-CA-C	-5.16	101.35	109.25
2	a	10	ILE	N-CA-CB	5.16	116.86	110.05
1	D	214	VAL	N-CA-C	5.13	116.06	111.90
2	j	10	ILE	N-CA-CB	5.13	116.82	110.05
1	B	174	ILE	N-CA-CB	5.12	116.54	110.55
2	k	10	ILE	N-CA-CB	5.12	116.81	110.05
1	L	113	ILE	CA-C-N	5.12	128.49	120.82
1	L	113	ILE	C-N-CA	5.12	128.49	120.82
1	Q	147	PRO	N-CA-C	5.11	119.27	111.34
1	E	174	ILE	N-CA-CB	5.09	116.51	110.55
1	I	148	PHE	CB-CA-C	5.08	118.27	110.14
1	A	76	SER	CA-C-N	5.07	127.07	120.28
1	A	76	SER	C-N-CA	5.07	127.07	120.28
1	E	174	ILE	CB-CA-C	-5.07	105.49	111.97
1	B	236	GLU	N-CA-C	5.06	116.60	111.14
1	D	122	PHE	CA-CB-CG	5.04	118.84	113.80
2	l	10	ILE	N-CA-CB	5.04	116.70	110.05
1	N	237	ASP	CA-CB-CG	5.04	117.64	112.60
1	H	237	ASP	CA-CB-CG	5.03	117.63	112.60
1	T	180	GLN	N-CA-C	5.01	117.03	109.41

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	1515	0	1539	16	0
1	B	1515	0	1539	15	0
1	C	1515	0	1539	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1515	0	1539	20	0
1	E	1515	0	1539	23	0
1	F	1515	0	1539	17	0
1	G	1515	0	1539	27	0
1	H	1515	0	1539	14	0
1	I	1515	0	1539	11	0
1	J	1515	0	1539	18	0
1	K	1515	0	1539	17	0
1	L	1515	0	1539	20	0
1	M	1515	0	1539	23	0
1	N	1515	0	1539	14	0
1	O	1515	0	1539	15	0
1	P	1515	0	1539	18	0
1	Q	1515	0	1539	18	0
1	R	1515	0	1539	21	0
1	S	1515	0	1539	23	0
1	T	1515	0	1539	16	0
2	a	678	0	679	6	0
2	b	678	0	679	6	0
2	c	678	0	679	19	0
2	d	678	0	679	13	0
2	e	678	0	679	8	0
2	f	669	0	673	5	0
2	g	678	0	679	6	0
2	h	678	0	679	6	0
2	i	678	0	679	8	0
2	j	678	0	679	7	0
2	k	678	0	679	9	0
2	l	678	0	679	6	0
2	m	678	0	679	6	0
2	n	678	0	679	10	0
2	o	678	0	679	10	0
2	p	678	0	680	5	0
2	q	678	0	679	6	0
2	r	678	0	679	7	0
2	s	678	0	680	7	0
2	t	678	0	679	11	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
3	K	1	0	0	0	0
3	L	1	0	0	0	0
3	M	1	0	0	0	0
3	N	1	0	0	0	0
3	O	1	0	0	0	0
3	P	1	0	0	0	0
3	Q	1	0	0	0	0
3	R	1	0	0	0	0
3	S	1	0	0	0	0
3	T	1	0	0	0	0
4	A	32	17	0	1	0
4	B	32	17	0	0	0
4	C	32	17	0	0	0
4	D	32	17	0	0	0
4	E	32	17	0	2	0
4	F	32	17	0	0	0
4	G	32	17	0	1	0
4	H	32	17	0	1	0
4	I	32	17	0	1	0
4	J	32	17	0	1	0
4	K	32	17	0	1	0
4	L	32	17	0	1	0
4	M	32	17	0	0	0
4	N	32	17	0	0	0
4	O	32	17	0	0	0
4	P	32	17	0	0	0
4	Q	32	17	0	0	0
4	R	32	17	0	0	0
4	S	32	17	0	2	0
4	T	32	17	0	1	0
5	A	34	26	26	5	0
5	B	17	13	13	1	0
5	D	17	13	13	2	0
5	E	17	13	13	2	0
5	F	17	13	13	0	0
5	G	17	13	13	2	0
5	H	17	13	13	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	I	34	26	26	2	0
5	K	17	13	13	2	0
5	L	34	26	26	4	0
5	M	17	13	13	0	0
5	O	17	13	13	2	0
5	P	17	13	13	4	0
5	Q	17	13	13	1	0
5	R	17	13	13	3	0
5	S	17	13	13	2	0
5	T	17	13	13	3	0
6	a	1	0	0	0	0
6	b	1	0	0	0	0
6	c	1	0	0	0	0
6	d	1	0	0	0	0
6	e	1	0	0	0	0
6	f	1	0	0	0	0
6	g	1	0	0	0	0
6	h	1	0	0	0	0
6	i	1	0	0	0	0
6	j	1	0	0	0	0
6	k	1	0	0	0	0
6	l	1	0	0	0	0
6	m	1	0	0	0	0
6	n	1	0	0	0	0
6	o	1	0	0	0	0
6	p	1	0	0	0	0
6	q	1	0	0	0	0
6	r	1	0	0	0	0
6	s	1	0	0	0	0
6	t	1	0	0	0	0
7	A	80	0	0	0	0
7	B	67	0	0	0	0
7	C	83	0	0	0	0
7	D	61	0	0	0	0
7	E	66	0	0	2	0
7	F	91	0	0	0	0
7	G	57	0	0	0	0
7	H	83	0	0	0	0
7	I	67	0	0	0	0
7	J	96	0	0	1	0
7	K	70	0	0	0	0
7	L	61	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	M	72	0	0	0	0
7	N	73	0	0	0	0
7	O	73	0	0	0	0
7	P	66	0	0	0	0
7	Q	82	0	0	0	0
7	R	72	0	0	0	0
7	S	68	0	0	0	0
7	T	76	0	0	0	0
7	a	39	0	0	0	0
7	b	24	0	0	0	0
7	c	15	0	0	0	0
7	d	27	0	0	0	0
7	e	24	0	0	0	0
7	f	33	0	0	0	0
7	g	35	0	0	0	0
7	h	24	0	0	1	0
7	i	35	0	0	1	0
7	j	34	0	0	1	0
7	k	45	0	0	1	0
7	l	31	0	0	0	0
7	m	37	0	0	1	0
7	n	42	0	0	1	0
7	o	55	0	0	0	0
7	p	24	0	0	0	0
7	q	32	0	0	0	0
7	r	42	0	0	0	0
7	s	29	0	0	0	0
7	t	24	0	0	0	0
All	All	46986	600	44616	407	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 5.

All (407) 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:84:GLU:HG2	1:B:91:LEU:HD11	1.60	0.83
1:K:116:VAL:HG21	1:K:174:ILE:HG12	1.69	0.75
1:M:221:MET:HG2	1:Q:221:MET:HE2	1.71	0.73
1:C:221:MET:HE2	1:G:221:MET:HE2	1.71	0.72
2:d:66:ARG:HH21	2:e:82:HIS:CE1	2.08	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:c:12:MET:HE2	2:d:5:LEU:HB3	1.75	0.69
1:I:163:LEU:HB2	1:I:197:LEU:HD11	1.74	0.69
1:C:116:VAL:HG21	1:C:174:ILE:HG12	1.75	0.69
1:L:187:LYS:HD2	1:M:126:HIS:HD2	1.57	0.69
1:R:249:ARG:NH1	1:S:249:ARG:HH11	1.91	0.68
1:B:215:MET:HG2	1:I:138:PHE:HB3	1.75	0.68
1:R:233:VAL:HG11	5:R:303:HBI:H113	1.76	0.67
1:D:215:MET:HG2	1:G:138:PHE:HB3	1.75	0.67
2:c:12:MET:HE1	2:d:78:VAL:HG13	1.78	0.66
2:c:31:HIS:HD2	2:c:32:LEU:HD23	1.60	0.66
1:E:71:LEU:HD13	1:F:81:SER:HB2	1.78	0.66
2:n:66:ARG:HH22	2:o:82:HIS:CE1	2.14	0.65
1:N:138:PHE:HB3	1:Q:215:MET:HG2	1.79	0.65
2:o:8:THR:HG21	2:o:53:PRO:HG3	1.78	0.65
2:c:70:MET:HE3	2:d:71:THR:HG22	1.79	0.64
1:P:207:GLU:HG3	1:P:226:VAL:HG22	1.78	0.64
2:j:52:PRO:HG2	2:j:55:ILE:HD13	1.80	0.64
1:P:157:LEU:HD13	5:P:303:HBI:H112	1.79	0.63
1:E:116:VAL:HG21	1:E:174:ILE:HG12	1.81	0.63
1:M:215:MET:HG2	1:R:138:PHE:HB3	1.81	0.63
1:E:224:LYS:NZ	7:E:401:HOH:O	2.33	0.62
1:T:116:VAL:HG21	1:T:174:ILE:HG12	1.81	0.62
1:R:84:GLU:O	1:R:86:PRO:HD3	2.00	0.62
2:a:8:THR:HG21	2:a:53:PRO:HG3	1.81	0.62
1:D:139:SER:HB3	1:D:176:SER:O	2.00	0.61
1:Q:116:VAL:HG11	1:Q:174:ILE:HD11	1.81	0.61
2:t:2:PRO:HA	2:t:83:LYS:HB2	1.82	0.61
2:k:66:ARG:HD3	7:k:424:HOH:O	1.99	0.61
1:G:157:LEU:HD13	5:G:303:HBI:H112	1.83	0.60
2:n:22:GLU:HG2	2:n:45:TYR:HB2	1.83	0.60
1:S:165:LEU:HG	4:S:302:QBQ:C	2.31	0.60
1:O:152:VAL:HG22	1:O:206:VAL:HG22	1.83	0.59
1:S:163:LEU:HB2	1:S:197:LEU:HD11	1.83	0.59
2:i:52:PRO:HG2	2:i:55:ILE:HD13	1.83	0.59
1:Q:116:VAL:HG21	1:Q:174:ILE:HG12	1.84	0.59
2:e:52:PRO:HG2	2:e:55:ILE:HD13	1.85	0.59
1:S:116:VAL:HG11	1:S:174:ILE:HD11	1.85	0.59
2:j:22:GLU:HG2	2:j:45:TYR:HB2	1.85	0.59
1:L:187:LYS:HD2	1:M:126:HIS:CD2	2.39	0.58
2:s:22:GLU:HG2	2:s:45:TYR:HB2	1.84	0.58
2:t:52:PRO:HG2	2:t:55:ILE:HD13	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:22:GLU:HG2	2:b:45:TYR:HB2	1.86	0.58
2:k:22:GLU:HG2	2:k:45:TYR:HB2	1.86	0.58
1:D:111:GLU:HB2	1:D:174:ILE:HG23	1.86	0.57
1:G:107:LYS:O	1:G:177:ARG:CB	2.52	0.57
2:i:70:MET:HE3	2:j:71:THR:HG22	1.87	0.57
2:l:22:GLU:HG2	2:l:45:TYR:HB2	1.86	0.57
1:L:163:LEU:HB2	1:L:197:LEU:HD11	1.86	0.57
2:i:22:GLU:HG2	2:i:45:TYR:HB2	1.86	0.57
2:a:22:GLU:HG2	2:a:45:TYR:HB2	1.85	0.57
2:g:22:GLU:HG2	2:g:45:TYR:HB2	1.86	0.57
1:F:96:TRP:CZ2	1:M:69:PRO:HB3	2.40	0.57
2:f:22:GLU:HG2	2:f:45:TYR:HB2	1.87	0.57
2:k:8:THR:HG21	2:k:53:PRO:HG3	1.87	0.57
2:c:31:HIS:CD2	2:c:32:LEU:HD23	2.40	0.56
1:G:107:LYS:O	1:G:177:ARG:HB2	2.05	0.56
1:R:152:VAL:HG22	1:R:206:VAL:HG22	1.86	0.56
1:F:66:LEU:HD11	1:M:93:LYS:HG2	1.86	0.56
1:G:233:VAL:HG11	5:G:303:HBI:H113	1.87	0.56
1:K:215:MET:HG2	1:T:138:PHE:HB3	1.87	0.56
1:M:221:MET:HG2	1:Q:221:MET:CE	2.34	0.56
2:b:8:THR:HG21	2:b:53:PRO:HG3	1.88	0.56
2:p:22:GLU:HG2	2:p:45:TYR:HB2	1.88	0.56
2:c:12:MET:CE	2:d:5:LEU:HB3	2.35	0.56
2:m:70:MET:HE3	2:n:71:THR:HG22	1.87	0.56
1:B:84:GLU:HG2	1:B:91:LEU:CD1	2.33	0.56
1:E:200:ALA:HB1	5:E:303:HBI:H111	1.87	0.56
1:H:163:LEU:HB2	1:H:197:LEU:HD11	1.86	0.56
1:P:200:ALA:HB1	5:P:303:HBI:H111	1.88	0.56
2:o:22:GLU:HG2	2:o:45:TYR:HB2	1.88	0.56
1:L:221:MET:HE2	1:R:221:MET:HE2	1.87	0.55
1:B:221:MET:HE1	1:H:221:MET:H	1.71	0.55
2:q:22:GLU:HG2	2:q:45:TYR:HB2	1.87	0.55
1:L:165:LEU:HG	4:L:302:QBQ:C	2.36	0.55
2:d:22:GLU:HG2	2:d:45:TYR:HB2	1.88	0.55
2:g:70:MET:HE3	2:h:71:THR:HG22	1.89	0.55
2:t:22:GLU:HG2	2:t:45:TYR:HB2	1.88	0.55
2:h:22:GLU:HG2	2:h:45:TYR:HB2	1.87	0.55
1:E:233:VAL:HG21	5:E:303:HBI:H113	1.88	0.54
1:A:215:MET:HG2	1:J:138:PHE:HB3	1.90	0.54
2:r:52:PRO:HG2	2:r:55:ILE:HD13	1.89	0.54
1:N:221:MET:H	1:P:221:MET:HE1	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:116:VAL:HG13	1:M:170:ARG:HB3	1.90	0.54
2:c:34:ALA:HB3	2:c:49:VAL:HA	1.89	0.54
2:c:14:VAL:HG22	2:c:15:GLY:H	1.71	0.53
1:D:221:MET:HE2	1:F:221:MET:HE2	1.90	0.53
1:J:105:PHE:CD2	1:J:140:MET:HE3	2.43	0.53
2:m:22:GLU:HG2	2:m:45:TYR:HB2	1.90	0.53
1:N:163:LEU:HB2	1:N:197:LEU:HD11	1.91	0.53
2:d:66:ARG:NH2	2:e:82:HIS:CE1	2.76	0.53
1:N:221:MET:HE1	1:P:221:MET:H	1.73	0.52
1:K:138:PHE:HB3	1:T:215:MET:HG2	1.91	0.52
2:f:71:THR:HG22	2:j:70:MET:HE3	1.90	0.52
2:r:22:GLU:HG2	2:r:45:TYR:HB2	1.92	0.52
1:A:138:PHE:HB3	1:J:215:MET:HG2	1.92	0.52
1:G:170:ARG:NH2	4:G:302:QBQ:O8	2.39	0.52
2:g:8:THR:HG21	2:g:53:PRO:HG3	1.90	0.52
1:B:147:PRO:O	1:B:211:MET:HG2	2.10	0.52
1:E:138:PHE:HB3	1:F:215:MET:HG2	1.92	0.52
1:G:152:VAL:HG22	1:G:206:VAL:HG22	1.92	0.52
1:I:200:ALA:HB1	5:I:303:HBI:H111	1.92	0.52
1:O:200:ALA:HB1	5:O:303:HBI:H111	1.90	0.52
1:L:157:LEU:HD13	5:L:303:HBI:H112	1.92	0.51
1:K:200:ALA:HB1	5:K:303:HBI:H111	1.92	0.51
2:c:2:PRO:HB3	2:c:83:LYS:HE2	1.92	0.51
2:n:8:THR:HG21	2:n:53:PRO:HG3	1.92	0.51
1:C:215:MET:HG2	1:H:138:PHE:HB3	1.91	0.51
1:H:116:VAL:HG11	1:H:174:ILE:HD11	1.92	0.51
1:N:215:MET:HG2	1:Q:138:PHE:HB3	1.93	0.51
1:T:200:ALA:HB1	5:T:303:HBI:H111	1.92	0.51
2:f:52:PRO:HG2	2:f:55:ILE:HD13	1.93	0.51
2:r:8:THR:HG21	2:r:53:PRO:HG3	1.92	0.51
1:D:116:VAL:HG11	1:D:174:ILE:HD11	1.91	0.51
1:F:187:LYS:HD2	1:G:126:HIS:CD2	2.45	0.51
1:R:163:LEU:HB2	1:R:197:LEU:HD11	1.93	0.51
1:A:163:LEU:HB2	1:A:197:LEU:HD11	1.93	0.51
1:E:221:MET:HE1	1:J:221:MET:H	1.76	0.51
2:o:31:HIS:CE1	2:o:63:ARG:NH1	2.79	0.50
2:q:70:MET:HE3	2:r:71:THR:HG22	1.92	0.50
1:S:116:VAL:HG21	1:S:174:ILE:HG12	1.94	0.50
1:G:85:ASN:O	1:G:88:ARG:HG3	2.10	0.50
2:c:10:ILE:HD11	2:d:73:VAL:HG11	1.92	0.50
1:S:143:HIS:HD2	4:T:302:QBQ:C4	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:ARG:HB3	1:B:110:GLN:HG2	1.93	0.50
1:G:116:VAL:HG11	1:G:174:ILE:HD11	1.94	0.50
2:k:71:THR:HG22	2:o:70:MET:HE3	1.94	0.50
1:E:71:LEU:HD13	1:F:81:SER:CB	2.42	0.50
1:P:84:GLU:CD	1:P:88:ARG:HH22	2.20	0.50
2:p:2:PRO:HG3	2:t:61:GLU:HG2	1.92	0.50
1:B:207:GLU:HB2	1:B:226:VAL:HG22	1.94	0.49
1:L:200:ALA:HB1	5:L:303:HBI:H111	1.93	0.49
1:L:215:MET:HG2	1:S:138:PHE:HB3	1.93	0.49
1:P:200:ALA:CB	5:P:303:HBI:H111	2.41	0.49
1:O:129:MET:HE2	1:O:234:PHE:CZ	2.48	0.49
2:n:66:ARG:NH2	2:o:82:HIS:CE1	2.79	0.49
1:M:163:LEU:HB2	1:M:197:LEU:HD11	1.94	0.49
1:A:116:VAL:HG21	1:A:174:ILE:HG12	1.94	0.49
1:A:118:ASN:ND2	4:A:302:QBQ:O2	2.46	0.49
1:H:161:GLN:HE21	1:H:161:GLN:N	2.11	0.49
1:K:221:MET:H	1:S:221:MET:HE1	1.78	0.49
1:R:200:ALA:HB1	5:R:303:HBI:H111	1.95	0.49
1:S:199:PRO:HG2	1:S:202:VAL:HG23	1.95	0.49
1:H:85:ASN:O	1:H:88:ARG:HG2	2.13	0.49
2:p:70:MET:HE3	2:q:71:THR:HG22	1.95	0.49
1:E:80:SER:O	1:E:82:LEU:O	2.30	0.49
1:T:116:VAL:HG11	1:T:174:ILE:HD11	1.94	0.49
1:B:97:ARG:NH2	1:I:143:HIS:HD2	2.10	0.48
2:q:52:PRO:HG2	2:q:55:ILE:HD13	1.95	0.48
1:G:150:GLY:HA3	1:G:207:GLU:O	2.12	0.48
1:M:102:MET:HG3	1:R:82:LEU:HD21	1.95	0.48
1:C:84:GLU:HG3	1:H:179:LEU:HD12	1.95	0.48
1:S:187:LYS:HD2	1:T:126:HIS:HD2	1.77	0.48
1:C:221:MET:HE2	1:G:221:MET:HB2	1.94	0.48
1:S:163:LEU:HD23	1:S:168:LEU:HD23	1.94	0.48
1:C:218:VAL:HG12	1:D:170:ARG:HG2	1.96	0.48
1:Q:146:VAL:HG22	1:Q:211:MET:HB2	1.94	0.48
2:p:8:THR:HG21	2:p:53:PRO:HG3	1.95	0.48
1:N:116:VAL:HG21	1:N:174:ILE:HG12	1.96	0.48
2:a:70:MET:HE3	2:b:71:THR:HG22	1.95	0.48
2:s:70:MET:HE3	2:t:71:THR:HG22	1.95	0.48
1:L:233:VAL:HG11	5:L:303:HBI:H113	1.94	0.48
1:A:200:ALA:CB	5:A:303:HBI:H111	2.44	0.48
1:D:163:LEU:HB2	1:D:197:LEU:HD11	1.95	0.48
2:c:10:ILE:HD11	2:d:73:VAL:CG1	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:146:VAL:HG21	1:J:212:CYS:HB3	1.95	0.48
1:M:84:GLU:HG3	1:R:179:LEU:HD12	1.96	0.48
1:O:84:GLU:HG3	1:P:179:LEU:HD12	1.96	0.47
2:m:8:THR:HG21	2:m:53:PRO:HG3	1.97	0.47
7:m:425:HOH:O	2:n:2:PRO:HB3	2.14	0.47
1:C:116:VAL:HG13	1:C:170:ARG:HB3	1.96	0.47
1:M:59:ARG:HB3	1:M:110:GLN:HG2	1.96	0.47
2:h:8:THR:HG21	2:h:53:PRO:HG3	1.96	0.47
1:D:63:ASP:O	1:D:66:LEU:O	2.33	0.47
1:L:221:MET:H	1:R:221:MET:HE1	1.79	0.47
2:a:71:THR:HG22	2:e:70:MET:HE3	1.96	0.47
2:b:24:SER:HB3	2:b:29:MET:HE3	1.97	0.47
2:c:8:THR:HG21	2:c:53:PRO:HG3	1.96	0.47
1:A:179:LEU:HD12	1:J:84:GLU:HG3	1.96	0.47
1:B:163:LEU:HD13	1:B:197:LEU:HD21	1.96	0.47
1:K:221:MET:HE2	1:S:221:MET:HB2	1.95	0.47
2:d:24:SER:HB3	2:d:29:MET:HE3	1.96	0.47
1:L:221:MET:HE2	1:R:221:MET:HB2	1.97	0.47
1:O:136:ASP:OD2	1:P:221:MET:HE3	2.15	0.47
1:A:221:MET:HE2	1:I:221:MET:HB2	1.97	0.47
1:G:104:PHE:O	1:G:107:LYS:HG2	2.14	0.47
1:P:187:LYS:HD2	1:Q:126:HIS:HD2	1.79	0.47
2:i:10:ILE:HD13	2:i:10:ILE:HA	1.69	0.47
2:q:8:THR:HG21	2:q:53:PRO:HG3	1.97	0.47
2:t:8:THR:HG21	2:t:53:PRO:HG3	1.95	0.47
1:L:200:ALA:CB	5:L:303:HBI:H111	2.45	0.47
1:P:84:GLU:OE1	1:P:88:ARG:NH2	2.47	0.47
2:i:8:THR:HG21	2:i:53:PRO:HG3	1.96	0.47
1:F:150:GLY:HA3	1:F:207:GLU:O	2.14	0.47
1:D:215:MET:HG2	1:G:138:PHE:CB	2.42	0.46
1:G:171:ILE:HA	1:G:174:ILE:HD12	1.97	0.46
2:r:70:MET:HE3	2:s:71:THR:HG22	1.97	0.46
2:s:10:ILE:HD11	2:t:73:VAL:CG1	2.45	0.46
1:N:187:LYS:HD2	1:O:126:HIS:HD2	1.80	0.46
2:a:27:GLU:O	2:a:30:GLN:HG3	2.15	0.46
2:r:31:HIS:CD2	2:r:63:ARG:HD2	2.51	0.46
2:e:63:ARG:HA	2:e:63:ARG:HD3	1.74	0.46
1:L:221:MET:CE	1:R:221:MET:HB2	2.45	0.46
2:d:70:MET:HE3	2:e:71:THR:HG22	1.97	0.46
2:p:71:THR:HG22	2:t:70:MET:HE3	1.98	0.46
1:R:200:ALA:CB	5:R:303:HBI:H111	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:303:HBI:H111	1:C:200:ALA:HB1	1.97	0.46
1:Q:116:VAL:HG13	1:Q:170:ARG:HB3	1.97	0.46
1:D:84:GLU:HG3	1:G:179:LEU:HD12	1.98	0.46
1:D:221:MET:HE2	1:D:221:MET:HB2	1.74	0.46
1:O:116:VAL:HG11	1:O:174:ILE:HD11	1.98	0.46
1:P:233:VAL:HG11	5:P:303:HBI:H113	1.97	0.46
1:S:184:ARG:O	1:S:188:GLN:HG3	2.16	0.46
1:K:112:THR:HG22	1:K:114:SER:H	1.80	0.46
2:b:11:ARG:HD3	2:b:11:ARG:HA	1.81	0.46
1:O:116:VAL:HG21	1:O:174:ILE:HG12	1.98	0.45
2:h:11:ARG:HB2	7:h:417:HOH:O	2.16	0.45
2:l:8:THR:HG21	2:l:53:PRO:HG3	1.98	0.45
1:G:113:ILE:HD13	1:G:174:ILE:HD13	1.98	0.45
2:c:12:MET:HE1	2:d:78:VAL:CG1	2.45	0.45
2:f:8:THR:HG21	2:f:53:PRO:HG3	1.97	0.45
1:Q:134:ASP:OD1	1:Q:153:HIS:HE1	1.99	0.45
2:m:10:ILE:HD11	2:n:73:VAL:CG1	2.46	0.45
1:B:116:VAL:HG21	1:B:174:ILE:HG12	1.98	0.45
1:E:81:SER:CB	1:F:71:LEU:HG	2.47	0.45
1:N:221:MET:HE2	1:P:221:MET:HE2	1.98	0.45
2:i:63:ARG:HA	2:i:63:ARG:HD3	1.79	0.45
1:L:221:MET:HE2	1:L:221:MET:HB2	1.72	0.45
2:g:82:HIS:ND1	2:g:84:GLU:OE1	2.29	0.45
1:E:198:ARG:HH12	2:e:38:ARG:NH1	2.15	0.45
1:F:122:PHE:HB2	1:F:162:VAL:HG13	1.99	0.45
1:I:85:ASN:HB3	1:I:88:ARG:HB2	1.98	0.45
1:I:116:VAL:HG11	1:I:174:ILE:HD11	1.98	0.45
1:L:245:LEU:HD11	1:M:243:GLU:HG3	1.99	0.45
1:M:193:ILE:HG23	1:M:197:LEU:HD12	1.98	0.45
1:N:221:MET:HB2	1:P:221:MET:HE2	1.99	0.45
1:O:221:MET:HE2	1:T:221:MET:HB2	1.98	0.45
1:G:107:LYS:O	1:G:177:ARG:HB3	2.15	0.45
1:K:126:HIS:HB3	1:O:187:LYS:HD2	1.98	0.45
2:c:22:GLU:HG3	2:c:45:TYR:HB2	1.98	0.45
2:f:63:ARG:HA	2:f:63:ARG:HD3	1.76	0.45
1:E:146:VAL:HG22	1:E:147:PRO:HD2	1.99	0.45
1:P:122:PHE:HB2	1:P:162:VAL:HG12	1.99	0.45
1:S:159:ASN:O	1:S:160:LYS:HB2	2.15	0.45
1:E:136:ASP:CG	1:F:221:MET:HE3	2.41	0.44
1:K:221:MET:HE3	1:T:136:ASP:CG	2.42	0.44
1:C:84:GLU:O	1:C:86:PRO:HD3	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:214:VAL:HG22	1:M:221:MET:HA	1.98	0.44
1:O:128:GLU:O	1:O:158:PRO:HD2	2.17	0.44
2:n:70:MET:HE3	2:o:71:THR:HG22	1.98	0.44
1:P:137:MET:HB2	1:P:152:VAL:HG23	1.98	0.44
1:H:161:GLN:HE21	1:H:161:GLN:H	1.66	0.44
1:J:99:ALA:O	1:J:103:GLN:HG3	2.16	0.44
1:H:200:ALA:HB1	5:H:303:HBI:H111	1.98	0.44
2:k:70:MET:HE3	2:l:71:THR:HG22	1.99	0.44
1:A:116:VAL:HG11	1:A:174:ILE:HD11	1.99	0.44
1:S:200:ALA:HB1	5:S:303:HBI:H111	2.00	0.44
2:c:63:ARG:HD3	2:c:63:ARG:HA	1.77	0.44
2:j:63:ARG:HD3	2:j:63:ARG:HA	1.78	0.44
2:k:10:ILE:HD13	2:k:10:ILE:HA	1.67	0.44
1:J:165:LEU:HG	4:J:302:QBQ:C	2.48	0.44
1:S:59:ARG:HB3	1:S:110:GLN:HG2	2.00	0.44
1:S:233:VAL:HG11	5:S:303:HBI:H113	2.00	0.44
2:a:10:ILE:HD13	2:a:10:ILE:HA	1.72	0.44
1:J:116:VAL:HG13	1:J:170:ARG:HB3	2.00	0.44
5:K:303:HBI:H71	1:O:235:ARG:NH1	2.32	0.44
1:I:165:LEU:HG	4:I:302:QBQ:C	2.48	0.43
1:M:123:ASP:H	1:S:89:GLN:HE22	1.65	0.43
1:M:216:ARG:HG2	1:R:105:PHE:CE1	2.53	0.43
5:A:304:HBI:H111	1:B:200:ALA:HB1	1.99	0.43
1:J:96:TRP:CD1	7:J:449:HOH:O	2.70	0.43
1:Q:200:ALA:HB1	5:Q:303:HBI:H111	2.00	0.43
1:B:191:VAL:O	1:B:195:GLU:HG3	2.19	0.43
1:C:117:LEU:HD11	1:C:171:ILE:HD11	2.00	0.43
1:D:142:GLU:O	1:G:94:THR:OG1	2.25	0.43
1:D:200:ALA:HB1	5:D:303:HBI:H111	2.01	0.43
1:D:221:MET:HE3	1:G:136:ASP:CG	2.44	0.43
1:G:124:GLU:OE2	1:G:126:HIS:CE1	2.71	0.43
1:N:221:MET:HG2	1:Q:138:PHE:HZ	1.83	0.43
1:Q:117:LEU:HD12	1:Q:117:LEU:HA	1.75	0.43
2:c:25:ASP:O	2:c:29:MET:HG2	2.18	0.43
2:d:25:ASP:O	2:d:29:MET:HG2	2.18	0.43
2:q:10:ILE:HD13	2:q:10:ILE:HA	1.68	0.43
1:A:136:ASP:HB2	1:J:221:MET:HE3	2.01	0.43
1:E:215:MET:HE3	1:F:138:PHE:HB3	2.01	0.43
1:O:138:PHE:HB3	1:P:215:MET:HG2	2.00	0.43
1:E:71:LEU:HB3	1:E:99:ALA:HB1	2.00	0.43
1:Q:184:ARG:O	1:Q:188:GLN:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:152:VAL:HG22	1:I:206:VAL:HG22	2.01	0.43
1:A:200:ALA:HB1	5:A:303:HBI:H111	2.01	0.43
1:B:221:MET:HE1	1:H:220:LYS:HA	2.00	0.43
1:D:138:PHE:HB3	1:G:215:MET:HG2	2.00	0.43
1:E:154:ILE:HG21	1:E:168:LEU:HD22	2.00	0.43
1:F:96:TRP:HZ3	1:M:73:ALA:HB2	1.84	0.43
2:c:10:ILE:HD13	2:c:10:ILE:HA	1.68	0.43
1:C:116:VAL:HG11	1:C:174:ILE:HD11	1.99	0.43
1:K:170:ARG:O	1:K:174:ILE:HG13	2.19	0.43
1:M:112:THR:HG22	1:M:114:SER:H	1.84	0.43
1:N:221:MET:N	1:P:221:MET:HE1	2.34	0.43
1:C:220:LYS:HG3	1:D:135:ILE:HG23	2.01	0.42
1:R:180:GLN:OE1	1:R:184:ARG:HD2	2.18	0.42
2:g:61:GLU:HG2	2:h:2:PRO:HG3	2.00	0.42
2:j:1:MET:HB3	7:j:401:HOH:O	2.19	0.42
2:n:66:ARG:NH2	2:o:82:HIS:ND1	2.67	0.42
2:o:10:ILE:HD13	2:o:10:ILE:HA	1.65	0.42
1:K:163:LEU:HB2	1:K:197:LEU:HD11	2.01	0.42
1:O:233:VAL:HG11	5:O:303:HBI:H113	2.00	0.42
1:Q:170:ARG:O	1:Q:174:ILE:HG13	2.19	0.42
1:T:200:ALA:CB	5:T:303:HBI:H111	2.48	0.42
2:i:11:ARG:HB2	7:i:420:HOH:O	2.19	0.42
1:D:136:ASP:OD1	1:G:221:MET:HE3	2.19	0.42
1:M:154:ILE:HG21	1:M:168:LEU:HD22	2.01	0.42
1:R:72:ALA:O	1:R:95:PRO:HB3	2.20	0.42
2:b:70:MET:HE3	2:c:71:THR:HG22	2.00	0.42
1:H:87:GLN:HE21	1:H:87:GLN:HB3	1.73	0.42
1:N:159:ASN:HB2	1:N:199:PRO:HA	2.01	0.42
1:R:116:VAL:HG13	1:R:170:ARG:HB3	2.01	0.42
2:l:70:MET:HE3	2:m:71:THR:HG22	2.01	0.42
1:C:150:GLY:HA3	1:C:207:GLU:O	2.19	0.42
1:J:163:LEU:HD23	1:J:168:LEU:HD23	2.01	0.42
1:R:144:HIS:NE2	4:S:302:QBQ:O5	2.48	0.42
2:s:10:ILE:HD11	2:t:73:VAL:HG11	2.00	0.42
1:S:152:VAL:HG22	1:S:206:VAL:HG22	2.01	0.42
1:E:166:SER:OG	4:E:302:QBQ:O9	2.26	0.42
1:H:165:LEU:HG	4:H:302:QBQ:C	2.50	0.42
2:s:10:ILE:HD13	2:s:10:ILE:HA	1.65	0.42
1:I:124:GLU:OE1	1:I:126:HIS:HE1	2.02	0.42
1:M:124:GLU:HB3	1:M:126:HIS:CE1	2.55	0.42
1:O:121:ILE:HG22	1:O:161:GLN:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:85:ASN:O	1:Q:88:ARG:HG2	2.20	0.42
2:o:25:ASP:O	2:o:29:MET:HG2	2.20	0.42
1:J:152:VAL:HG22	1:J:206:VAL:HG22	2.02	0.41
2:r:25:ASP:O	2:r:29:MET:HG2	2.20	0.41
1:A:116:VAL:HG13	1:A:170:ARG:HB3	2.01	0.41
1:D:62:GLU:HG2	1:D:66:LEU:HD12	2.02	0.41
1:E:180:GLN:OE1	1:E:184:ARG:HD2	2.20	0.41
1:F:99:ALA:O	1:F:103:GLN:HG3	2.20	0.41
1:I:117:LEU:HD11	1:I:171:ILE:HD11	2.02	0.41
1:K:82:LEU:HD11	1:T:102:MET:HG3	2.02	0.41
1:M:183:GLU:OE2	1:M:183:GLU:N	2.50	0.41
1:T:170:ARG:O	1:T:174:ILE:HG13	2.20	0.41
2:n:22:GLU:HG3	7:n:418:HOH:O	2.20	0.41
5:A:304:HBI:H113	1:B:233:VAL:HG11	2.02	0.41
1:F:247:LEU:HB3	1:J:226:VAL:HG11	2.03	0.41
1:Q:112:THR:HG22	1:Q:115:ASP:H	1.85	0.41
2:l:63:ARG:HD3	2:l:63:ARG:HA	1.92	0.41
1:C:170:ARG:O	1:C:174:ILE:HG13	2.21	0.41
1:L:82:LEU:HD11	1:S:102:MET:HG3	2.03	0.41
1:A:150:GLY:HA3	1:A:207:GLU:O	2.20	0.41
1:B:221:MET:HE1	1:H:221:MET:N	2.32	0.41
1:C:221:MET:H	1:G:221:MET:HE1	1.85	0.41
1:D:82:LEU:HD22	1:G:106:THR:HG21	2.03	0.41
1:E:118:ASN:HA	7:E:438:HOH:O	2.21	0.41
1:T:116:VAL:HG13	1:T:170:ARG:HB3	2.03	0.41
1:A:221:MET:HE2	1:A:221:MET:HB2	1.91	0.41
1:J:150:GLY:HA3	1:J:207:GLU:O	2.21	0.41
1:K:137:MET:HE3	1:K:137:MET:HB3	2.01	0.41
2:m:25:ASP:O	2:m:29:MET:HG2	2.21	0.41
1:C:82:LEU:HD21	1:H:102:MET:HG3	2.03	0.41
1:C:146:VAL:CG2	1:C:212:CYS:HB3	2.50	0.41
1:K:165:LEU:HG	4:K:302:QBQ:C	2.51	0.41
1:S:117:LEU:HD11	1:S:171:ILE:HD11	2.03	0.41
1:G:221:MET:HE2	1:G:221:MET:HB2	1.83	0.41
1:K:116:VAL:HG11	1:K:174:ILE:HD11	2.02	0.41
1:R:116:VAL:HG11	1:R:174:ILE:HD11	2.02	0.41
2:c:34:ALA:O	2:c:35:SER:HB2	2.20	0.41
1:A:163:LEU:HD13	1:A:197:LEU:HD21	2.02	0.41
1:A:235:ARG:NH1	5:A:304:HBI:H71	2.36	0.41
1:E:221:MET:H	1:J:221:MET:HE1	1.85	0.41
1:E:248:ILE:HG13	1:E:249:ARG:HD2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:241:ARG:NH1	1:N:243:GLU:OE2	2.54	0.41
1:R:237:ASP:HB3	1:R:240:THR:HB	2.03	0.41
1:T:85:ASN:O	1:T:88:ARG:HG2	2.21	0.41
1:T:157:LEU:HD13	5:T:303:HBI:H112	2.02	0.41
1:T:163:LEU:HD23	1:T:168:LEU:CD2	2.50	0.41
2:h:25:ASP:O	2:h:29:MET:HG2	2.20	0.41
2:k:63:ARG:HA	2:k:63:ARG:HD3	1.78	0.41
2:s:8:THR:HG21	2:s:53:PRO:HG3	2.02	0.41
1:E:165:LEU:HG	4:E:302:QBQ:C	2.51	0.41
1:J:163:LEU:HD23	1:J:168:LEU:CD2	2.51	0.41
5:I:304:HBI:H112	1:J:157:LEU:HD13	2.02	0.40
1:K:221:MET:HE3	1:T:136:ASP:OD1	2.20	0.40
1:N:221:MET:HE3	1:Q:136:ASP:CG	2.46	0.40
1:S:62:GLU:O	1:S:65:GLU:HG3	2.21	0.40
2:k:66:ARG:HH21	2:l:82:HIS:CE1	2.39	0.40
1:F:137:MET:HB2	1:F:152:VAL:HG23	2.04	0.40
1:L:72:ALA:O	1:L:95:PRO:HB3	2.21	0.40
1:L:126:HIS:HB3	1:L:128:GLU:HG2	2.04	0.40
1:L:185:LEU:O	1:L:189:ILE:HG13	2.21	0.40
2:e:25:ASP:O	2:e:29:MET:HG2	2.22	0.40
2:t:63:ARG:HA	2:t:63:ARG:HD3	1.80	0.40
1:C:146:VAL:HG21	1:C:212:CYS:HB3	2.04	0.40
1:E:140:MET:HE2	1:E:147:PRO:HG3	2.04	0.40
1:F:116:VAL:HG21	1:F:174:ILE:HG12	2.03	0.40
1:K:167:LYS:N	1:K:167:LYS:HD3	2.35	0.40
1:L:93:LYS:HB2	1:L:97:ARG:CZ	2.52	0.40
2:i:25:ASP:O	2:i:29:MET:HG2	2.21	0.40
2:j:25:ASP:O	2:j:29:MET:HG2	2.21	0.40
2:k:25:ASP:O	2:k:29:MET:HG2	2.21	0.40
2:t:25:ASP:O	2:t:29:MET:HG2	2.21	0.40
1:D:200:ALA:CB	5:D:303:HBI:H111	2.52	0.40
1:S:198:ARG:HA	1:S:198:ARG:HD3	1.90	0.40
2:g:83:LYS:HE3	2:g:83:LYS:HB3	1.93	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	190/209 (91%)	187 (98%)	3 (2%)	0	100	100
1	B	190/209 (91%)	186 (98%)	4 (2%)	0	100	100
1	C	190/209 (91%)	186 (98%)	4 (2%)	0	100	100
1	D	190/209 (91%)	186 (98%)	4 (2%)	0	100	100
1	E	190/209 (91%)	184 (97%)	6 (3%)	0	100	100
1	F	190/209 (91%)	186 (98%)	4 (2%)	0	100	100
1	G	190/209 (91%)	185 (97%)	4 (2%)	1 (0%)	24	27
1	H	190/209 (91%)	185 (97%)	5 (3%)	0	100	100
1	I	190/209 (91%)	183 (96%)	7 (4%)	0	100	100
1	J	190/209 (91%)	186 (98%)	4 (2%)	0	100	100
1	K	190/209 (91%)	187 (98%)	3 (2%)	0	100	100
1	L	190/209 (91%)	188 (99%)	2 (1%)	0	100	100
1	M	190/209 (91%)	187 (98%)	3 (2%)	0	100	100
1	N	190/209 (91%)	183 (96%)	7 (4%)	0	100	100
1	O	190/209 (91%)	185 (97%)	5 (3%)	0	100	100
1	P	190/209 (91%)	184 (97%)	6 (3%)	0	100	100
1	Q	190/209 (91%)	185 (97%)	5 (3%)	0	100	100
1	R	190/209 (91%)	185 (97%)	4 (2%)	1 (0%)	24	27
1	S	190/209 (91%)	186 (98%)	4 (2%)	0	100	100
1	T	190/209 (91%)	185 (97%)	5 (3%)	0	100	100
2	a	82/87 (94%)	79 (96%)	2 (2%)	1 (1%)	10	8
2	b	82/87 (94%)	78 (95%)	3 (4%)	1 (1%)	10	8
2	c	82/87 (94%)	76 (93%)	3 (4%)	3 (4%)	2	1
2	d	82/87 (94%)	77 (94%)	4 (5%)	1 (1%)	10	8
2	e	82/87 (94%)	81 (99%)	0	1 (1%)	10	8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	f	81/87 (93%)	79 (98%)	1 (1%)	1 (1%)	10	8
2	g	82/87 (94%)	79 (96%)	2 (2%)	1 (1%)	10	8
2	h	82/87 (94%)	80 (98%)	1 (1%)	1 (1%)	10	8
2	i	82/87 (94%)	80 (98%)	1 (1%)	1 (1%)	10	8
2	j	82/87 (94%)	79 (96%)	2 (2%)	1 (1%)	10	8
2	k	82/87 (94%)	80 (98%)	1 (1%)	1 (1%)	10	8
2	l	82/87 (94%)	79 (96%)	2 (2%)	1 (1%)	10	8
2	m	82/87 (94%)	79 (96%)	2 (2%)	1 (1%)	10	8
2	n	82/87 (94%)	79 (96%)	2 (2%)	1 (1%)	10	8
2	o	82/87 (94%)	81 (99%)	0	1 (1%)	10	8
2	p	82/87 (94%)	79 (96%)	2 (2%)	1 (1%)	10	8
2	q	82/87 (94%)	80 (98%)	1 (1%)	1 (1%)	10	8
2	r	82/87 (94%)	81 (99%)	0	1 (1%)	10	8
2	s	82/87 (94%)	81 (99%)	0	1 (1%)	10	8
2	t	82/87 (94%)	80 (98%)	1 (1%)	1 (1%)	10	8
All	All	5439/5920 (92%)	5296 (97%)	119 (2%)	24 (0%)	30	34

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	a	11	ARG
2	b	11	ARG
2	c	11	ARG
2	c	35	SER
2	d	11	ARG
2	e	11	ARG
2	f	11	ARG
2	g	11	ARG
2	h	11	ARG
2	i	11	ARG
2	j	11	ARG
2	k	11	ARG
2	l	11	ARG
2	m	11	ARG
2	n	11	ARG
2	o	11	ARG
2	p	11	ARG

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Mol	Chain	Res	Type
2	q	11	ARG
2	r	11	ARG
2	s	11	ARG
2	t	11	ARG
1	G	125	ASP
2	c	14	VAL
1	R	123	ASP

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	169/181 (93%)	164 (97%)	5 (3%)	36	49
1	B	169/181 (93%)	164 (97%)	5 (3%)	36	49
1	C	169/181 (93%)	159 (94%)	10 (6%)	18	22
1	D	169/181 (93%)	160 (95%)	9 (5%)	20	26
1	E	169/181 (93%)	157 (93%)	12 (7%)	13	16
1	F	169/181 (93%)	162 (96%)	7 (4%)	27	37
1	G	169/181 (93%)	159 (94%)	10 (6%)	18	22
1	H	169/181 (93%)	163 (96%)	6 (4%)	31	42
1	I	169/181 (93%)	161 (95%)	8 (5%)	23	31
1	J	169/181 (93%)	162 (96%)	7 (4%)	27	37
1	K	169/181 (93%)	162 (96%)	7 (4%)	27	37
1	L	169/181 (93%)	162 (96%)	7 (4%)	27	37
1	M	169/181 (93%)	163 (96%)	6 (4%)	31	42
1	N	169/181 (93%)	162 (96%)	7 (4%)	27	37
1	O	169/181 (93%)	161 (95%)	8 (5%)	23	31
1	P	169/181 (93%)	163 (96%)	6 (4%)	31	42
1	Q	169/181 (93%)	161 (95%)	8 (5%)	23	31
1	R	169/181 (93%)	163 (96%)	6 (4%)	31	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	S	169/181 (93%)	161 (95%)	8 (5%)	23	31
1	T	169/181 (93%)	166 (98%)	3 (2%)	51	68
2	a	75/77 (97%)	72 (96%)	3 (4%)	28	38
2	b	75/77 (97%)	70 (93%)	5 (7%)	15	17
2	c	75/77 (97%)	66 (88%)	9 (12%)	5	4
2	d	75/77 (97%)	70 (93%)	5 (7%)	15	17
2	e	75/77 (97%)	70 (93%)	5 (7%)	15	17
2	f	74/77 (96%)	69 (93%)	5 (7%)	14	17
2	g	75/77 (97%)	72 (96%)	3 (4%)	28	38
2	h	75/77 (97%)	71 (95%)	4 (5%)	20	26
2	i	75/77 (97%)	71 (95%)	4 (5%)	20	26
2	j	75/77 (97%)	71 (95%)	4 (5%)	20	26
2	k	75/77 (97%)	72 (96%)	3 (4%)	28	38
2	l	75/77 (97%)	72 (96%)	3 (4%)	28	38
2	m	75/77 (97%)	71 (95%)	4 (5%)	20	26
2	n	75/77 (97%)	71 (95%)	4 (5%)	20	26
2	o	75/77 (97%)	72 (96%)	3 (4%)	28	38
2	p	75/77 (97%)	70 (93%)	5 (7%)	15	17
2	q	75/77 (97%)	70 (93%)	5 (7%)	15	17
2	r	75/77 (97%)	72 (96%)	3 (4%)	28	38
2	s	75/77 (97%)	70 (93%)	5 (7%)	15	17
2	t	75/77 (97%)	71 (95%)	4 (5%)	20	26
All	All	4879/5160 (95%)	4648 (95%)	231 (5%)	23	31

All (231) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	117	LEU
1	A	123	ASP
1	A	161	GLN
1	A	162	VAL
1	A	198	ARG
1	B	66	LEU
1	B	122	PHE

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Mol	Chain	Res	Type
1	B	166	SER
1	B	207	GLU
1	B	221	MET
1	C	66	LEU
1	C	89	GLN
1	C	111	GLU
1	C	114	SER
1	C	117	LEU
1	C	160	LYS
1	C	174	ILE
1	C	198	ARG
1	C	214	VAL
1	C	221	MET
1	D	66	LEU
1	D	89	GLN
1	D	112	THR
1	D	114	SER
1	D	117	LEU
1	D	122	PHE
1	D	139	SER
1	D	174	ILE
1	D	221	MET
1	E	66	LEU
1	E	89	GLN
1	E	114	SER
1	E	117	LEU
1	E	121	ILE
1	E	151	LYS
1	E	162	VAL
1	E	163	LEU
1	E	174	ILE
1	E	198	ARG
1	E	221	MET
1	E	249	ARG
1	F	100	SER
1	F	113	ILE
1	F	114	SER
1	F	123	ASP
1	F	162	VAL
1	F	198	ARG
1	F	242	GLU
1	G	66	LEU

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Mol	Chain	Res	Type
1	G	79	LEU
1	G	106	THR
1	G	116	VAL
1	G	123	ASP
1	G	141	CYS
1	G	162	VAL
1	G	198	ARG
1	G	214	VAL
1	G	221	MET
1	H	87	GLN
1	H	117	LEU
1	H	125	ASP
1	H	161	GLN
1	H	198	ARG
1	H	207	GLU
1	I	66	LEU
1	I	89	GLN
1	I	116	VAL
1	I	117	LEU
1	I	161	GLN
1	I	207	GLU
1	I	214	VAL
1	I	224	LYS
1	J	114	SER
1	J	117	LEU
1	J	123	ASP
1	J	151	LYS
1	J	198	ARG
1	J	207	GLU
1	J	221	MET
1	K	65	GLU
1	K	68	LEU
1	K	113	ILE
1	K	126	HIS
1	K	162	VAL
1	K	167	LYS
1	K	174	ILE
1	L	60	SER
1	L	114	SER
1	L	116	VAL
1	L	117	LEU
1	L	141	CYS

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Mol	Chain	Res	Type
1	L	207	GLU
1	L	221	MET
1	M	87	GLN
1	M	119	ASP
1	M	151	LYS
1	M	161	GLN
1	M	162	VAL
1	M	216	ARG
1	N	92	LEU
1	N	114	SER
1	N	117	LEU
1	N	125	ASP
1	N	159	ASN
1	N	207	GLU
1	N	221	MET
1	O	92	LEU
1	O	96	TRP
1	O	117	LEU
1	O	141	CYS
1	O	161	GLN
1	O	198	ARG
1	O	207	GLU
1	O	221	MET
1	P	61	GLU
1	P	88	ARG
1	P	112	THR
1	P	117	LEU
1	P	162	VAL
1	P	221	MET
1	Q	66	LEU
1	Q	112	THR
1	Q	117	LEU
1	Q	123	ASP
1	Q	161	GLN
1	Q	198	ARG
1	Q	221	MET
1	Q	249	ARG
1	R	93	LYS
1	R	114	SER
1	R	117	LEU
1	R	160	LYS
1	R	187	LYS

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Mol	Chain	Res	Type
1	R	221	MET
1	S	65	GLU
1	S	100	SER
1	S	114	SER
1	S	116	VAL
1	S	117	LEU
1	S	125	ASP
1	S	146	VAL
1	S	221	MET
1	T	89	GLN
1	T	111	GLU
1	T	117	LEU
2	a	10	ILE
2	a	30	GLN
2	a	77	LEU
2	b	10	ILE
2	b	28	LEU
2	b	30	GLN
2	b	61	GLU
2	b	77	LEU
2	c	10	ILE
2	c	11	ARG
2	c	32	LEU
2	c	36	LYS
2	c	55	ILE
2	c	56	VAL
2	c	61	GLU
2	c	63	ARG
2	c	83	LYS
2	d	8	THR
2	d	10	ILE
2	d	61	GLU
2	d	77	LEU
2	d	83	LYS
2	e	8	THR
2	e	10	ILE
2	e	23	GLN
2	e	63	ARG
2	e	77	LEU
2	f	10	ILE
2	f	30	GLN
2	f	61	GLU

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Mol	Chain	Res	Type
2	f	63	ARG
2	f	77	LEU
2	g	10	ILE
2	g	61	GLU
2	g	77	LEU
2	h	10	ILE
2	h	55	ILE
2	h	61	GLU
2	h	77	LEU
2	i	10	ILE
2	i	61	GLU
2	i	63	ARG
2	i	77	LEU
2	j	10	ILE
2	j	61	GLU
2	j	63	ARG
2	j	77	LEU
2	k	10	ILE
2	k	63	ARG
2	k	77	LEU
2	l	10	ILE
2	l	61	GLU
2	l	77	LEU
2	m	10	ILE
2	m	30	GLN
2	m	61	GLU
2	m	77	LEU
2	n	10	ILE
2	n	61	GLU
2	n	66	ARG
2	n	77	LEU
2	o	10	ILE
2	o	77	LEU
2	o	83	LYS
2	p	10	ILE
2	p	24	SER
2	p	38	ARG
2	p	61	GLU
2	p	77	LEU
2	q	10	ILE
2	q	61	GLU
2	q	63	ARG

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Mol	Chain	Res	Type
2	q	66	ARG
2	q	77	LEU
2	r	10	ILE
2	r	62	ARG
2	r	77	LEU
2	s	8	THR
2	s	10	ILE
2	s	61	GLU
2	s	77	LEU
2	s	84	GLU
2	t	10	ILE
2	t	61	GLU
2	t	63	ARG
2	t	77	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (105) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	ASN
1	B	70	ASN
1	B	161	GLN
1	C	67	ASN
1	C	70	ASN
1	C	126	HIS
1	C	143	HIS
1	C	161	GLN
1	E	70	ASN
1	E	143	HIS
1	E	219	GLN
1	F	70	ASN
1	F	126	HIS
1	F	161	GLN
1	F	180	GLN
1	F	188	GLN
1	F	219	GLN
1	G	64	ASN
1	G	67	ASN
1	G	70	ASN
1	G	126	HIS
1	G	161	GLN
1	H	67	ASN
1	H	70	ASN

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Mol	Chain	Res	Type
1	H	85	ASN
1	H	87	GLN
1	H	89	GLN
1	H	126	HIS
1	H	161	GLN
1	H	180	GLN
1	I	70	ASN
1	I	85	ASN
1	I	161	GLN
1	J	67	ASN
1	J	85	ASN
1	J	89	GLN
1	J	126	HIS
1	K	70	ASN
1	K	126	HIS
1	K	222	ASN
1	L	67	ASN
1	L	70	ASN
1	L	126	HIS
1	L	143	HIS
1	M	67	ASN
1	M	70	ASN
1	M	126	HIS
1	N	70	ASN
1	N	87	GLN
1	N	126	HIS
1	O	67	ASN
1	O	126	HIS
1	O	159	ASN
1	P	70	ASN
1	P	180	GLN
1	P	188	GLN
1	P	219	GLN
1	Q	70	ASN
1	Q	126	HIS
1	Q	219	GLN
1	R	67	ASN
1	R	70	ASN
1	R	85	ASN
1	R	126	HIS
1	S	70	ASN
1	S	87	GLN

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Mol	Chain	Res	Type
1	S	89	GLN
1	S	143	HIS
1	S	219	GLN
1	S	222	ASN
1	T	67	ASN
1	T	70	ASN
1	T	85	ASN
1	T	126	HIS
2	b	30	GLN
2	c	31	HIS
2	d	75	GLN
2	e	9	GLN
2	e	23	GLN
2	e	75	GLN
2	f	9	GLN
2	f	30	GLN
2	f	43	ASN
2	f	75	GLN
2	h	9	GLN
2	h	43	ASN
2	i	9	GLN
2	i	75	GLN
2	j	9	GLN
2	k	9	GLN
2	l	9	GLN
2	l	31	HIS
2	m	9	GLN
2	n	9	GLN
2	n	30	GLN
2	n	75	GLN
2	o	9	GLN
2	p	9	GLN
2	p	31	HIS
2	q	9	GLN
2	q	43	ASN
2	r	9	GLN
2	r	31	HIS
2	s	9	GLN
2	s	43	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 80 ligands modelled in this entry, 40 are monoatomic - leaving 40 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
4	QBQ	K	302	-	33,34,34	0.80	1 (3%)	47,54,54	0.67	0
5	HBI	Q	303	-	15,18,18	1.32	2 (13%)	14,26,26	1.23	2 (14%)
5	HBI	P	303	-	15,18,18	1.20	1 (6%)	14,26,26	1.44	3 (21%)
5	HBI	T	303	-	15,18,18	1.42	3 (20%)	14,26,26	1.20	2 (14%)
4	QBQ	J	302	-	33,34,34	0.47	0	47,54,54	0.79	0
4	QBQ	H	302	-	33,34,34	0.45	0	47,54,54	0.84	1 (2%)
5	HBI	F	303	-	15,18,18	1.35	1 (6%)	14,26,26	1.43	3 (21%)
4	QBQ	O	302	-	33,34,34	0.46	0	47,54,54	0.80	0
4	QBQ	A	302	-	33,34,34	0.46	0	47,54,54	0.84	0
4	QBQ	F	302	-	33,34,34	0.43	0	47,54,54	0.83	1 (2%)
4	QBQ	T	302	-	33,34,34	0.46	0	47,54,54	0.85	0
5	HBI	E	303	-	15,18,18	1.45	2 (13%)	14,26,26	1.36	2 (14%)
4	QBQ	S	302	-	33,34,34	0.44	0	47,54,54	0.82	1 (2%)
5	HBI	L	303	-	15,18,18	1.45	4 (26%)	14,26,26	1.68	4 (28%)
5	HBI	M	303	-	15,18,18	1.53	2 (13%)	14,26,26	1.36	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	HBI	D	303	-	15,18,18	1.38	3 (20%)	14,26,26	1.38	4 (28%)
4	QBQ	L	302	-	33,34,34	0.48	0	47,54,54	0.86	0
4	QBQ	D	302	-	33,34,34	0.44	0	47,54,54	0.81	0
5	HBI	A	303	-	15,18,18	1.16	2 (13%)	14,26,26	1.21	2 (14%)
4	QBQ	M	302	-	33,34,34	0.48	0	47,54,54	0.80	0
5	HBI	G	303	-	15,18,18	1.16	2 (13%)	14,26,26	1.49	4 (28%)
4	QBQ	I	302	-	33,34,34	0.46	0	47,54,54	0.81	1 (2%)
5	HBI	S	303	-	15,18,18	1.33	1 (6%)	14,26,26	1.20	1 (7%)
5	HBI	L	304	-	15,18,18	1.30	2 (13%)	14,26,26	1.48	4 (28%)
4	QBQ	E	302	-	33,34,34	0.93	1 (3%)	47,54,54	0.68	0
4	QBQ	Q	302	-	33,34,34	0.93	2 (6%)	47,54,54	0.72	0
5	HBI	O	303	-	15,18,18	1.50	3 (20%)	14,26,26	1.29	2 (14%)
4	QBQ	P	302	-	33,34,34	0.50	0	47,54,54	0.88	0
5	HBI	B	303	-	15,18,18	1.31	3 (20%)	14,26,26	1.30	3 (21%)
4	QBQ	C	302	-	33,34,34	0.42	0	47,54,54	0.74	0
5	HBI	I	304	-	15,18,18	1.44	2 (13%)	14,26,26	1.43	4 (28%)
4	QBQ	B	302	-	33,34,34	1.22	3 (9%)	47,54,54	0.77	1 (2%)
5	HBI	I	303	-	15,18,18	1.25	2 (13%)	14,26,26	1.33	2 (14%)
5	HBI	H	303	-	15,18,18	1.19	3 (20%)	14,26,26	1.26	2 (14%)
5	HBI	A	304	-	15,18,18	1.26	2 (13%)	14,26,26	1.65	4 (28%)
4	QBQ	G	302	-	33,34,34	0.43	0	47,54,54	0.80	0
5	HBI	R	303	-	15,18,18	1.41	2 (13%)	14,26,26	1.36	2 (14%)
5	HBI	K	303	-	15,18,18	1.29	2 (13%)	14,26,26	1.24	2 (14%)
4	QBQ	N	302	-	33,34,34	1.02	2 (6%)	47,54,54	0.70	0
4	QBQ	R	302	-	33,34,34	0.49	0	47,54,54	0.76	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
4	QBQ	K	302	-	-	8/22/38/38	0/3/3/3
5	HBI	Q	303	-	-	0/4/17/17	0/2/2/2
5	HBI	P	303	-	-	0/4/17/17	0/2/2/2
5	HBI	T	303	-	-	0/4/17/17	0/2/2/2
4	QBQ	J	302	-	-	6/22/38/38	0/3/3/3
4	QBQ	H	302	-	-	2/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	HBI	F	303	-	-	0/4/17/17	0/2/2/2
4	QBQ	O	302	-	-	5/22/38/38	0/3/3/3
4	QBQ	A	302	-	-	5/22/38/38	0/3/3/3
4	QBQ	F	302	-	-	5/22/38/38	0/3/3/3
4	QBQ	T	302	-	-	5/22/38/38	0/3/3/3
5	HBI	E	303	-	-	0/4/17/17	0/2/2/2
4	QBQ	S	302	-	-	5/22/38/38	0/3/3/3
5	HBI	L	303	-	-	0/4/17/17	0/2/2/2
5	HBI	M	303	-	-	0/4/17/17	0/2/2/2
5	HBI	D	303	-	-	0/4/17/17	0/2/2/2
4	QBQ	L	302	-	-	4/22/38/38	0/3/3/3
4	QBQ	D	302	-	-	5/22/38/38	0/3/3/3
5	HBI	A	303	-	-	0/4/17/17	0/2/2/2
4	QBQ	M	302	-	-	4/22/38/38	0/3/3/3
5	HBI	G	303	-	-	0/4/17/17	0/2/2/2
4	QBQ	I	302	-	-	2/22/38/38	0/3/3/3
5	HBI	S	303	-	-	0/4/17/17	0/2/2/2
5	HBI	L	304	-	-	0/4/17/17	0/2/2/2
4	QBQ	E	302	-	-	6/22/38/38	0/3/3/3
4	QBQ	Q	302	-	-	11/22/38/38	0/3/3/3
5	HBI	O	303	-	-	0/4/17/17	0/2/2/2
4	QBQ	P	302	-	-	6/22/38/38	0/3/3/3
5	HBI	B	303	-	-	0/4/17/17	0/2/2/2
4	QBQ	C	302	-	-	7/22/38/38	0/3/3/3
5	HBI	I	304	-	-	0/4/17/17	0/2/2/2
4	QBQ	B	302	-	-	6/22/38/38	0/3/3/3
5	HBI	I	303	-	-	0/4/17/17	0/2/2/2
5	HBI	H	303	-	-	0/4/17/17	0/2/2/2
5	HBI	A	304	-	-	0/4/17/17	0/2/2/2
4	QBQ	G	302	-	-	5/22/38/38	0/3/3/3
5	HBI	R	303	-	-	0/4/17/17	0/2/2/2
5	HBI	K	303	-	-	0/4/17/17	0/2/2/2
4	QBQ	N	302	-	-	4/22/38/38	0/3/3/3
4	QBQ	R	302	-	-	3/22/38/38	0/3/3/3

All (53) bond length outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	303	HBI	C4-N3	3.99	1.46	1.38
5	F	303	HBI	C4-N3	3.62	1.45	1.38
5	K	303	HBI	C8A-N1	3.55	1.41	1.36
4	B	302	QBQ	P2-O10	-3.55	1.39	1.50
5	I	304	HBI	C4-N3	3.48	1.45	1.38
5	R	303	HBI	C4-N3	3.47	1.45	1.38
5	M	303	HBI	C4-N3	3.41	1.45	1.38
5	D	303	HBI	C4-N3	3.19	1.44	1.38
5	O	303	HBI	C8A-N1	3.13	1.41	1.36
5	T	303	HBI	C8A-N1	3.10	1.41	1.36
5	I	304	HBI	C8A-N1	3.09	1.40	1.36
5	P	303	HBI	C4-N3	3.08	1.44	1.38
4	N	302	QBQ	P2-O10	-3.07	1.40	1.50
5	L	304	HBI	C4-N3	3.07	1.44	1.38
5	L	303	HBI	C4-N3	3.01	1.44	1.38
5	Q	303	HBI	C8A-N1	2.99	1.40	1.36
5	B	303	HBI	C8A-N1	2.99	1.40	1.36
4	E	302	QBQ	P2-O10	-2.98	1.41	1.50
5	R	303	HBI	C8A-N1	2.95	1.40	1.36
5	S	303	HBI	C8A-N1	2.94	1.40	1.36
5	Q	303	HBI	C4-N3	2.93	1.44	1.38
5	A	304	HBI	C4-N3	2.80	1.44	1.38
5	E	303	HBI	C8A-N1	2.79	1.40	1.36
5	I	303	HBI	C4-N3	2.78	1.44	1.38
5	O	303	HBI	C4-N3	2.72	1.43	1.38
4	B	302	QBQ	P2-O9	-2.72	1.44	1.54
4	Q	302	QBQ	P2-O10	-2.64	1.42	1.50
5	D	303	HBI	C2-N2	2.63	1.40	1.34
5	T	303	HBI	C4-N3	2.62	1.43	1.38
5	M	303	HBI	C4A-N5	2.57	1.43	1.37
4	B	302	QBQ	C2-C1	-2.55	1.38	1.45
5	H	303	HBI	C2-N2	2.55	1.40	1.34
5	G	303	HBI	C4-N3	2.46	1.43	1.38
5	L	303	HBI	O4-C4	-2.33	1.19	1.23
5	L	304	HBI	C8A-N1	2.29	1.39	1.36
5	D	303	HBI	C8A-N1	2.27	1.39	1.36
5	I	303	HBI	C8A-N1	2.24	1.39	1.36
5	A	303	HBI	C2-N2	2.23	1.39	1.34
5	L	303	HBI	C2-N2	2.23	1.39	1.34
4	N	302	QBQ	C2-C1	-2.20	1.39	1.45
5	L	303	HBI	C8A-N1	2.19	1.39	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	303	HBI	C8A-N1	2.19	1.39	1.36
5	B	303	HBI	C4A-N5	2.16	1.42	1.37
4	Q	302	QBQ	C2-C1	-2.11	1.39	1.45
5	H	303	HBI	C4-N3	2.10	1.42	1.38
5	B	303	HBI	C4-N3	2.08	1.42	1.38
5	A	303	HBI	C4-N3	2.07	1.42	1.38
5	O	303	HBI	C2-N2	2.04	1.39	1.34
5	A	304	HBI	C4A-N5	2.03	1.41	1.37
5	K	303	HBI	C4-N3	2.03	1.42	1.38
5	T	303	HBI	C2-N2	2.01	1.38	1.34
5	H	303	HBI	C8A-N1	2.01	1.39	1.36
4	K	302	QBQ	C2-C1	-2.01	1.40	1.45

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	304	HBI	O4-C4-N3	-3.09	114.30	120.11
5	L	303	HBI	N2-C2-N3	2.91	122.90	116.76
5	L	303	HBI	N2-C2-N1	-2.78	114.24	119.67
5	G	303	HBI	O4-C4-N3	-2.75	114.94	120.11
5	I	303	HBI	O4-C4-N3	-2.63	115.16	120.11
5	L	303	HBI	O4-C4-N3	-2.59	115.24	120.11
5	M	303	HBI	N2-C2-N1	-2.56	114.67	119.67
5	T	303	HBI	O4-C4-N3	-2.56	115.30	120.11
5	F	303	HBI	N2-C2-N1	-2.52	114.75	119.67
5	B	303	HBI	O4-C4-N3	-2.48	115.45	120.11
5	Q	303	HBI	O4-C4-N3	-2.47	115.47	120.11
5	P	303	HBI	O9-C9-C6	2.46	113.98	109.00
5	K	303	HBI	O4-C4-N3	-2.44	115.53	120.11
5	L	303	HBI	O9-C9-C6	2.44	113.94	109.00
5	L	304	HBI	N2-C2-N1	-2.42	114.94	119.67
5	L	304	HBI	O4-C4-N3	-2.42	115.57	120.11
5	A	304	HBI	N2-C2-N1	-2.40	114.99	119.67
5	R	303	HBI	O9-C9-C6	2.37	113.81	109.00
5	I	304	HBI	O9-C9-C6	2.34	113.75	109.00
5	D	303	HBI	O9-C9-C6	2.34	113.73	109.00
5	H	303	HBI	O4-C4-N3	-2.33	115.73	120.11
5	R	303	HBI	N2-C2-N1	-2.33	115.12	119.67
5	P	303	HBI	N2-C2-N1	-2.30	115.17	119.67
5	S	303	HBI	O4-C4-N3	-2.30	115.79	120.11
5	O	303	HBI	O4-C4-N3	-2.29	115.80	120.11
5	G	303	HBI	N2-C2-N1	-2.28	115.22	119.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	302	QBQ	C10-C2-C1	-2.27	116.94	118.35
5	A	303	HBI	O4-C4-N3	-2.27	115.85	120.11
5	A	304	HBI	C2-N3-C4	-2.23	121.06	125.11
5	F	303	HBI	N2-C2-N3	2.23	121.47	116.76
5	G	303	HBI	O9-C9-C6	2.23	113.51	109.00
5	A	303	HBI	O9-C9-C6	2.22	113.50	109.00
5	I	304	HBI	O4-C4-N3	-2.22	115.95	120.11
5	I	304	HBI	N2-C2-N1	-2.21	115.36	119.67
5	B	303	HBI	O9-C9-C6	2.21	113.47	109.00
5	I	303	HBI	O9-C9-C6	2.20	113.47	109.00
4	F	302	QBQ	C10-C2-C1	-2.20	116.99	118.35
5	L	304	HBI	C2-N3-C4	-2.20	121.13	125.11
5	T	303	HBI	O9-C9-C6	2.16	113.37	109.00
5	I	304	HBI	C2-N3-C4	-2.15	121.22	125.11
5	L	304	HBI	O9-C9-C6	2.14	113.34	109.00
5	E	303	HBI	N2-C2-N1	-2.14	115.50	119.67
5	H	303	HBI	O9-C9-C6	2.13	113.32	109.00
5	O	303	HBI	N2-C2-N1	-2.13	115.52	119.67
4	S	302	QBQ	C10-C2-C1	-2.12	117.03	118.35
5	F	303	HBI	O9-C9-C6	2.12	113.30	109.00
5	E	303	HBI	O9-C9-C6	2.12	113.29	109.00
5	G	303	HBI	C2-N3-C4	-2.10	121.30	125.11
5	B	303	HBI	C2-N3-C4	-2.08	121.34	125.11
5	D	303	HBI	N2-C2-N1	-2.08	115.62	119.67
5	D	303	HBI	O4-C4-N3	-2.05	116.26	120.11
5	P	303	HBI	C2-N3-C4	-2.05	121.40	125.11
4	I	302	QBQ	C10-C2-C1	-2.05	117.08	118.35
4	B	302	QBQ	C6-O-C5	-2.04	104.95	109.47
5	A	304	HBI	O9-C9-C6	2.04	113.13	109.00
5	D	303	HBI	N2-C2-N3	2.03	121.05	116.76
5	Q	303	HBI	O9-C9-C6	2.01	113.06	109.00
5	K	303	HBI	O9-C9-C6	2.00	113.06	109.00

There are no chirality outliers.

All (104) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	302	QBQ	P1-O7-P2-O8
4	B	302	QBQ	P1-O7-P2-O8
4	C	302	QBQ	P1-O7-P2-O8
4	C	302	QBQ	P1-O7-P2-O9
4	D	302	QBQ	P1-O7-P2-O8

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Mol	Chain	Res	Type	Atoms
4	E	302	QBQ	C7-O1-P-O3
4	F	302	QBQ	P1-O7-P2-O8
4	G	302	QBQ	P1-O7-P2-O8
4	H	302	QBQ	P1-O7-P2-O9
4	J	302	QBQ	P1-O7-P2-O8
4	K	302	QBQ	P1-O7-P2-O8
4	K	302	QBQ	C7-O1-P-O3
4	L	302	QBQ	P1-O7-P2-O8
4	M	302	QBQ	P1-O7-P2-O8
4	O	302	QBQ	P1-O7-P2-O8
4	P	302	QBQ	P1-O7-P2-O8
4	P	302	QBQ	P1-O7-P2-O9
4	Q	302	QBQ	P1-O7-P2-O8
4	R	302	QBQ	P1-O7-P2-O8
4	R	302	QBQ	P1-O7-P2-O9
4	S	302	QBQ	P1-O7-P2-O8
4	T	302	QBQ	P1-O7-P2-O8
4	Q	302	QBQ	C8-C6-C7-O1
4	Q	302	QBQ	O-C6-C7-O1
4	A	302	QBQ	P1-O4-P-O3
4	B	302	QBQ	P1-O4-P-O3
4	D	302	QBQ	P1-O4-P-O3
4	I	302	QBQ	P1-O4-P-O3
4	J	302	QBQ	P1-O4-P-O3
4	M	302	QBQ	P1-O4-P-O3
4	T	302	QBQ	P1-O4-P-O3
4	E	302	QBQ	O-C6-C7-O1
4	P	302	QBQ	O-C6-C7-O1
4	T	302	QBQ	P1-O7-P2-O10
4	B	302	QBQ	P1-O7-P2-O9
4	O	302	QBQ	P1-O7-P2-O9
4	Q	302	QBQ	P1-O7-P2-O9
4	S	302	QBQ	P1-O7-P2-O9
4	K	302	QBQ	O-C6-C7-O1
4	C	302	QBQ	P1-O4-P-O2
4	E	302	QBQ	P1-O4-P-O2
4	O	302	QBQ	P1-O4-P-O3
4	S	302	QBQ	P1-O4-P-O3
4	K	302	QBQ	C9-C5-N2-C4
4	P	302	QBQ	C7-O1-P-O3
4	Q	302	QBQ	C7-O1-P-O3
4	Q	302	QBQ	C7-O1-P-O4

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Mol	Chain	Res	Type	Atoms
4	Q	302	QBQ	C7-O1-P-O2
4	A	302	QBQ	P1-O4-P-O2
4	D	302	QBQ	P1-O4-P-O2
4	I	302	QBQ	P1-O4-P-O2
4	K	302	QBQ	P1-O4-P-O2
4	L	302	QBQ	P1-O4-P-O3
4	N	302	QBQ	P1-O4-P-O2
4	Q	302	QBQ	P1-O4-P-O2
4	T	302	QBQ	P1-O4-P-O2
4	A	302	QBQ	C9-C5-N2-C4
4	D	302	QBQ	C9-C5-N2-C4
4	E	302	QBQ	C9-C5-N2-C4
4	J	302	QBQ	C9-C5-N2-C4
4	Q	302	QBQ	C9-C5-N2-C4
4	C	302	QBQ	C9-C5-N2-C4
4	T	302	QBQ	C9-C5-N2-C4
4	B	302	QBQ	P1-O4-P-O2
4	G	302	QBQ	P1-O4-P-O3
4	J	302	QBQ	P1-O4-P-O2
4	S	302	QBQ	P1-O4-P-O2
4	E	302	QBQ	C8-C6-C7-O1
4	B	302	QBQ	P1-O7-P2-O10
4	F	302	QBQ	P1-O7-P2-O10
4	K	302	QBQ	P1-O7-P2-O10
4	Q	302	QBQ	P1-O7-P2-O10
4	S	302	QBQ	P1-O7-P2-O10
4	D	302	QBQ	P1-O7-P2-O9
4	F	302	QBQ	P1-O7-P2-O9
4	G	302	QBQ	P1-O7-P2-O9
4	J	302	QBQ	P1-O7-P2-O9
4	K	302	QBQ	P1-O7-P2-O9
4	L	302	QBQ	P1-O7-P2-O9
4	M	302	QBQ	P1-O7-P2-O9
4	N	302	QBQ	C9-C5-N2-C4
4	H	302	QBQ	O-C6-C7-O1
4	E	302	QBQ	P1-O4-P-O3
4	G	302	QBQ	P1-O4-P-O2
4	L	302	QBQ	P1-O4-P-O2
4	M	302	QBQ	P1-O4-P-O2
4	O	302	QBQ	P1-O4-P-O2
4	Q	302	QBQ	P1-O4-P-O3
4	R	302	QBQ	P1-O4-P-O2

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Mol	Chain	Res	Type	Atoms
4	B	302	QBQ	C9-C5-N2-C4
4	P	302	QBQ	C8-C6-C7-O1
4	A	302	QBQ	P1-O7-P2-O10
4	C	302	QBQ	P1-O7-P2-O10
4	J	302	QBQ	P1-O7-P2-O10
4	O	302	QBQ	P1-O7-P2-O10
4	F	302	QBQ	C9-C5-N2-C4
4	G	302	QBQ	C9-C5-N2-C4
4	P	302	QBQ	C9-C5-N2-C4
4	F	302	QBQ	O-C6-C7-O1
4	K	302	QBQ	C8-C6-C7-O1
4	N	302	QBQ	O-C6-C7-O1
4	C	302	QBQ	P1-O4-P-O3
4	N	302	QBQ	P1-O4-P-O3
4	C	302	QBQ	O-C6-C7-O1

There are no ring outliers.

27 monomers are involved in 48 short contacts:

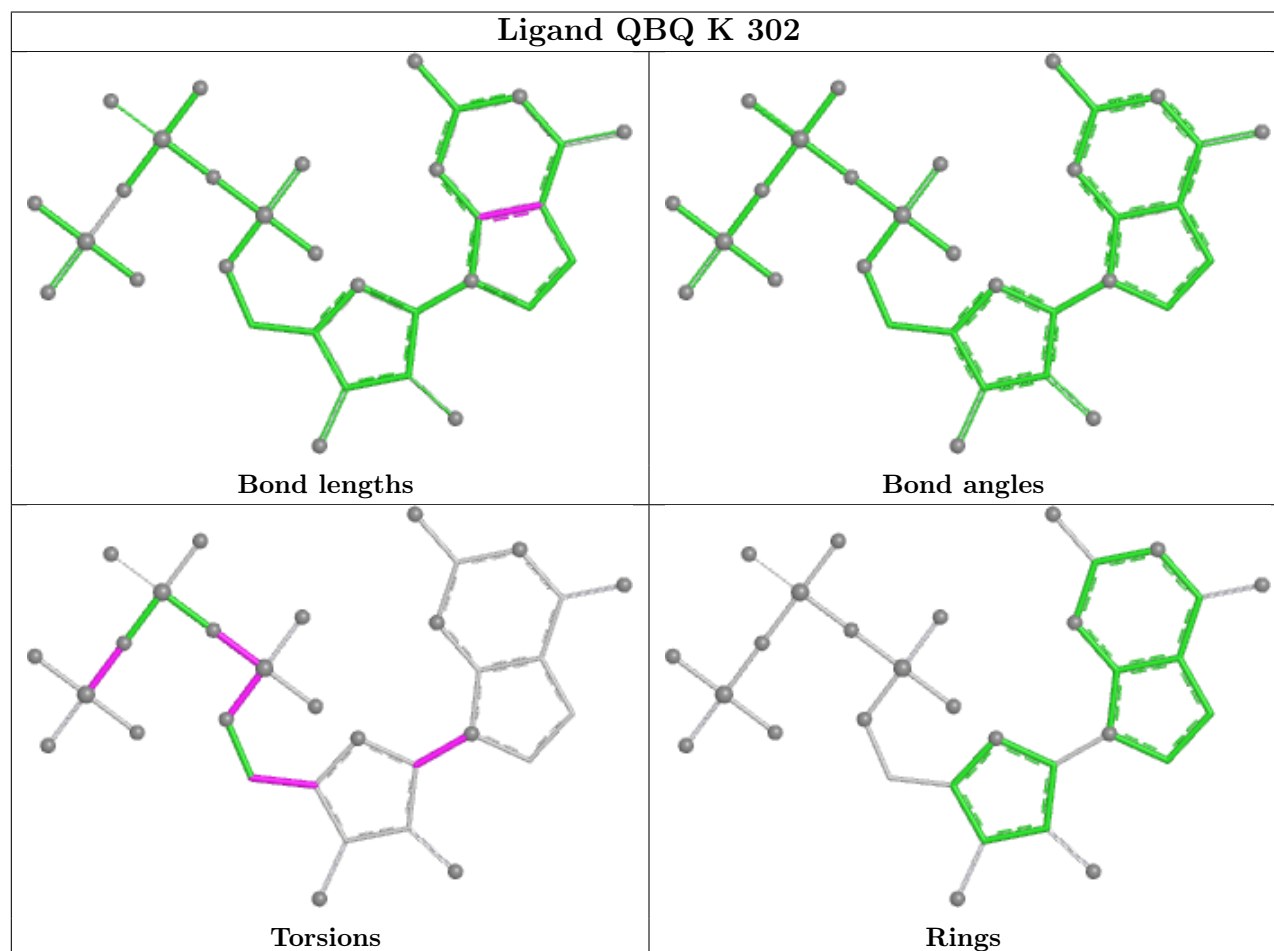
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	K	302	QBQ	1	0
5	Q	303	HBI	1	0
5	P	303	HBI	4	0
5	T	303	HBI	3	0
4	J	302	QBQ	1	0
4	H	302	QBQ	1	0
4	A	302	QBQ	1	0
4	T	302	QBQ	1	0
5	E	303	HBI	2	0
4	S	302	QBQ	2	0
5	L	303	HBI	4	0
5	D	303	HBI	2	0
4	L	302	QBQ	1	0
5	A	303	HBI	2	0
5	G	303	HBI	2	0
4	I	302	QBQ	1	0
5	S	303	HBI	2	0
4	E	302	QBQ	2	0
5	O	303	HBI	2	0
5	B	303	HBI	1	0
5	I	304	HBI	1	0
5	I	303	HBI	1	0

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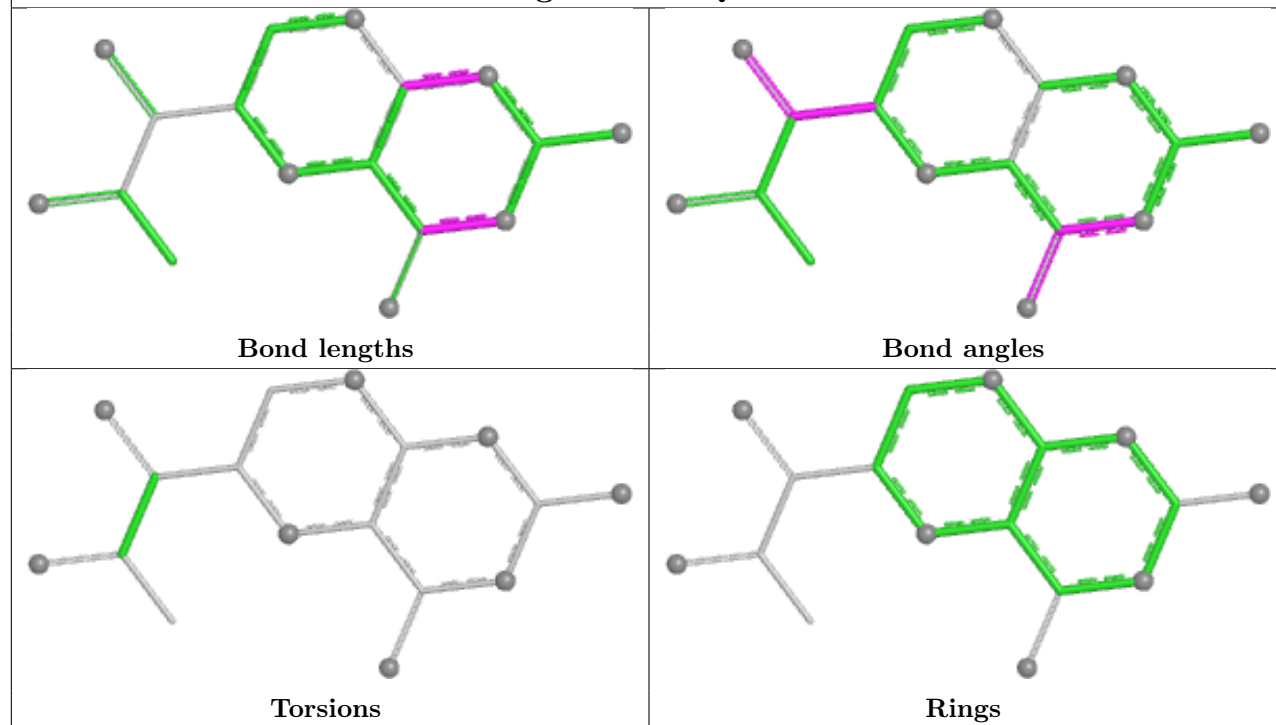
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	H	303	HBI	1	0
5	A	304	HBI	3	0
4	G	302	QBQ	1	0
5	R	303	HBI	3	0
5	K	303	HBI	2	0

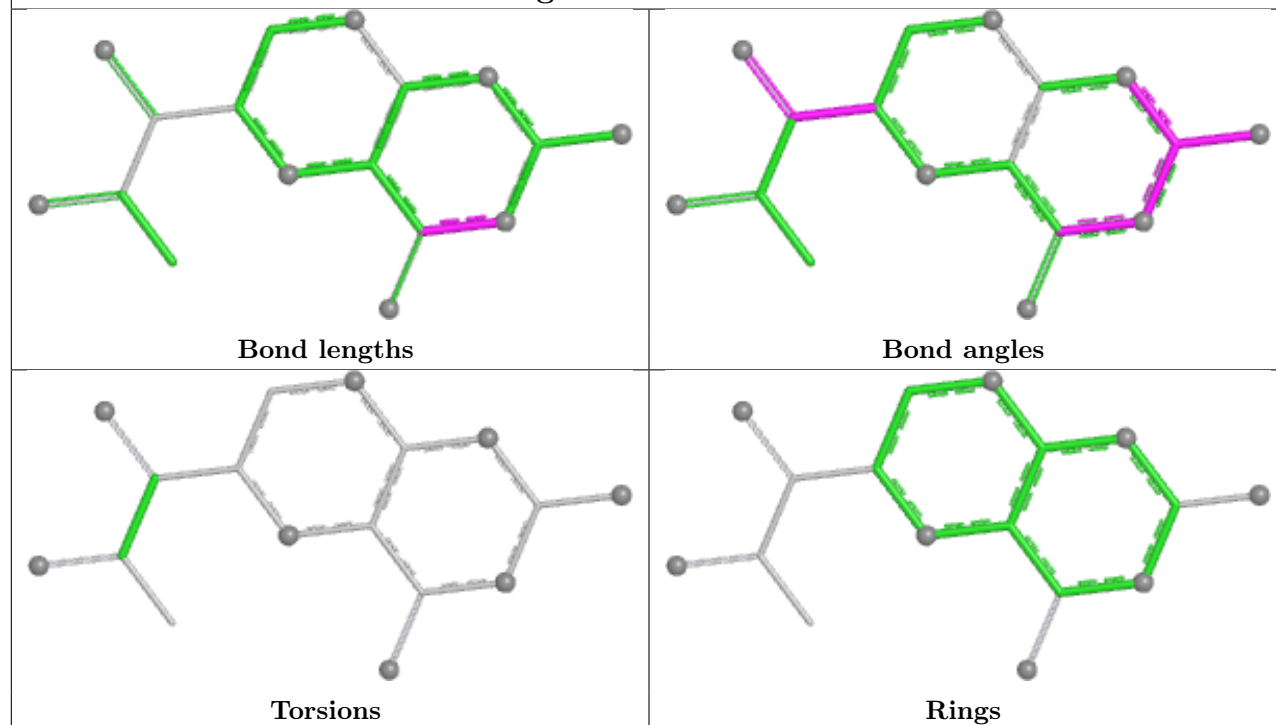
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



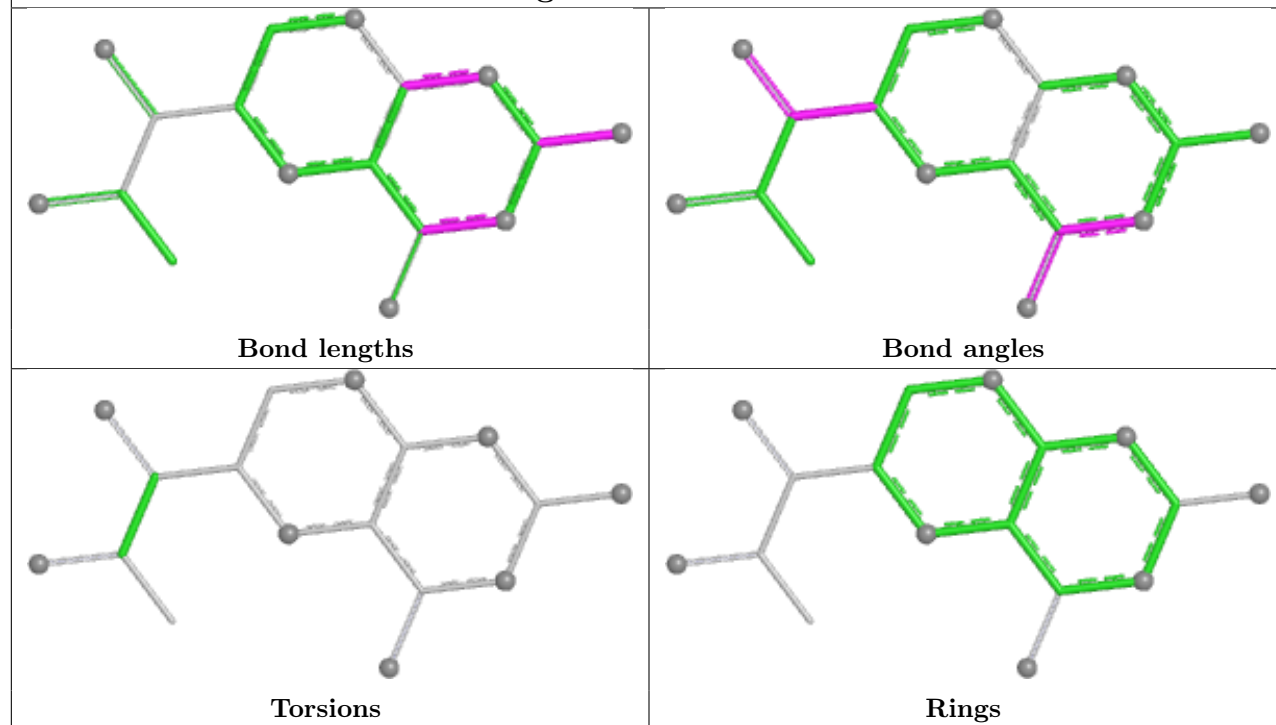
Ligand HBI Q 303



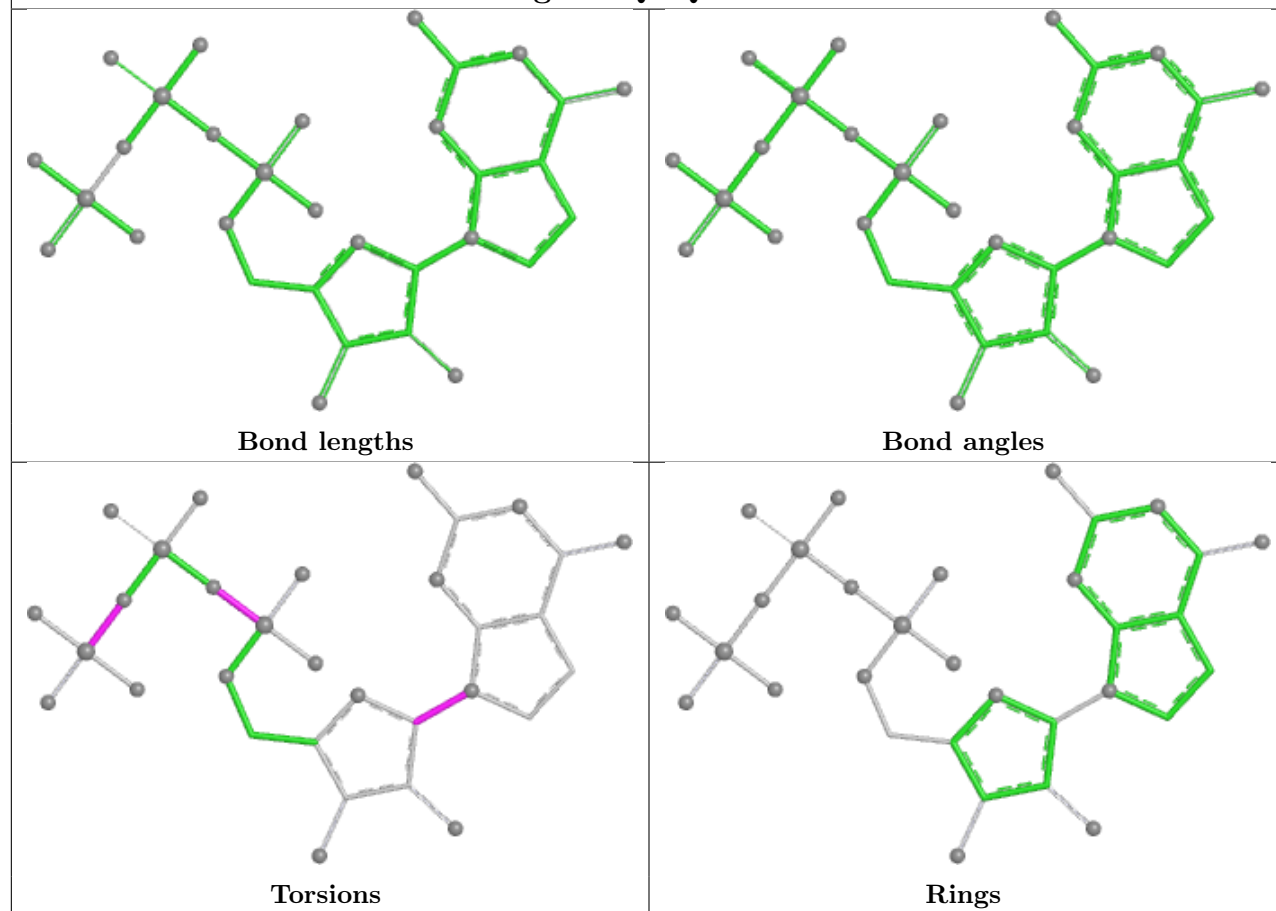
Ligand HBI P 303

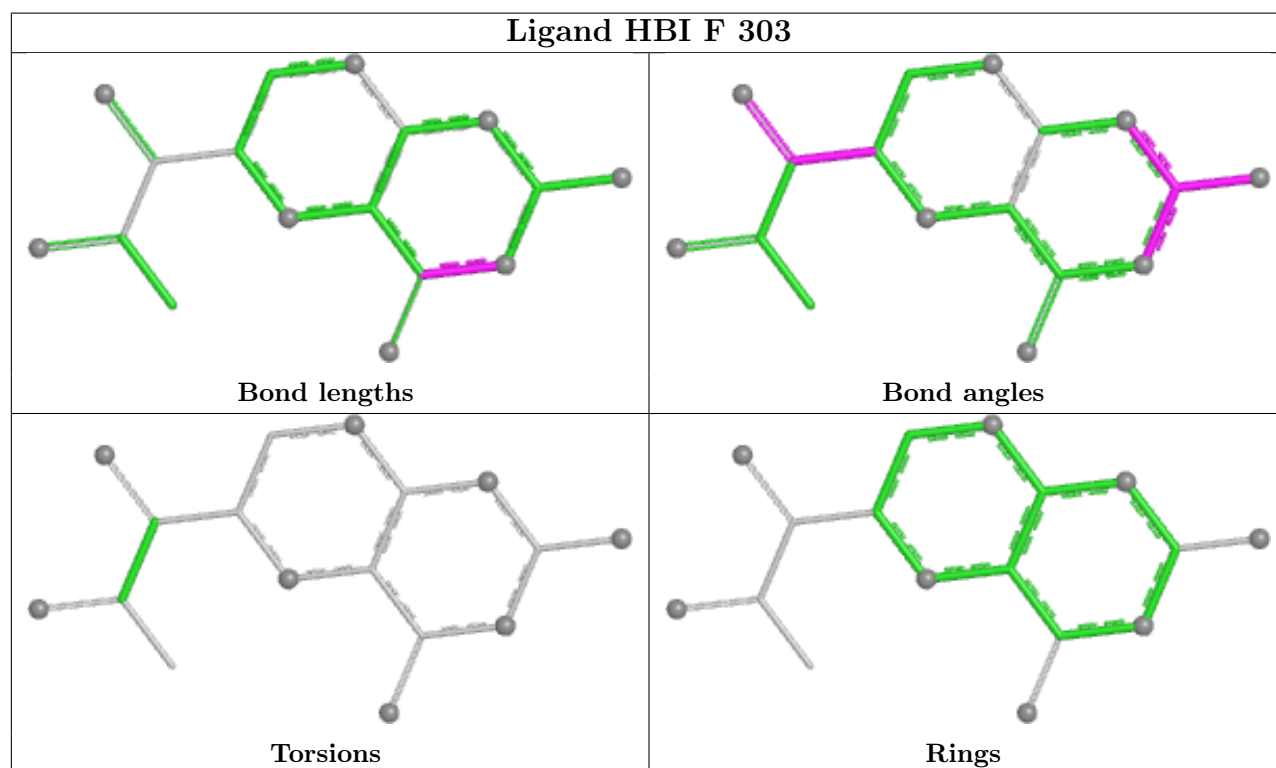
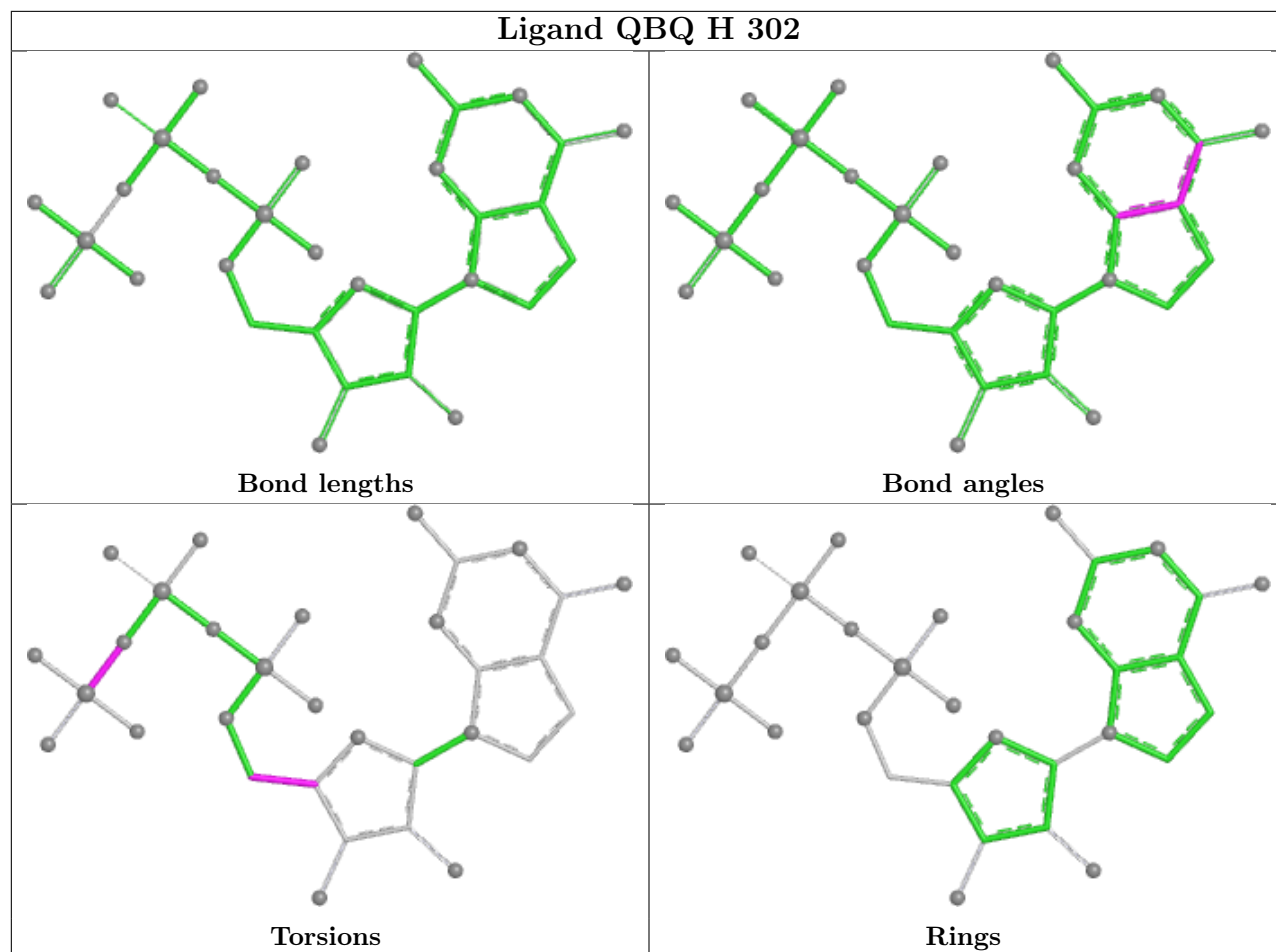


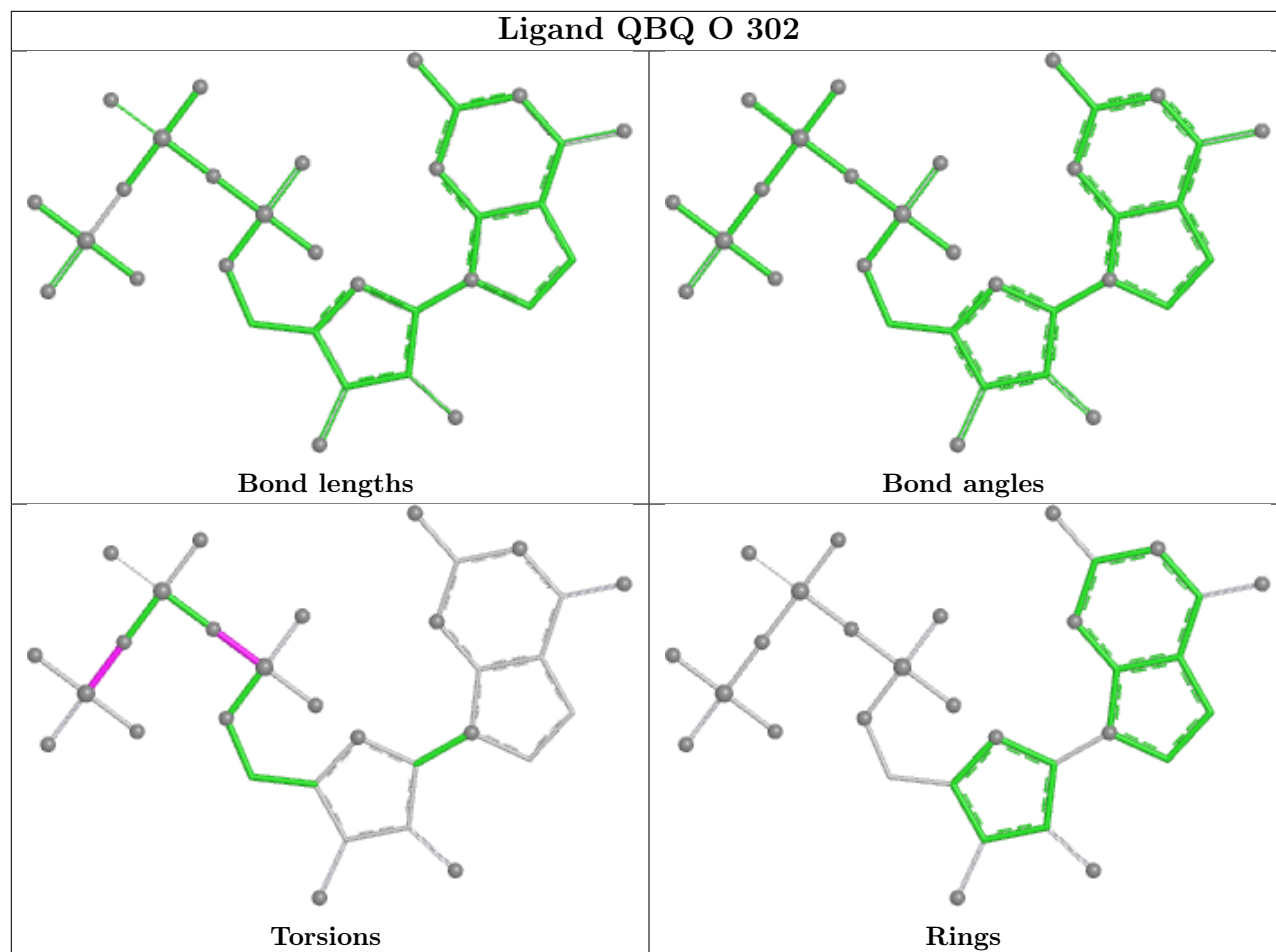
Ligand HBI T 303

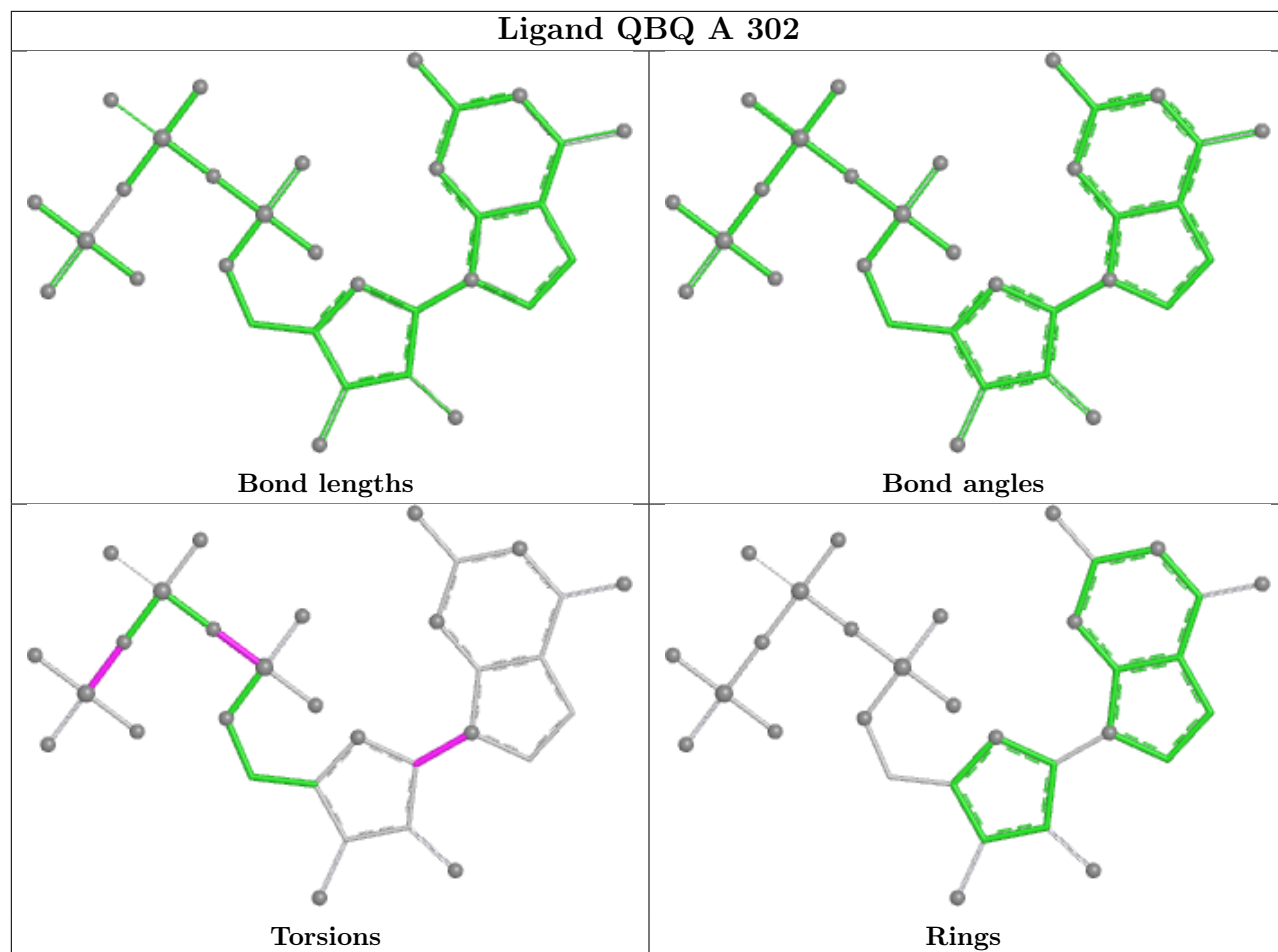


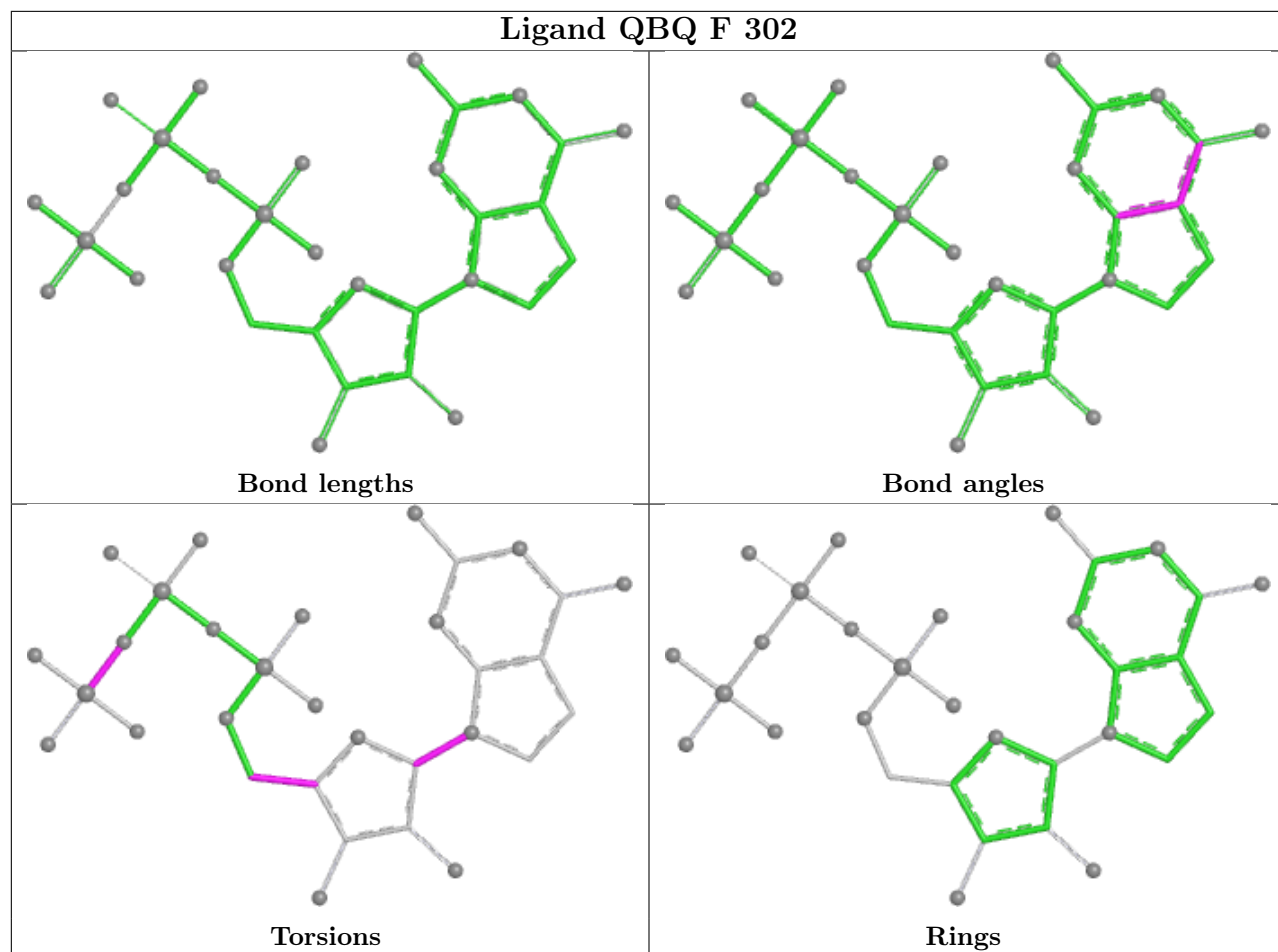
Ligand QBQ J 302

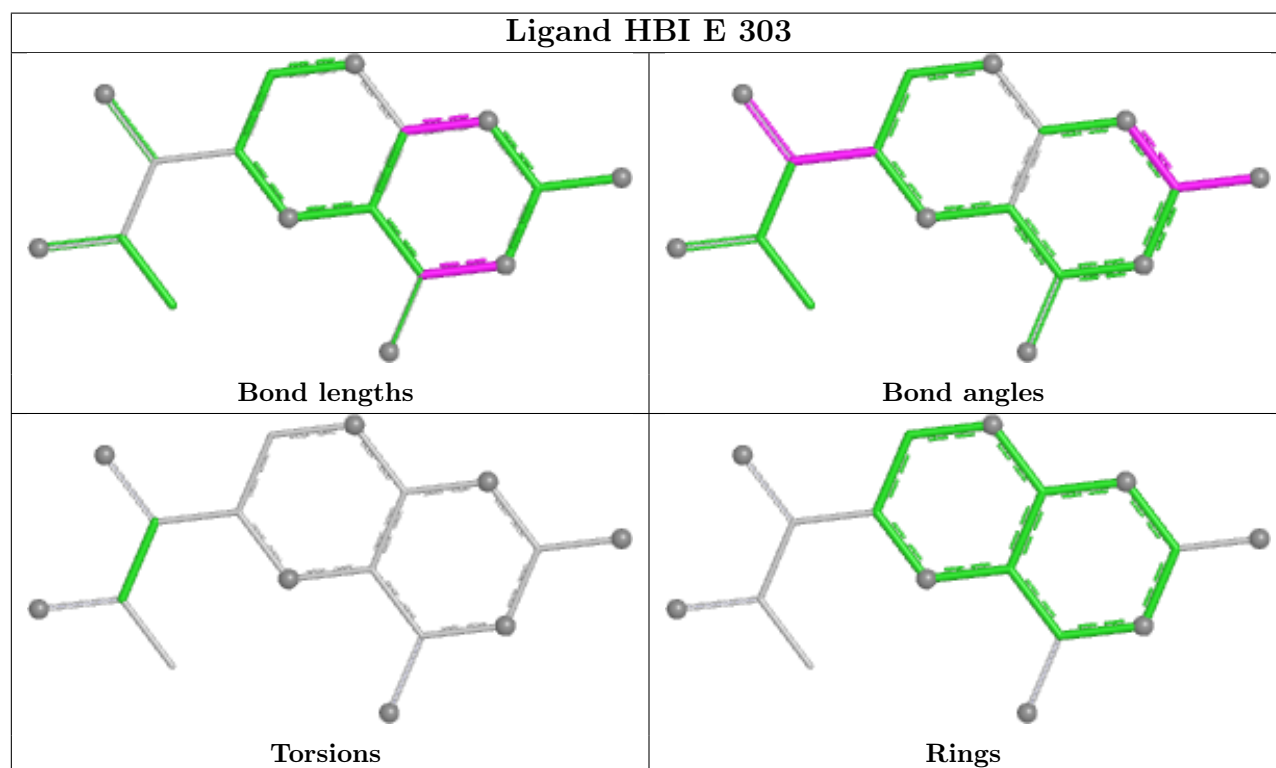
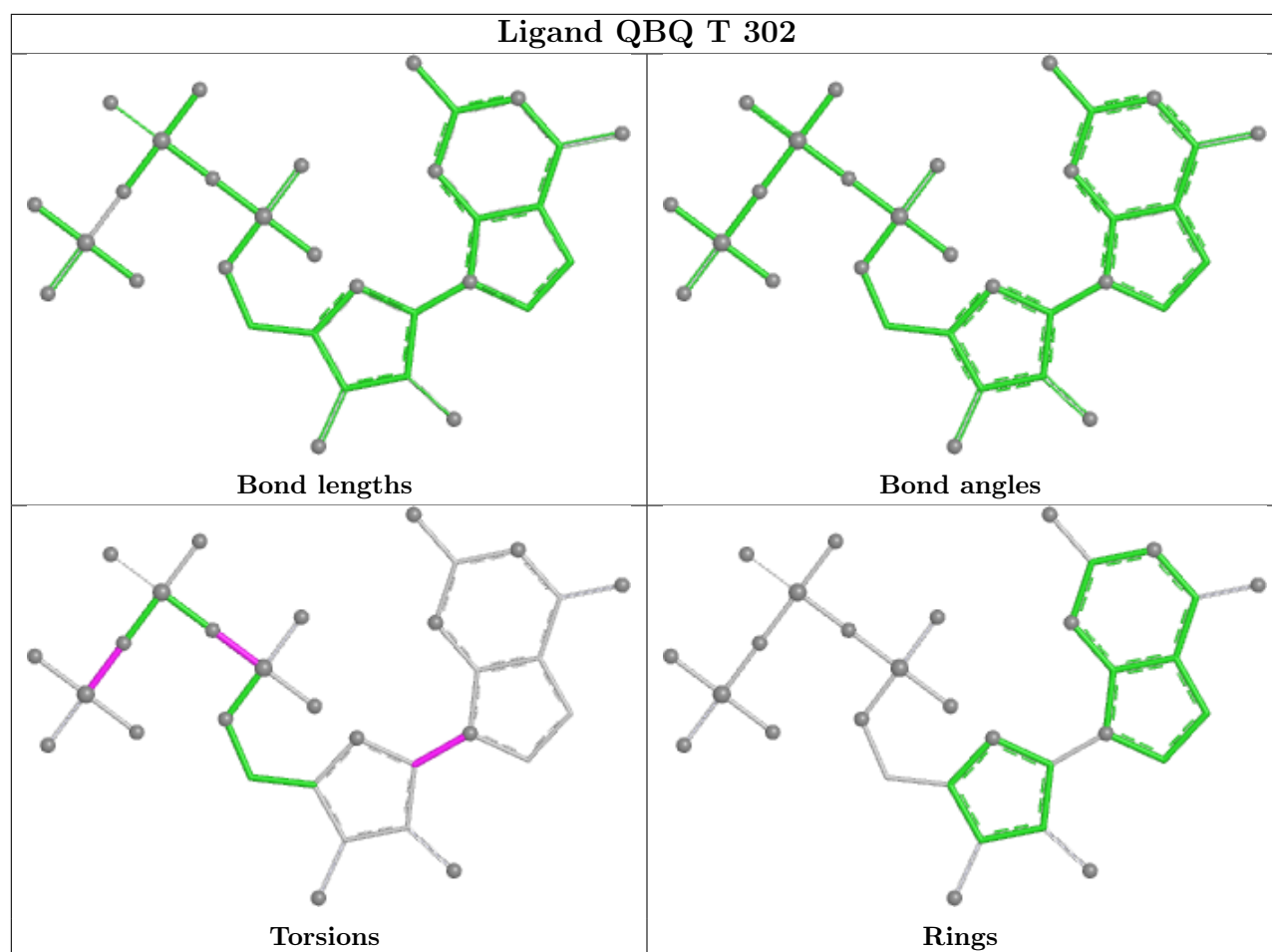




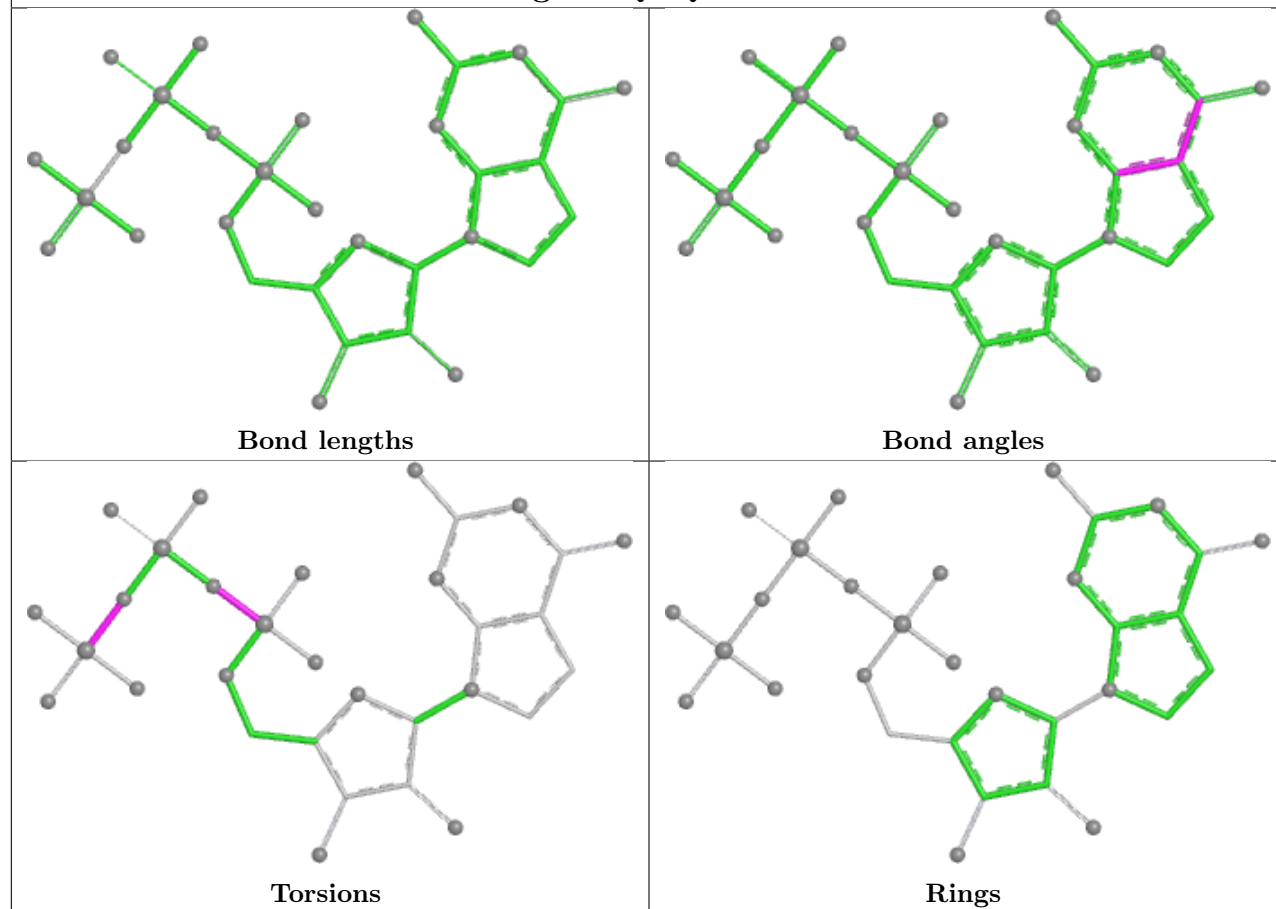




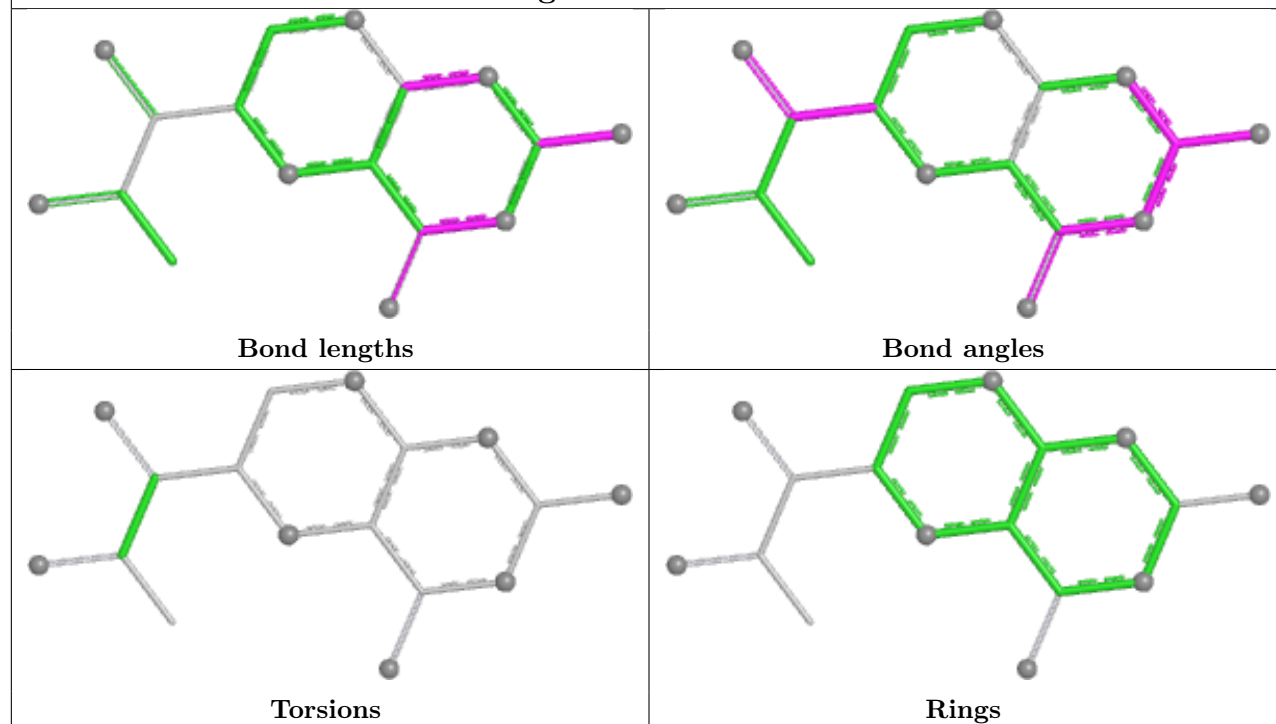




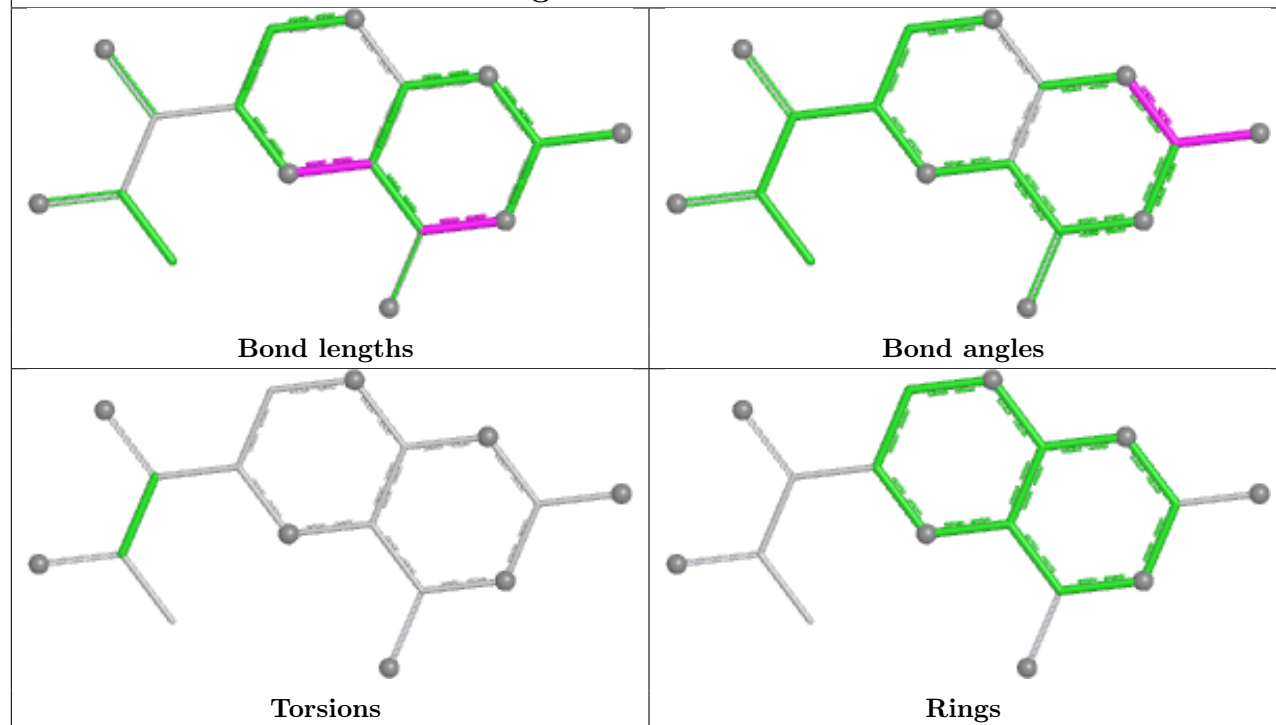
Ligand QBQ S 302



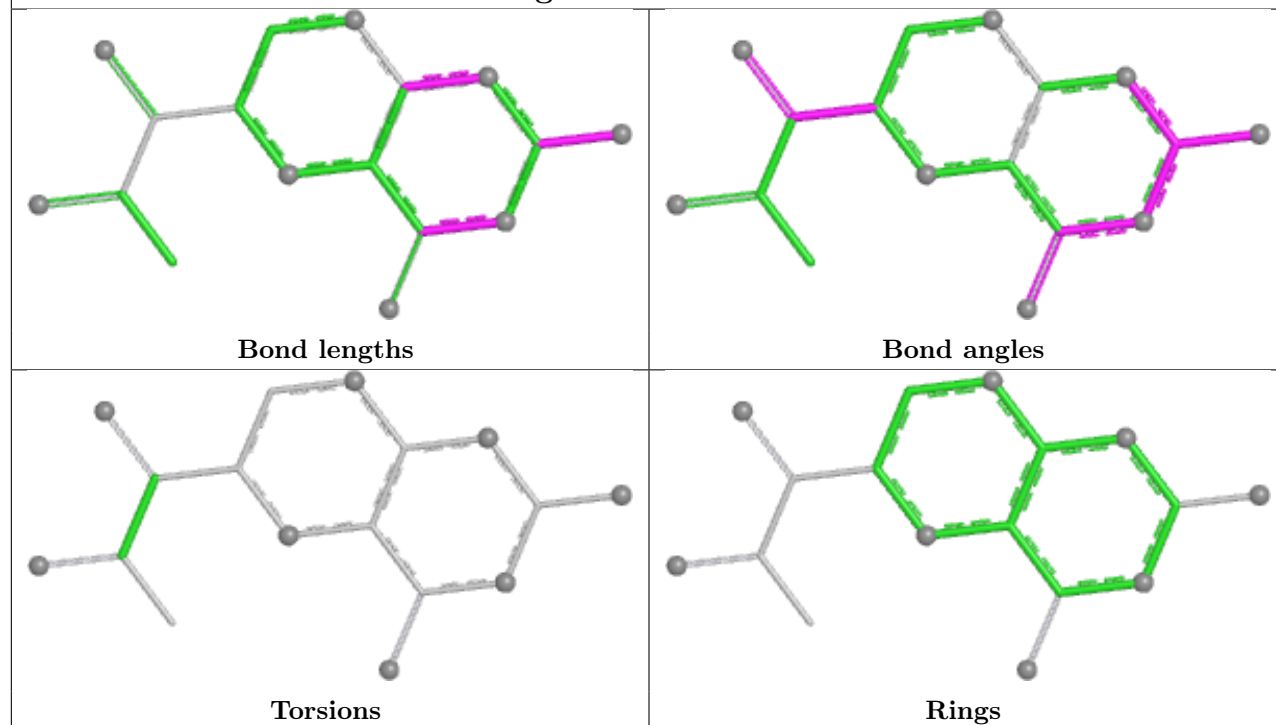
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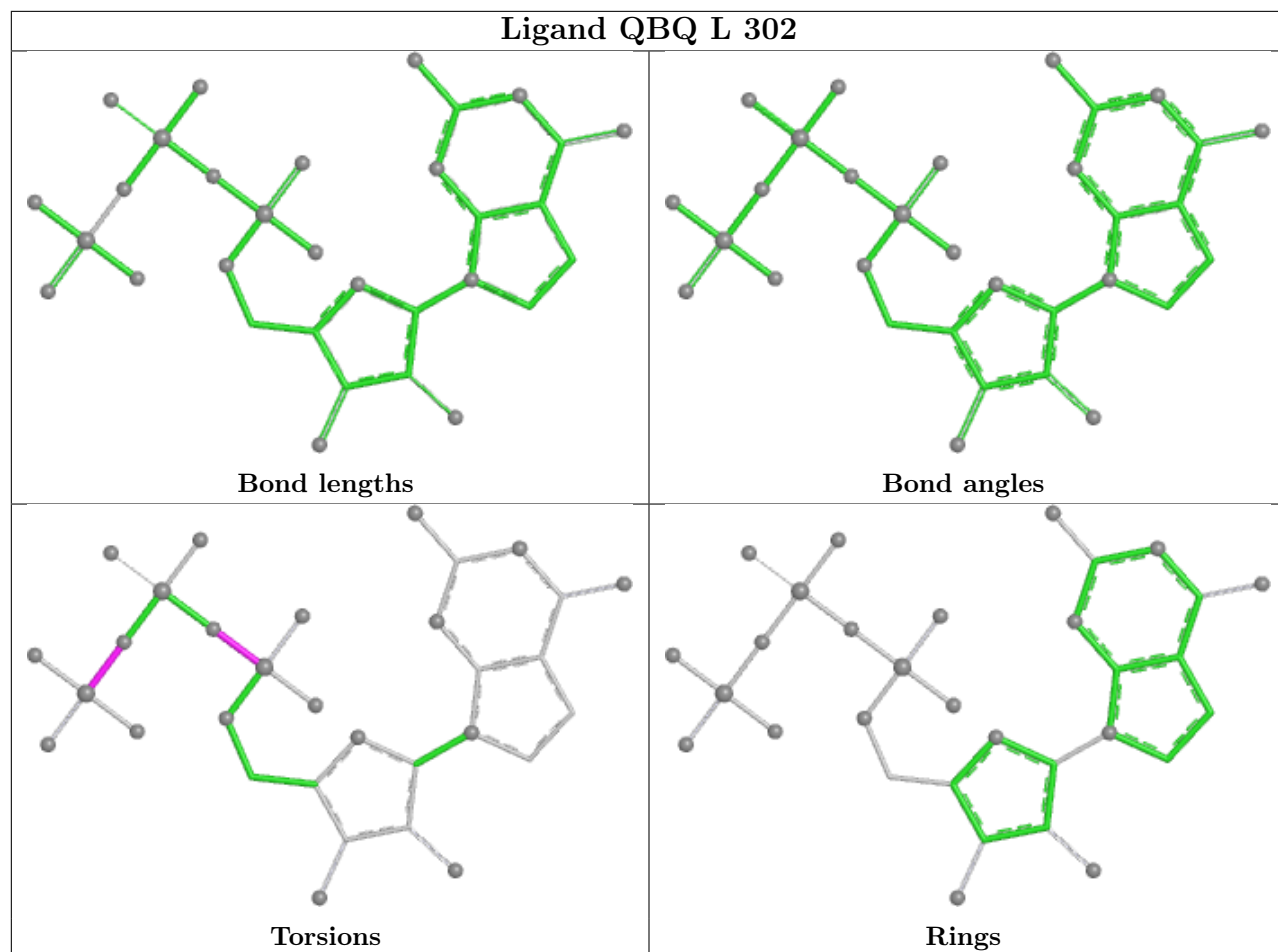


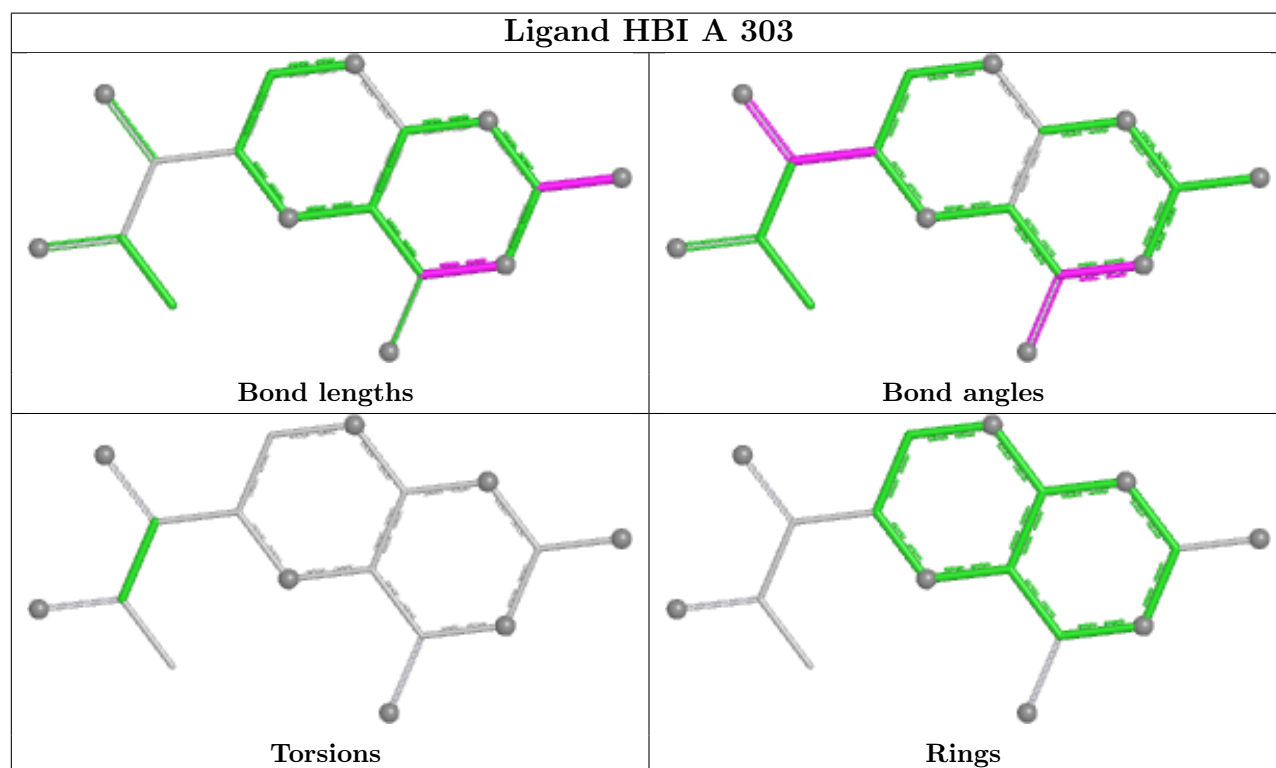
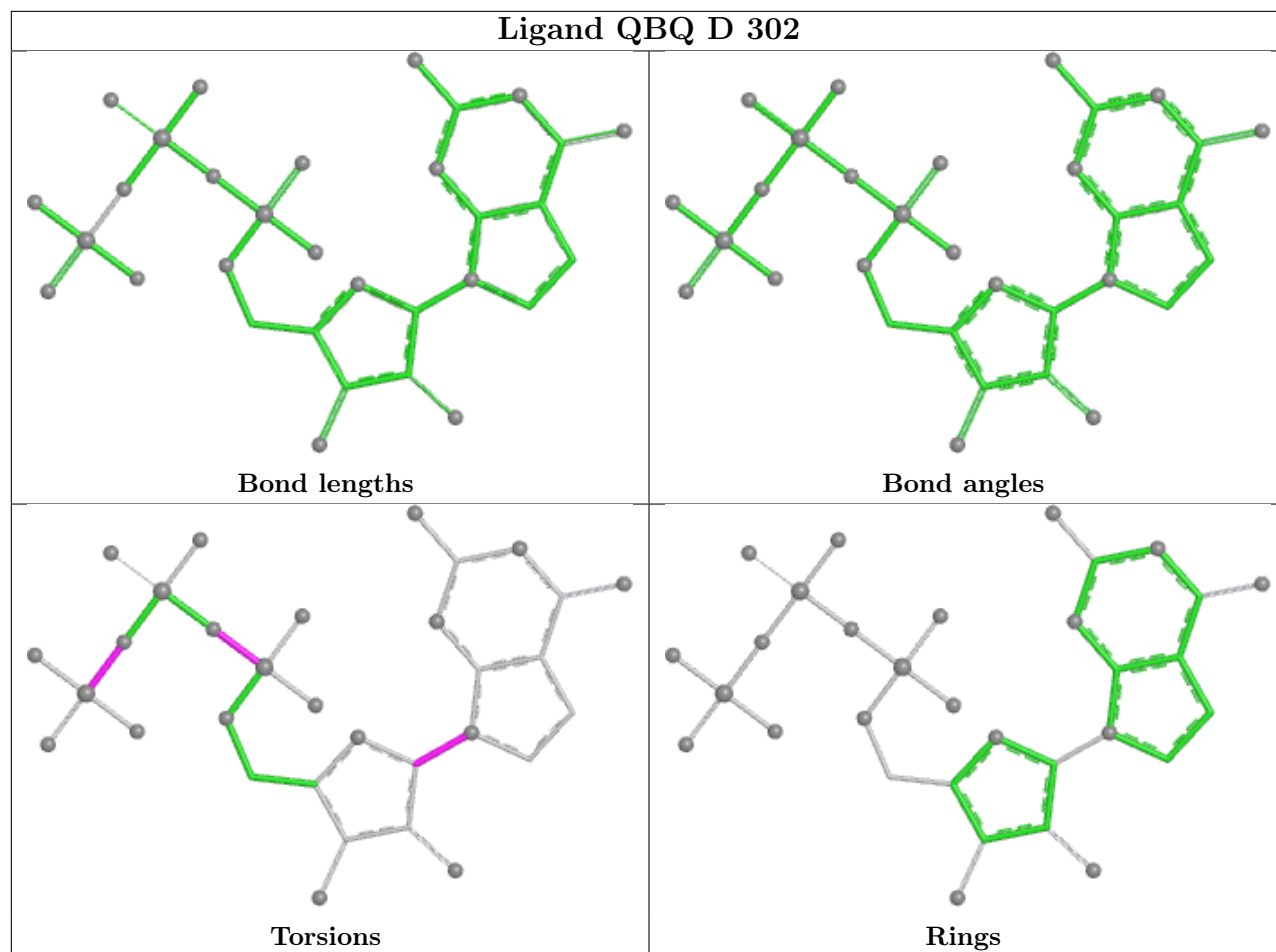
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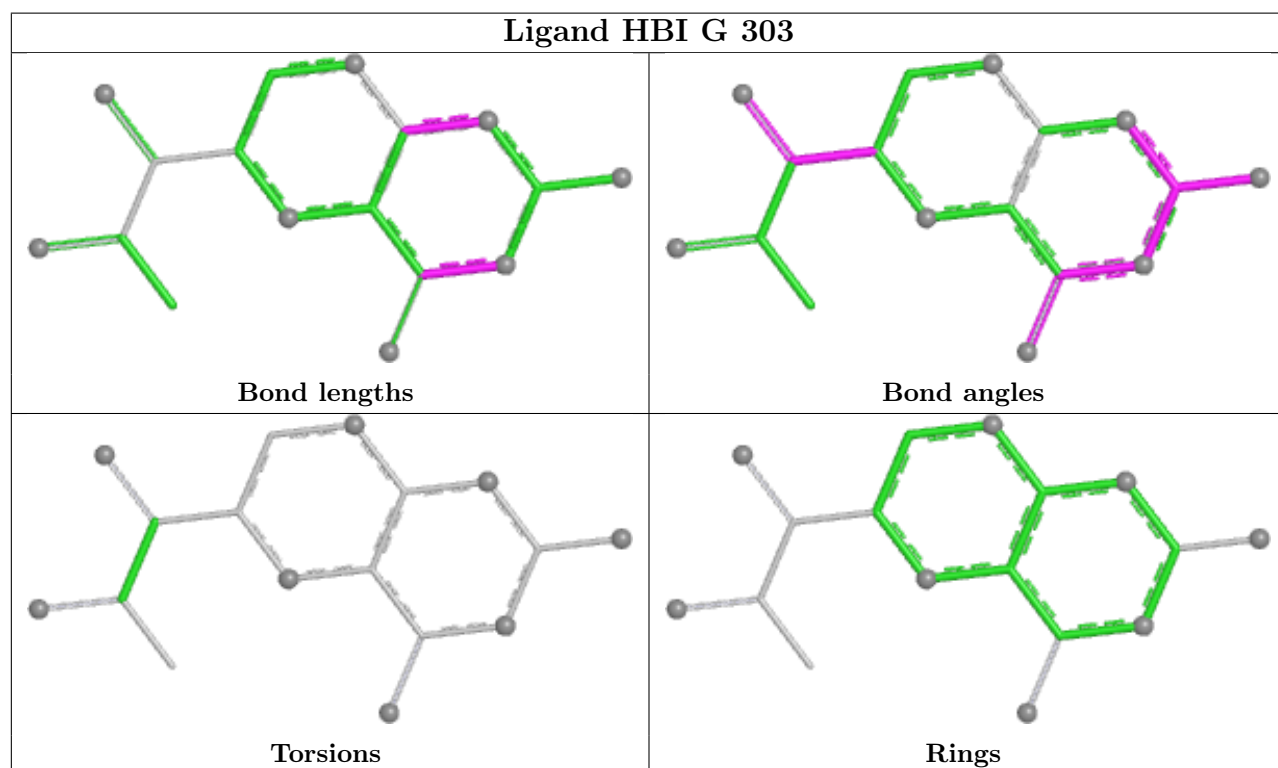
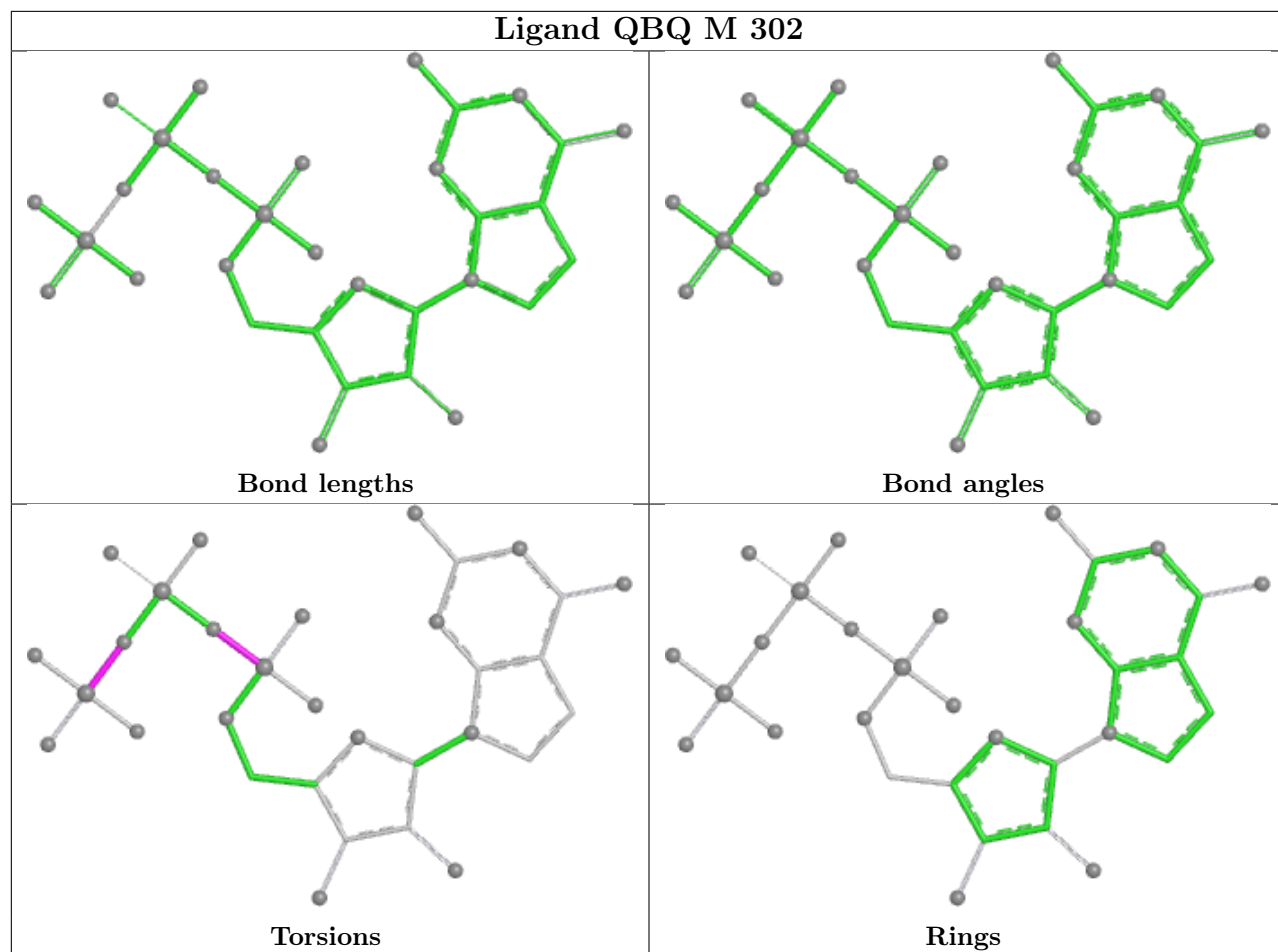


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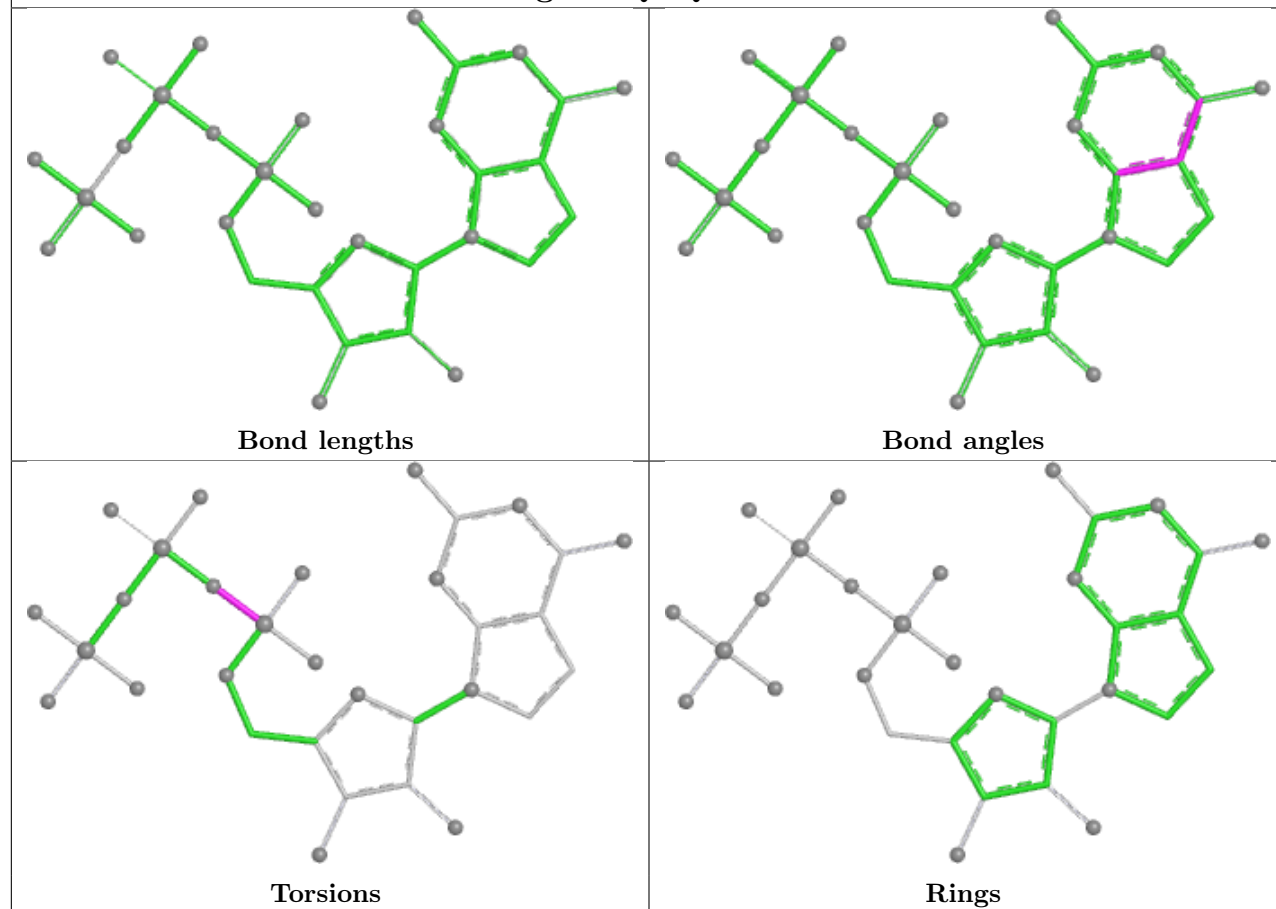




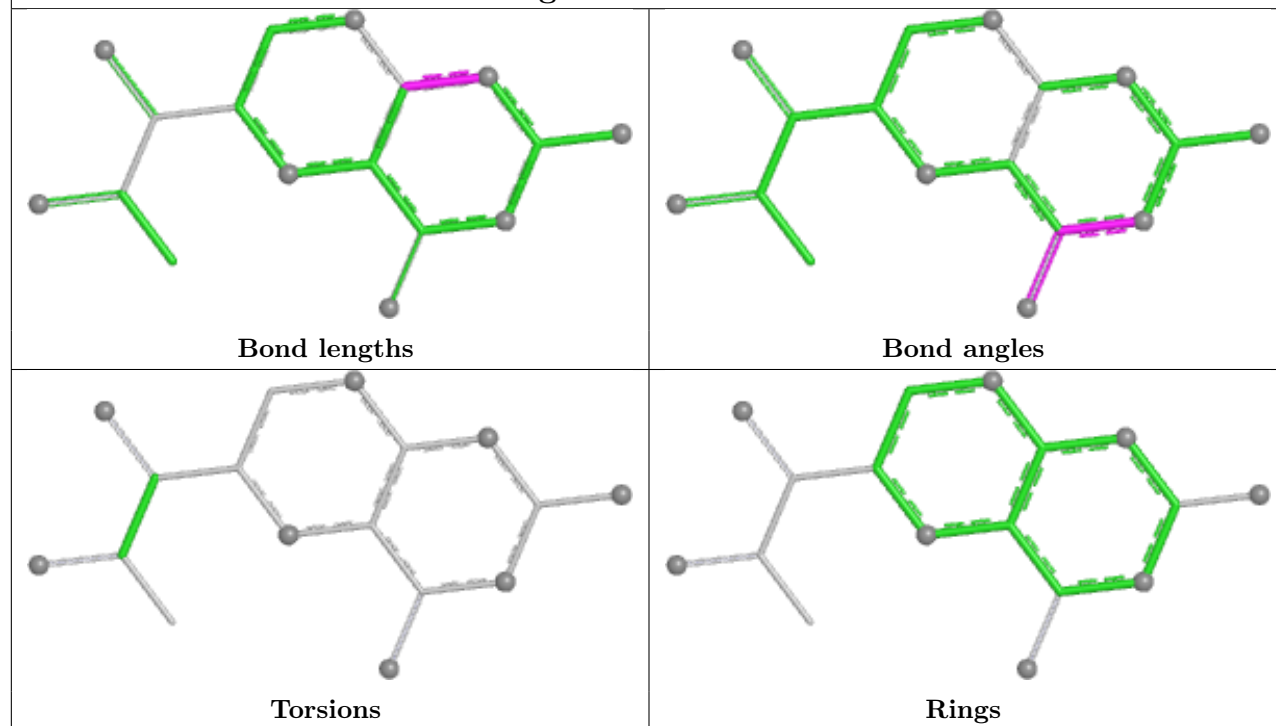




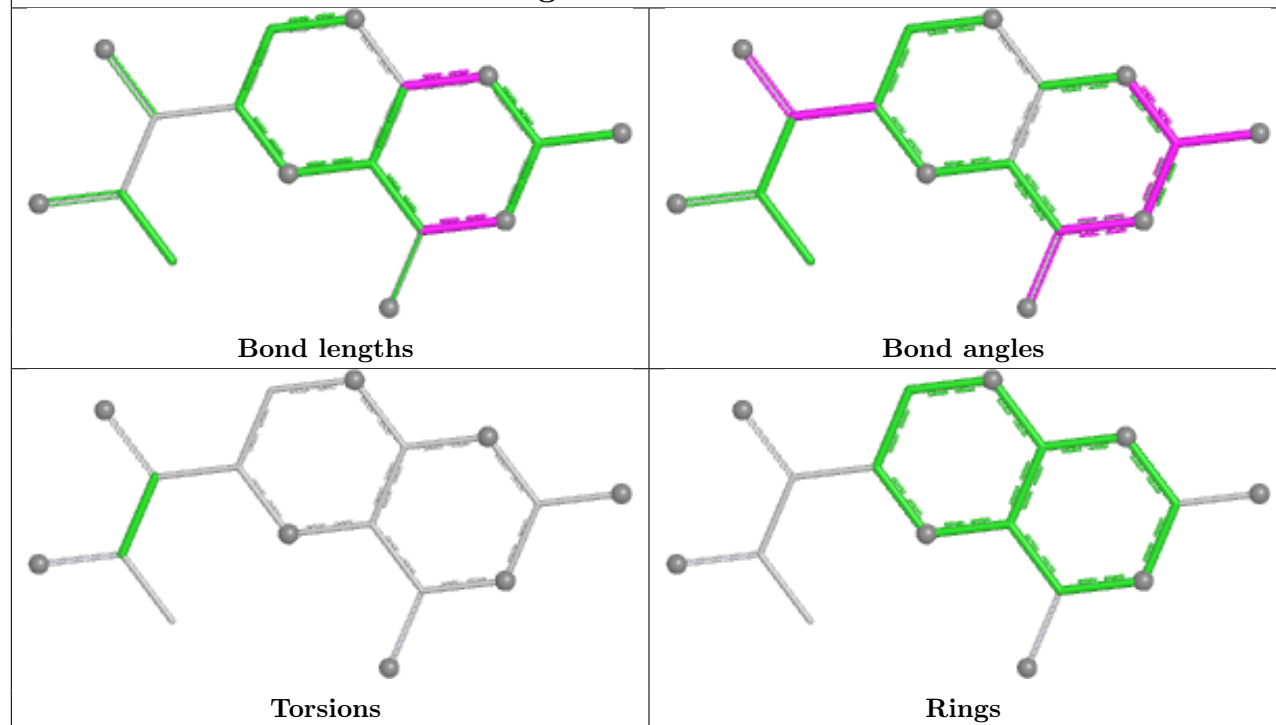
Ligand QBQ I 302



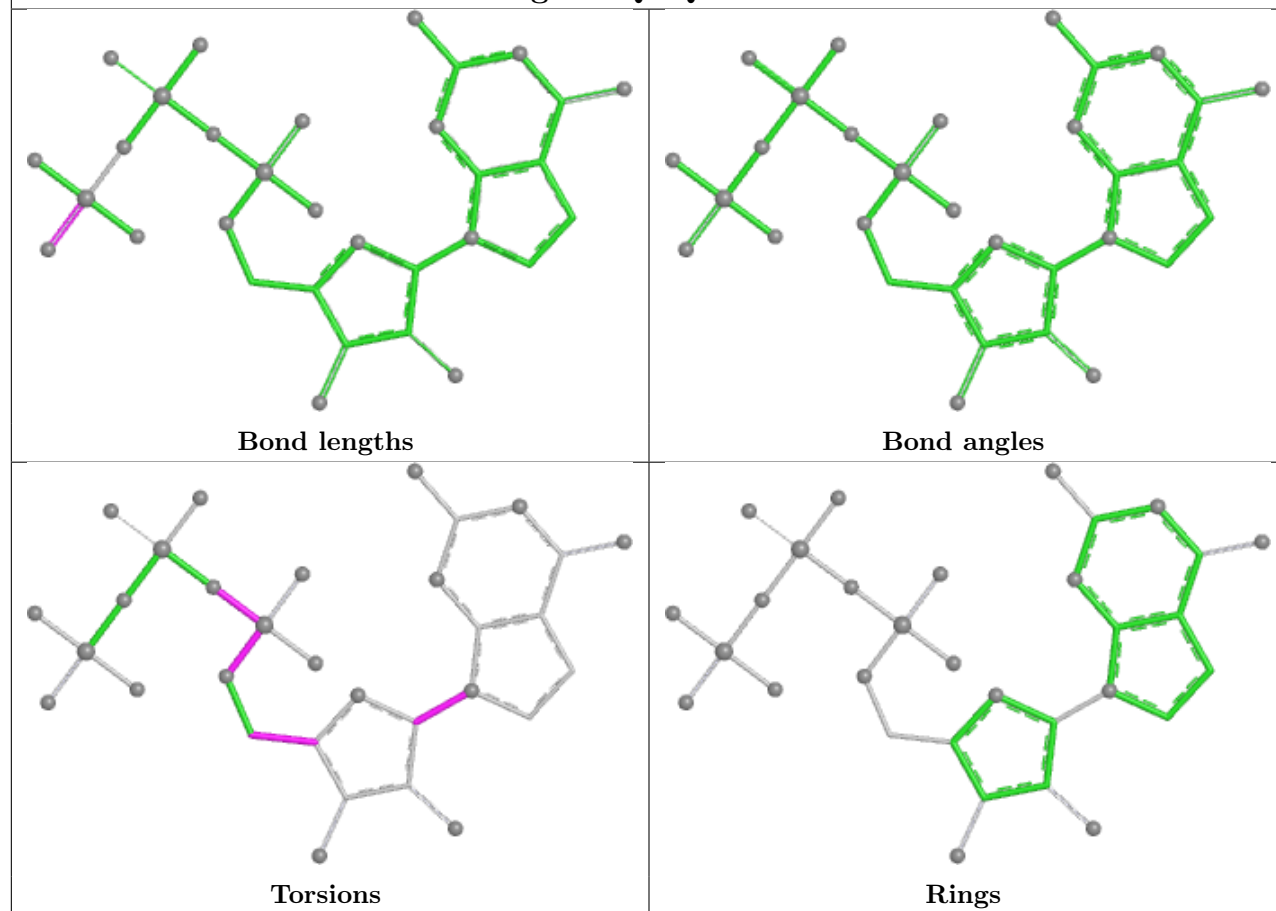
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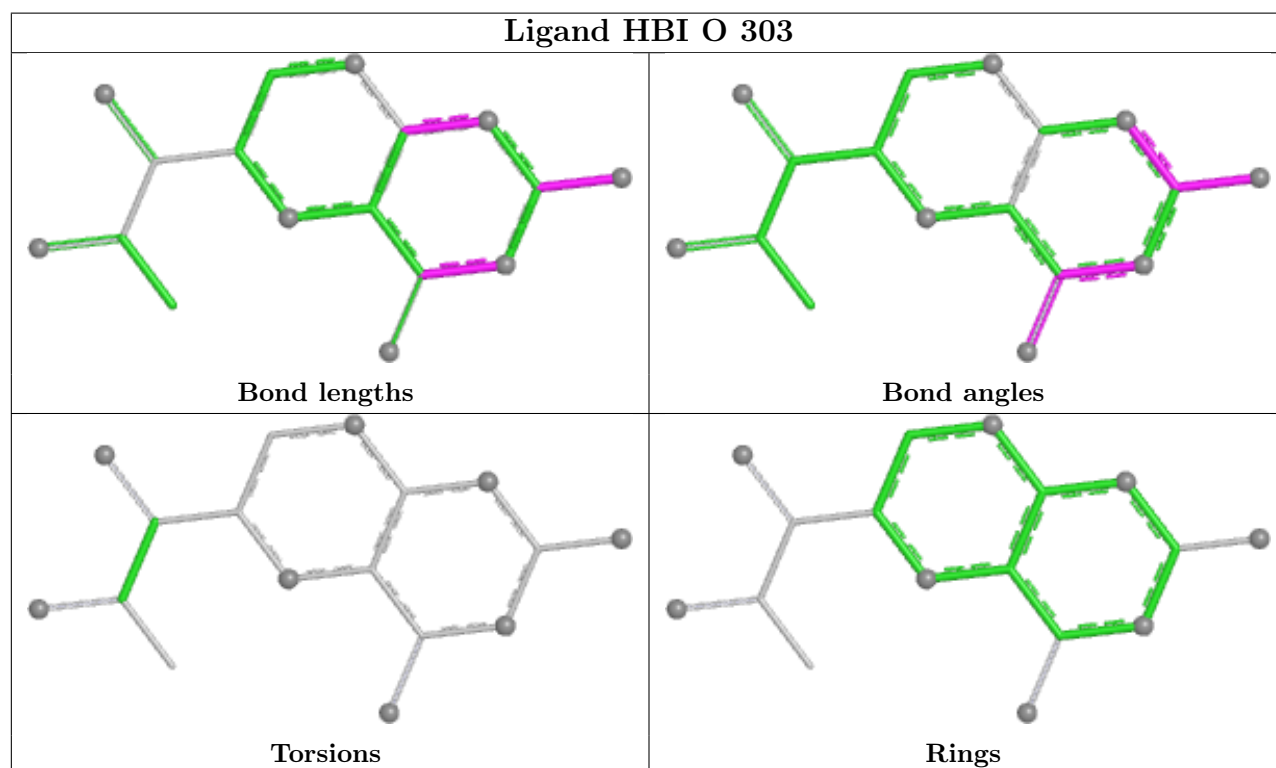
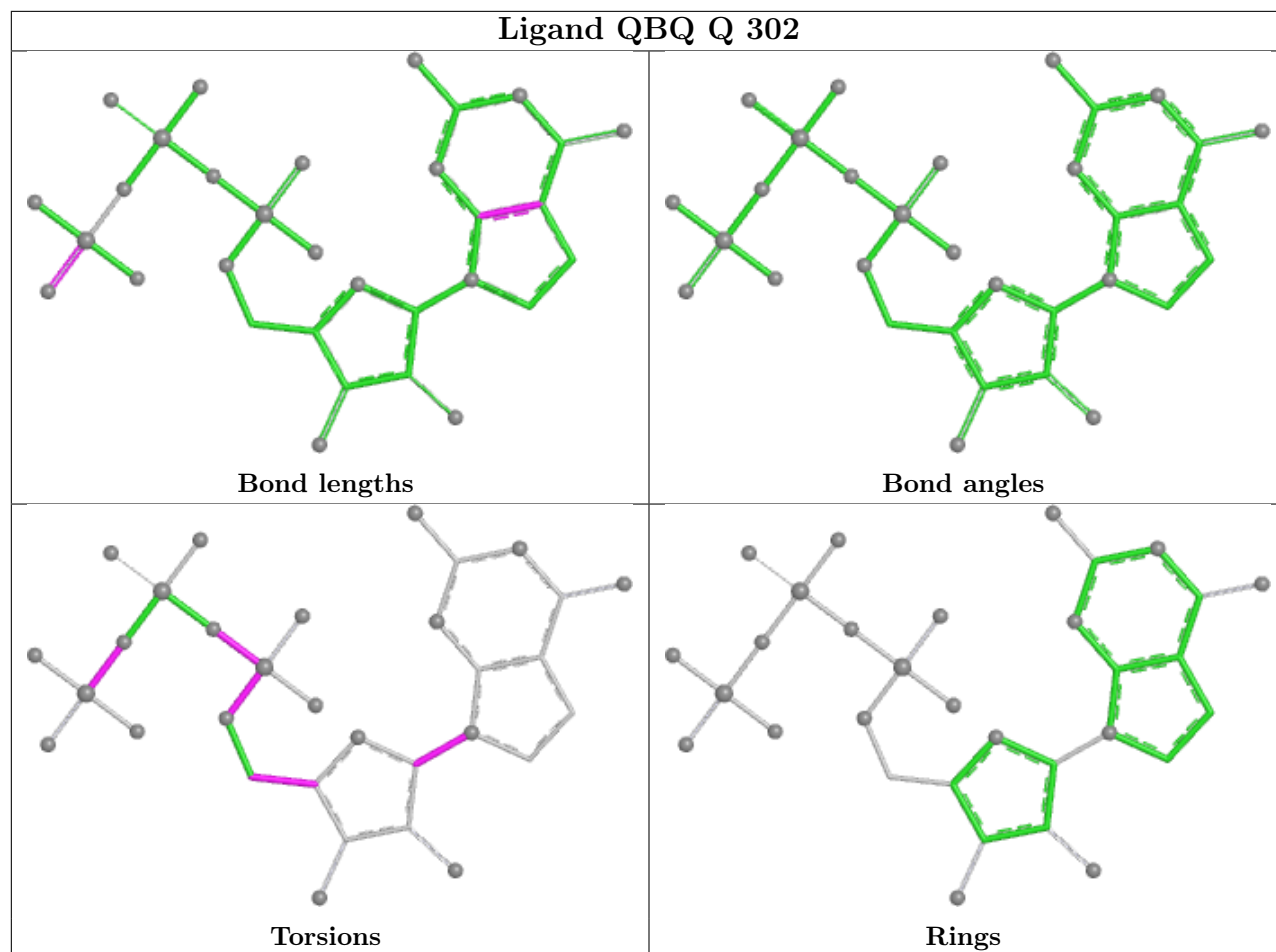


Ligand HBI L 304

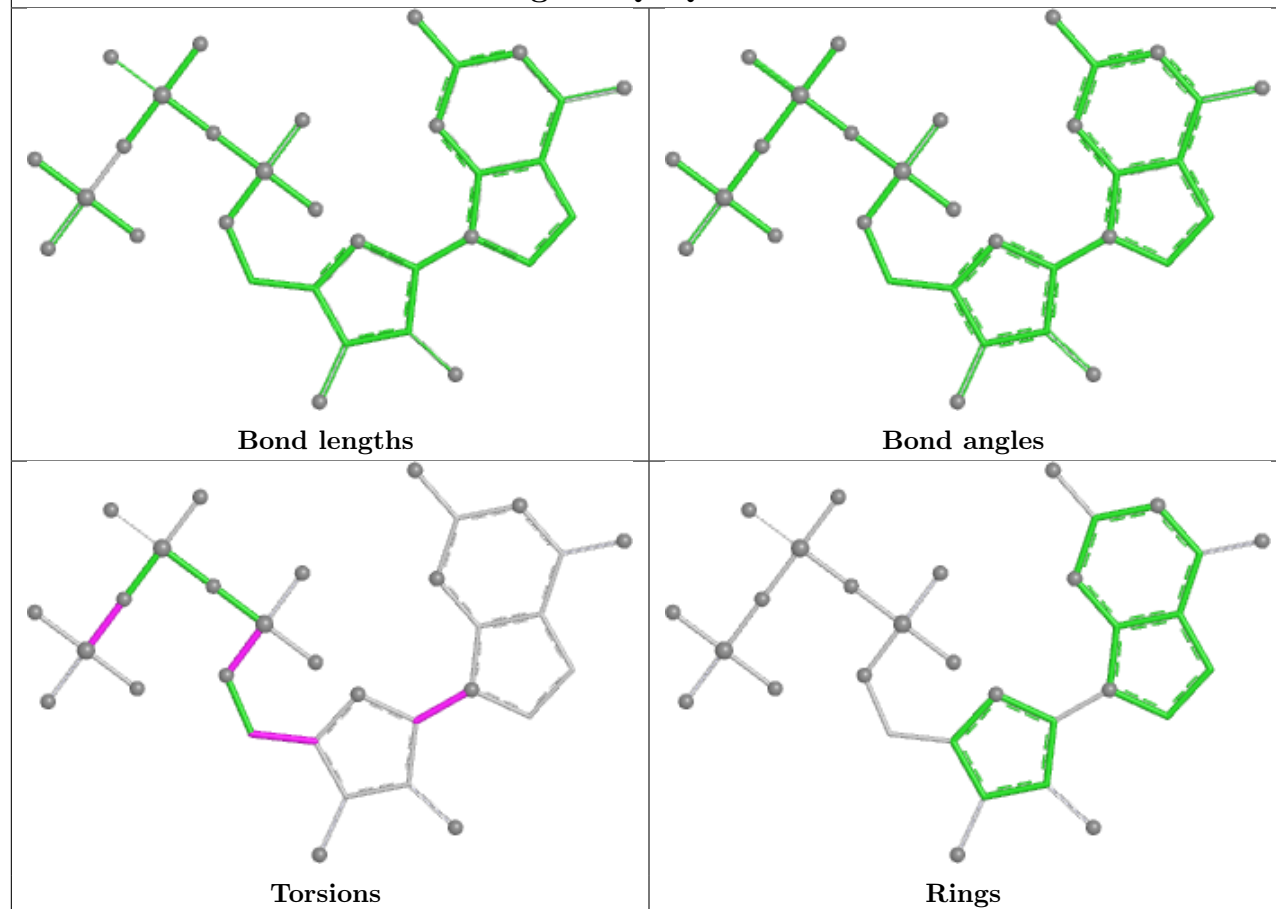


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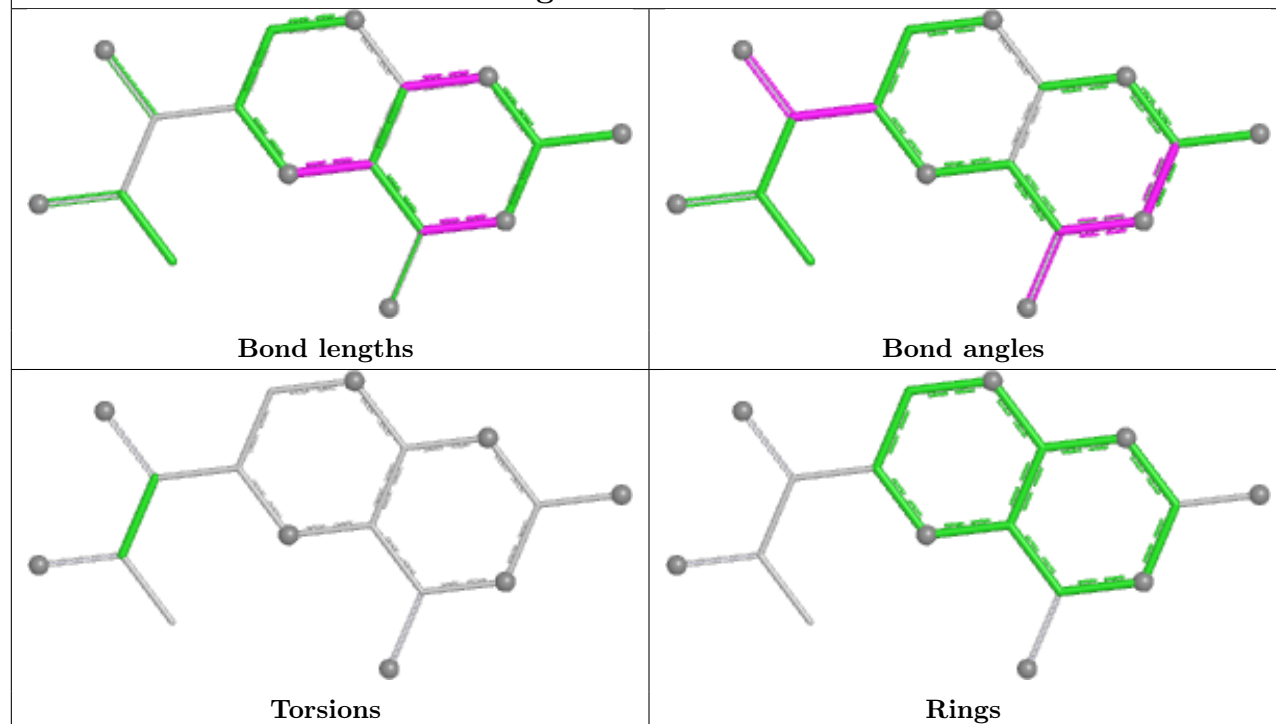


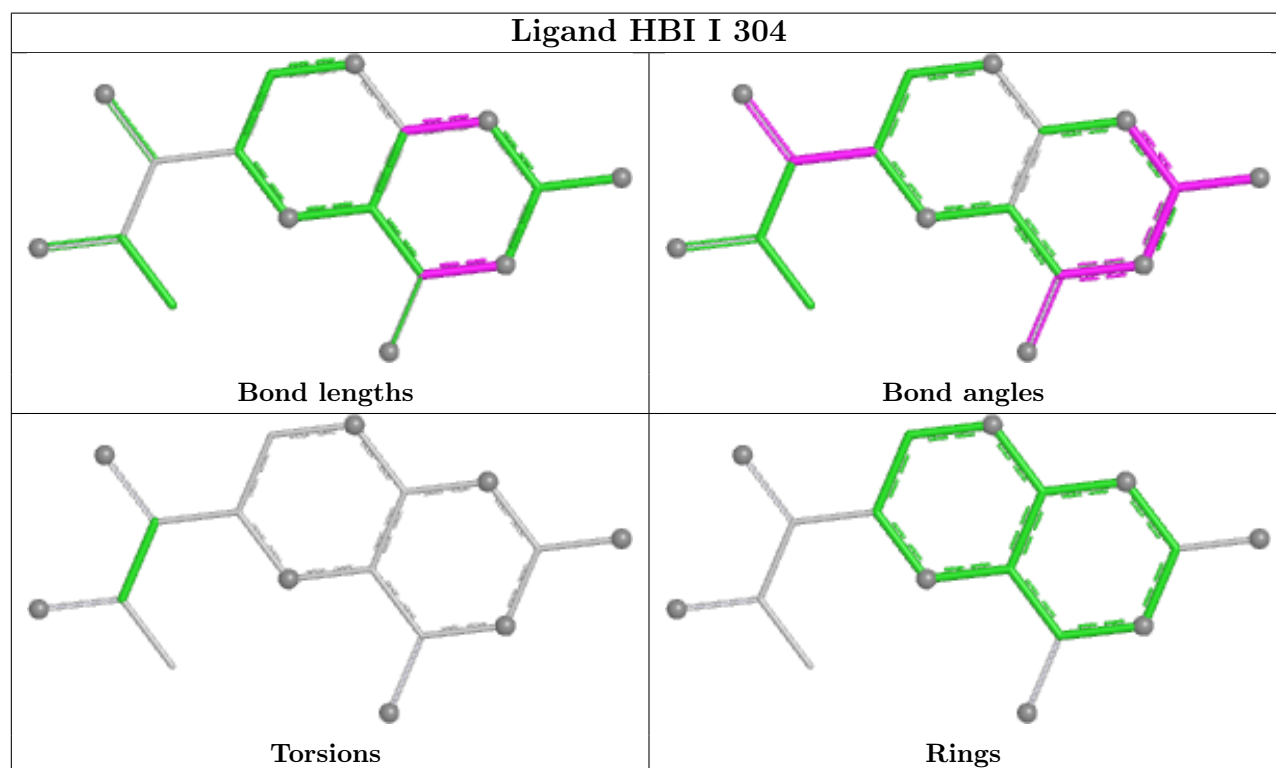
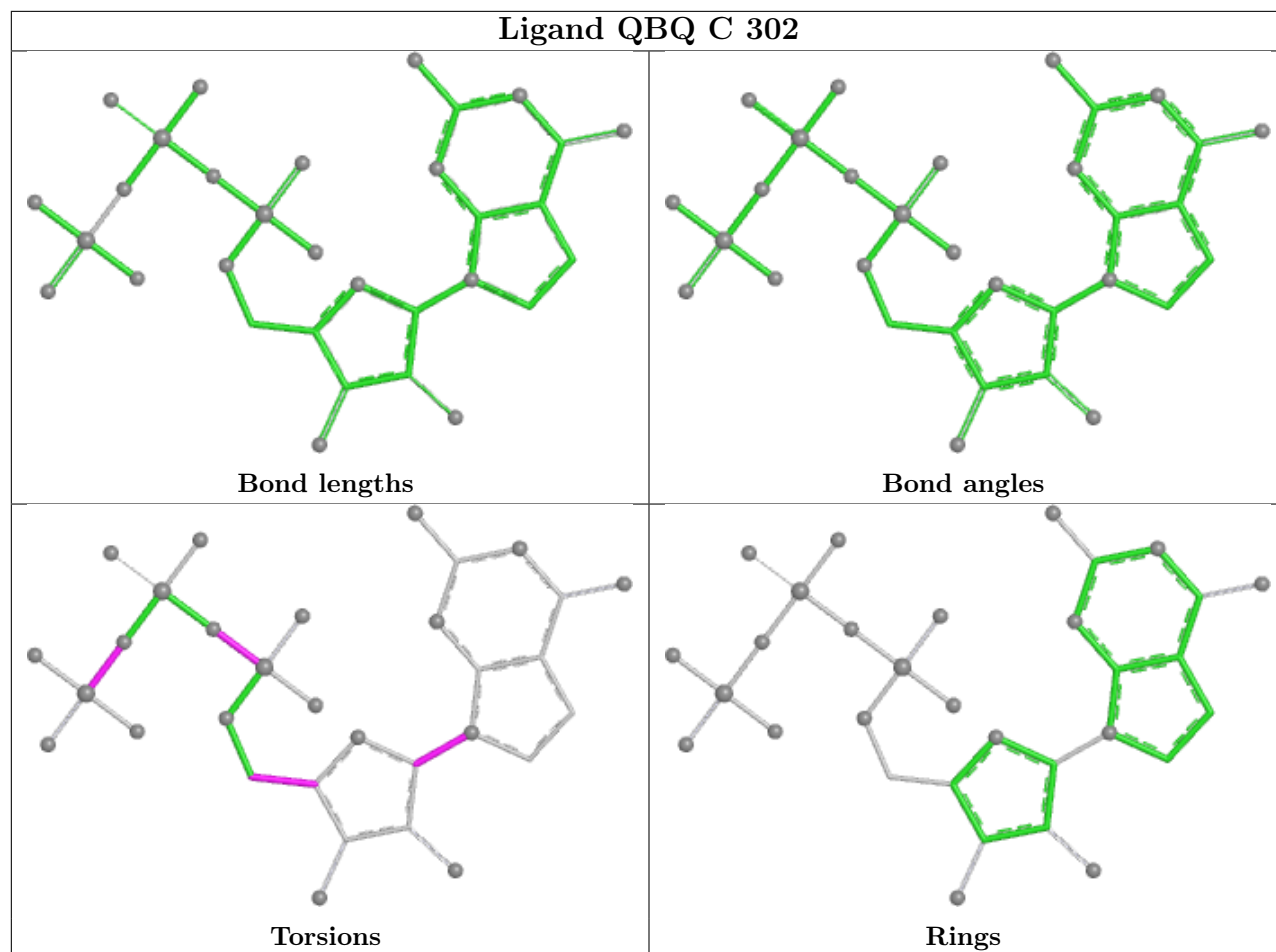


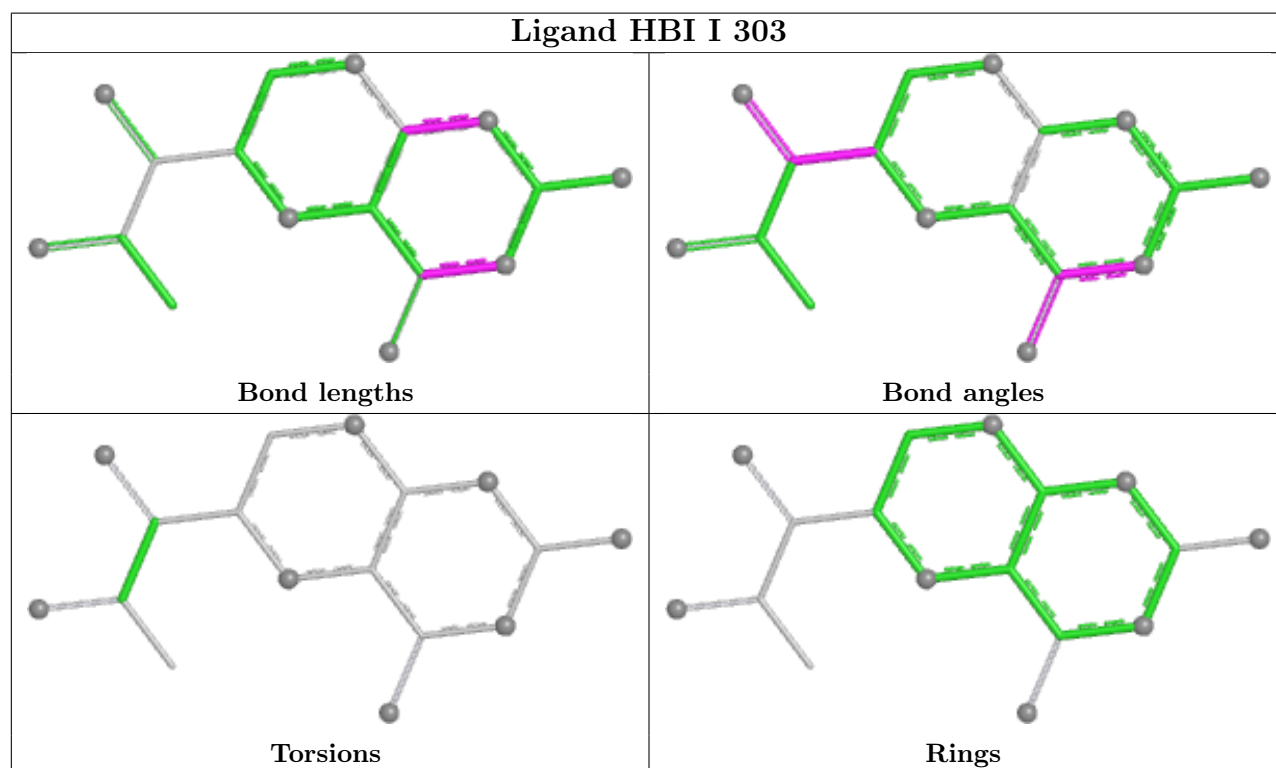
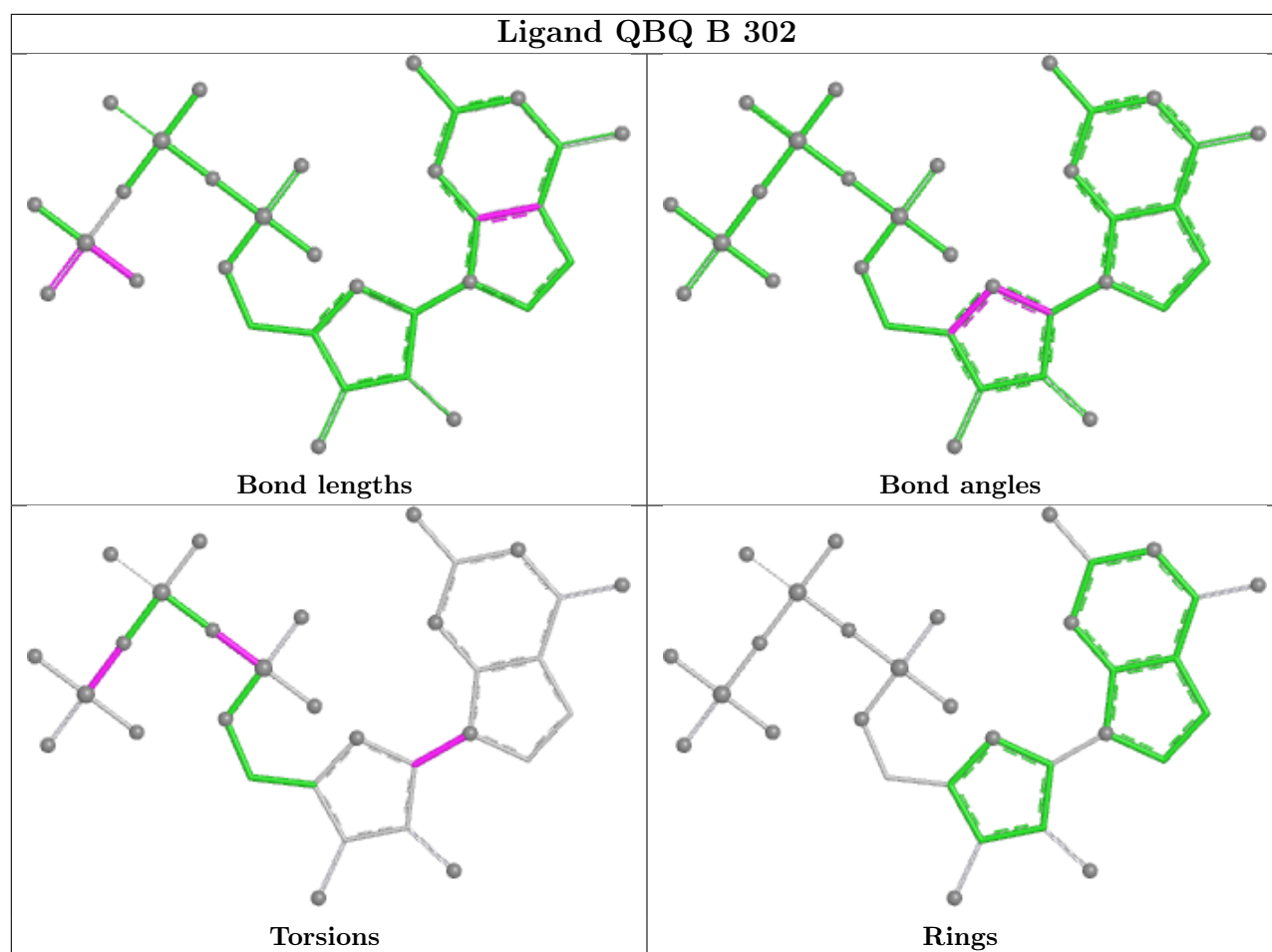
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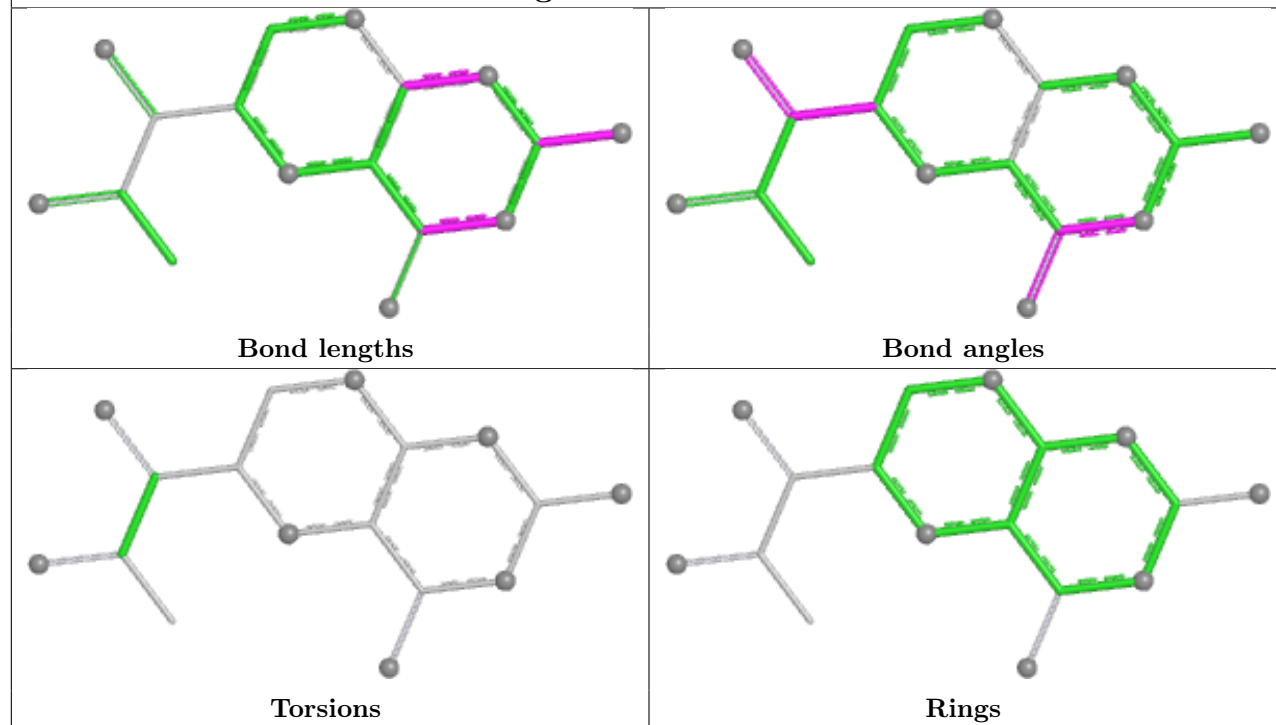
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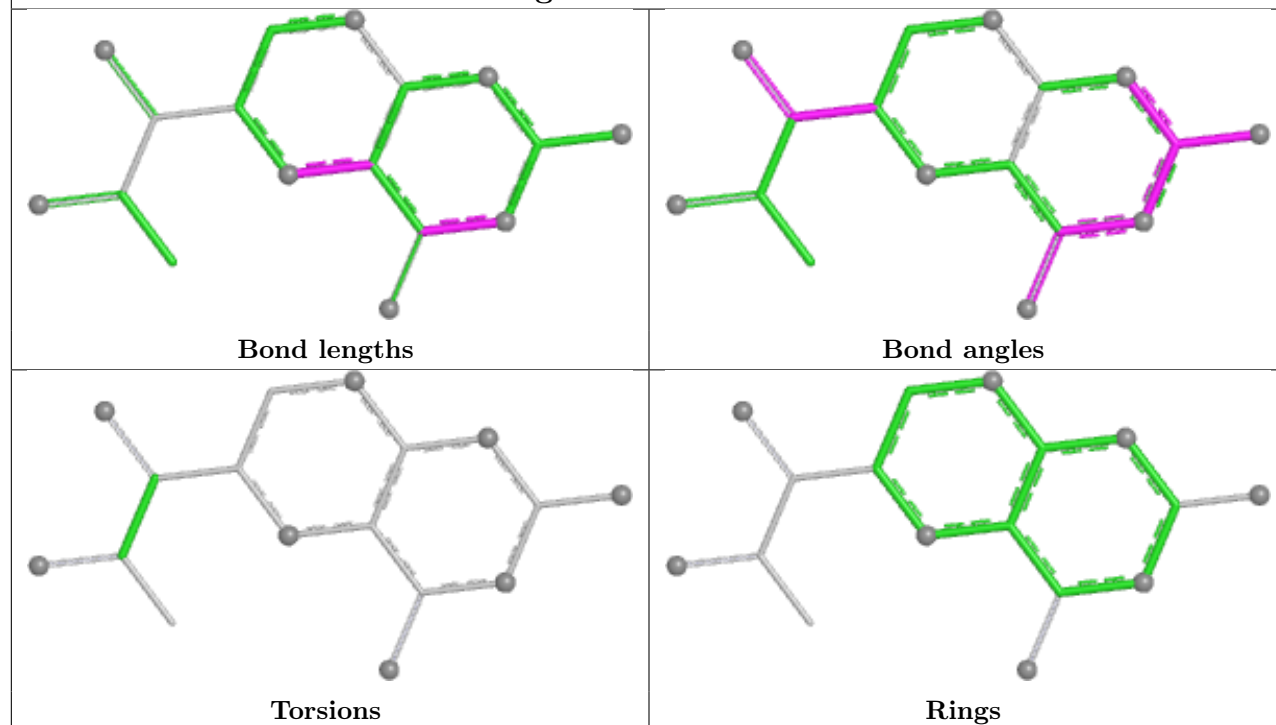


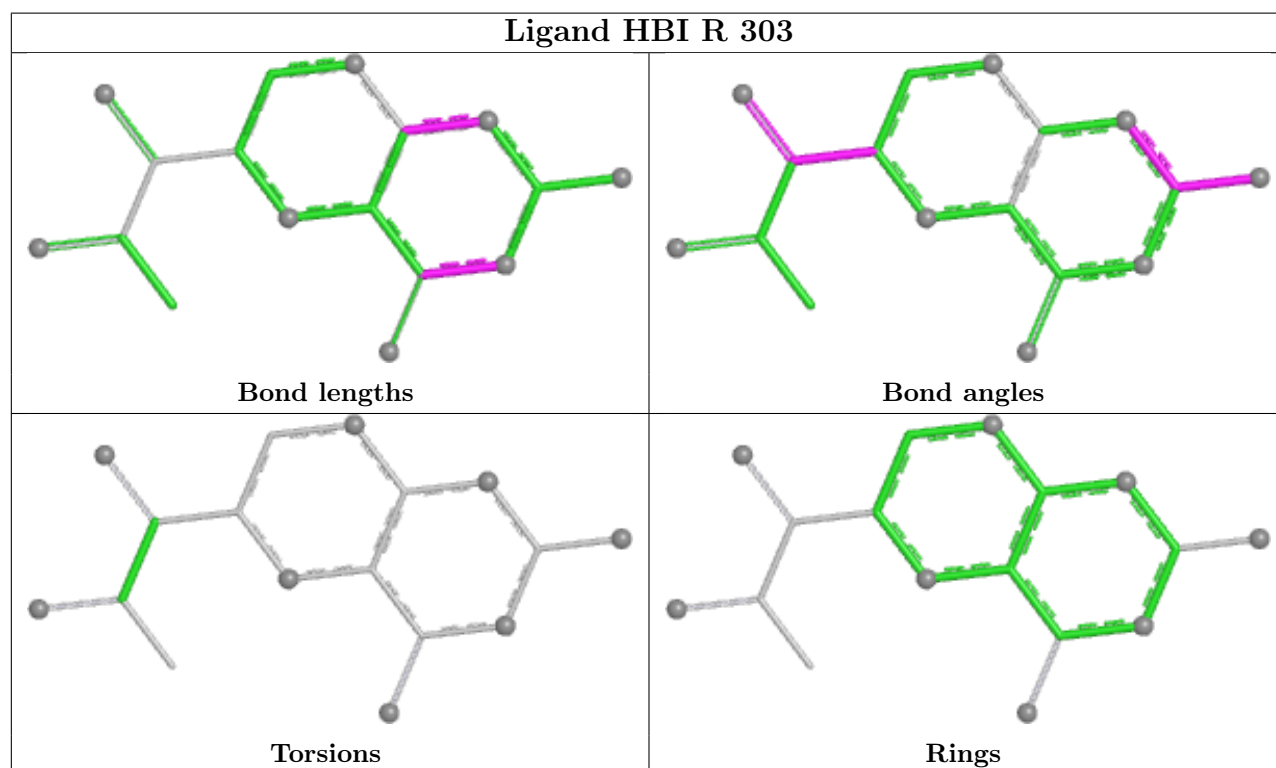
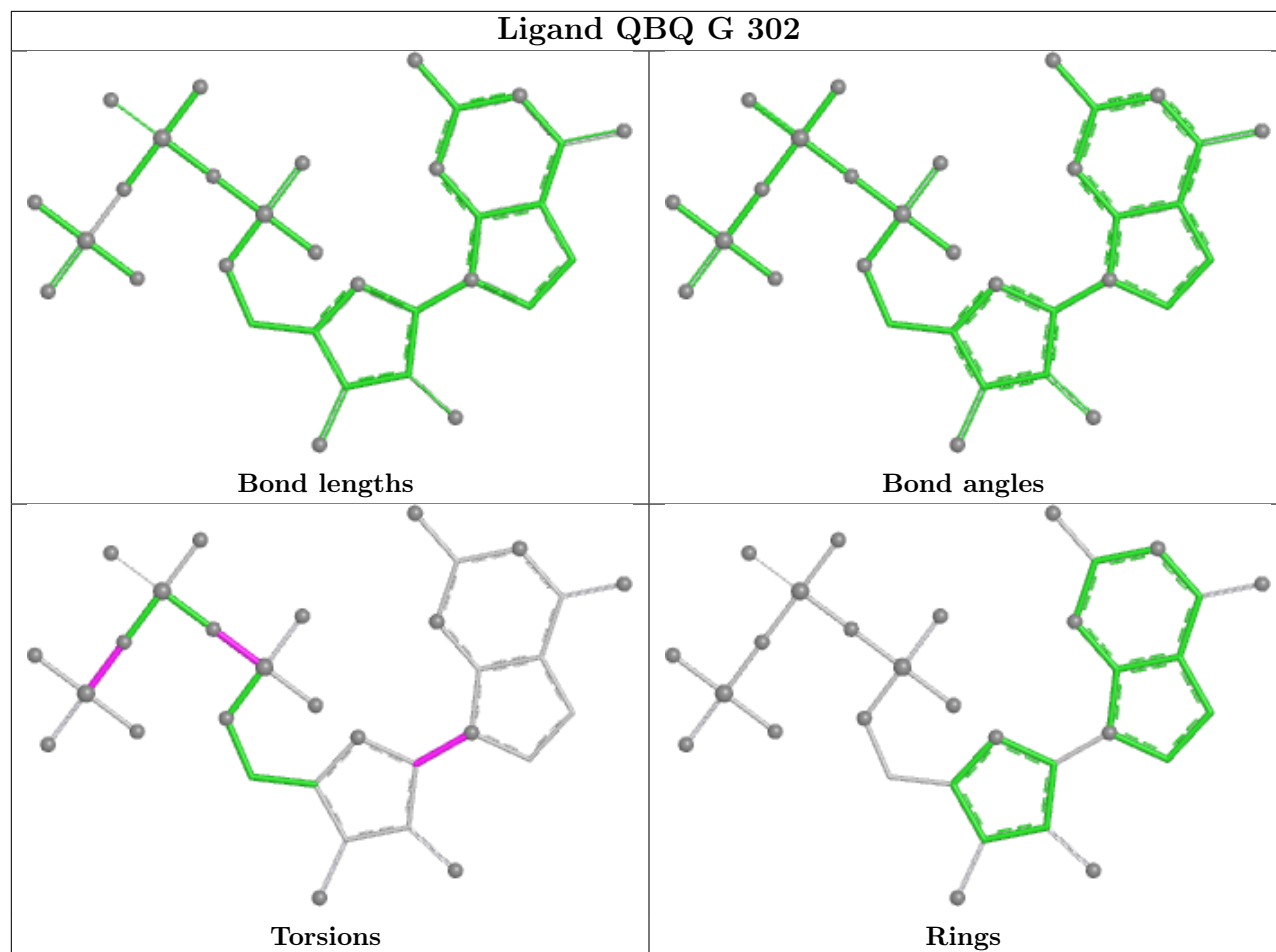


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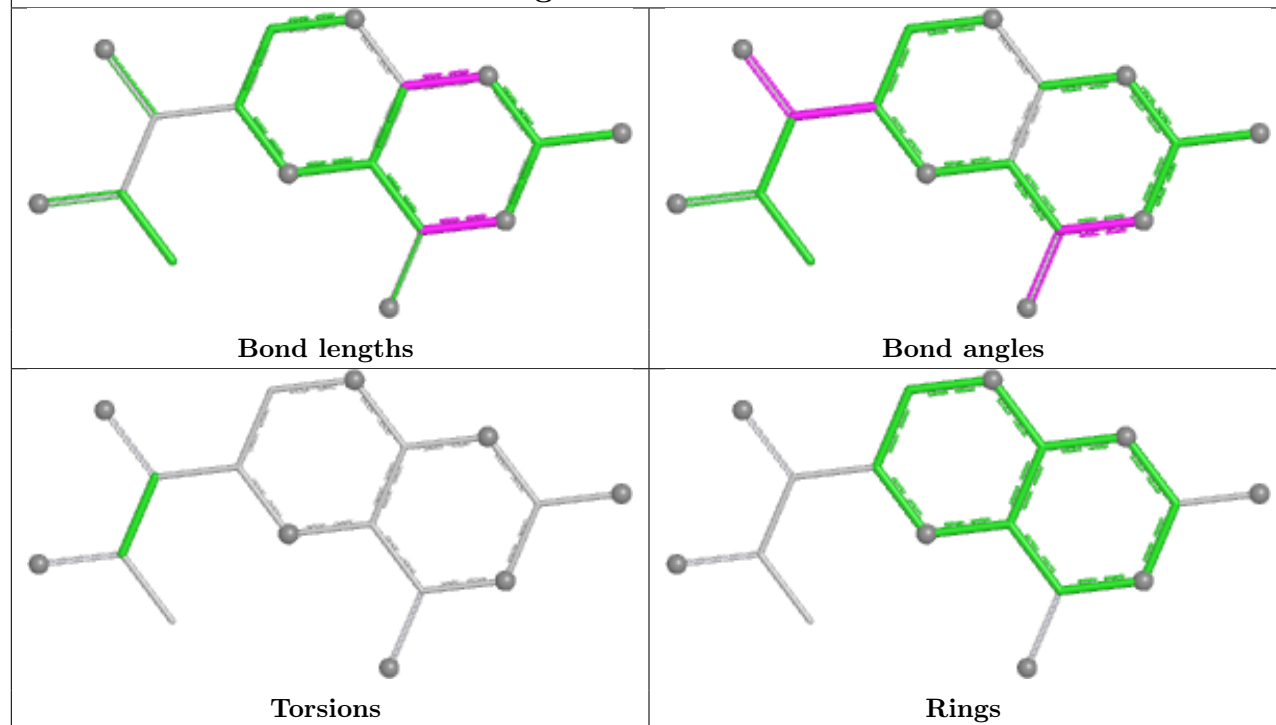


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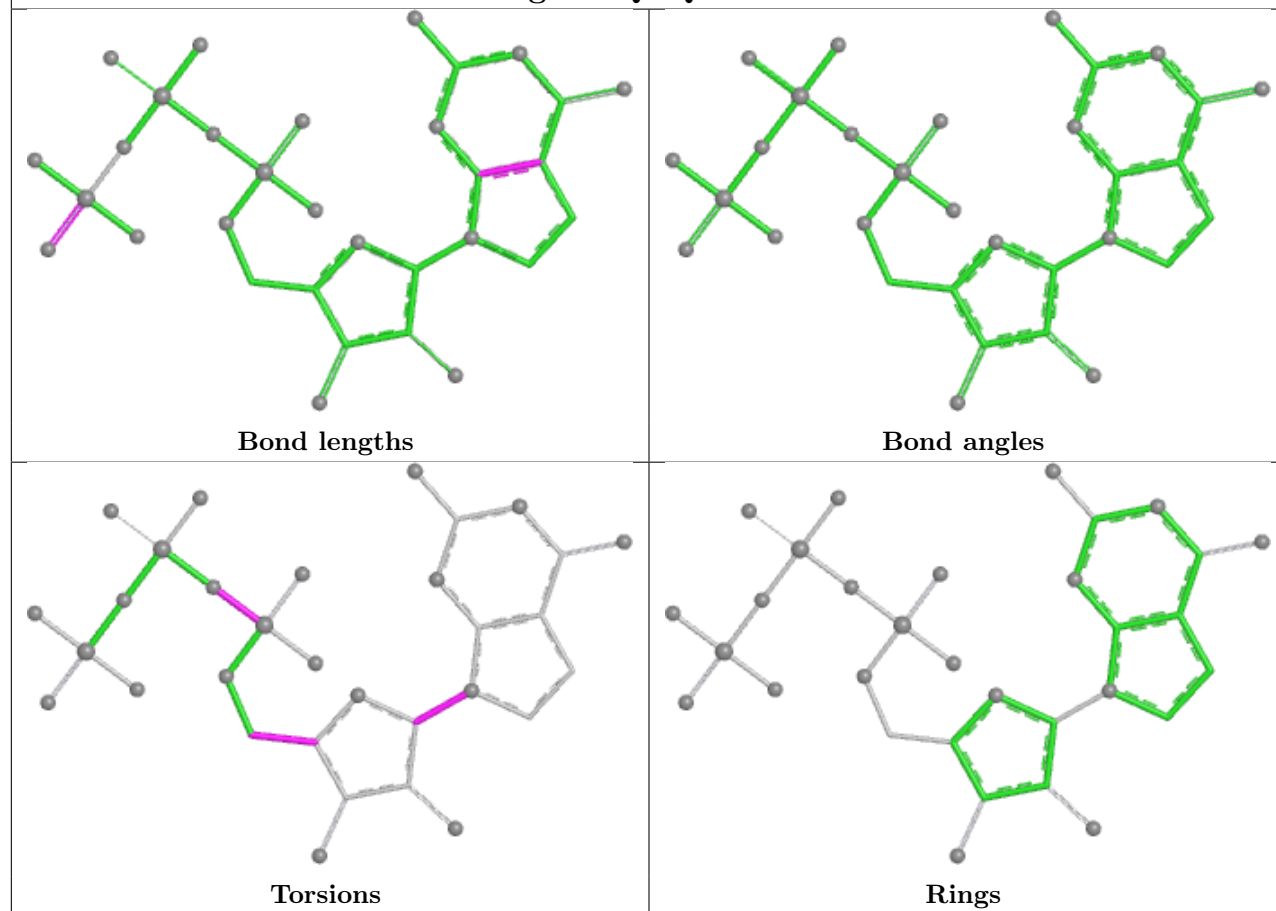


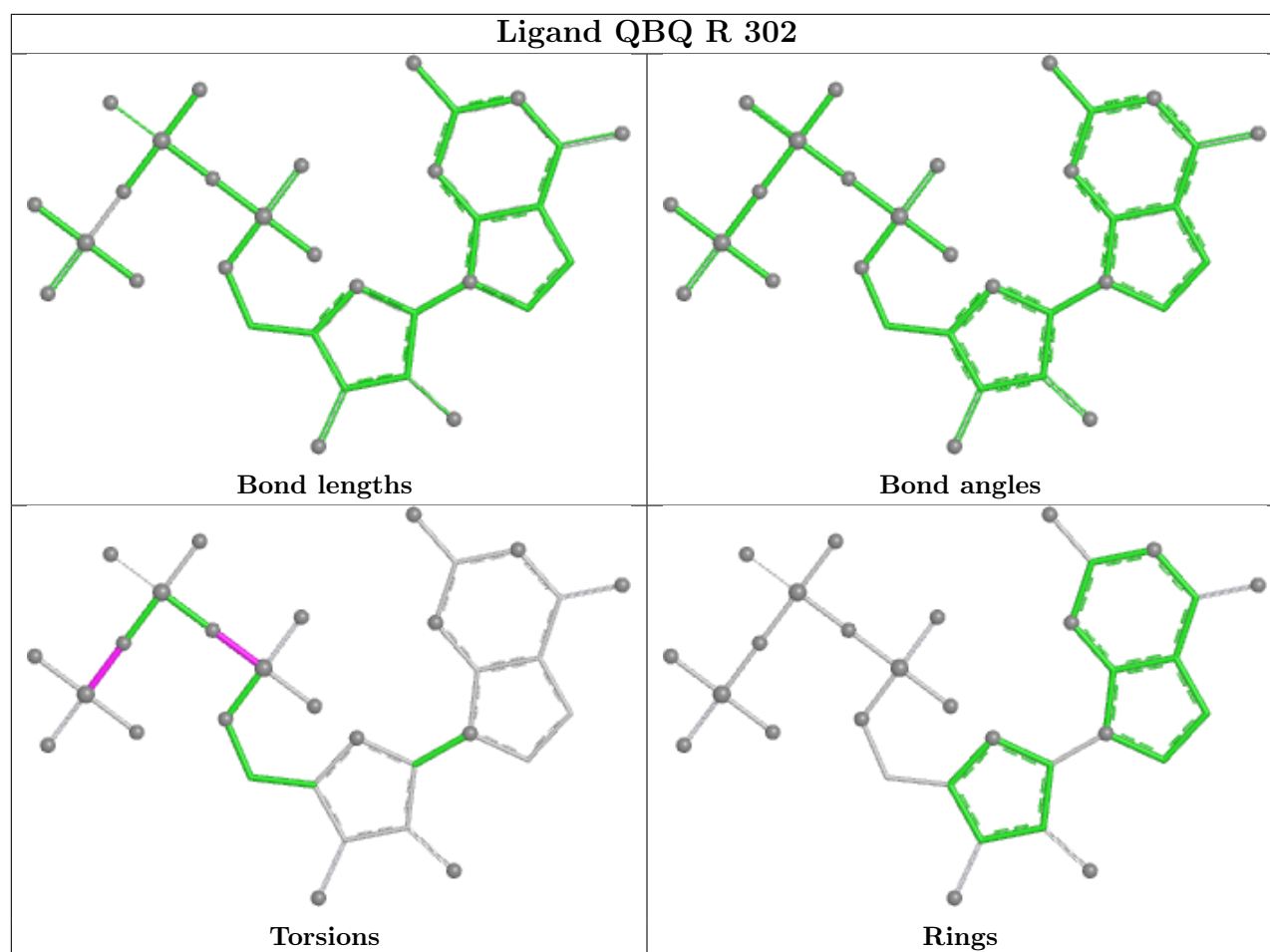


Ligand HBI K 303



Ligand QBQ N 302





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	192/209 (91%)	-0.28	3 (1%) 70 67	22, 34, 64, 77	0
1	B	192/209 (91%)	-0.07	5 (2%) 57 54	24, 39, 65, 76	0
1	C	192/209 (91%)	-0.13	4 (2%) 63 60	25, 36, 64, 76	0
1	D	192/209 (91%)	0.06	4 (2%) 63 60	24, 41, 72, 83	0
1	E	192/209 (91%)	-0.10	7 (3%) 46 43	25, 37, 62, 80	0
1	F	192/209 (91%)	-0.18	6 (3%) 51 48	23, 37, 62, 77	0
1	G	192/209 (91%)	0.08	7 (3%) 46 43	25, 40, 73, 88	0
1	H	192/209 (91%)	-0.23	5 (2%) 57 54	25, 35, 65, 82	0
1	I	192/209 (91%)	-0.00	8 (4%) 40 37	25, 39, 77, 89	0
1	J	192/209 (91%)	-0.25	3 (1%) 70 67	24, 34, 61, 80	0
1	K	192/209 (91%)	-0.17	3 (1%) 70 67	26, 38, 60, 69	0
1	L	192/209 (91%)	-0.02	7 (3%) 46 43	25, 40, 73, 87	0
1	M	192/209 (91%)	-0.14	3 (1%) 70 67	23, 36, 66, 88	0
1	N	192/209 (91%)	-0.25	4 (2%) 63 60	24, 35, 64, 79	0
1	O	192/209 (91%)	-0.01	6 (3%) 51 48	25, 40, 70, 82	0
1	P	192/209 (91%)	0.06	7 (3%) 46 43	26, 42, 78, 90	0
1	Q	192/209 (91%)	-0.11	4 (2%) 63 60	23, 36, 67, 77	0
1	R	192/209 (91%)	-0.13	6 (3%) 51 48	24, 36, 66, 85	0
1	S	192/209 (91%)	-0.05	4 (2%) 63 60	25, 40, 68, 80	0
1	T	192/209 (91%)	-0.09	5 (2%) 57 54	24, 39, 68, 78	0
2	a	84/87 (96%)	0.47	2 (2%) 59 56	40, 56, 78, 83	0
2	b	84/87 (96%)	0.61	3 (3%) 46 43	41, 60, 77, 82	0
2	c	84/87 (96%)	0.93	9 (10%) 11 8	47, 66, 88, 95	0
2	d	84/87 (96%)	0.68	6 (7%) 22 19	43, 64, 87, 93	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
2	e	84/87 (96%)	0.46	3 (3%) 46 43	37, 56, 76, 87	0
2	f	83/87 (95%)	0.18	2 (2%) 59 56	32, 47, 65, 74	0
2	g	84/87 (96%)	0.26	2 (2%) 59 56	36, 47, 63, 68	0
2	h	84/87 (96%)	0.39	1 (1%) 76 74	35, 55, 73, 77	0
2	i	84/87 (96%)	0.25	2 (2%) 59 56	34, 53, 72, 83	0
2	j	84/87 (96%)	0.27	3 (3%) 46 43	36, 50, 70, 78	0
2	k	84/87 (96%)	-0.03	0 100 100	31, 42, 58, 66	0
2	l	84/87 (96%)	0.29	2 (2%) 59 56	32, 51, 66, 68	0
2	m	84/87 (96%)	0.29	4 (4%) 35 32	34, 48, 70, 78	0
2	n	84/87 (96%)	0.00	1 (1%) 76 74	32, 43, 63, 74	0
2	o	84/87 (96%)	-0.12	2 (2%) 59 56	29, 40, 54, 64	0
2	p	84/87 (96%)	0.52	5 (5%) 27 24	38, 55, 74, 77	0
2	q	84/87 (96%)	0.43	3 (3%) 46 43	37, 53, 74, 82	0
2	r	84/87 (96%)	0.17	1 (1%) 76 74	36, 46, 67, 80	0
2	s	84/87 (96%)	0.31	1 (1%) 76 74	41, 53, 70, 78	0
2	t	84/87 (96%)	0.59	4 (4%) 35 32	46, 60, 82, 90	0
All	All	5519/5920 (93%)	0.04	157 (2%) 55 52	22, 42, 73, 95	0

All (157) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	c	34	ALA	6.8
1	J	96	TRP	4.8
2	c	33	GLY	4.1
2	c	1	MET	4.1
2	t	10	ILE	4.0
1	P	58	PRO	3.9
2	m	1	MET	3.9
1	T	125	ASP	3.9
2	q	1	MET	3.7
2	t	1	MET	3.6
2	d	1	MET	3.5
2	b	1	MET	3.4
2	n	1	MET	3.4
2	c	32	LEU	3.4
2	p	1	MET	3.4

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Mol	Chain	Res	Type	RSRZ
1	T	122	PHE	3.4
1	P	123	ASP	3.3
2	h	1	MET	3.2
1	H	125	ASP	3.2
1	E	120	ALA	3.2
1	P	96	TRP	3.1
2	f	10	ILE	3.1
2	c	35	SER	3.1
1	L	117	LEU	3.1
2	r	1	MET	3.1
1	L	125	ASP	3.1
1	O	122	PHE	3.0
1	J	122	PHE	3.0
1	T	126	HIS	3.0
1	R	121	ILE	2.9
1	A	249	ARG	2.9
2	g	22	GLU	2.9
2	i	1	MET	2.9
1	C	125	ASP	2.9
2	o	1	MET	2.8
1	B	126	HIS	2.8
1	O	126	HIS	2.8
2	f	1	MET	2.8
1	D	96	TRP	2.8
1	Q	126	HIS	2.8
1	I	122	PHE	2.8
1	D	126	HIS	2.8
1	F	126	HIS	2.8
1	R	126	HIS	2.8
1	R	122	PHE	2.8
1	E	119	ASP	2.7
1	I	123	ASP	2.7
2	l	1	MET	2.7
1	K	126	HIS	2.7
1	C	126	HIS	2.7
1	P	122	PHE	2.7
2	l	10	ILE	2.7
1	N	126	HIS	2.6
1	P	126	HIS	2.6
1	O	58	PRO	2.6
1	G	126	HIS	2.6
1	M	66	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	T	117	LEU	2.6
1	S	122	PHE	2.6
1	L	113	ILE	2.6
2	e	10	ILE	2.6
1	I	126	HIS	2.6
2	b	10	ILE	2.6
2	q	10	ILE	2.6
2	t	84	GLU	2.6
1	S	96	TRP	2.6
2	a	1	MET	2.5
2	c	83	LYS	2.5
2	d	83	LYS	2.5
2	p	22	GLU	2.5
1	C	249	ARG	2.5
1	G	125	ASP	2.5
1	J	126	HIS	2.5
1	Q	122	PHE	2.5
2	p	10	ILE	2.5
2	i	84	GLU	2.5
2	e	84	GLU	2.5
2	a	10	ILE	2.5
2	p	3	TYR	2.5
1	F	124	GLU	2.4
2	j	62	ARG	2.4
1	B	96	TRP	2.4
1	I	159	ASN	2.4
1	E	249	ARG	2.4
1	G	59	ARG	2.4
1	H	124	GLU	2.4
2	p	33	GLY	2.4
1	F	122	PHE	2.4
1	L	122	PHE	2.4
1	N	122	PHE	2.4
2	g	10	ILE	2.4
1	M	126	HIS	2.4
2	j	10	ILE	2.4
1	O	96	TRP	2.4
1	F	125	ASP	2.4
1	G	96	TRP	2.4
1	Q	120	ALA	2.3
1	P	121	ILE	2.3
2	s	10	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
2	d	62	ARG	2.3
1	I	124	GLU	2.3
1	O	82	LEU	2.3
1	S	58	PRO	2.3
2	d	10	ILE	2.3
1	O	66	LEU	2.3
2	b	33	GLY	2.3
1	H	122	PHE	2.2
2	t	60	LEU	2.2
2	m	2	PRO	2.2
1	L	126	HIS	2.2
1	A	122	PHE	2.2
1	E	118	ASN	2.2
1	G	58	PRO	2.2
1	L	58	PRO	2.2
2	j	1	MET	2.2
1	F	62	GLU	2.2
1	B	117	LEU	2.2
2	c	4	LEU	2.2
1	D	122	PHE	2.2
1	D	125	ASP	2.2
1	T	58	PRO	2.2
1	F	249	ARG	2.2
1	G	66	LEU	2.2
2	m	10	ILE	2.2
2	o	10	ILE	2.2
2	m	62	ARG	2.2
1	L	123	ASP	2.2
1	N	124	GLU	2.2
2	c	10	ILE	2.1
1	C	159	ASN	2.1
1	B	122	PHE	2.1
1	H	126	HIS	2.1
1	R	120	ALA	2.1
1	Q	117	LEU	2.1
1	E	125	ASP	2.1
1	H	123	ASP	2.1
1	I	125	ASP	2.1
1	R	123	ASP	2.1
1	A	126	HIS	2.1
2	d	67	VAL	2.1
1	K	125	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	S	116	VAL	2.1
1	I	113	ILE	2.1
1	G	116	VAL	2.1
1	E	83	GLY	2.1
2	d	64	GLY	2.1
2	q	62	ARG	2.1
2	e	1	MET	2.0
1	K	62	GLU	2.0
1	P	124	GLU	2.0
1	I	117	LEU	2.0
1	N	117	LEU	2.0
2	c	62	ARG	2.0
1	E	117	LEU	2.0
1	B	121	ILE	2.0
1	M	58	PRO	2.0
1	R	58	PRO	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	QBQ	K	302	32/32	0.88	0.12	63,66,90,92	17
5	HBI	S	303	17/17	0.88	0.12	43,54,62,63	13
4	QBQ	E	302	32/32	0.89	0.12	54,64,88,91	17
6	K	c	301	1/1	0.89	0.11	97,97,97,97	0
5	HBI	P	303	17/17	0.90	0.12	50,55,67,68	13
5	HBI	D	303	17/17	0.91	0.12	47,55,66,68	13
5	HBI	L	303	17/17	0.91	0.09	32,38,46,49	13

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	HBI	L	304	17/17	0.91	0.11	48,55,67,68	13
5	HBI	M	303	17/17	0.92	0.11	42,51,60,61	13
5	HBI	O	303	17/17	0.92	0.10	38,47,62,62	13
5	HBI	I	303	17/17	0.92	0.09	44,52,63,64	13
5	HBI	A	304	17/17	0.92	0.11	41,46,51,52	13
5	HBI	F	303	17/17	0.92	0.10	41,49,59,59	13
6	K	p	301	1/1	0.92	0.12	94,94,94,94	0
5	HBI	H	303	17/17	0.93	0.09	39,46,51,52	13
4	QBQ	T	302	32/32	0.93	0.09	58,60,85,88	17
5	HBI	I	304	17/17	0.93	0.10	38,46,53,53	13
5	HBI	Q	303	17/17	0.93	0.09	44,52,65,66	13
5	HBI	R	303	17/17	0.93	0.09	34,39,49,50	13
5	HBI	K	303	17/17	0.93	0.09	38,45,54,55	13
5	HBI	E	303	17/17	0.93	0.09	44,50,58,59	13
6	K	e	301	1/1	0.93	0.14	76,76,76,76	0
4	QBQ	Q	302	32/32	0.93	0.09	51,55,82,85	17
6	K	t	301	1/1	0.93	0.08	74,74,74,74	0
4	QBQ	A	302	32/32	0.94	0.09	48,53,77,81	17
5	HBI	T	303	17/17	0.94	0.10	38,47,54,55	13
4	QBQ	C	302	32/32	0.94	0.09	53,58,83,85	17
6	K	d	301	1/1	0.94	0.08	75,75,75,75	0
5	HBI	A	303	17/17	0.94	0.09	40,48,56,57	13
6	K	g	301	1/1	0.94	0.09	74,74,74,74	0
6	K	i	301	1/1	0.94	0.08	72,72,72,72	0
6	K	l	301	1/1	0.94	0.08	71,71,71,71	0
6	K	m	301	1/1	0.94	0.07	71,71,71,71	0
5	HBI	G	303	17/17	0.94	0.09	45,53,65,66	13
6	K	s	301	1/1	0.94	0.14	78,78,78,78	0
4	QBQ	L	302	32/32	0.94	0.08	48,62,91,102	17
3	ZN	D	301	1/1	0.95	0.06	73,73,73,73	0
4	QBQ	S	302	32/32	0.95	0.08	43,47,70,75	17
4	QBQ	F	302	32/32	0.95	0.07	41,48,69,74	17
4	QBQ	H	302	32/32	0.95	0.08	41,48,72,74	17
4	QBQ	J	302	32/32	0.95	0.09	48,53,77,79	17
6	K	h	301	1/1	0.95	0.08	76,76,76,76	0
5	HBI	B	303	17/17	0.95	0.09	45,53,63,64	13
6	K	j	301	1/1	0.95	0.07	66,66,66,66	0
3	ZN	P	301	1/1	0.95	0.07	75,75,75,75	0
4	QBQ	D	302	32/32	0.95	0.08	44,52,76,84	17
4	QBQ	N	302	32/32	0.95	0.08	45,51,73,78	17
4	QBQ	O	302	32/32	0.95	0.08	45,51,73,79	17
4	QBQ	P	302	32/32	0.95	0.08	46,54,80,90	17

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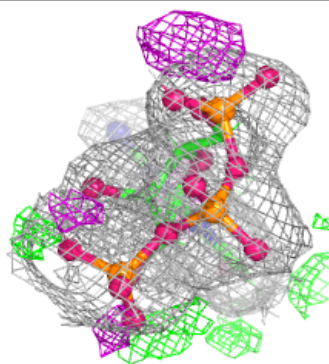
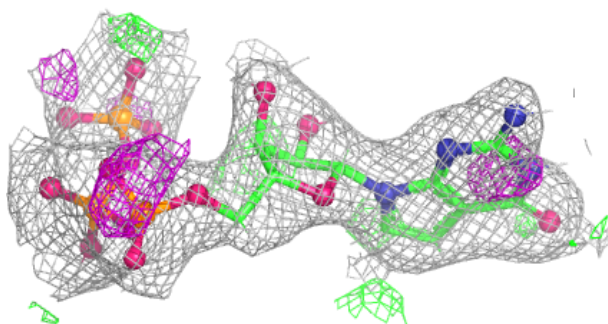
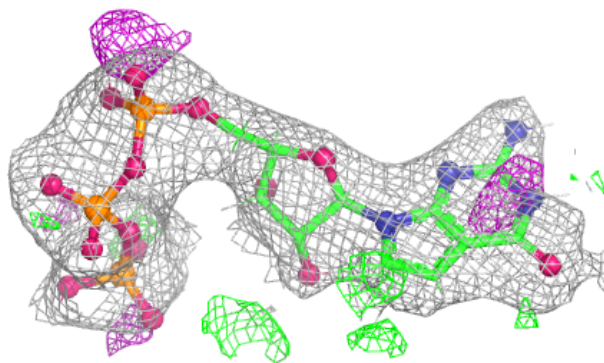
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	QBQ	B	302	32/32	0.96	0.07	40,45,65,70	17
6	K	a	301	1/1	0.96	0.07	76,76,76,76	0
6	K	k	301	1/1	0.96	0.05	63,63,63,63	0
3	ZN	A	301	1/1	0.96	0.07	59,59,59,59	0
4	QBQ	R	302	32/32	0.96	0.07	44,48,69,73	17
6	K	n	301	1/1	0.96	0.06	64,64,64,64	0
4	QBQ	G	302	32/32	0.96	0.07	47,52,75,79	17
3	ZN	O	301	1/1	0.96	0.08	78,78,78,78	0
4	QBQ	I	302	32/32	0.96	0.07	47,55,82,88	17
4	QBQ	M	302	32/32	0.97	0.06	42,48,65,73	17
3	ZN	L	301	1/1	0.97	0.07	104,104,104,104	0
6	K	f	301	1/1	0.97	0.06	72,72,72,72	0
3	ZN	M	301	1/1	0.97	0.07	78,78,78,78	0
6	K	o	301	1/1	0.97	0.09	56,56,56,56	0
3	ZN	G	301	1/1	0.97	0.08	85,85,85,85	0
6	K	q	301	1/1	0.97	0.04	69,69,69,69	0
6	K	r	301	1/1	0.97	0.08	63,63,63,63	0
6	K	b	301	1/1	0.97	0.10	76,76,76,76	0
3	ZN	K	301	1/1	0.97	0.07	66,66,66,66	0
3	ZN	E	301	1/1	0.98	0.07	65,65,65,65	0
3	ZN	Q	301	1/1	0.98	0.06	74,74,74,74	0
3	ZN	S	301	1/1	0.98	0.07	70,70,70,70	0
3	ZN	T	301	1/1	0.98	0.06	61,61,61,61	0
3	ZN	C	301	1/1	0.98	0.06	75,75,75,75	0
3	ZN	I	301	1/1	0.98	0.07	73,73,73,73	0
3	ZN	N	301	1/1	0.98	0.06	65,65,65,65	0
3	ZN	J	301	1/1	0.98	0.04	63,63,63,63	0
3	ZN	H	301	1/1	0.99	0.07	70,70,70,70	0
3	ZN	R	301	1/1	0.99	0.06	73,73,73,73	0
3	ZN	F	301	1/1	0.99	0.04	69,69,69,69	0
3	ZN	B	301	1/1	0.99	0.04	73,73,73,73	0

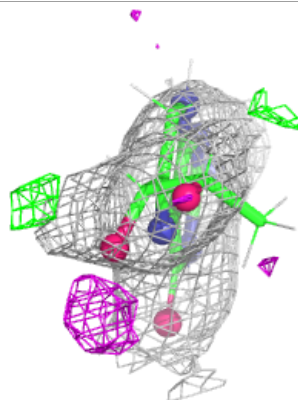
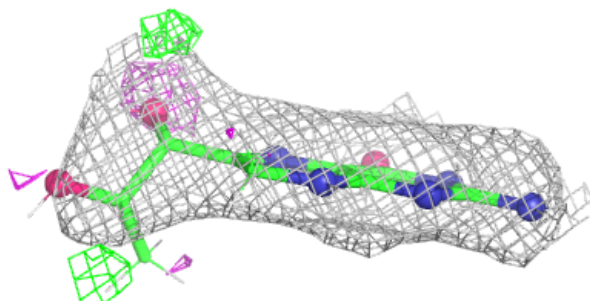
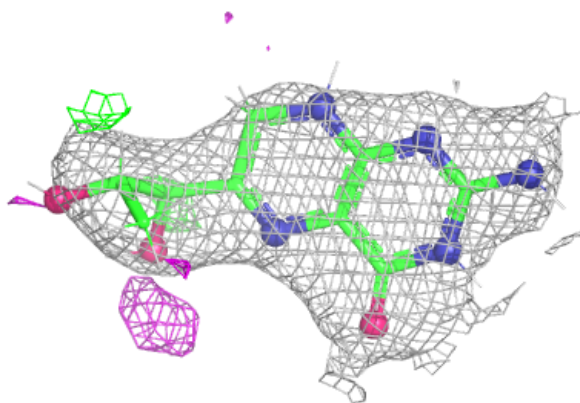
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around QBQ K 302:

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

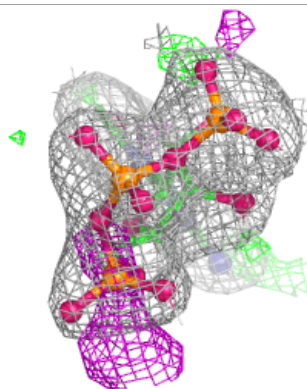
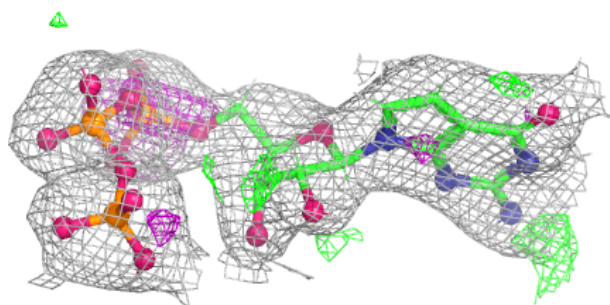
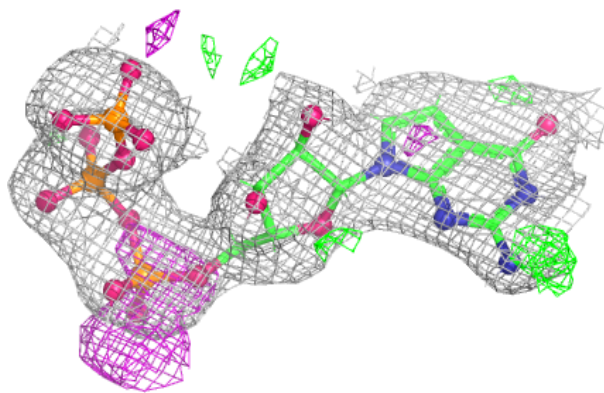
**Electron density around HBI S 303:**

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



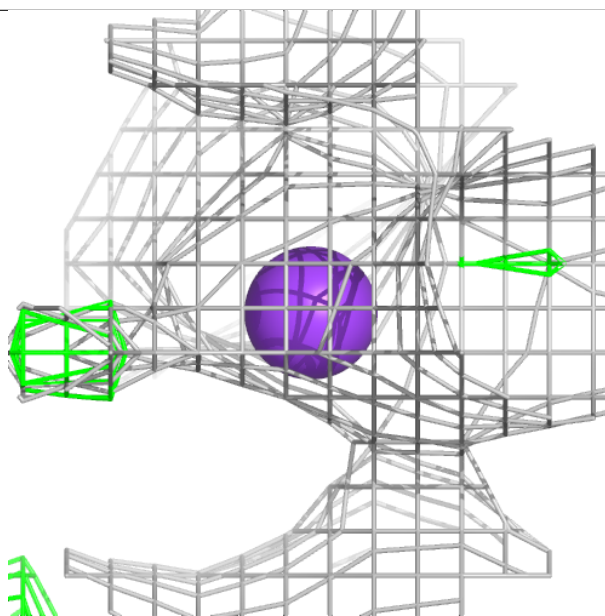
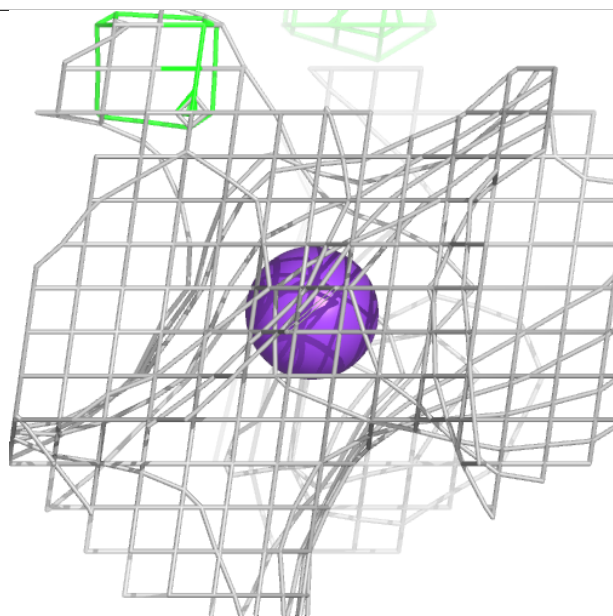
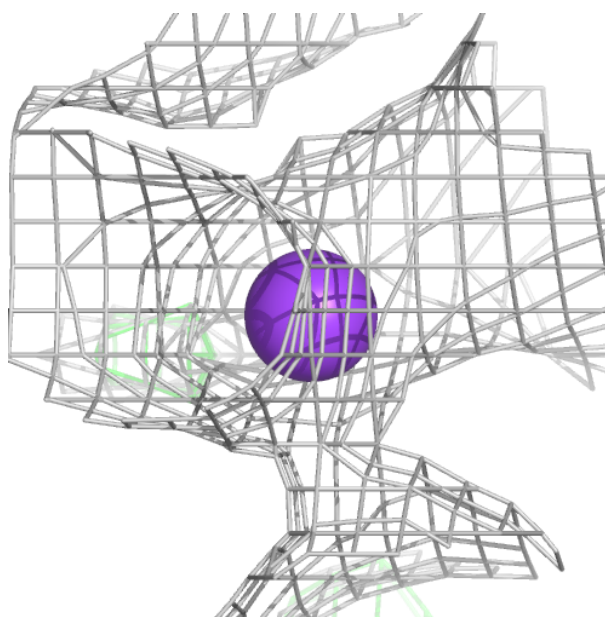
Electron density around QBQ E 302:

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



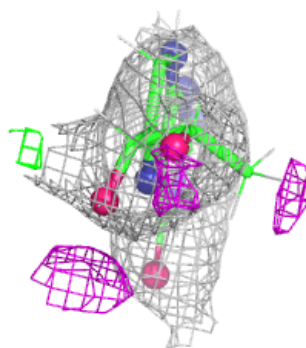
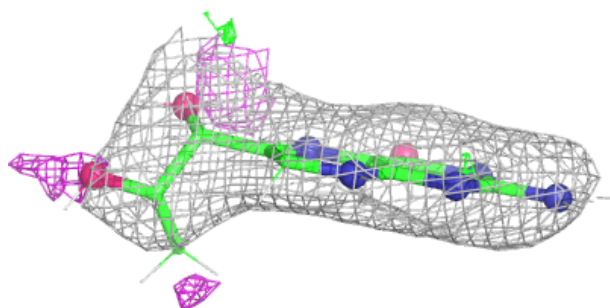
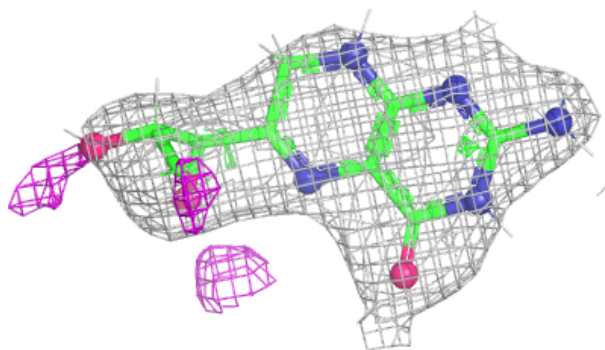
Electron density around K c 301:

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

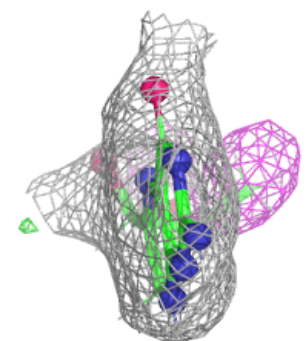
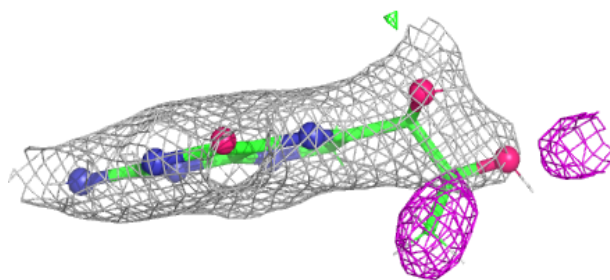
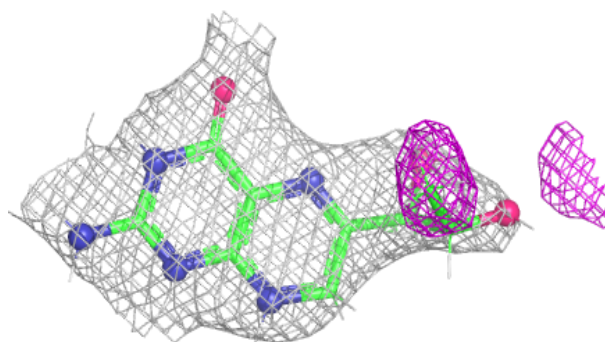


Electron density around HBI P 303:

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

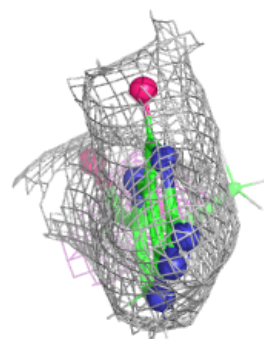
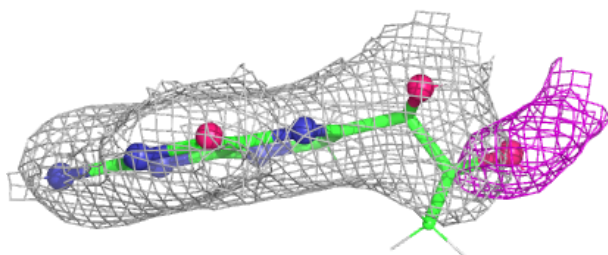
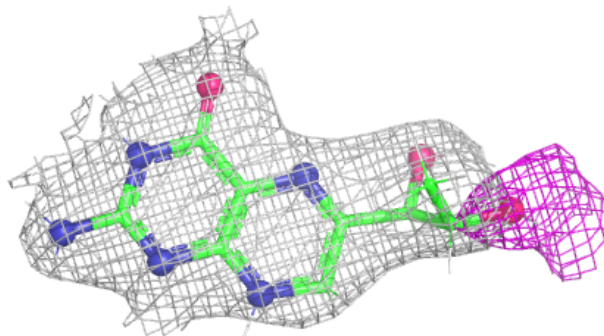
**Electron density around HBI D 303:**

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

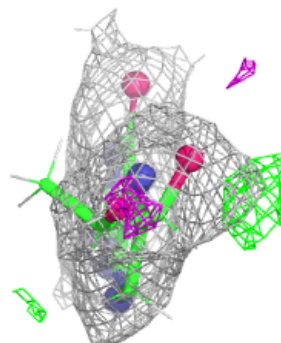
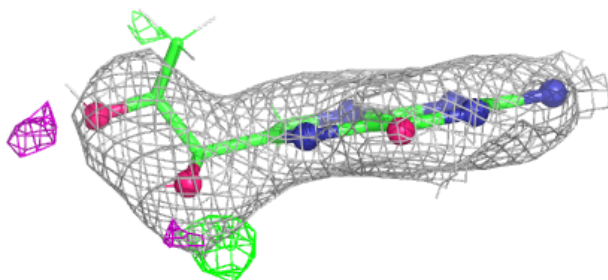
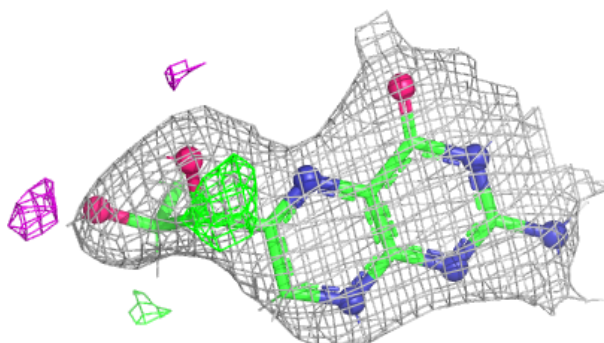


Electron density around HBI L 303:

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

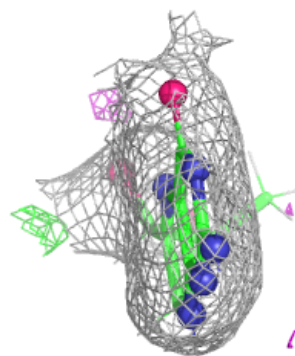
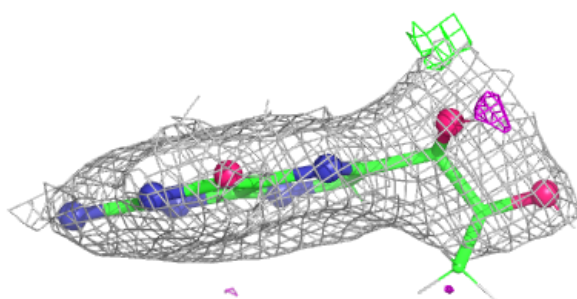
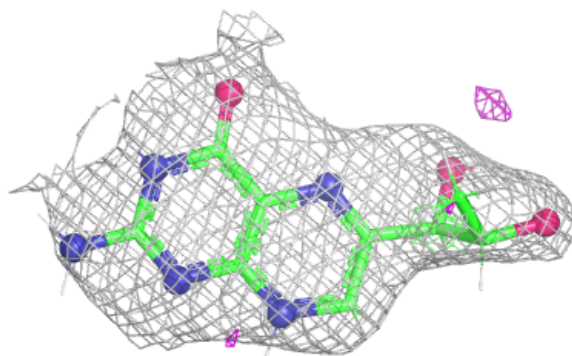
**Electron density around HBI L 304:**

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

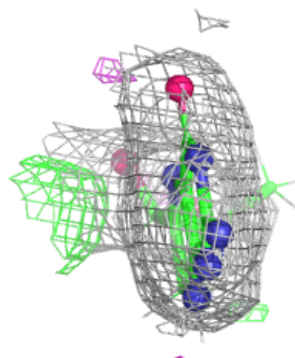
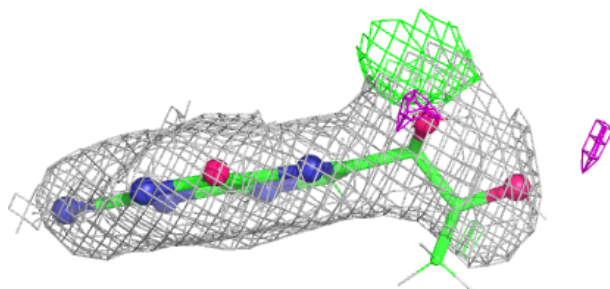
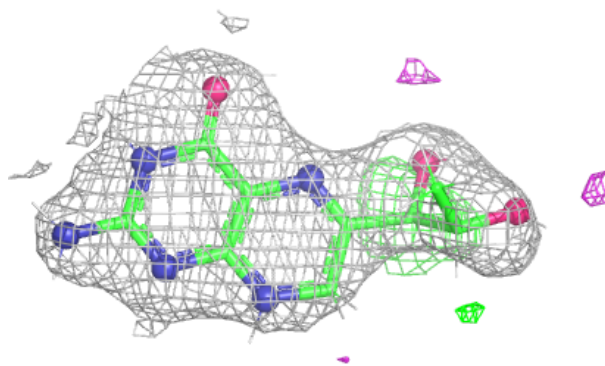


Electron density around HBI M 303:

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

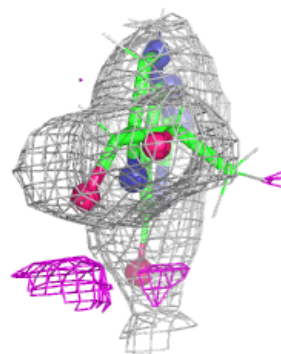
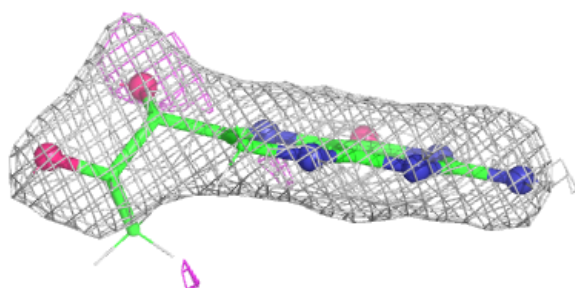
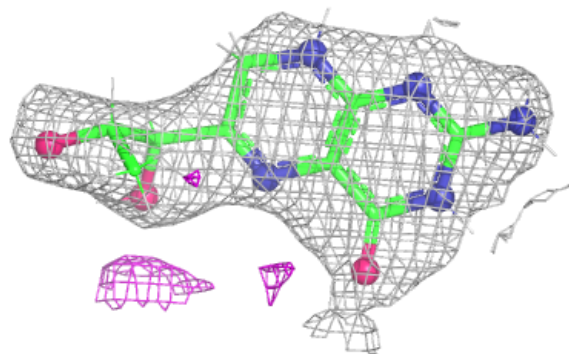
**Electron density around HBI O 303:**

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

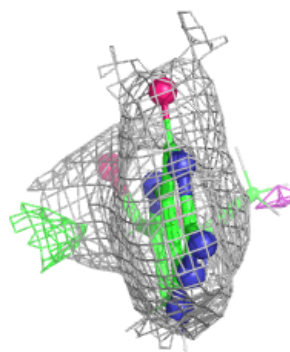
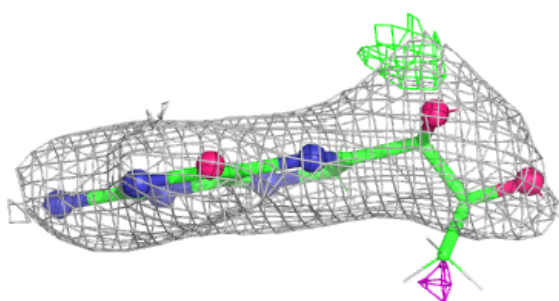
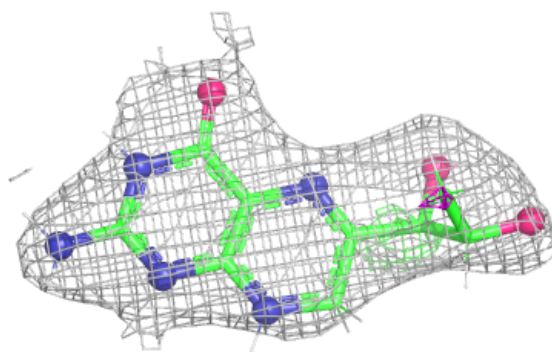


Electron density around HBI I 303:

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

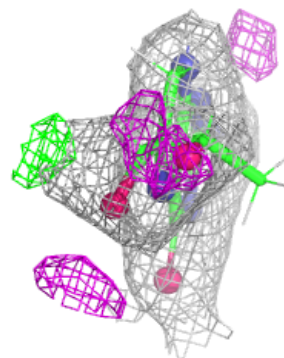
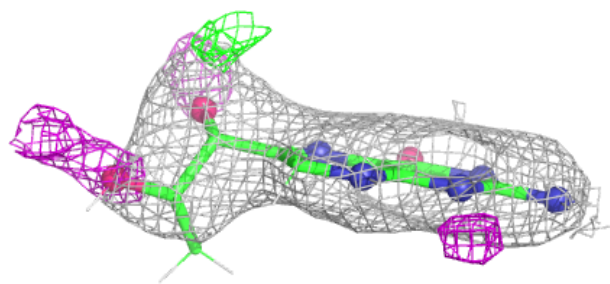
**Electron density around HBI A 304:**

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



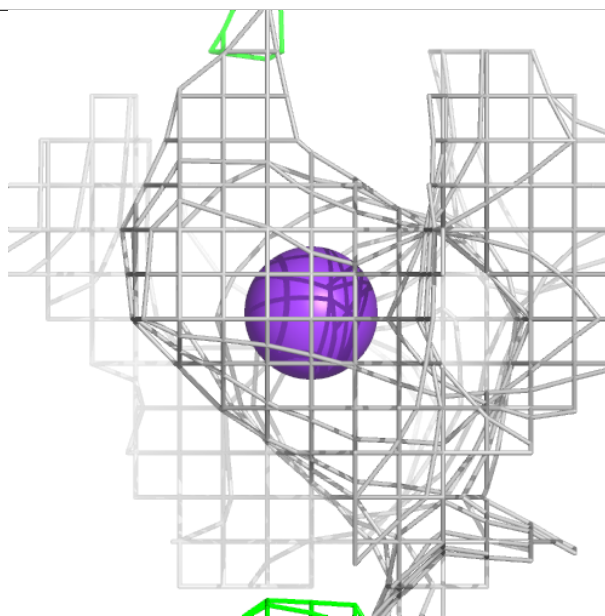
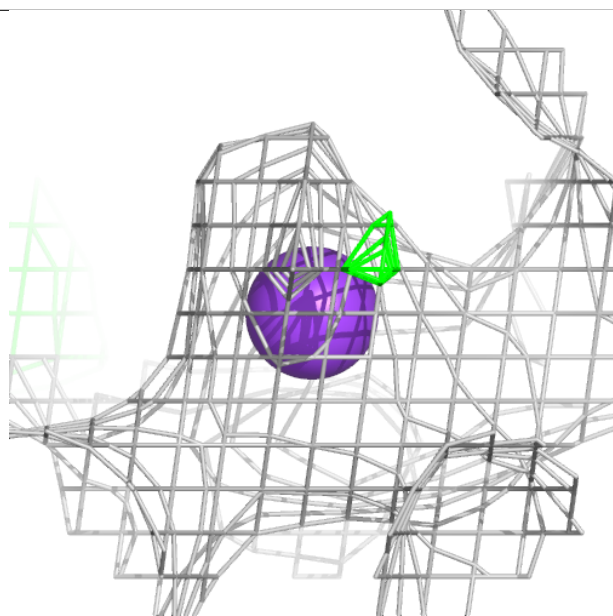
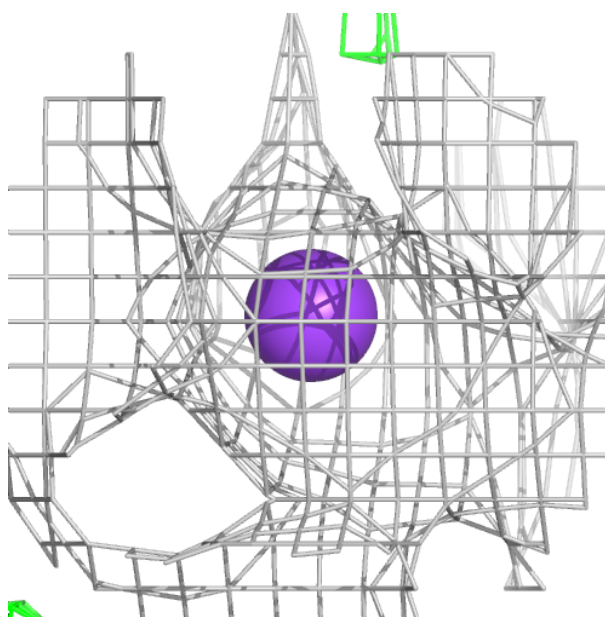
Electron density around HBI F 303:

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



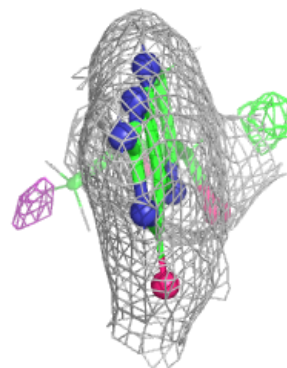
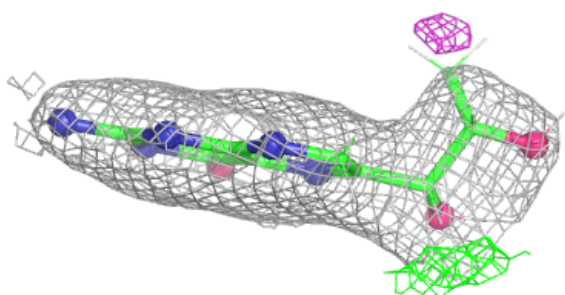
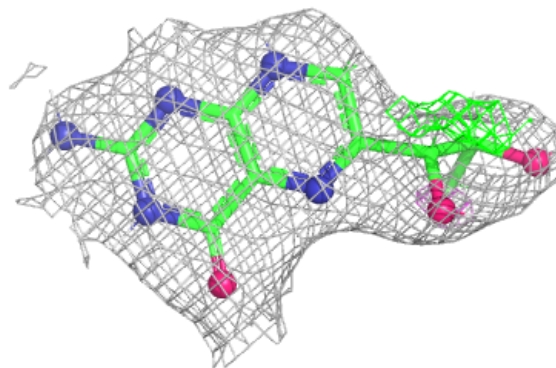
Electron density around K p 301:

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

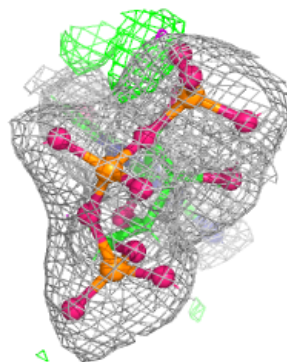
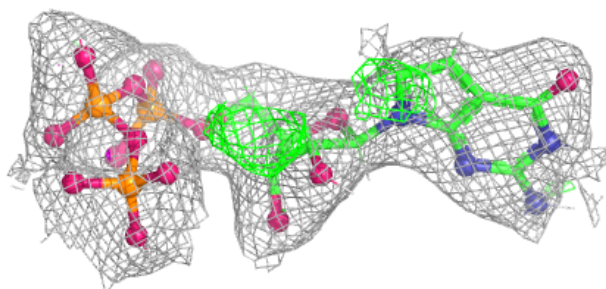
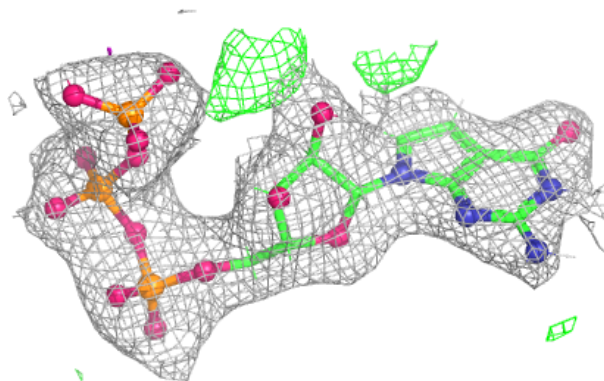


Electron density around HBI H 303:

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

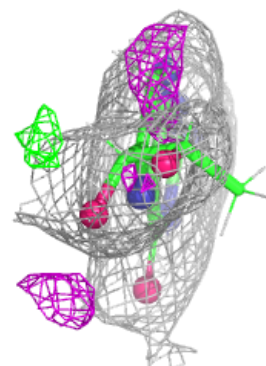
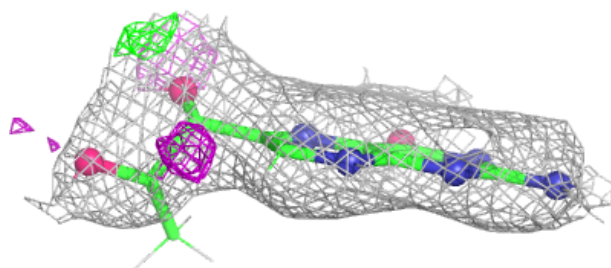
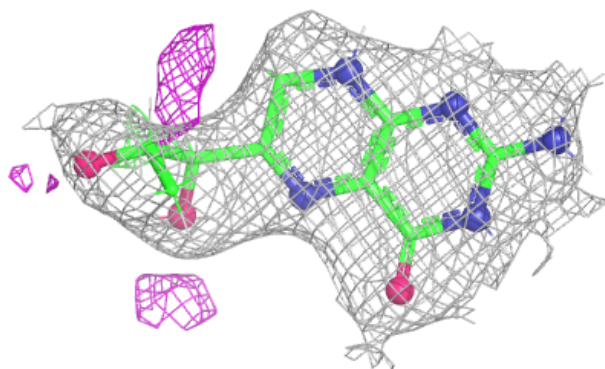
**Electron density around QBQ T 302:**

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

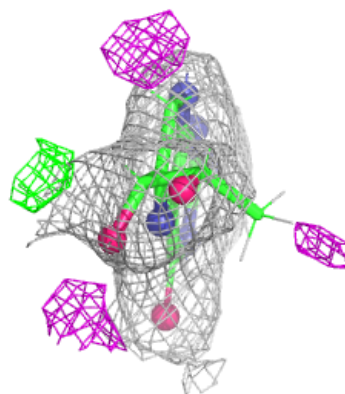
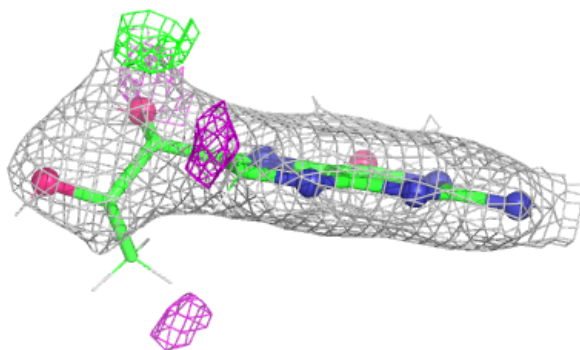
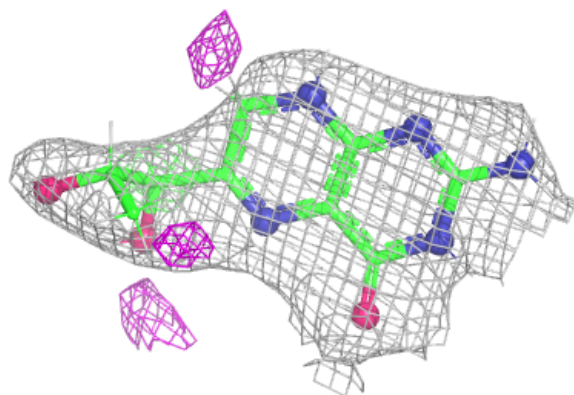


Electron density around HBI I 304:

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

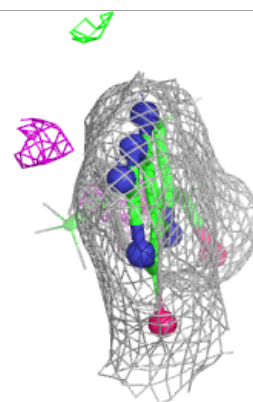
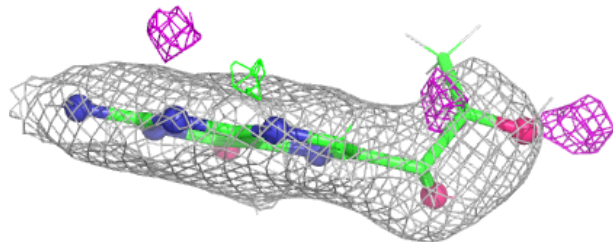
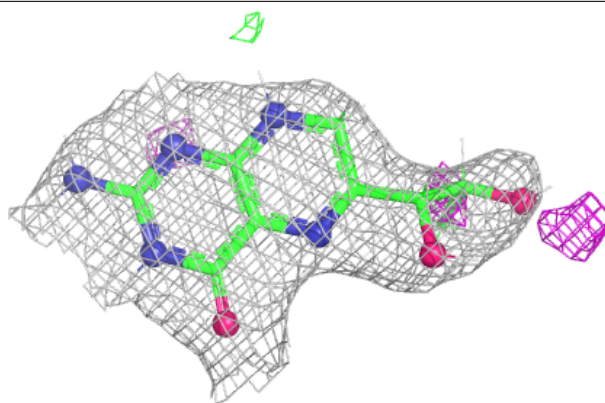
**Electron density around HBI Q 303:**

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

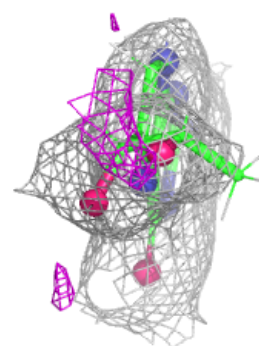
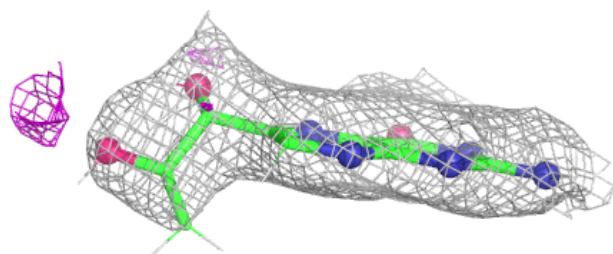
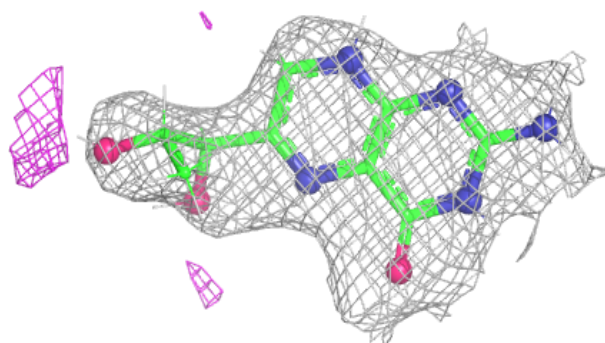


Electron density around HBI R 303:

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

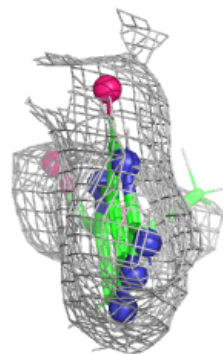
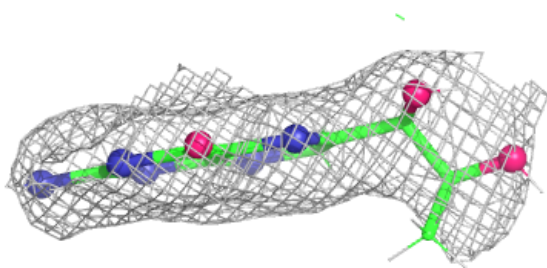
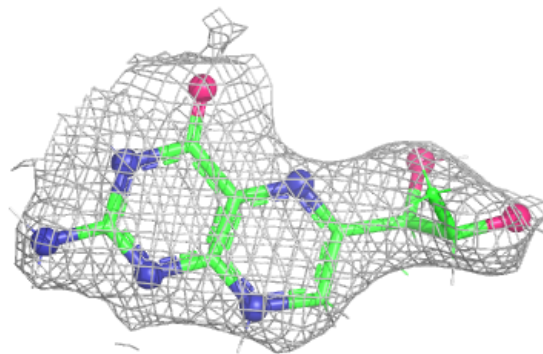
**Electron density around HBI K 303:**

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



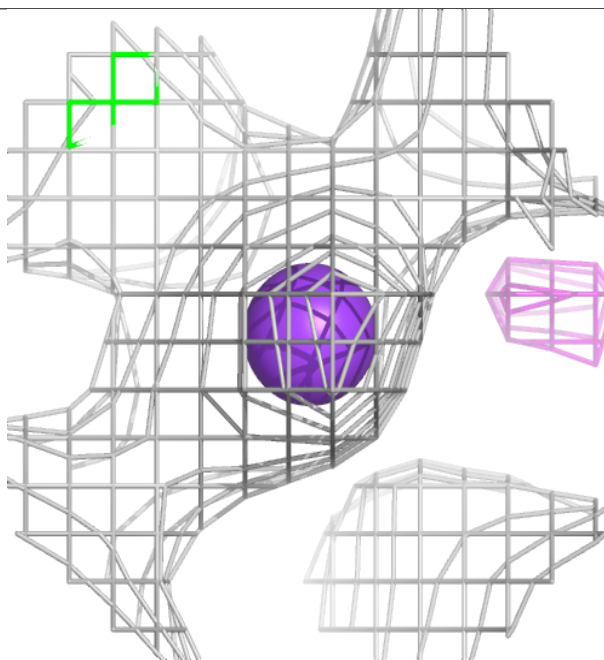
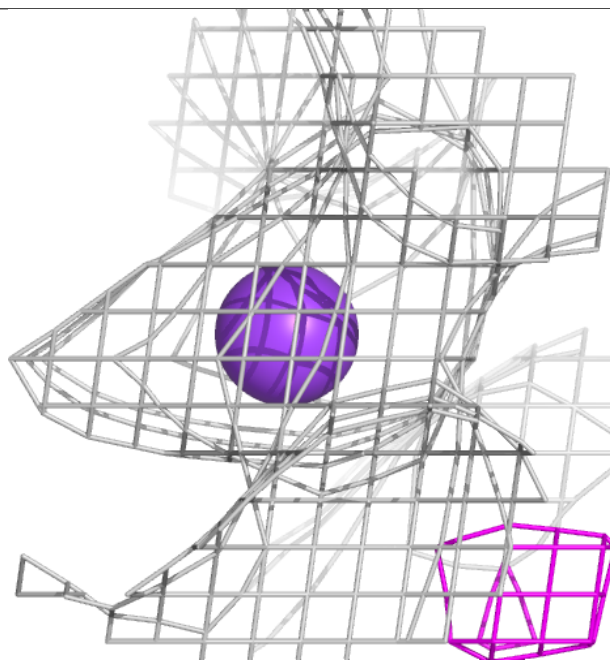
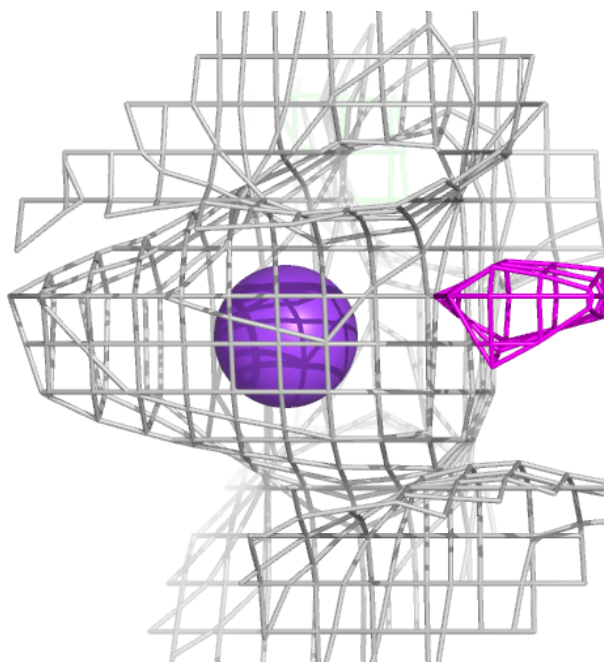
Electron density around HBI E 303:

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



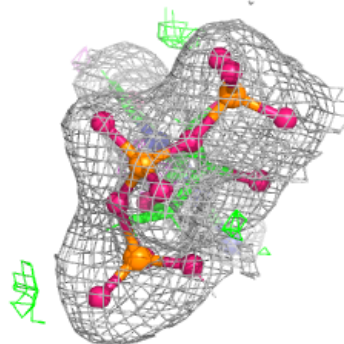
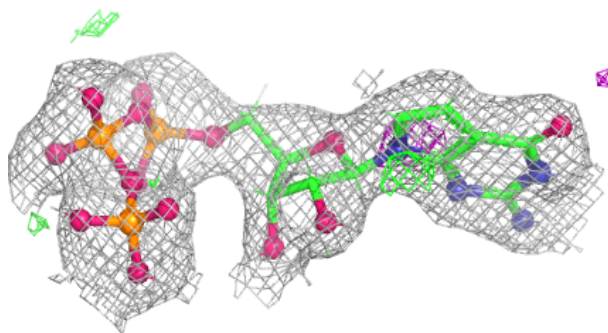
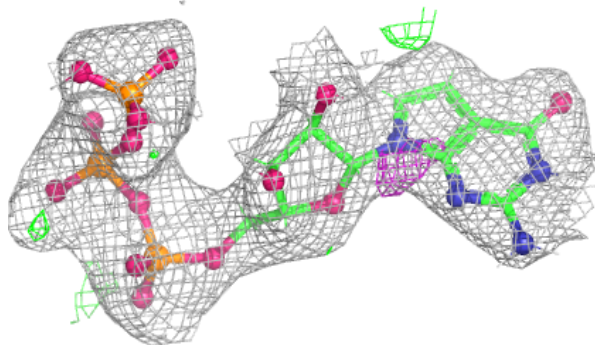
Electron density around K e 301:

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



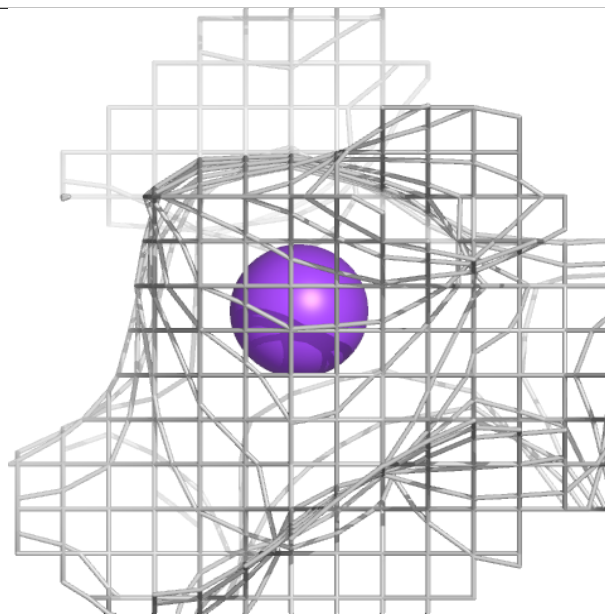
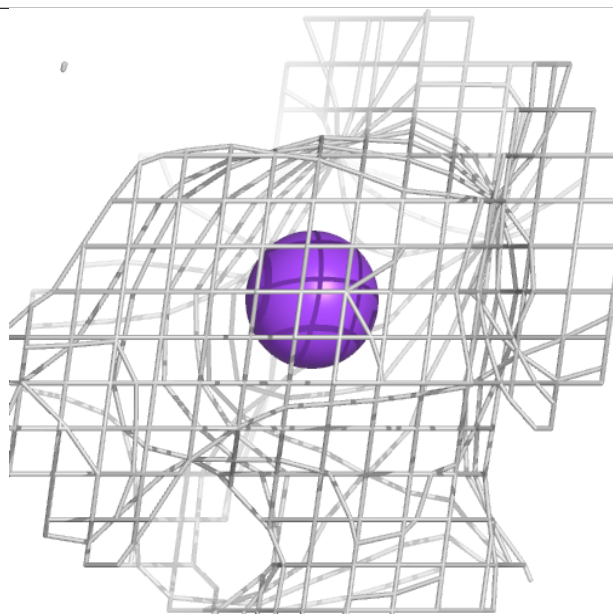
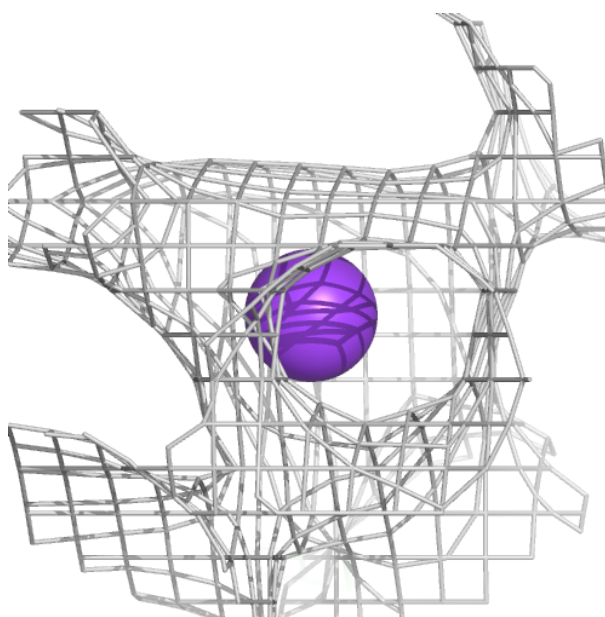
Electron density around QBQ Q 302:

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



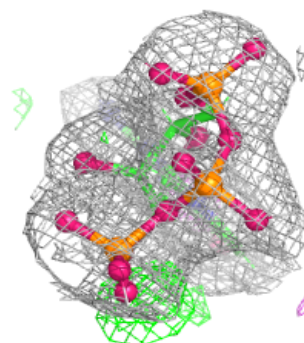
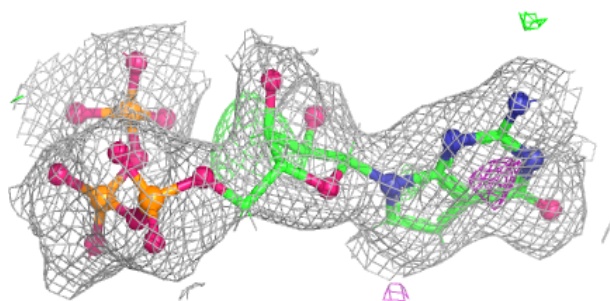
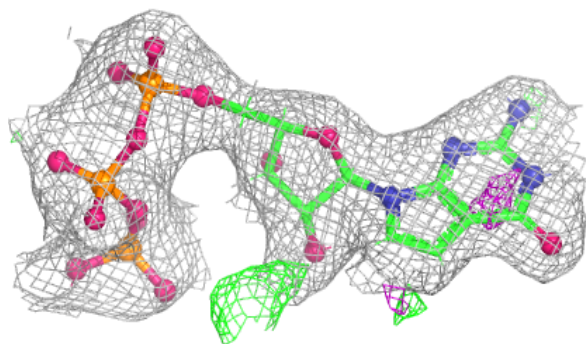
Electron density around K t 301:

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

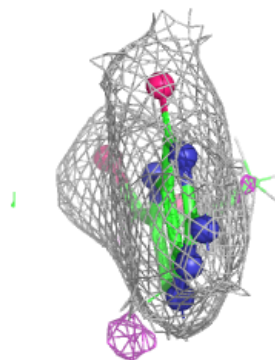
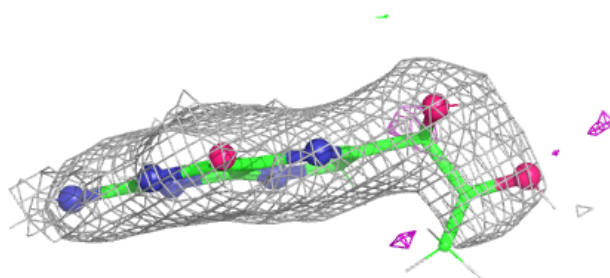
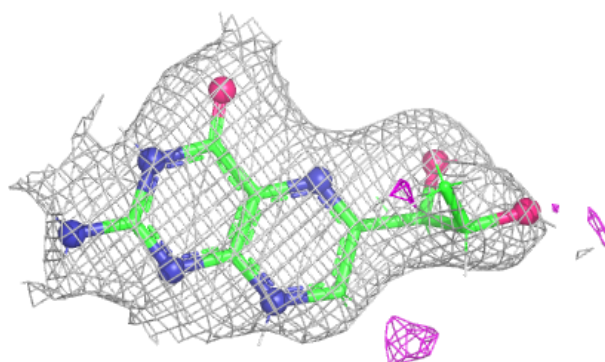


Electron density around QBQ A 302:

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

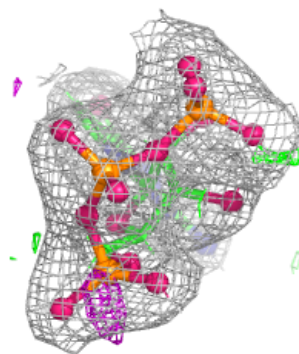
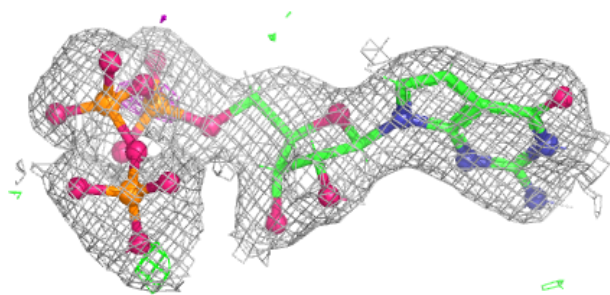
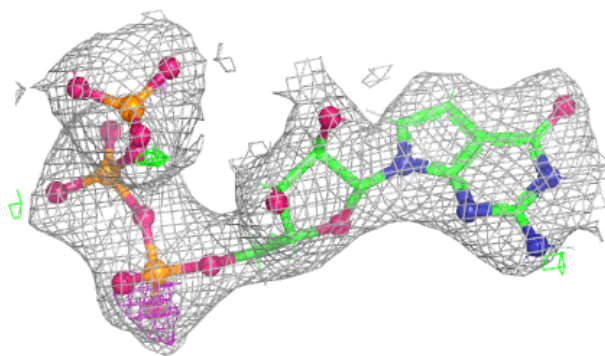
**Electron density around HBI T 303:**

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



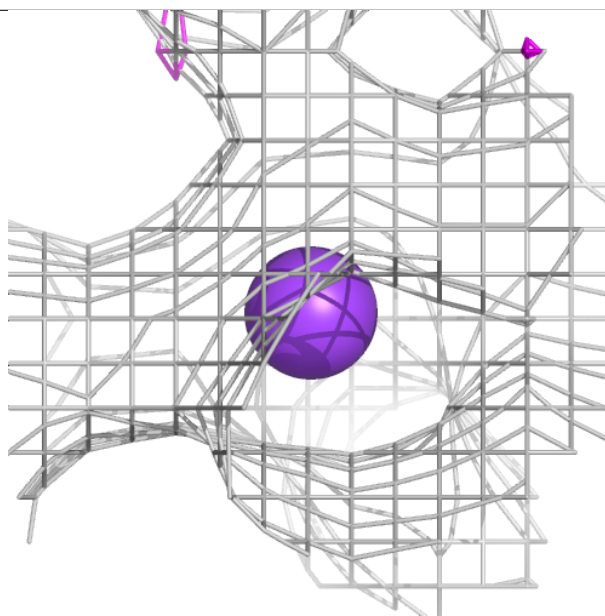
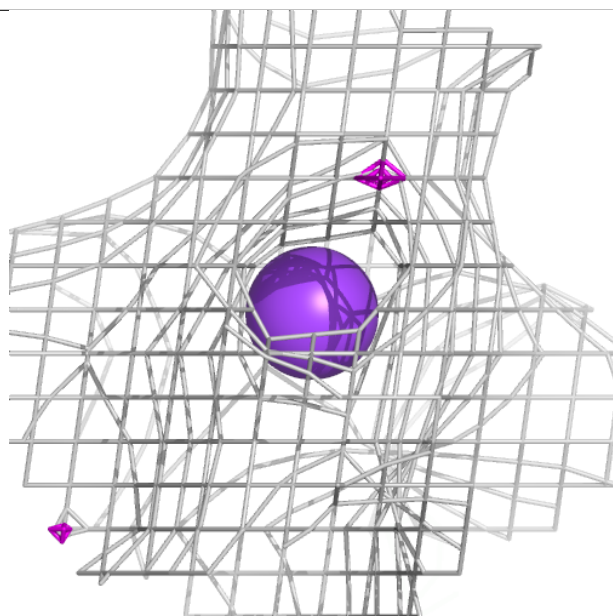
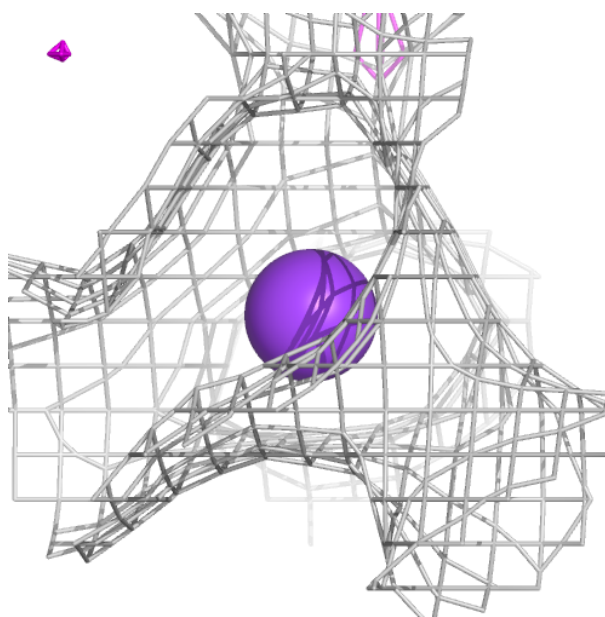
Electron density around QBQ C 302:

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



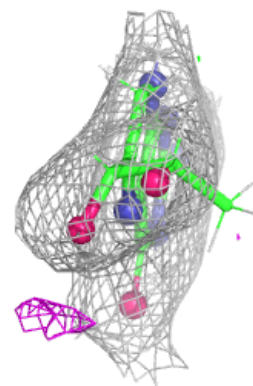
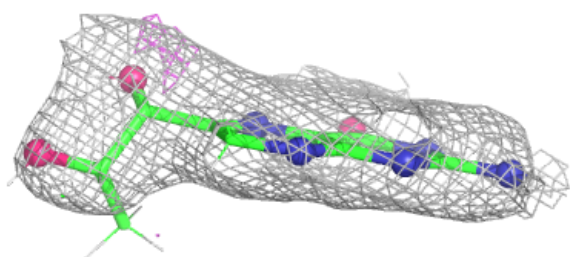
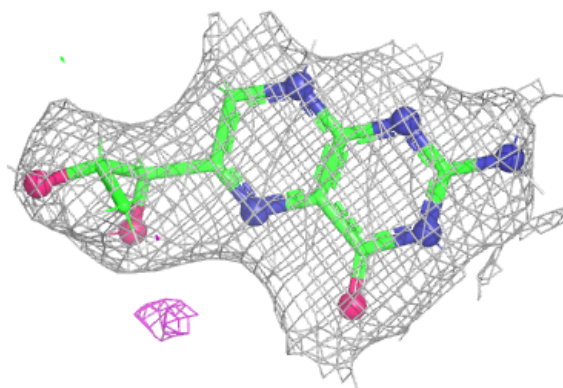
Electron density around K d 301:

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



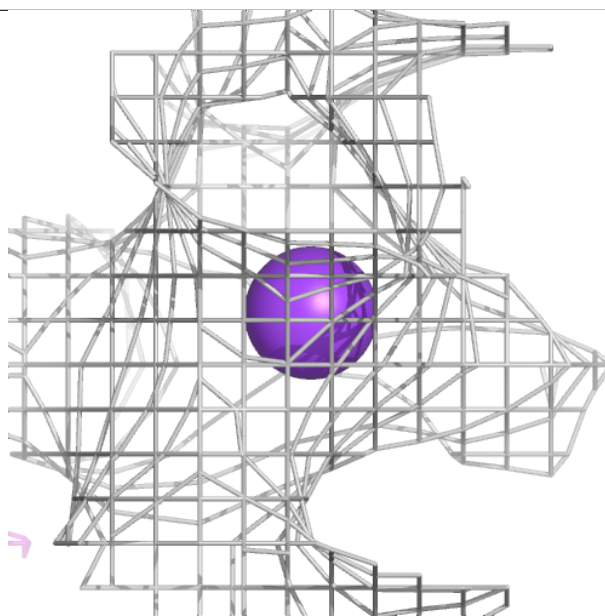
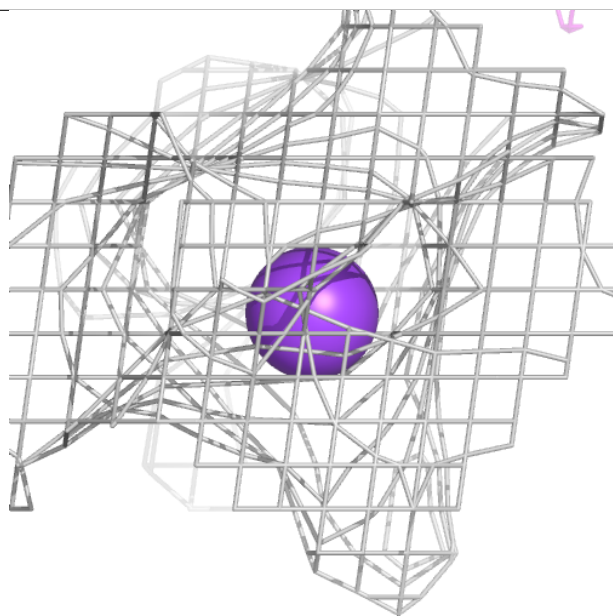
Electron density around HBI A 303:

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



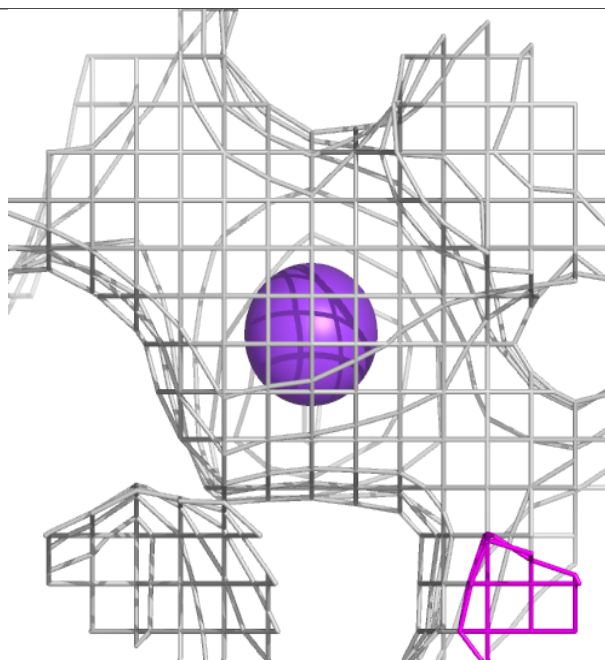
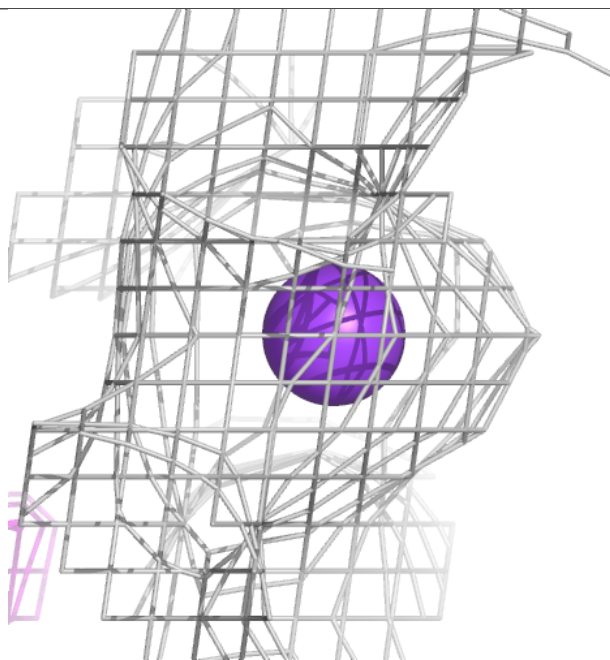
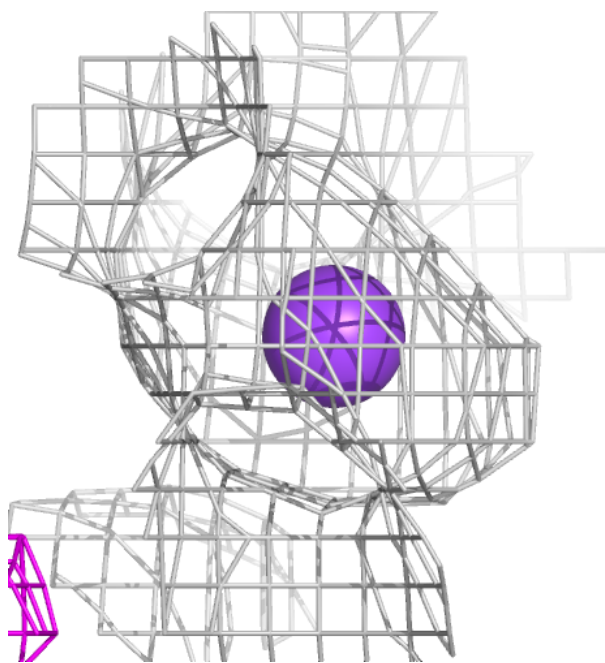
Electron density around K g 301:

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



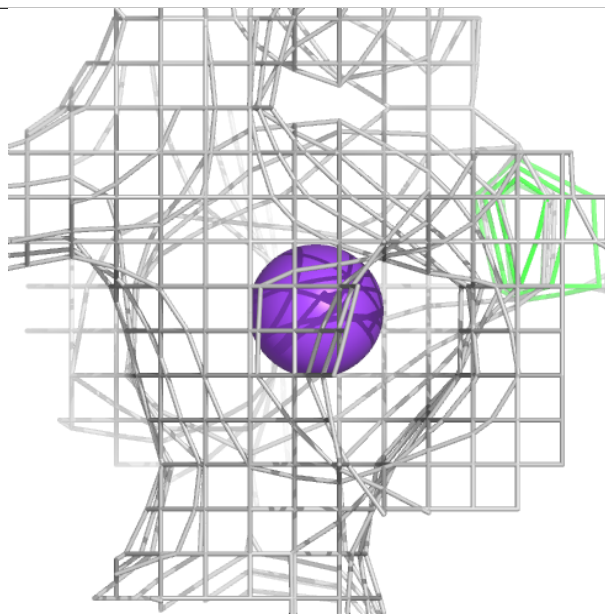
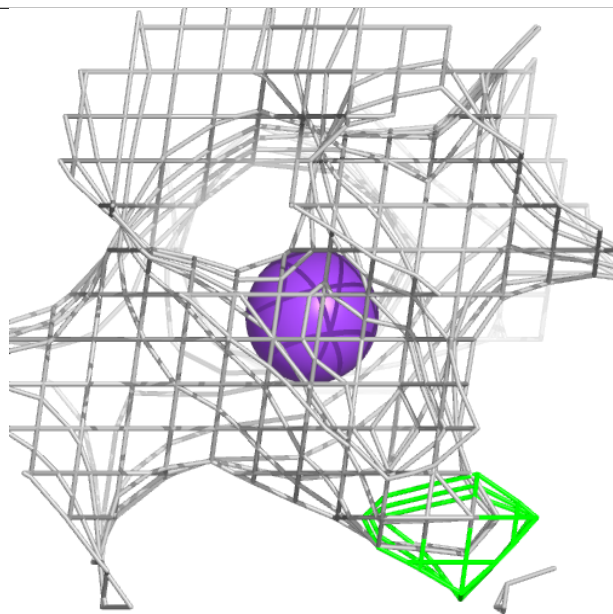
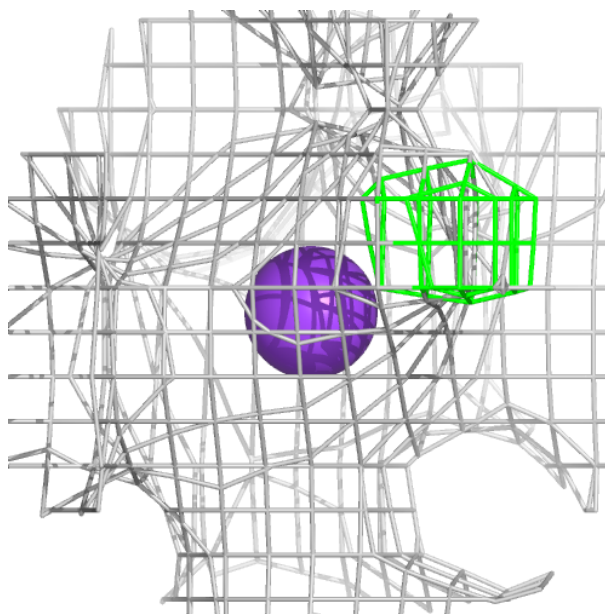
Electron density around K i 301:

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



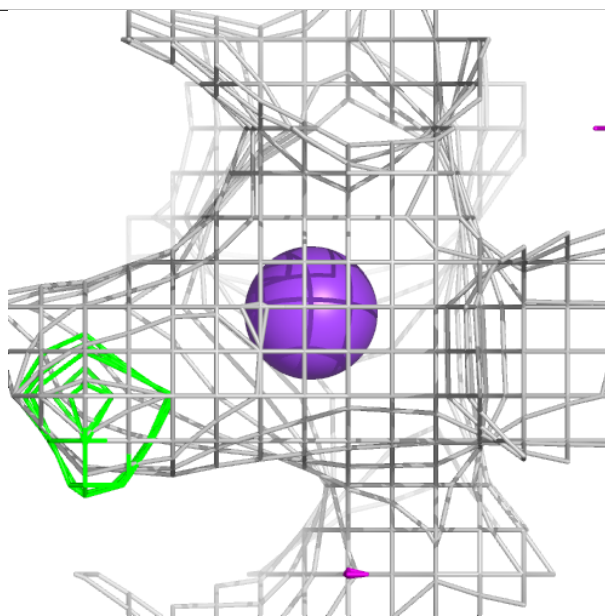
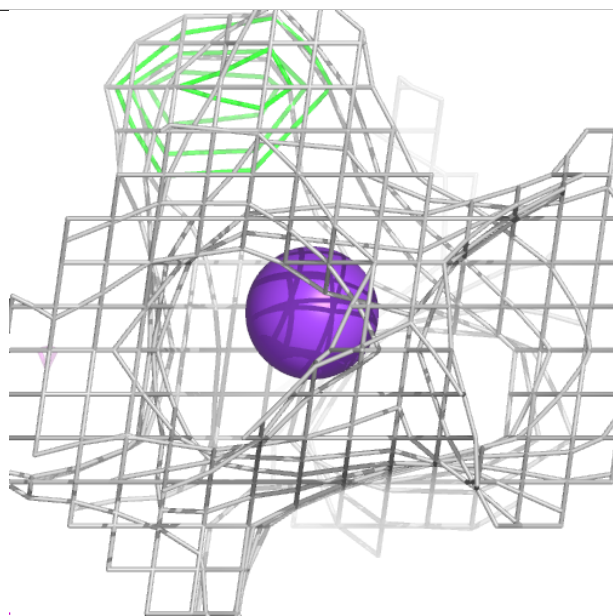
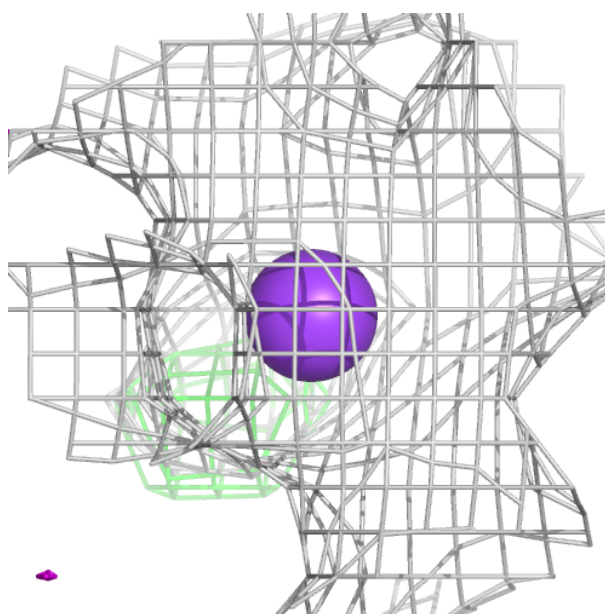
Electron density around K 1 301:

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



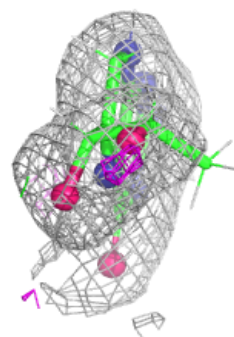
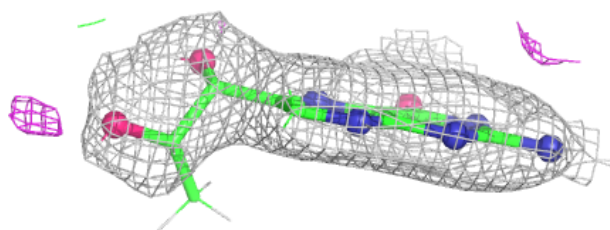
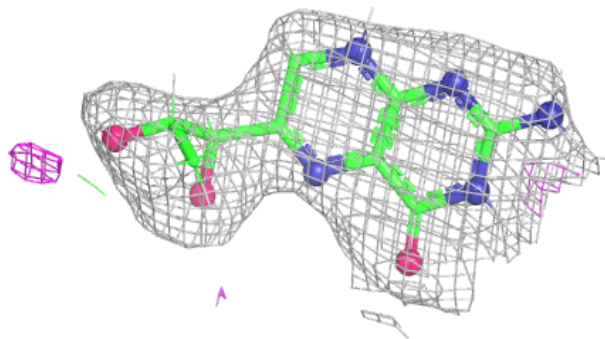
Electron density around K m 301:

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



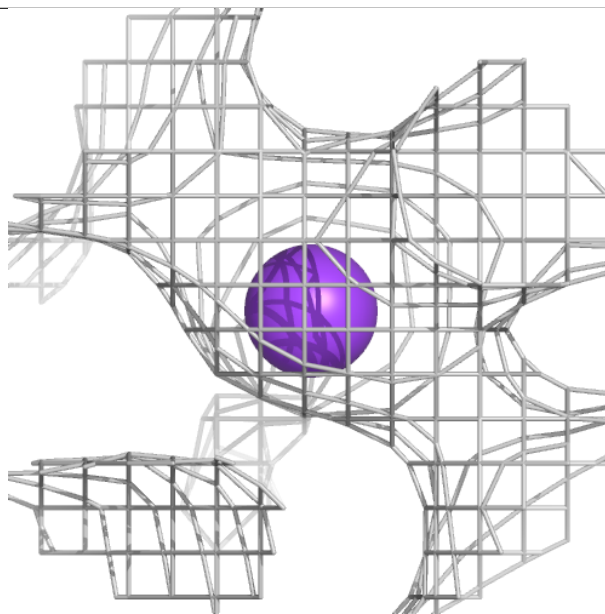
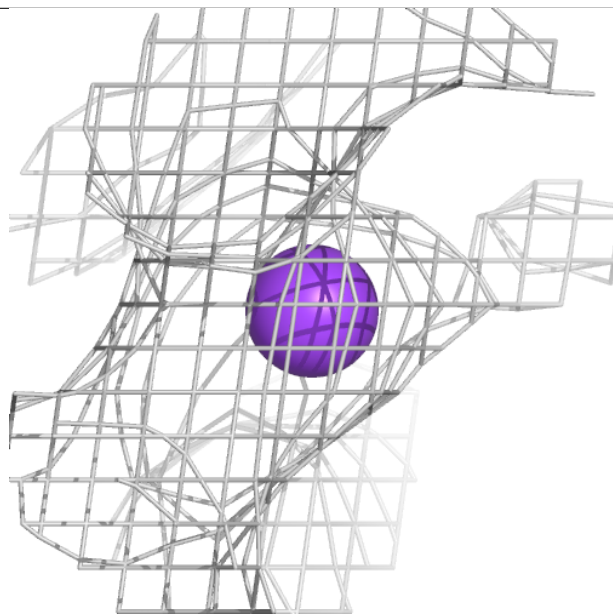
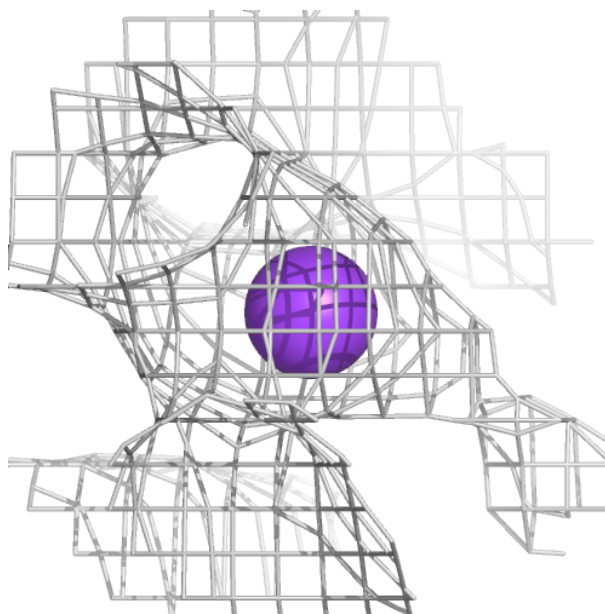
Electron density around HBI G 303:

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



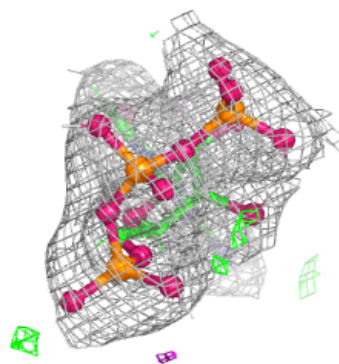
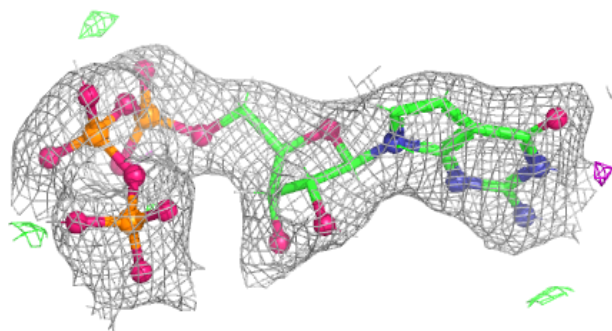
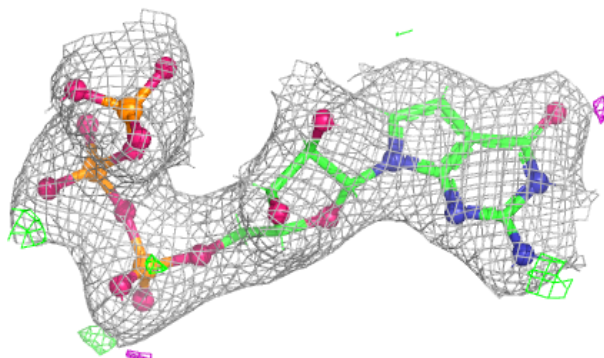
Electron density around K s 301:

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



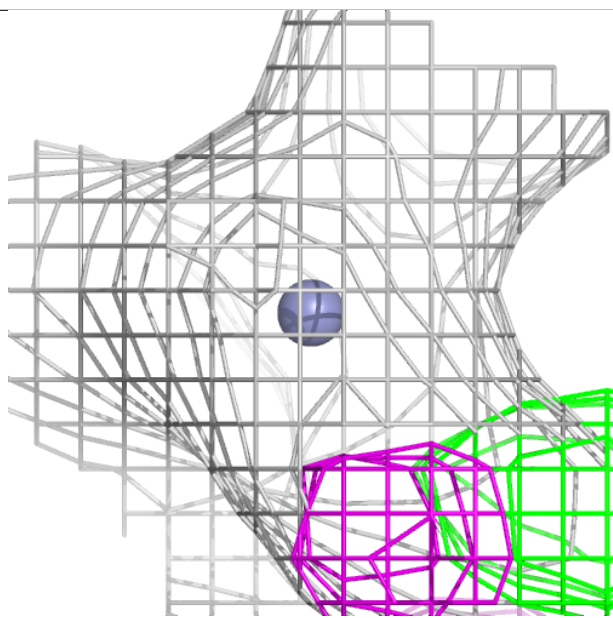
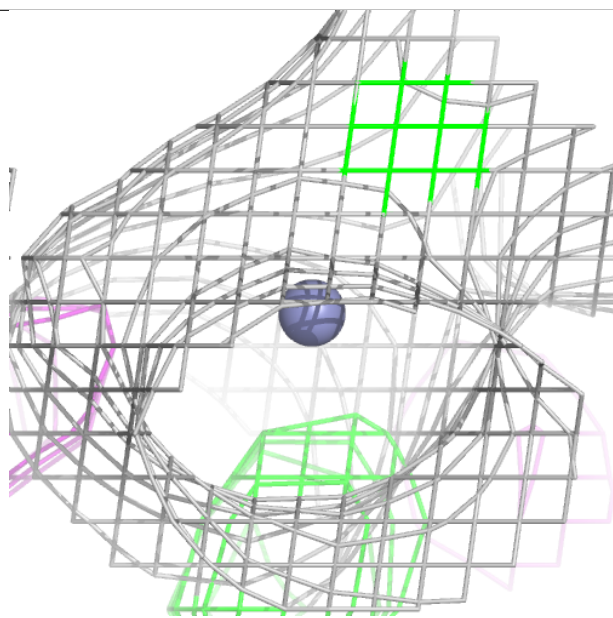
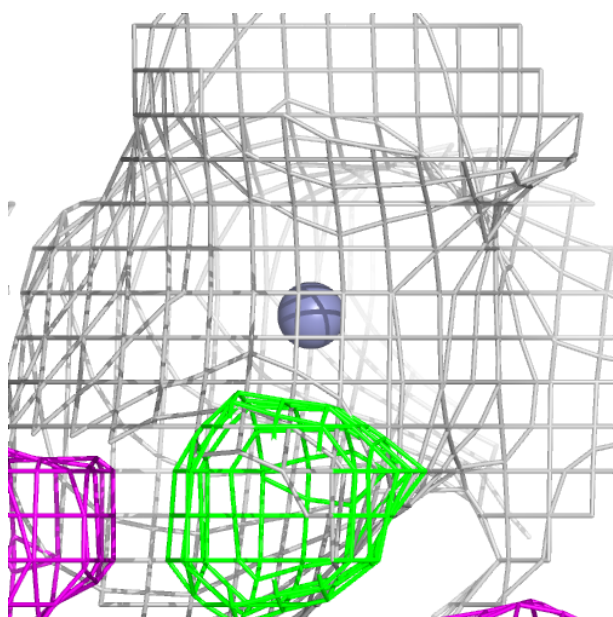
Electron density around QBQ L 302:

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



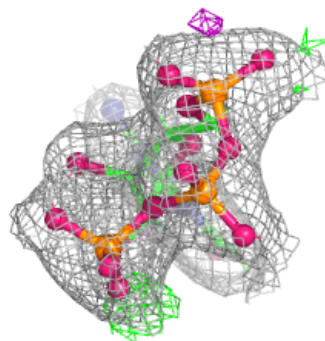
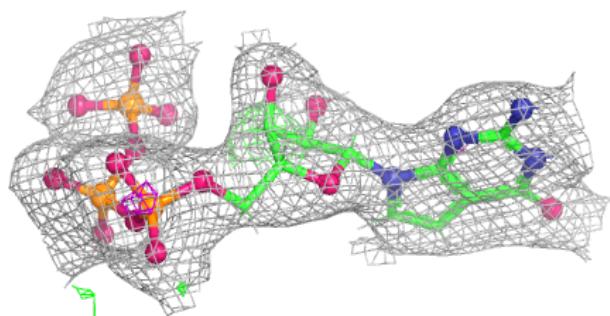
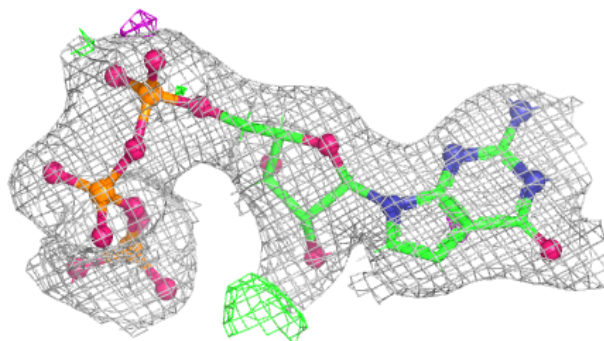
Electron density around ZN D 301:

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

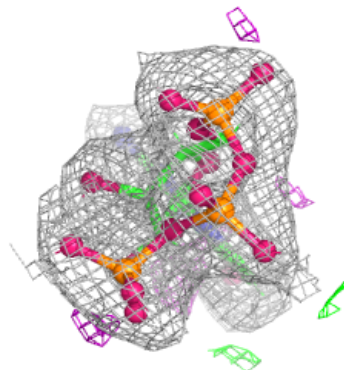
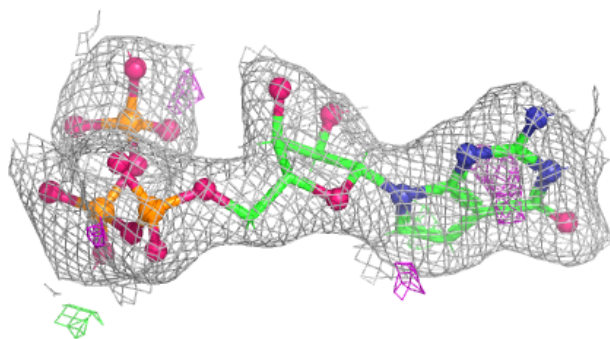
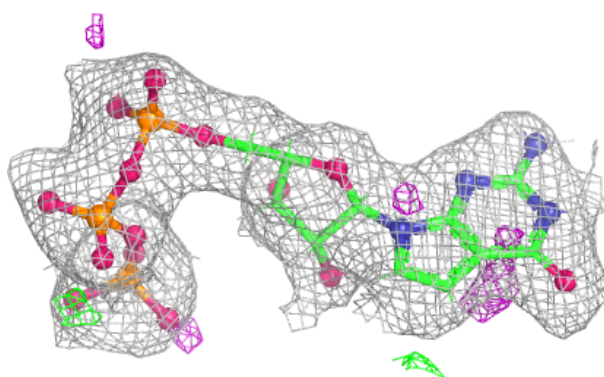


Electron density around QBQ S 302:

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

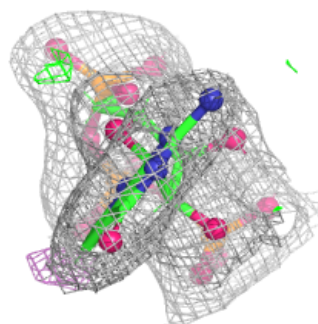
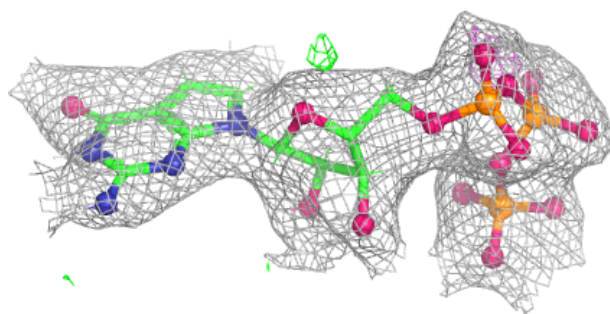
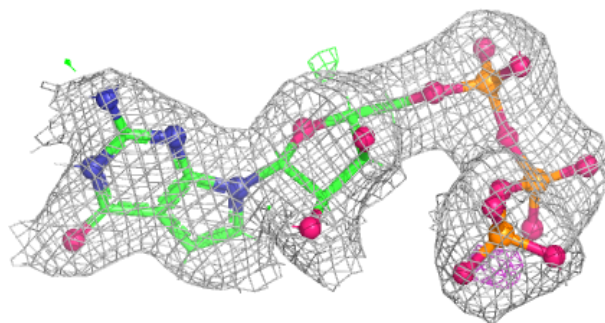
**Electron density around QBQ F 302:**

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

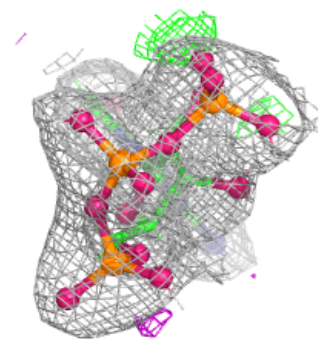
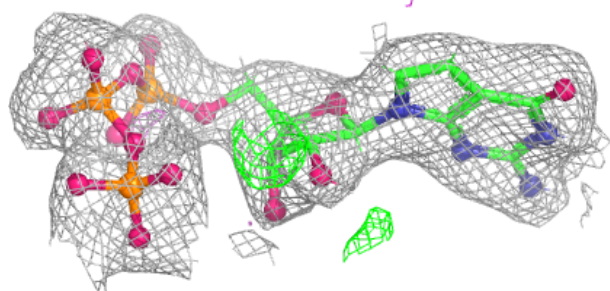
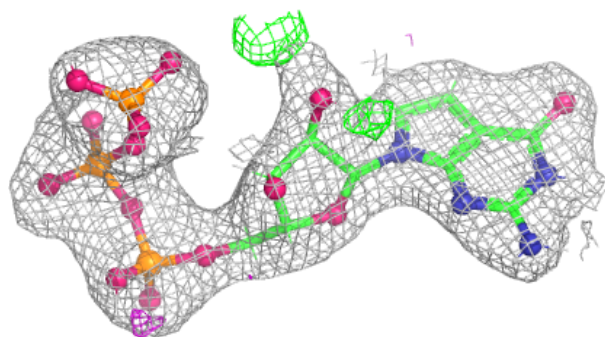


Electron density around QBQ H 302:

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

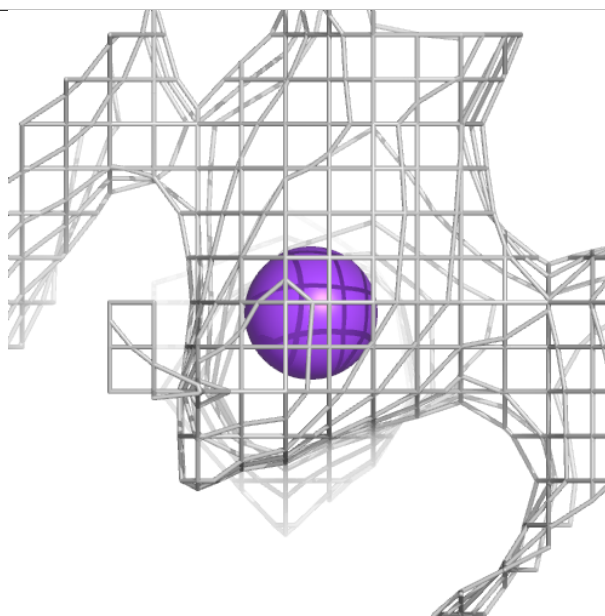
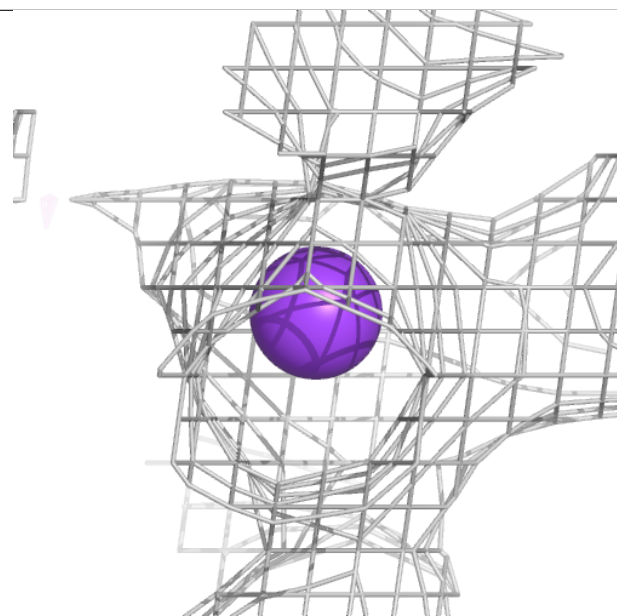
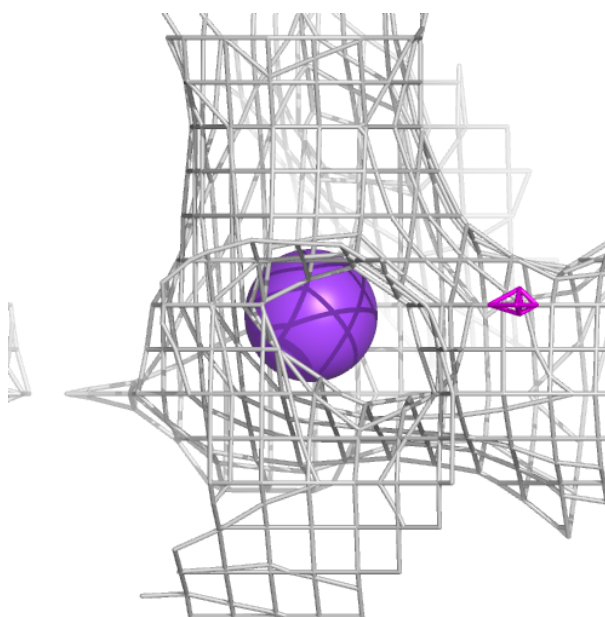
**Electron density around QBQ J 302:**

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



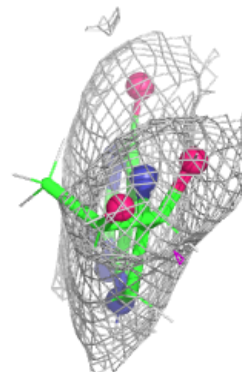
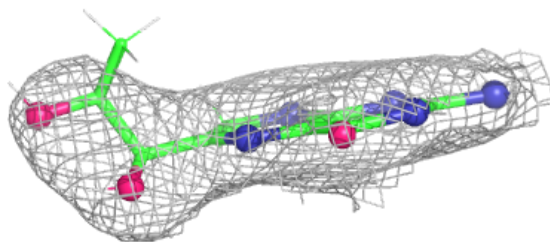
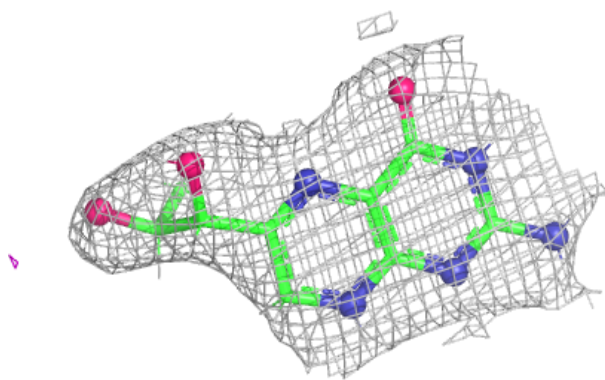
Electron density around K h 301:

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



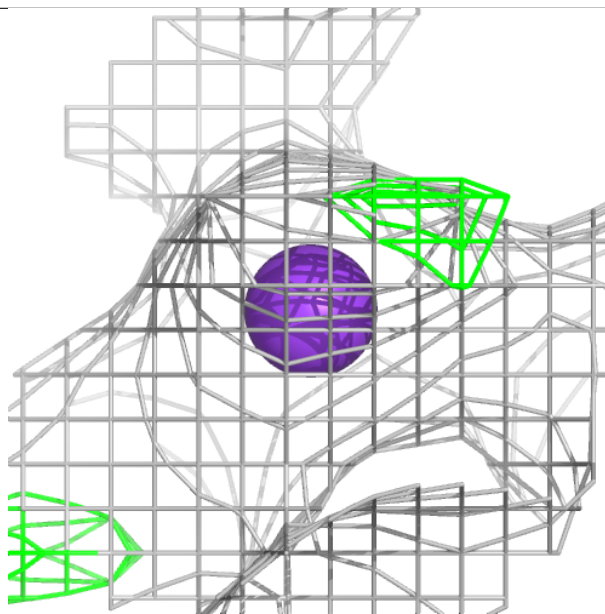
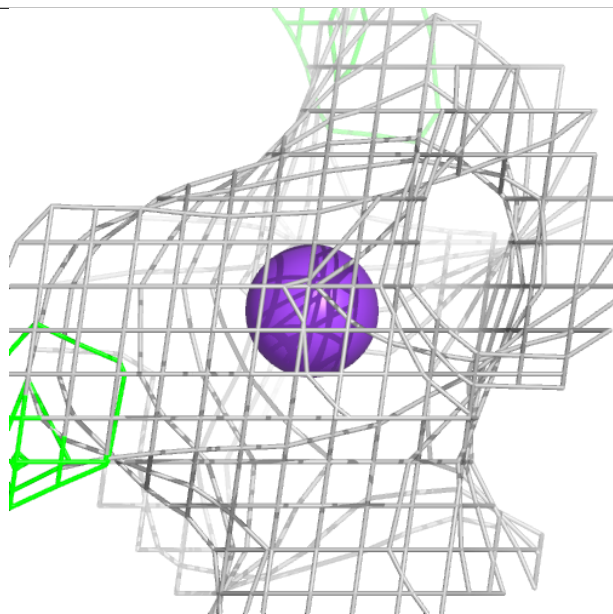
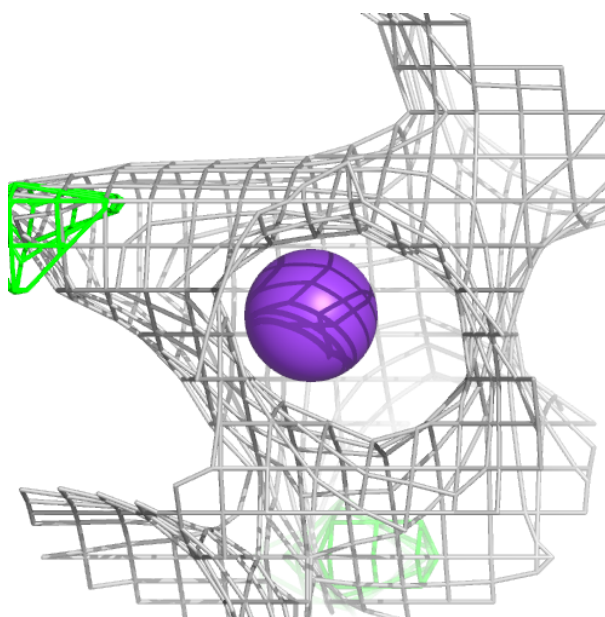
Electron density around HBI B 303:

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



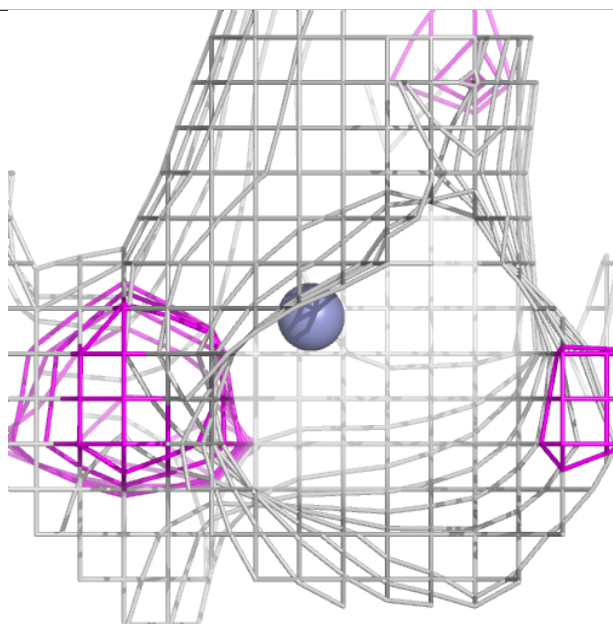
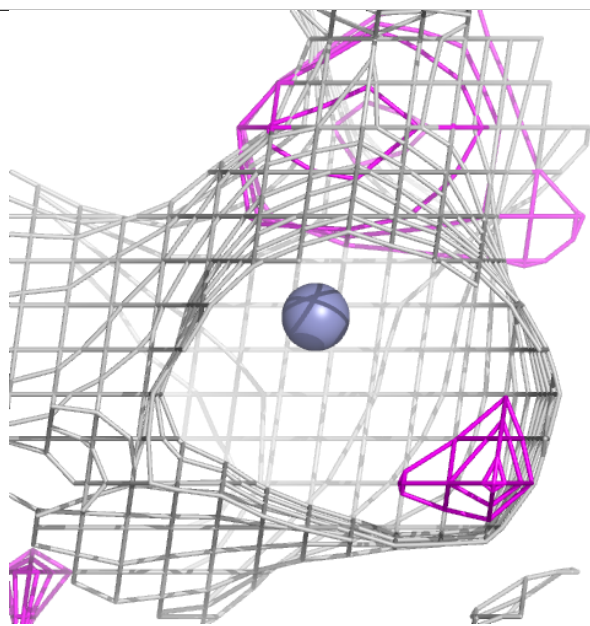
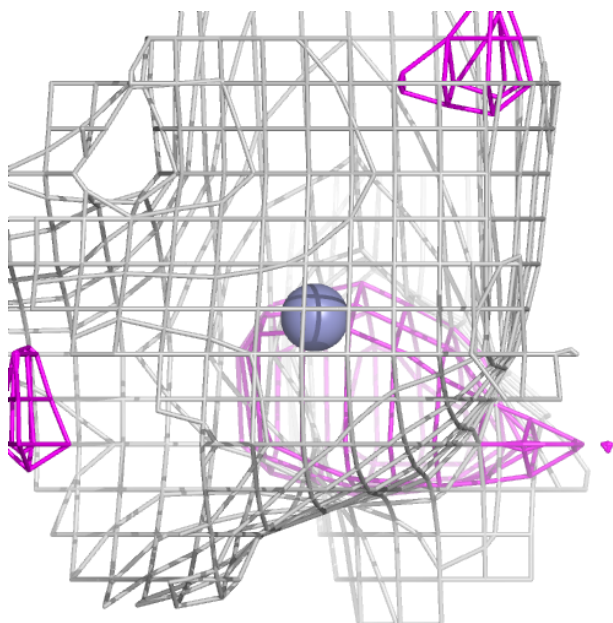
Electron density around K j 301:

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



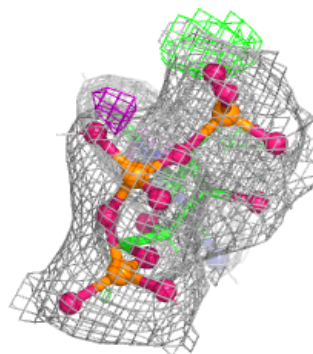
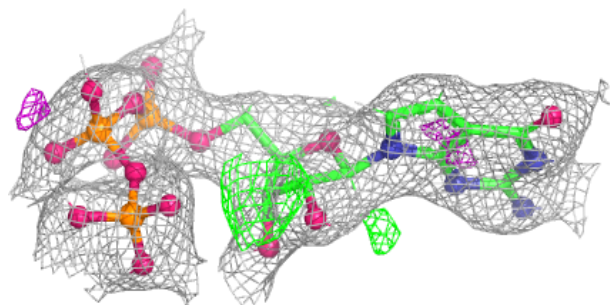
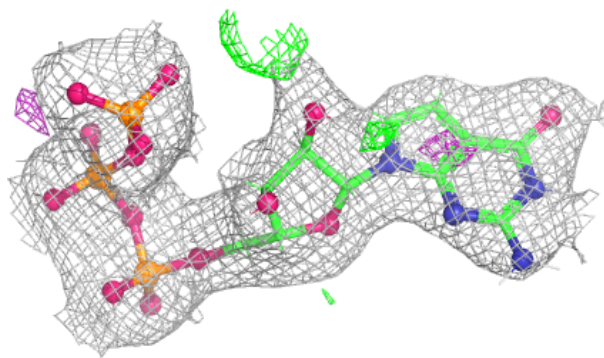
Electron density around ZN P 301:

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

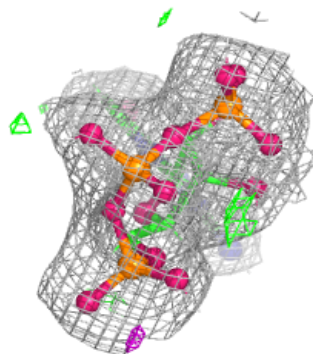
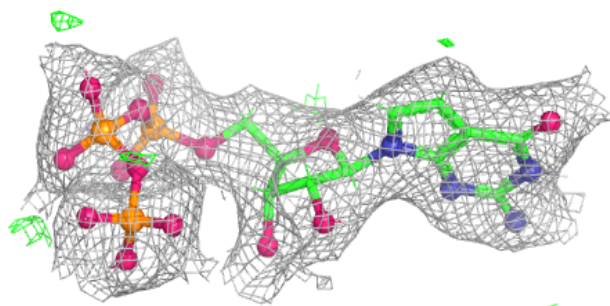
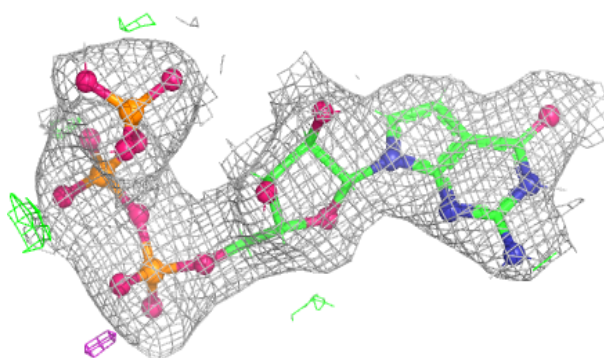


Electron density around QBQ D 302:

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

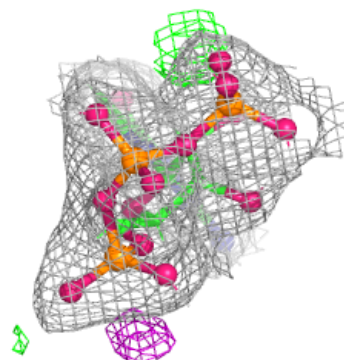
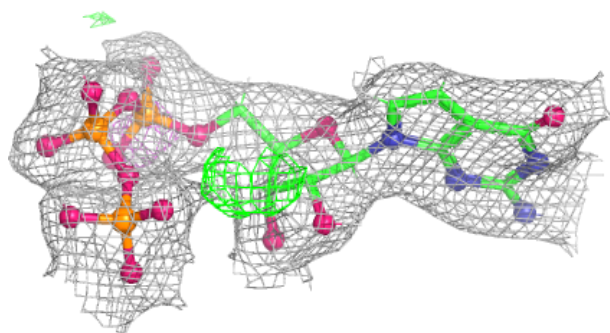
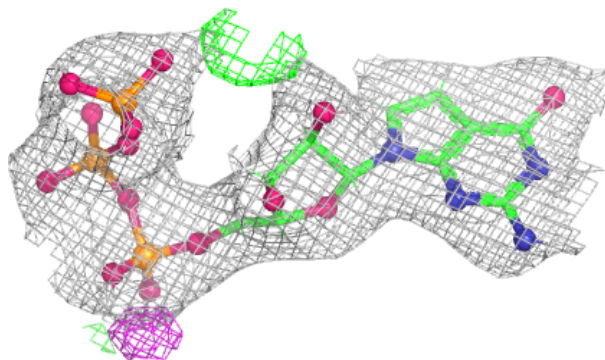
**Electron density around QBQ N 302:**

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

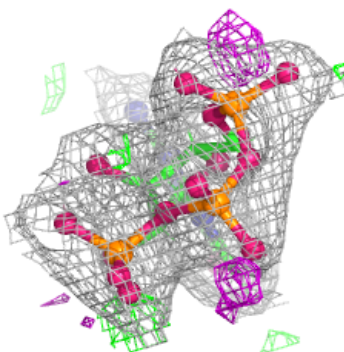
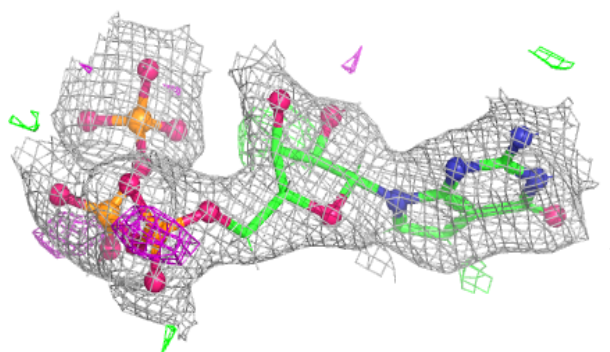
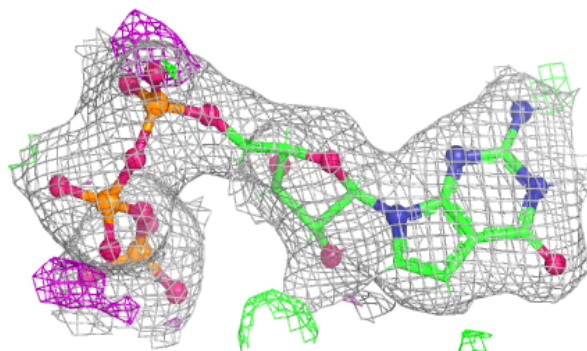


Electron density around QBQ O 302:

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

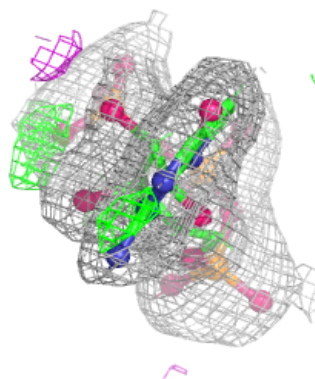
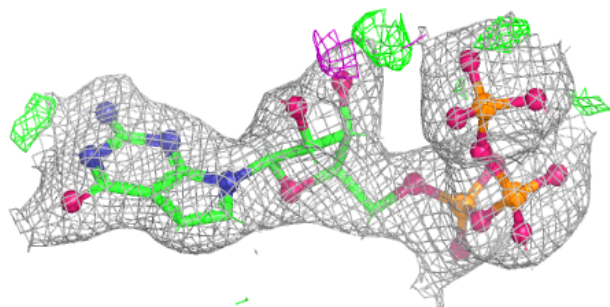
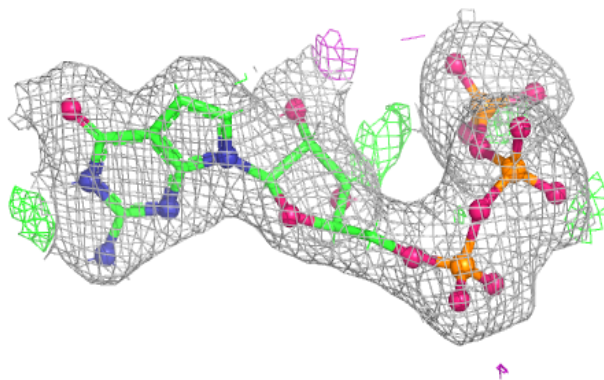
**Electron density around QBQ P 302:**

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



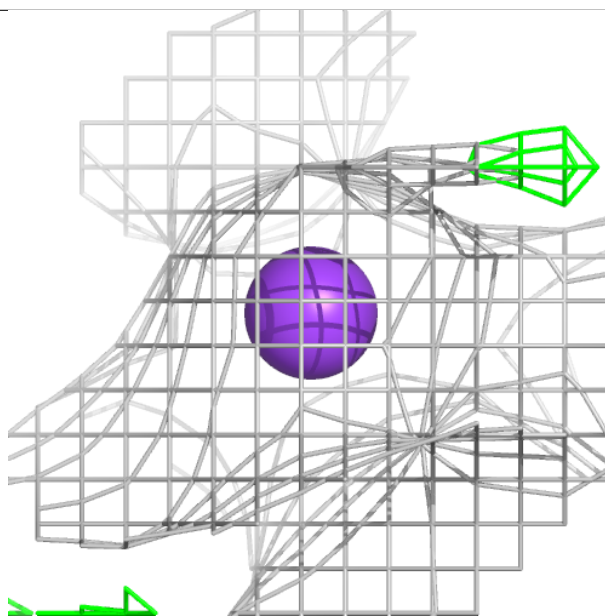
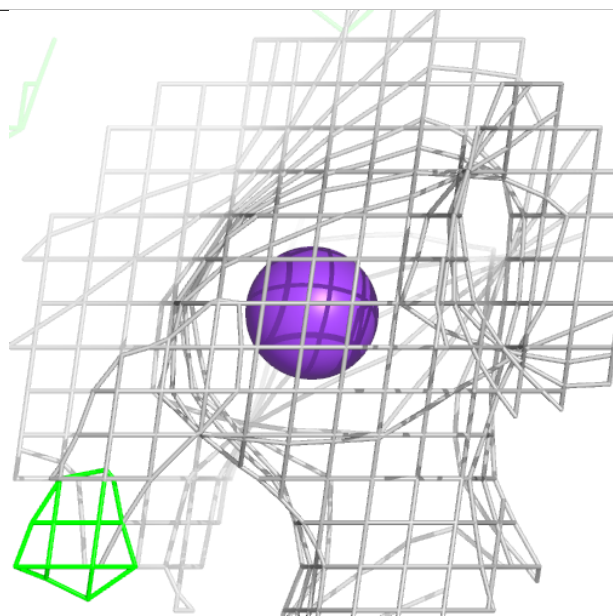
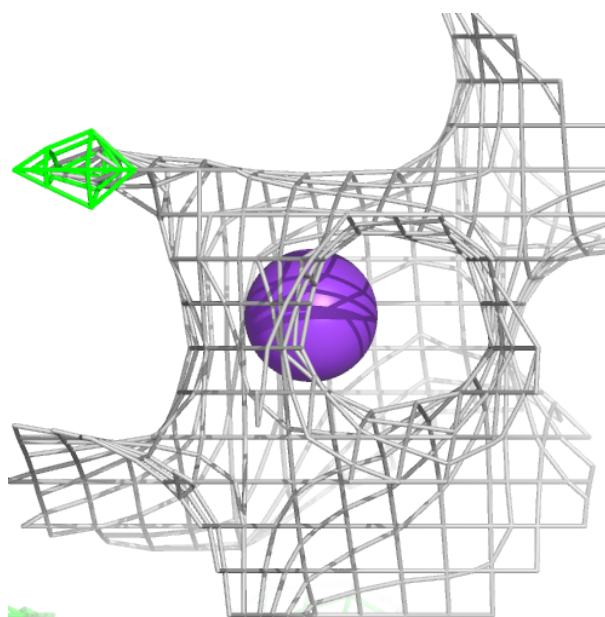
Electron density around QBQ B 302:

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



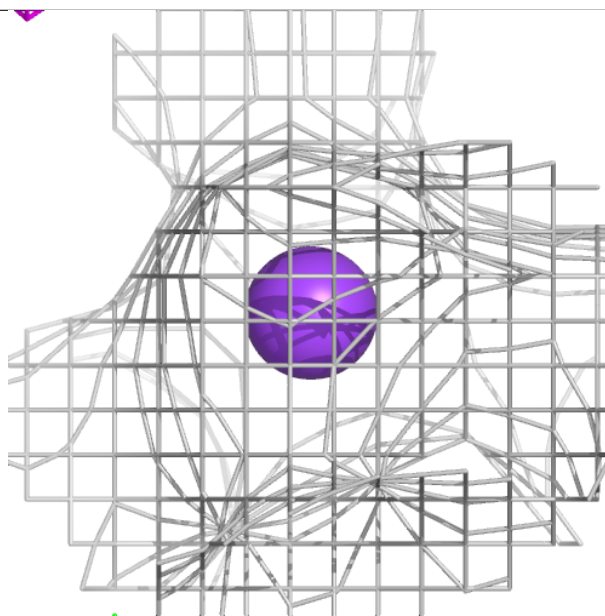
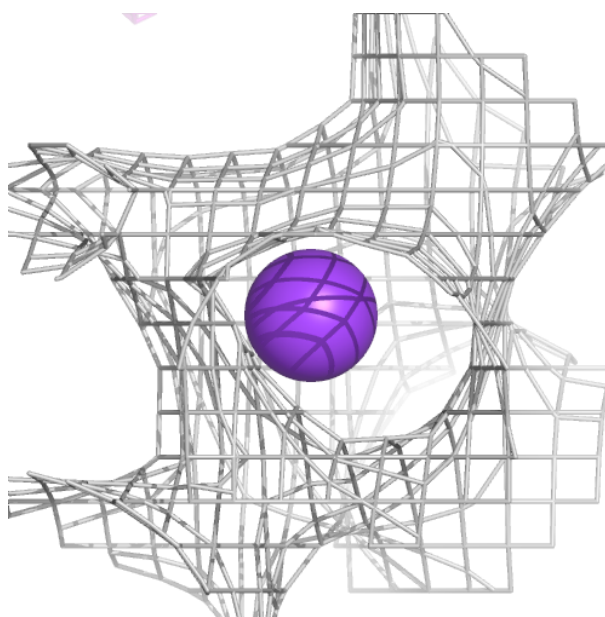
Electron density around K a 301:

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



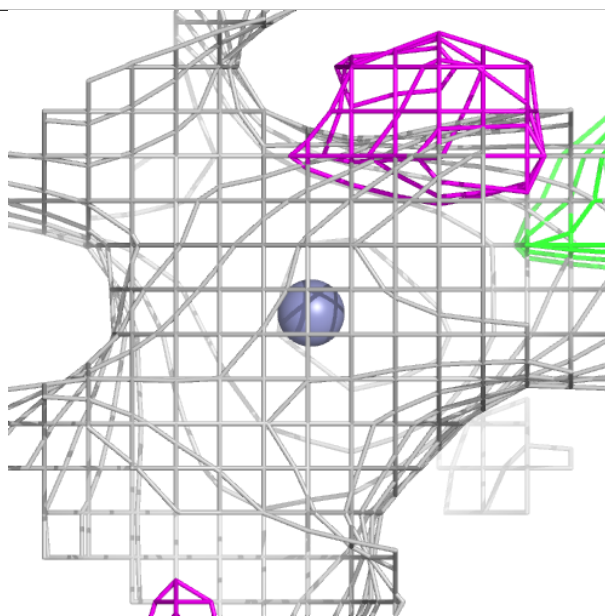
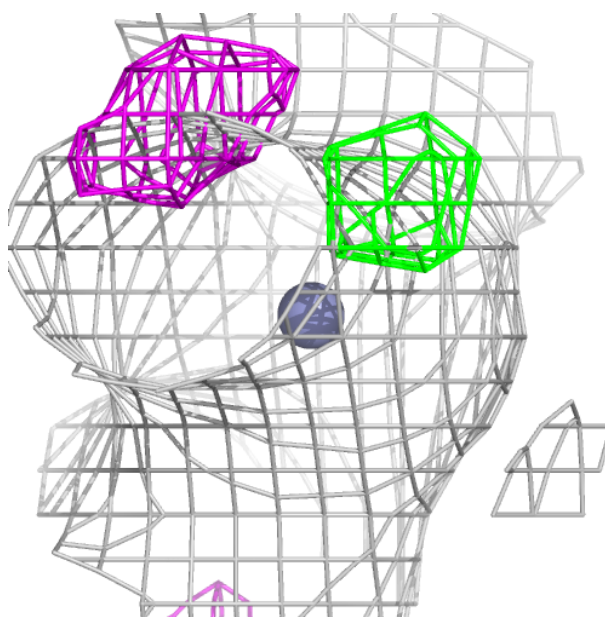
Electron density around K k 301:

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



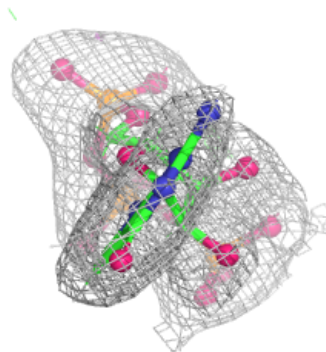
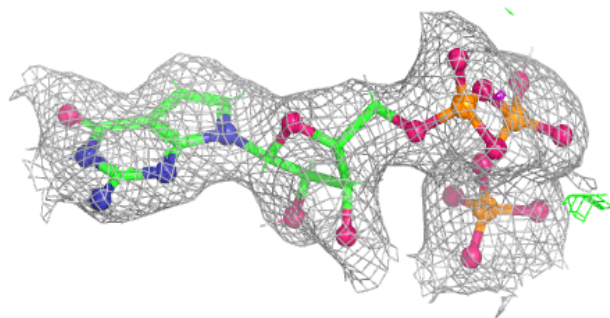
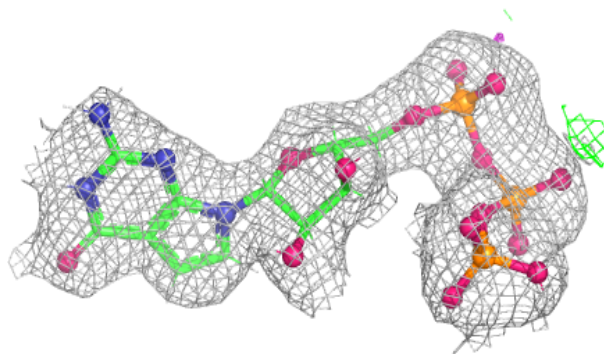
Electron density around ZN A 301:

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



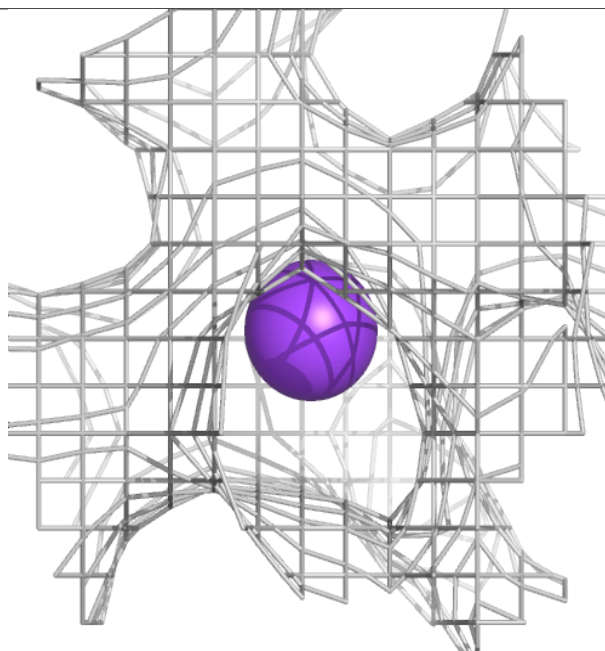
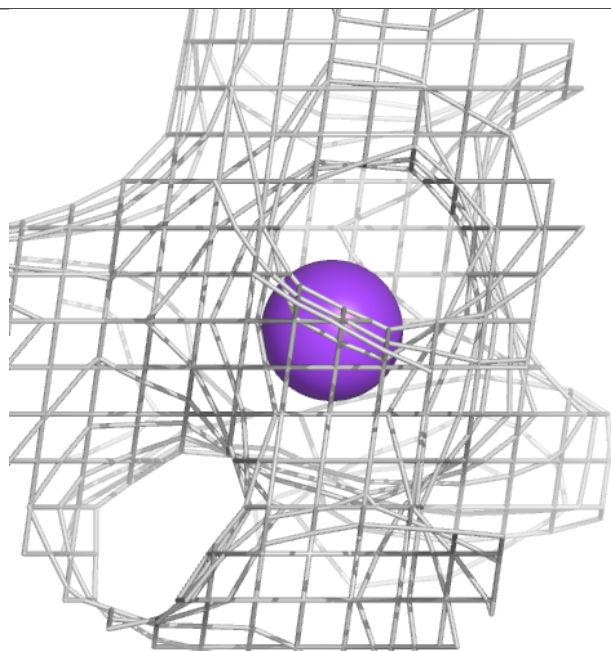
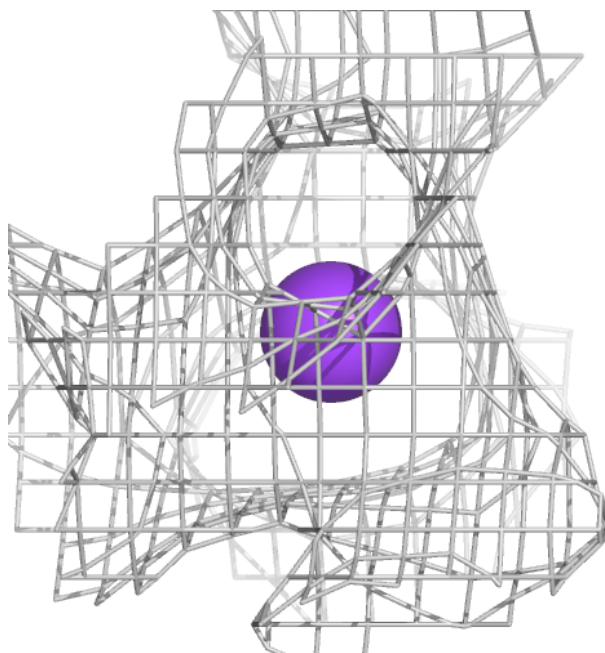
Electron density around QBQ R 302:

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



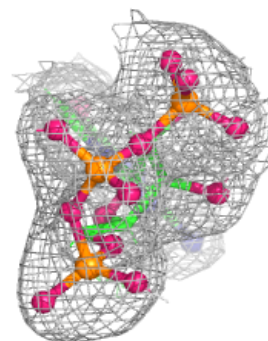
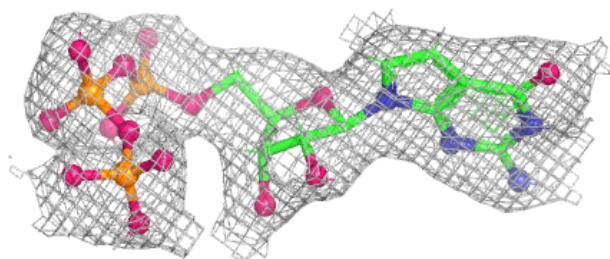
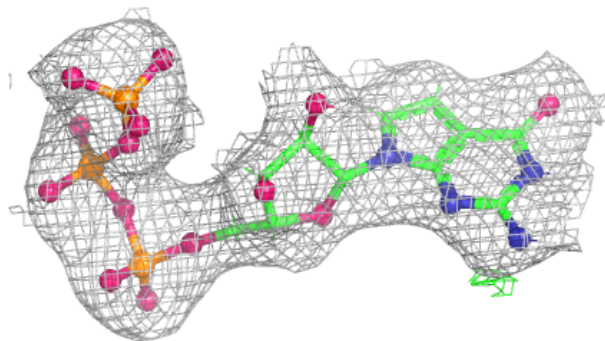
Electron density around K n 301:

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



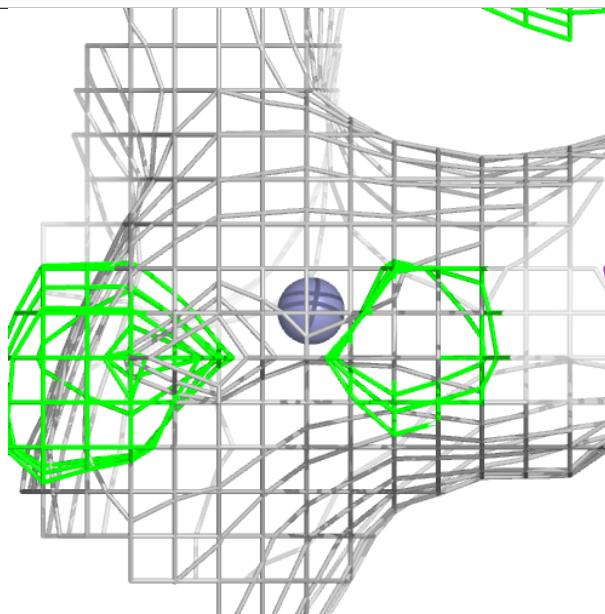
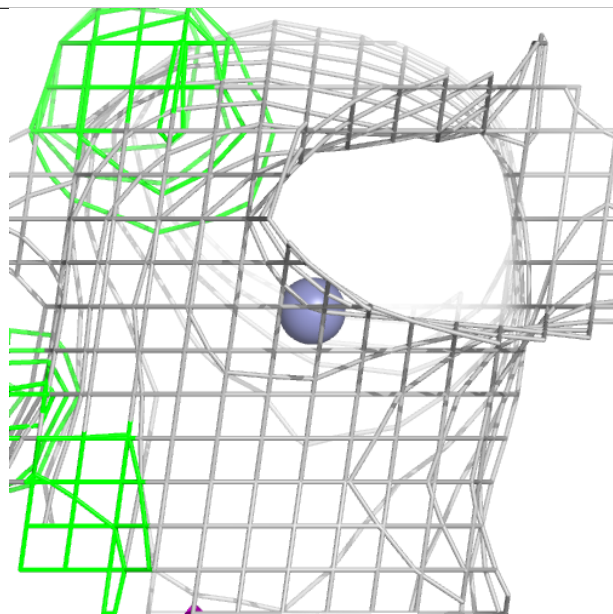
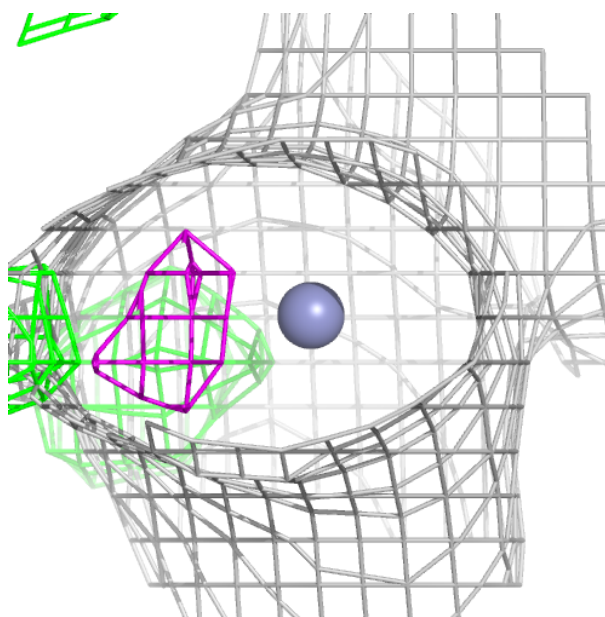
Electron density around QBQ G 302:

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



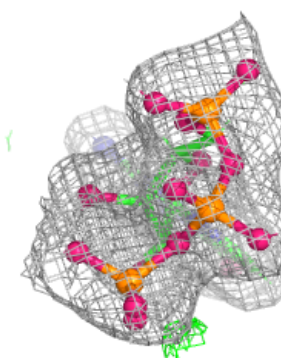
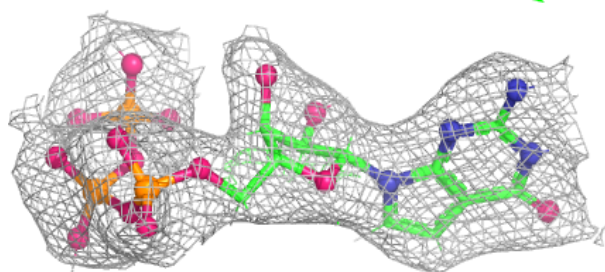
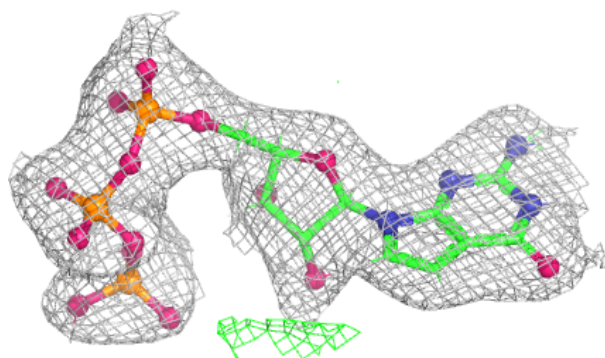
Electron density around ZN O 301:

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

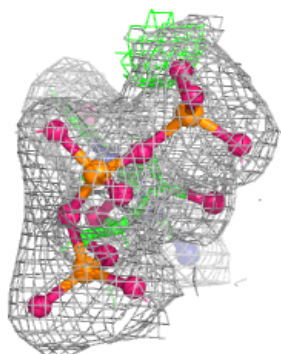
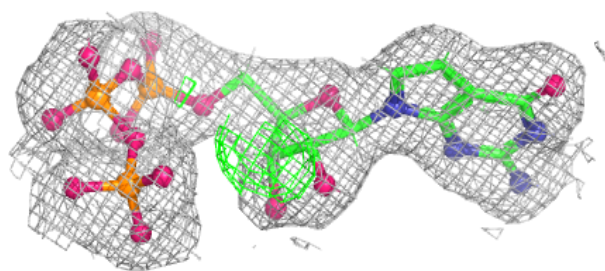
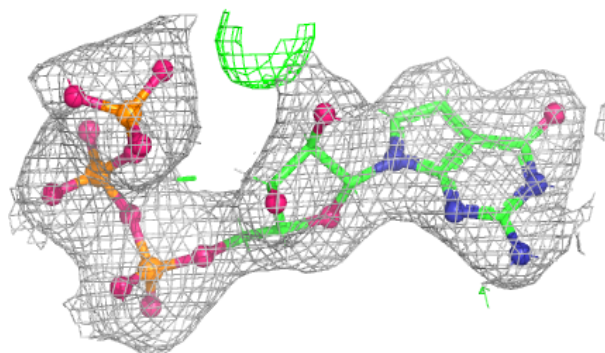


Electron density around QBQ I 302:

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

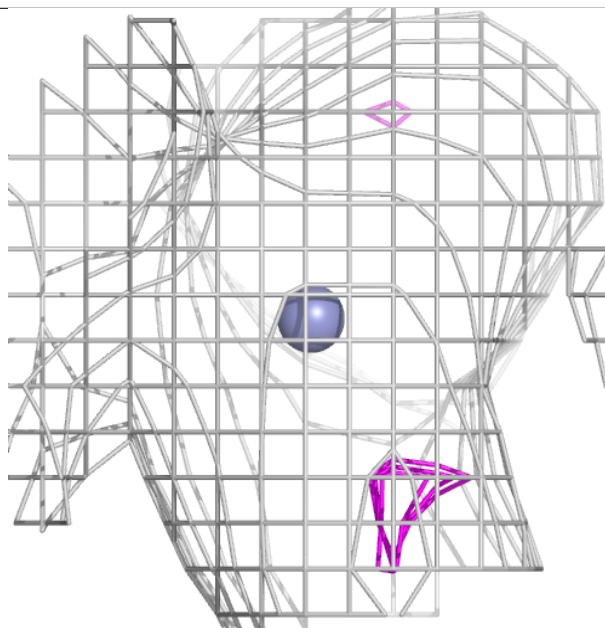
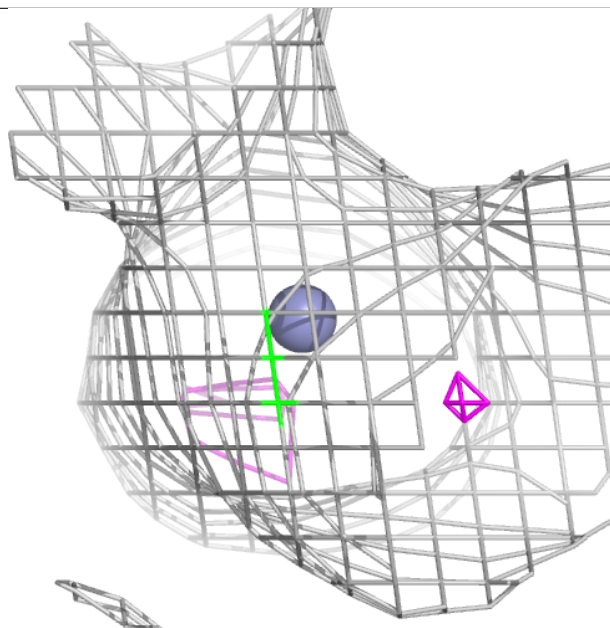
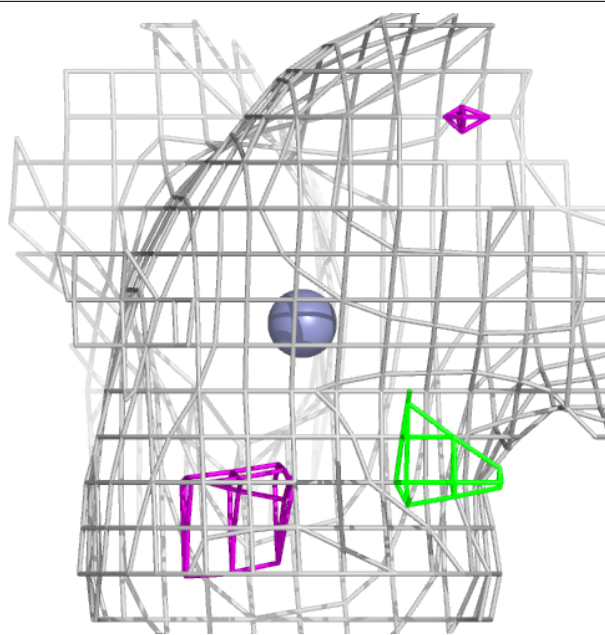
**Electron density around QBQ M 302:**

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



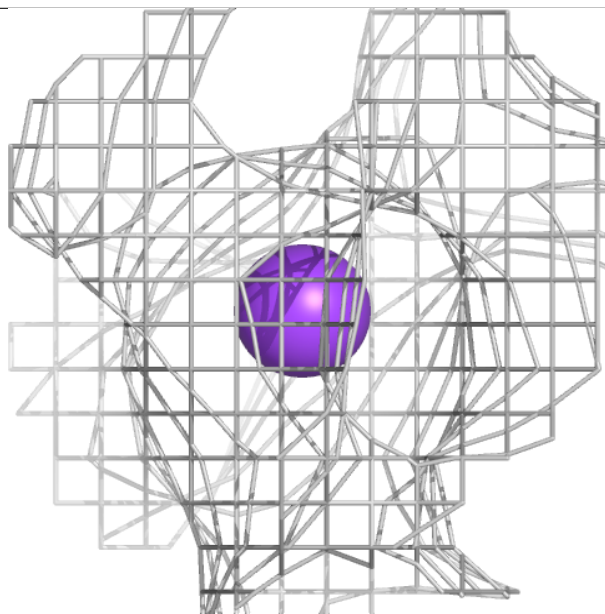
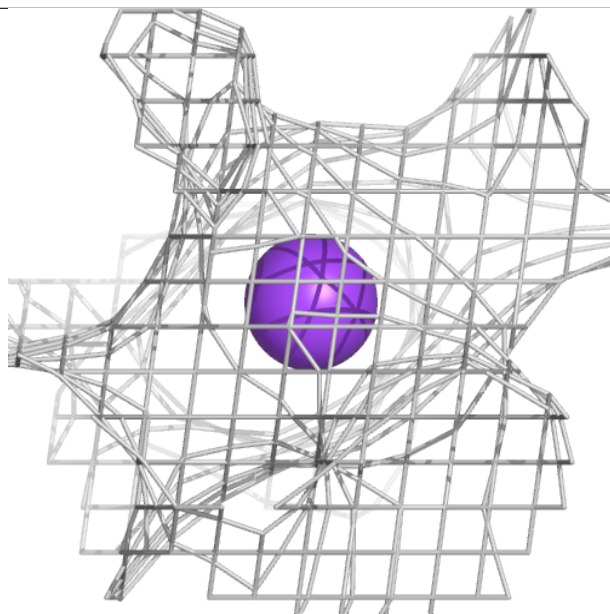
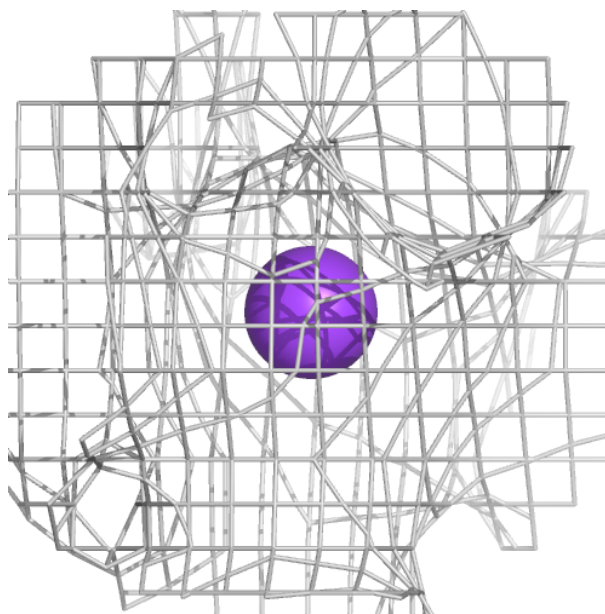
Electron density around ZN L 301:

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



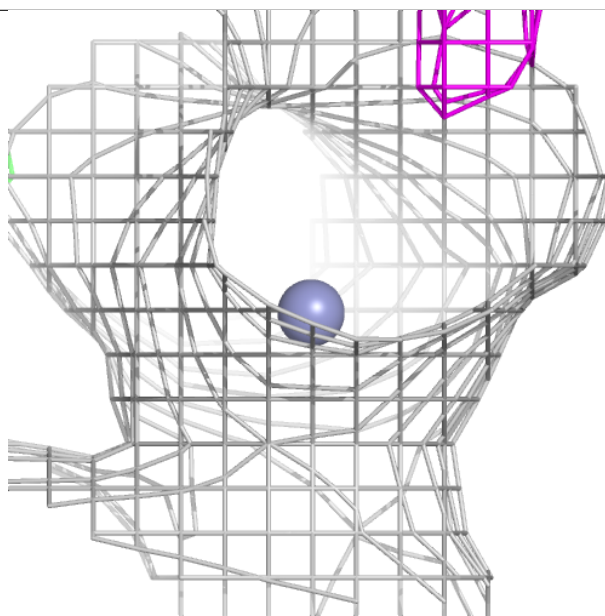
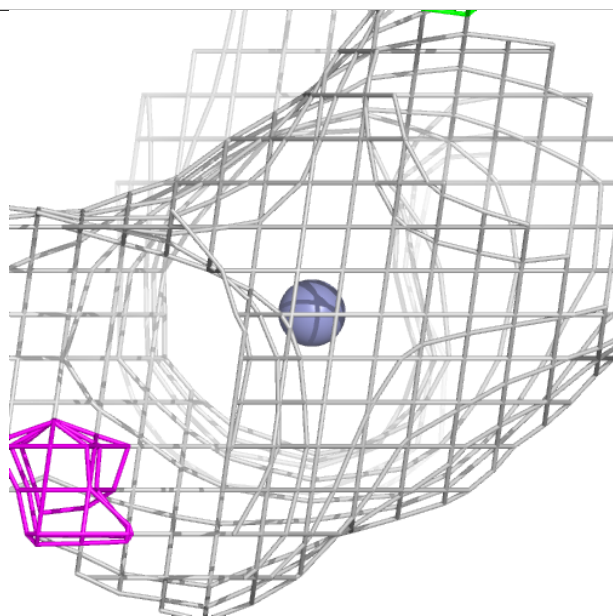
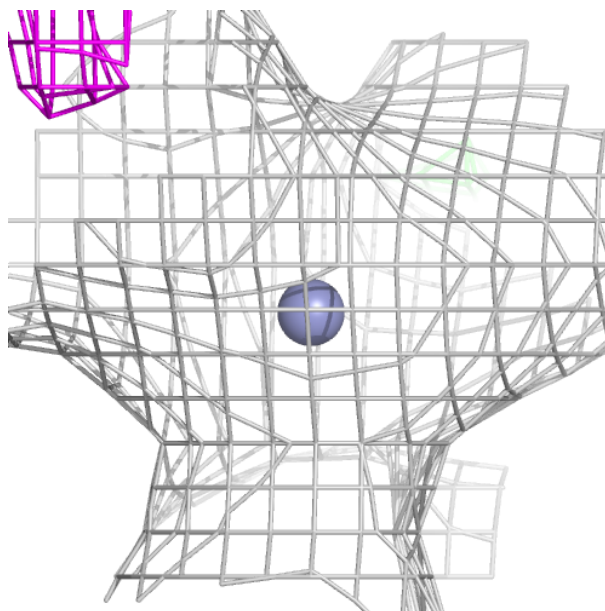
Electron density around K f 301:

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



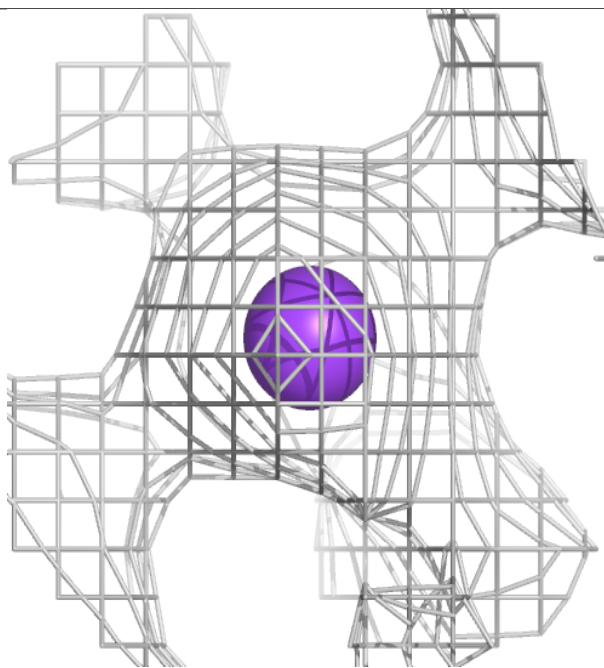
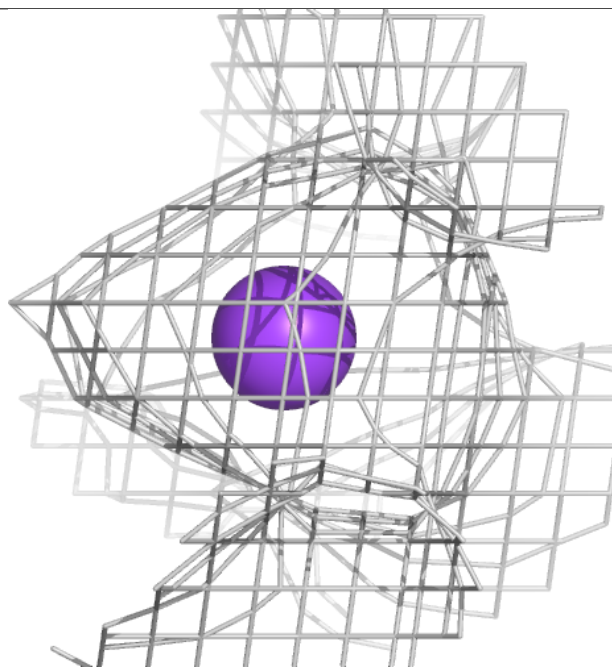
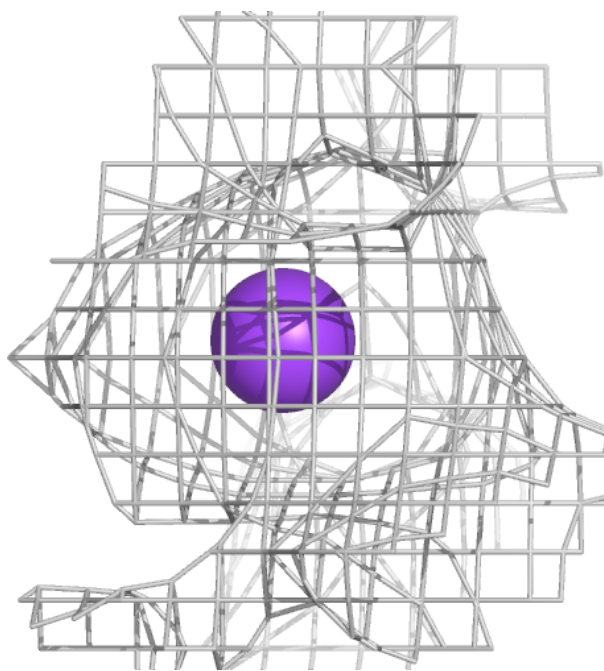
Electron density around ZN M 301:

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



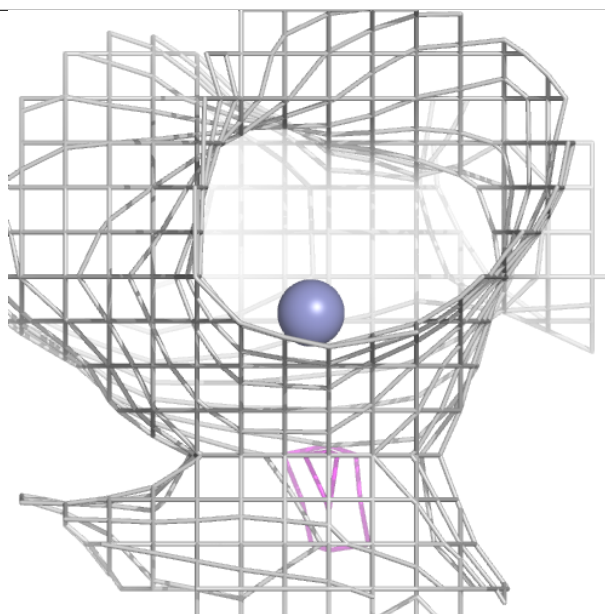
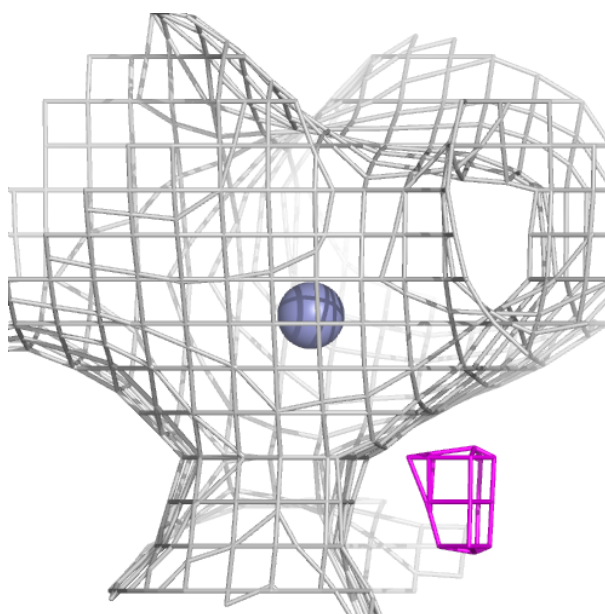
Electron density around K o 301:

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



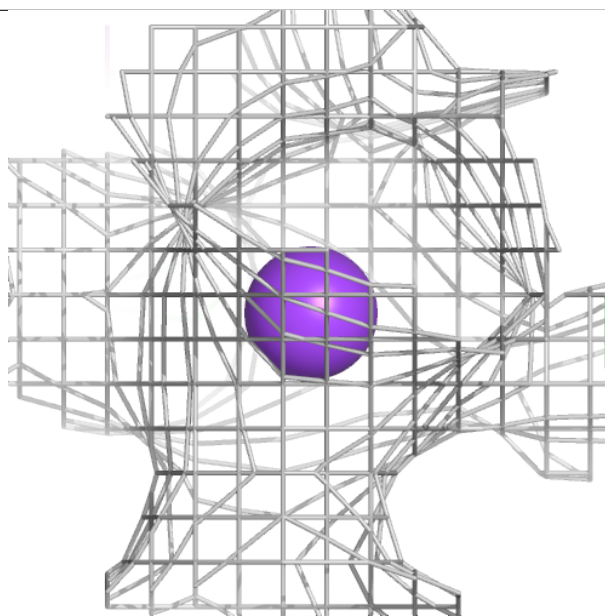
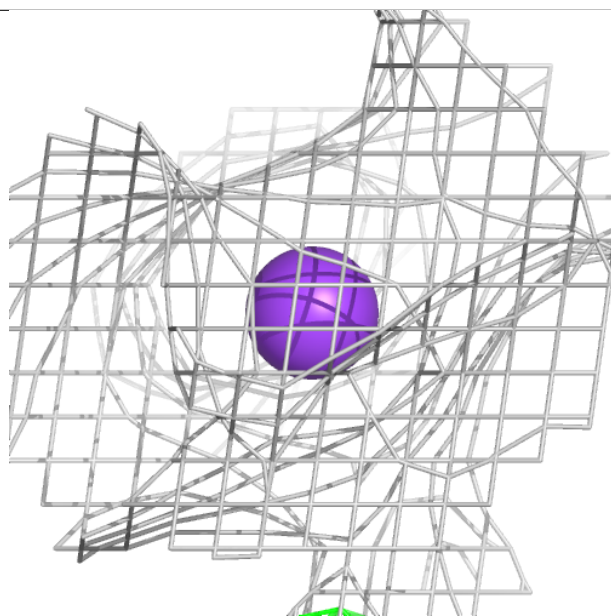
Electron density around ZN G 301:

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



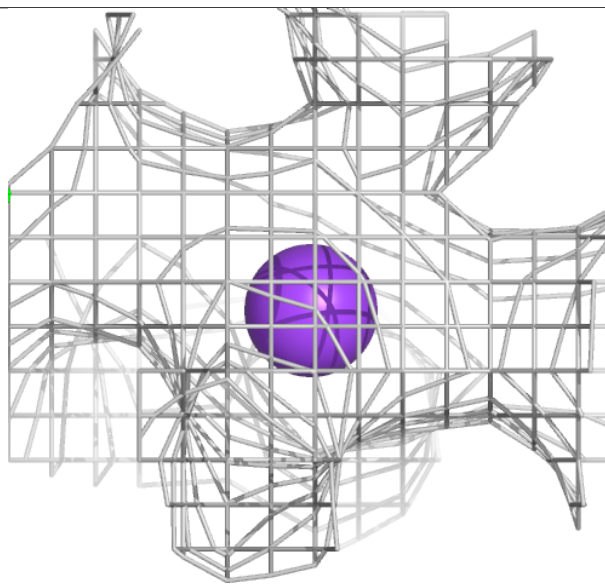
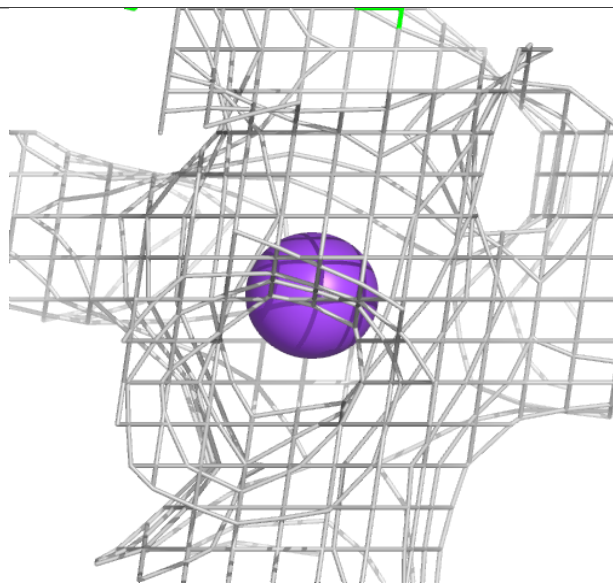
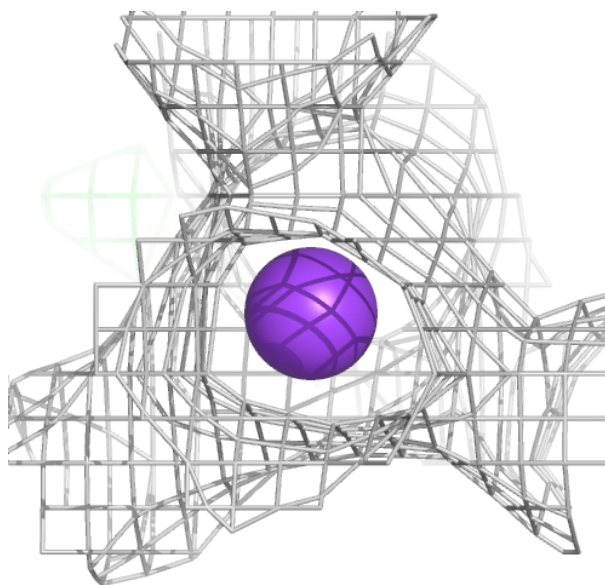
Electron density around K q 301:

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



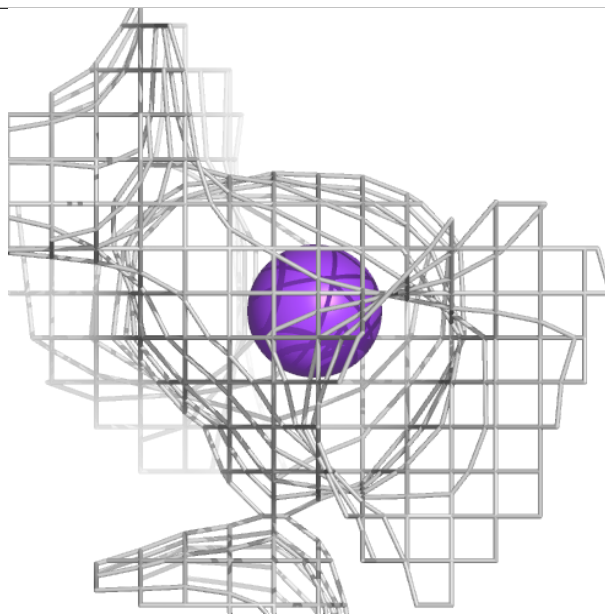
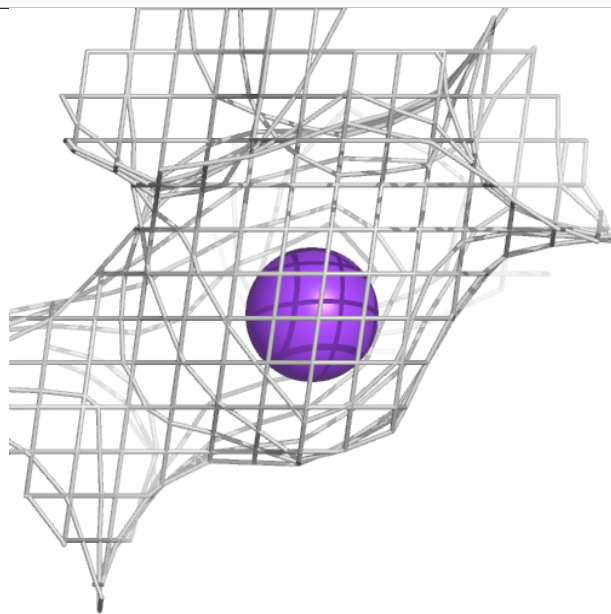
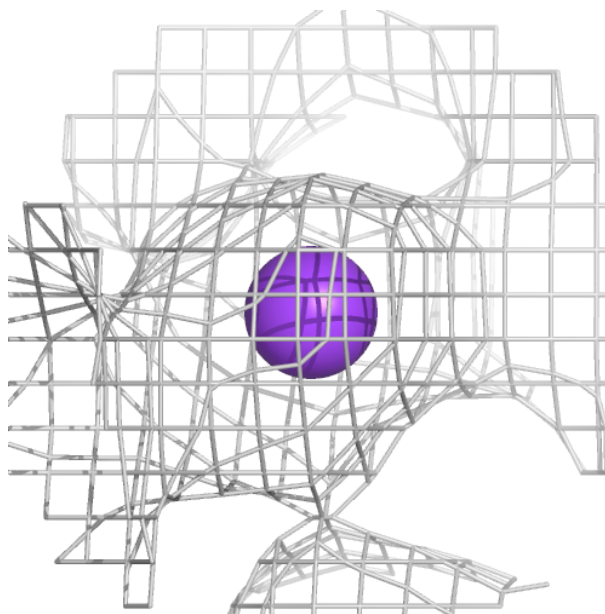
Electron density around K r 301:

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



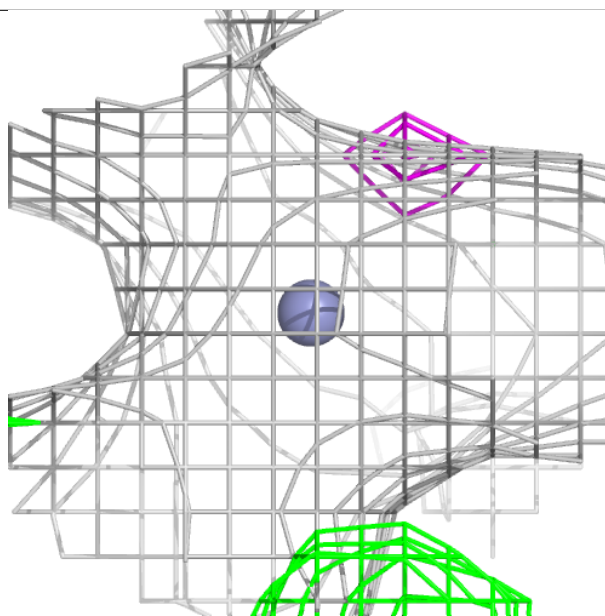
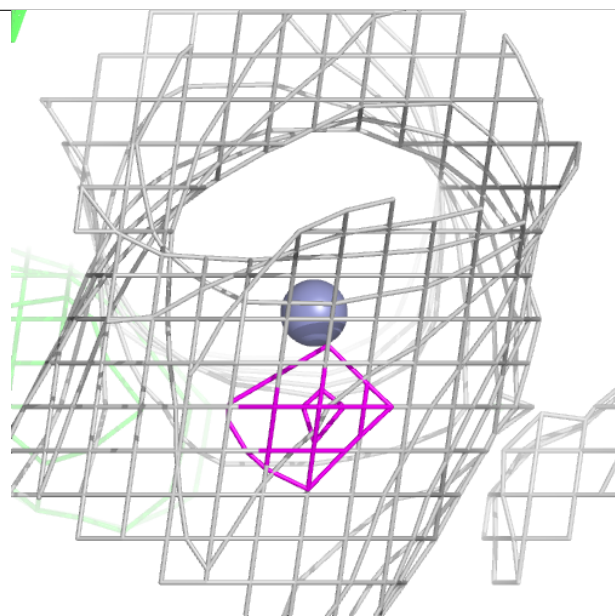
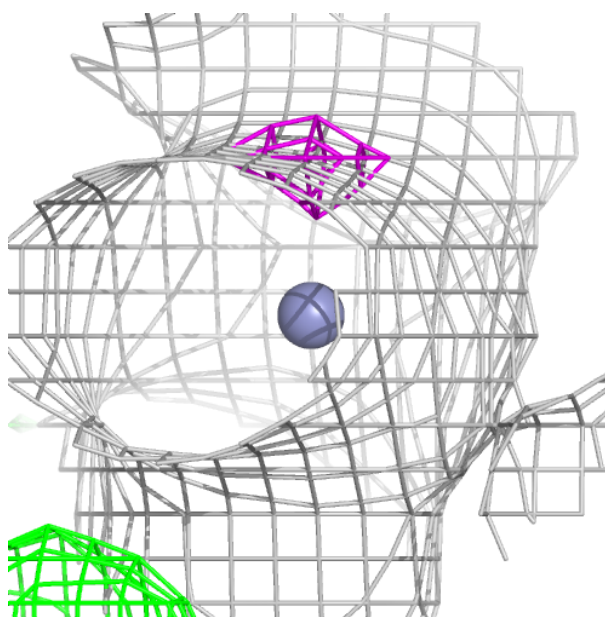
Electron density around K b 301:

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



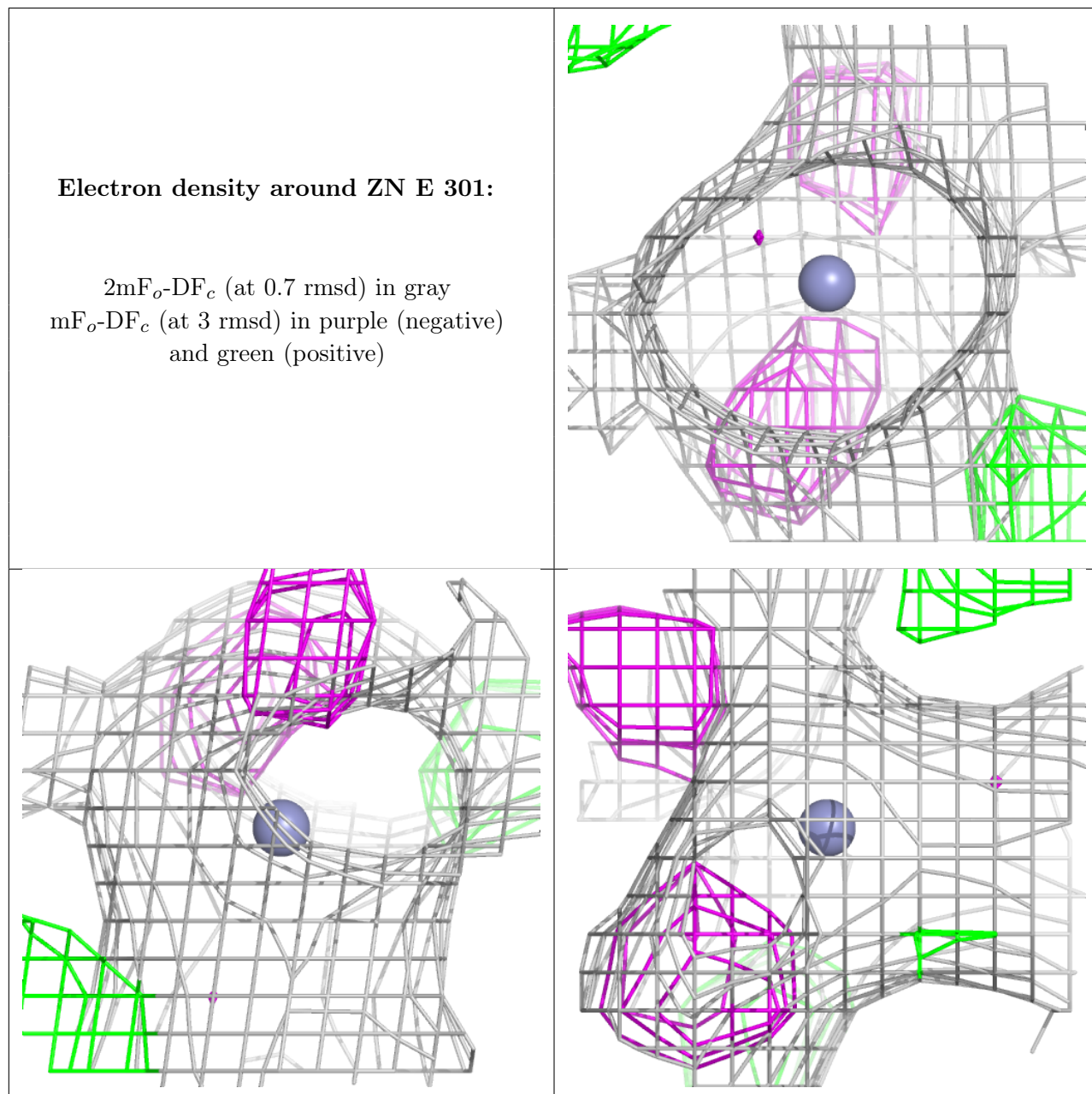
Electron density around ZN K 301:

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



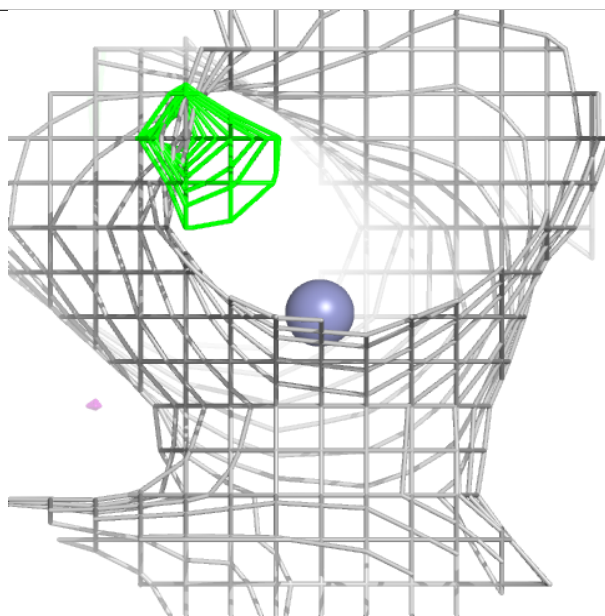
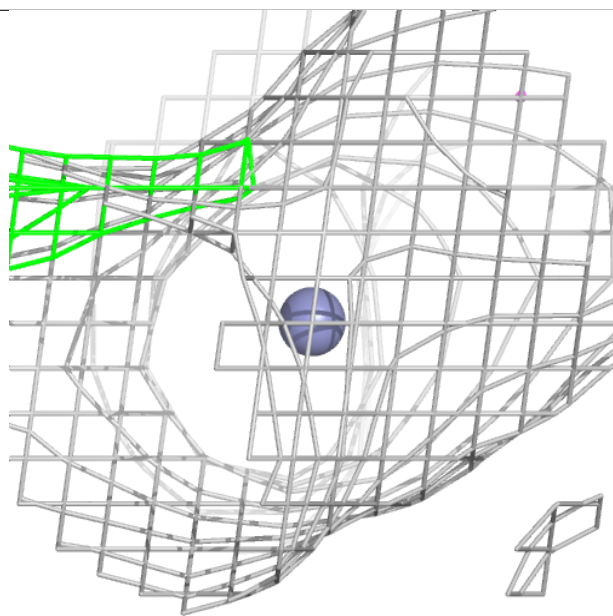
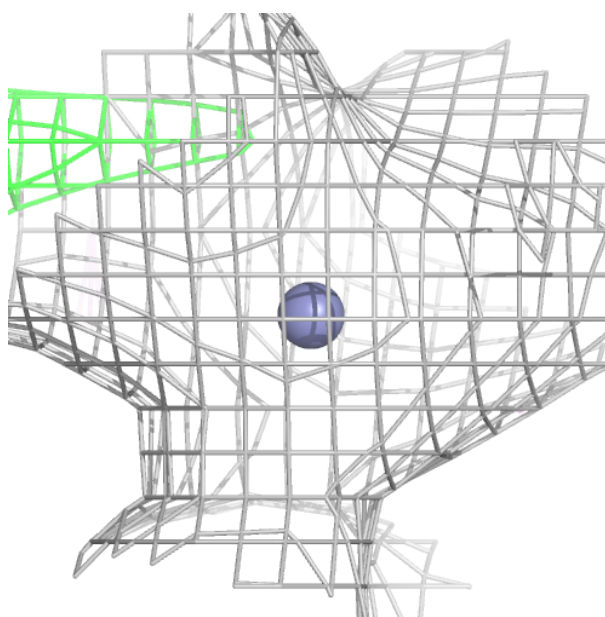
Electron density around ZN E 301:

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



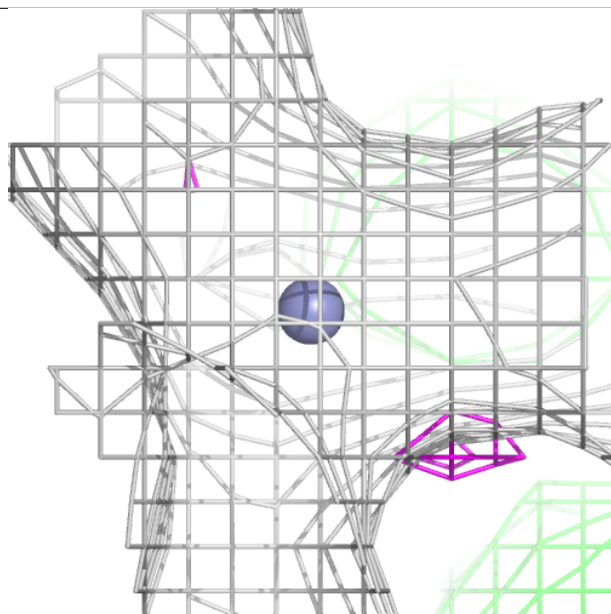
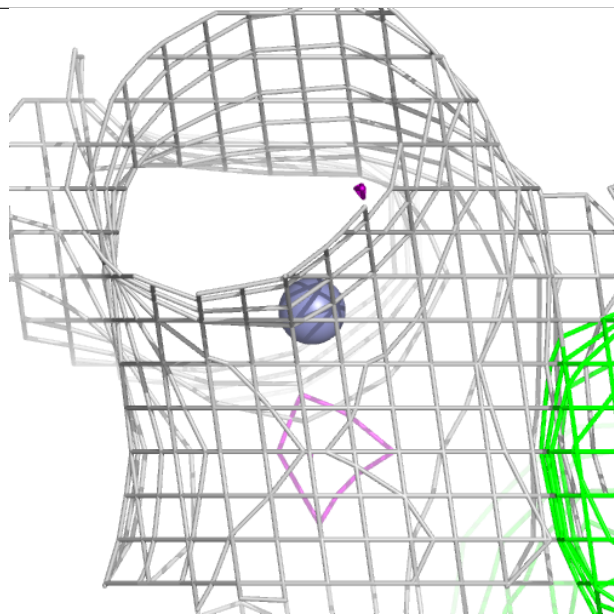
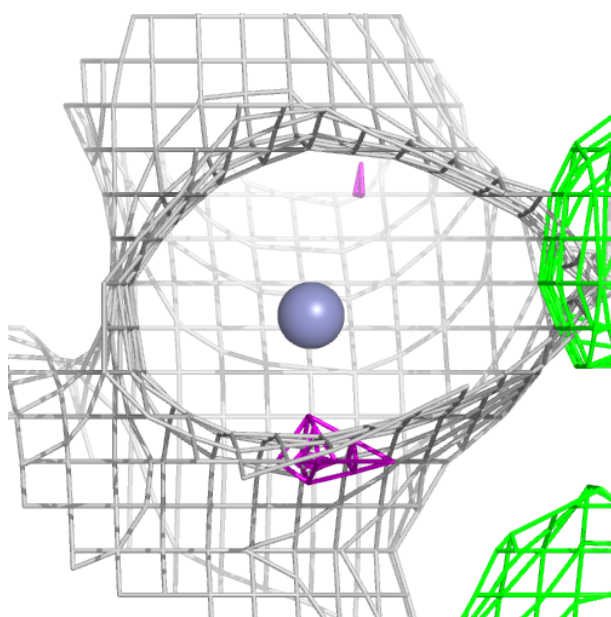
Electron density around ZN Q 301:

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



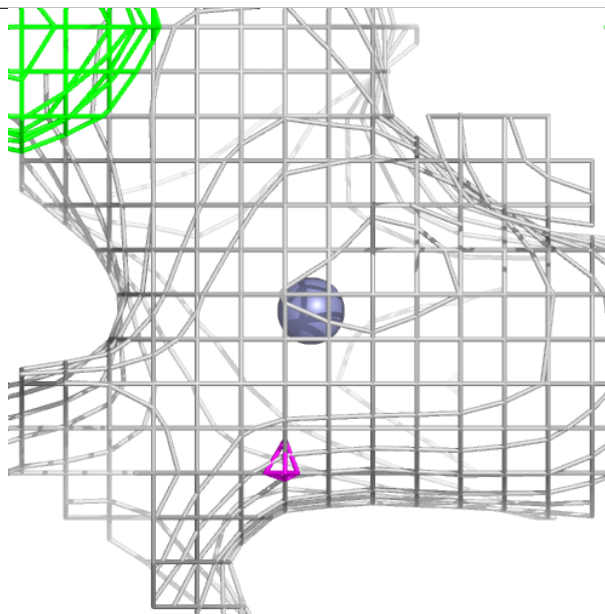
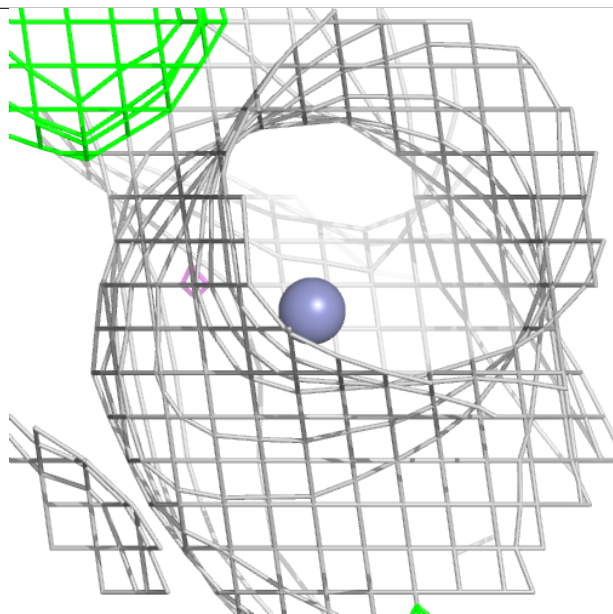
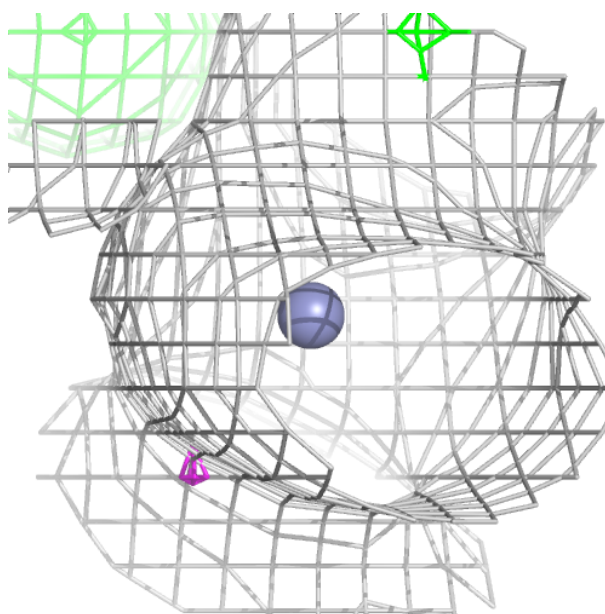
Electron density around ZN S 301:

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



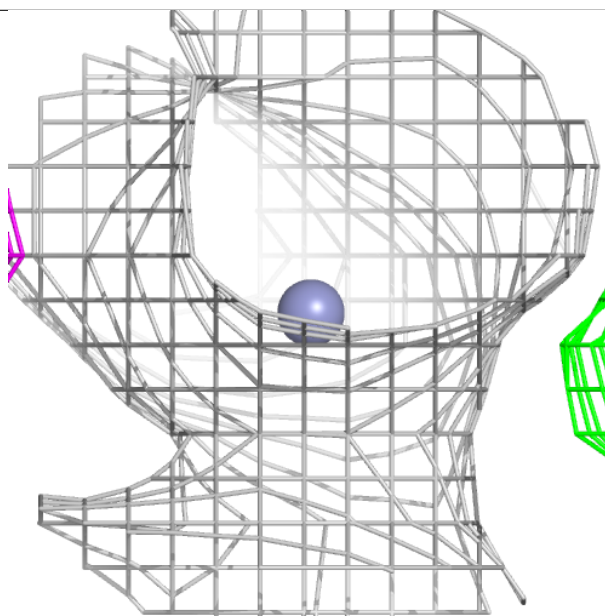
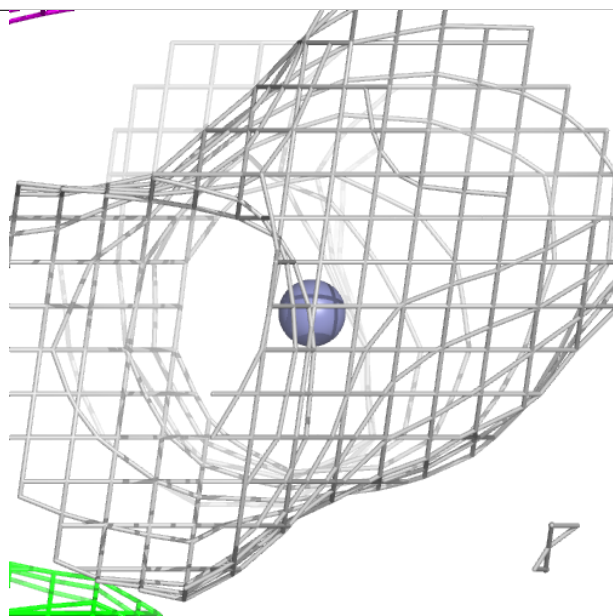
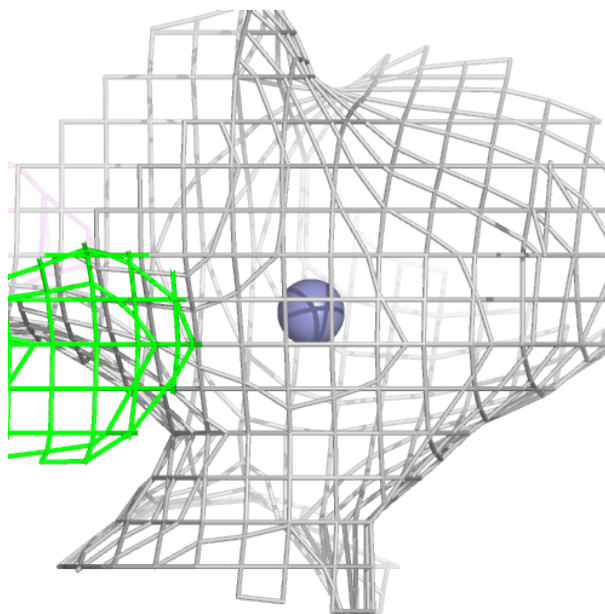
Electron density around ZN T 301:

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



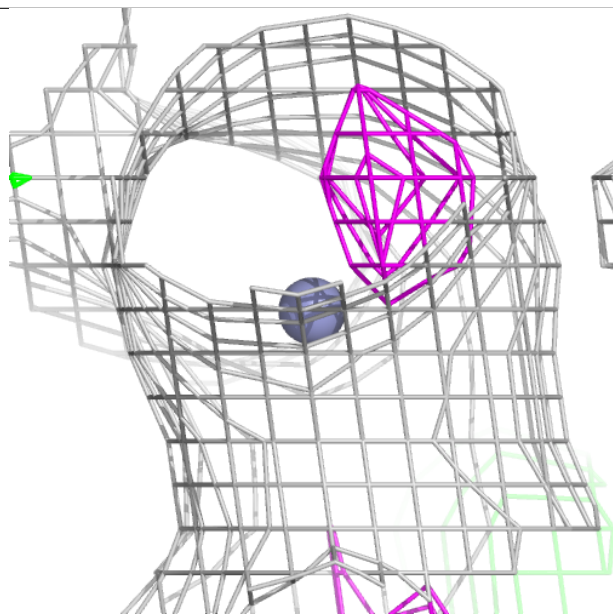
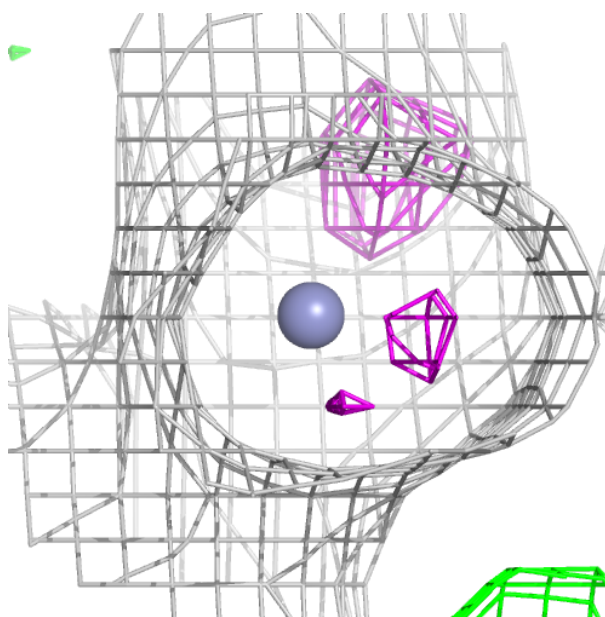
Electron density around ZN C 301:

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



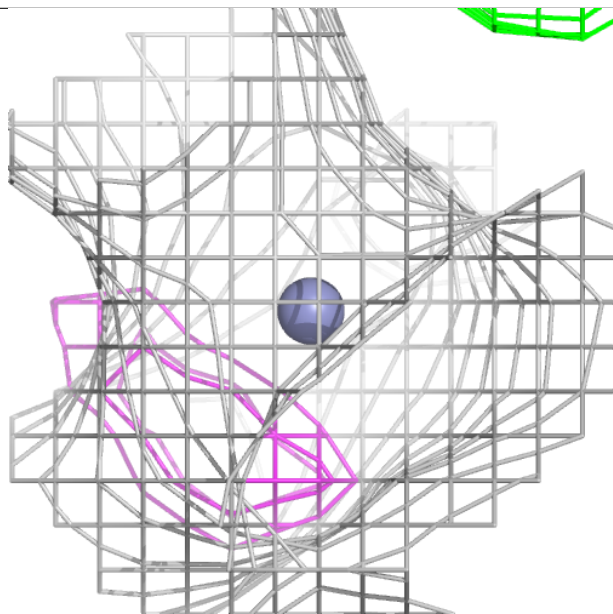
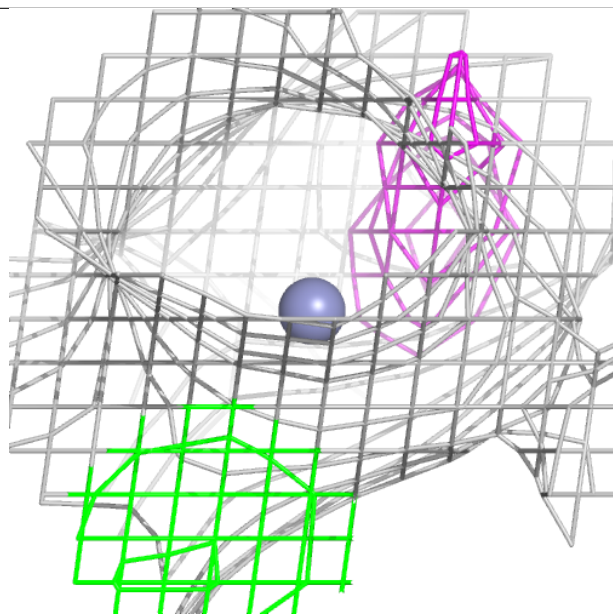
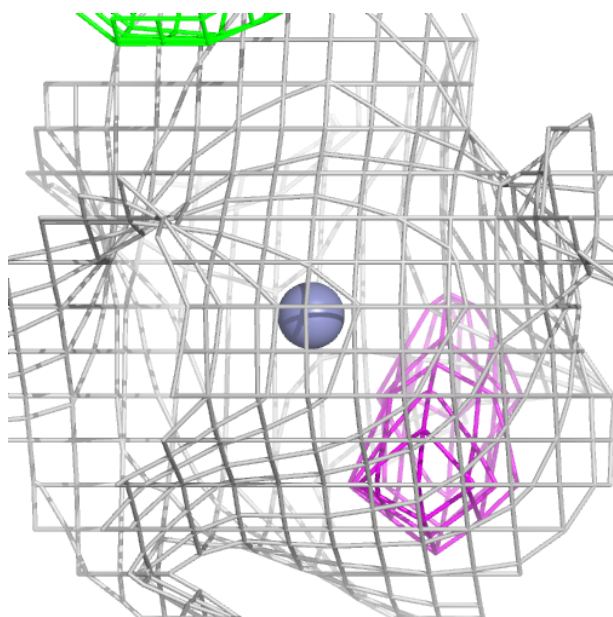
Electron density around ZN I 301:

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



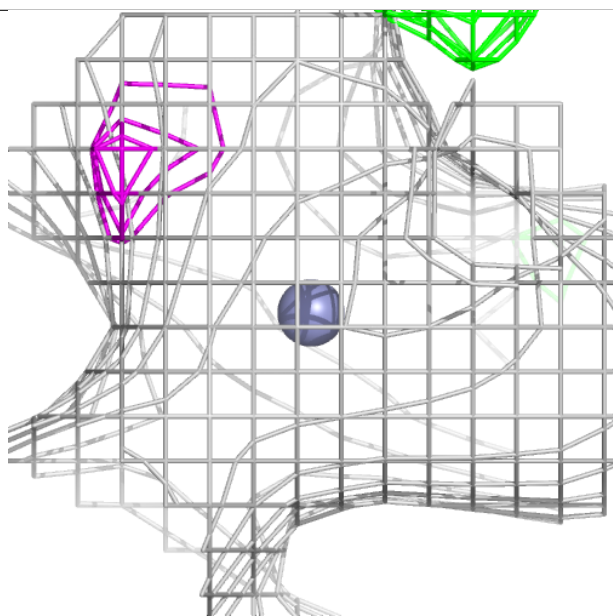
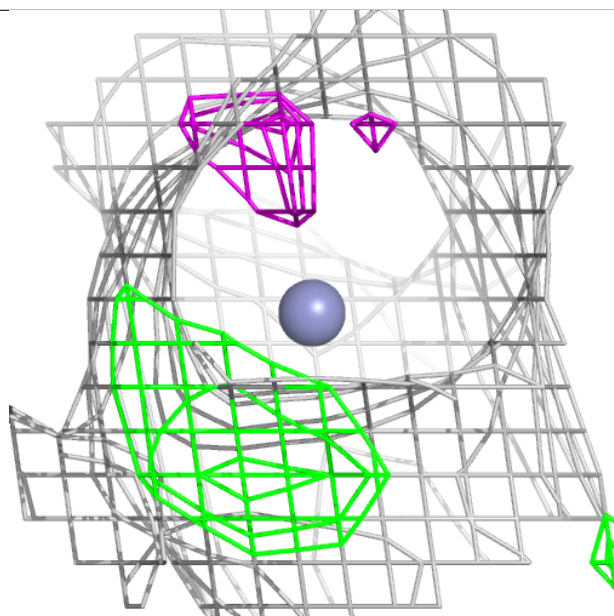
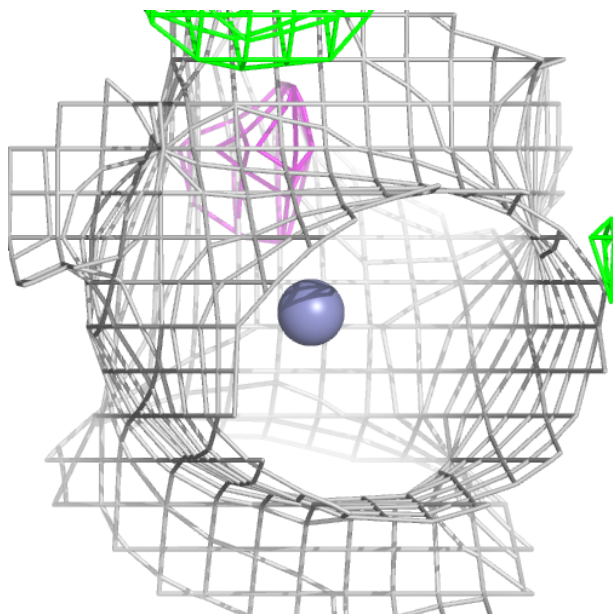
Electron density around ZN N 301:

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



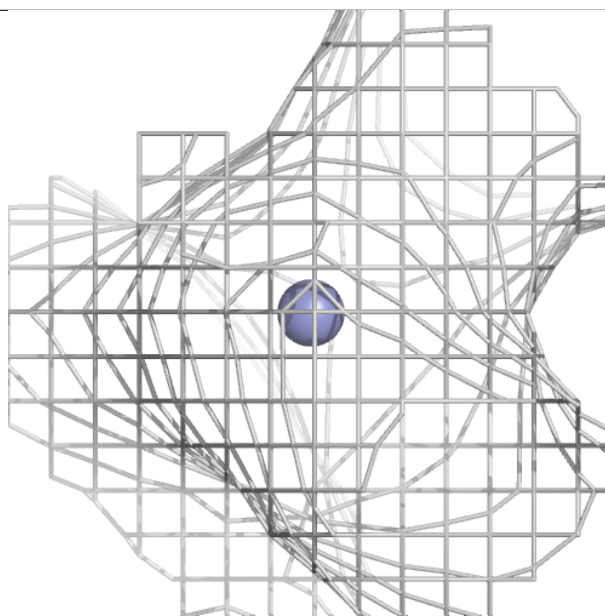
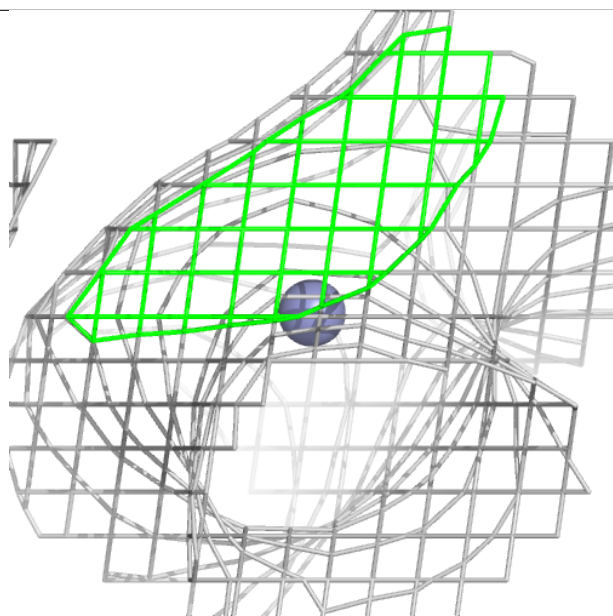
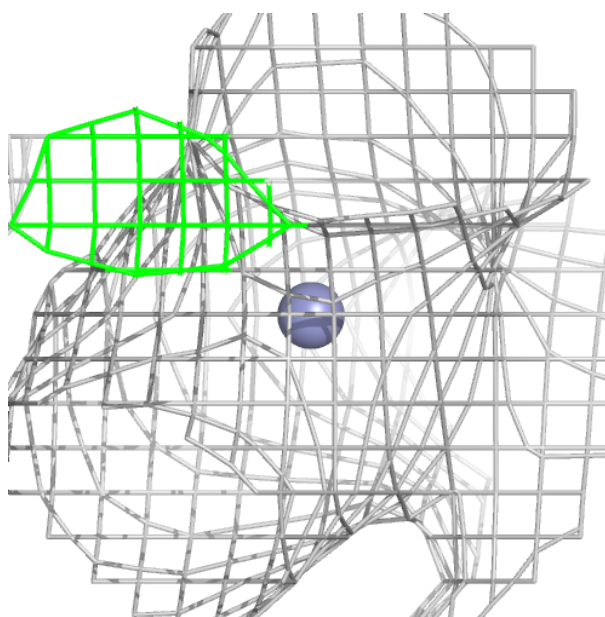
Electron density around ZN J 301:

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



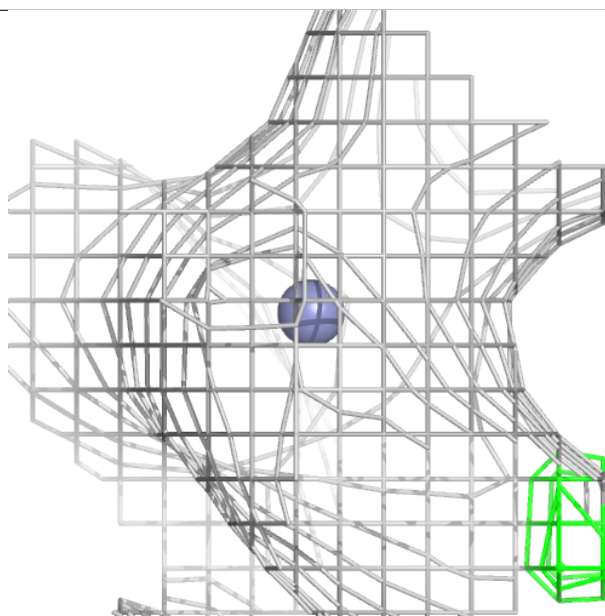
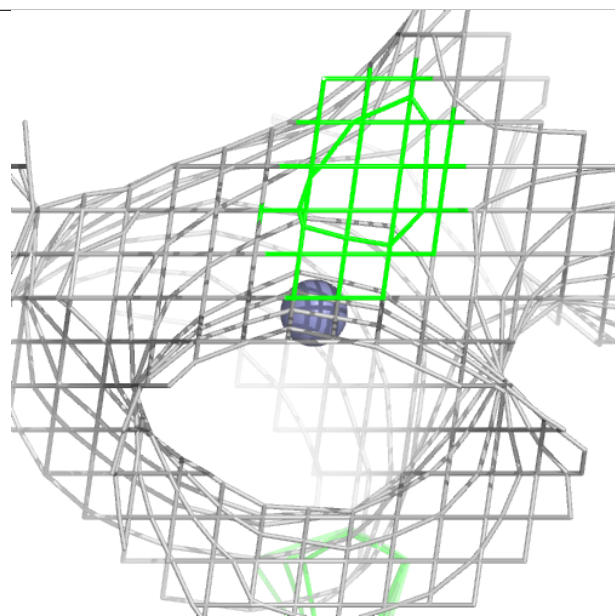
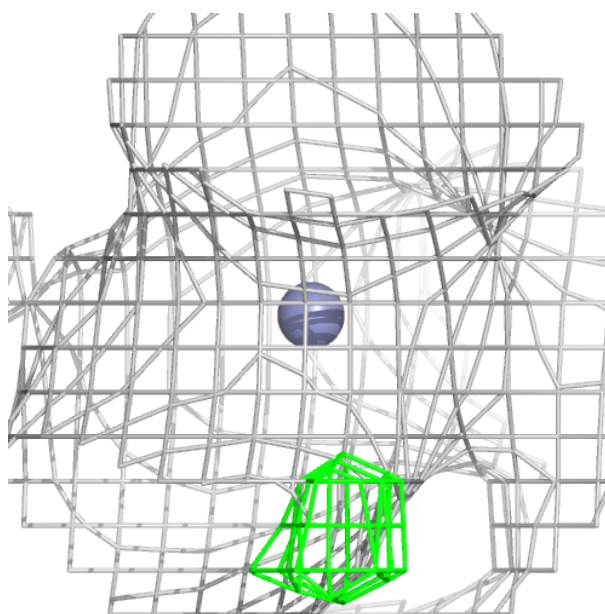
Electron density around ZN H 301:

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



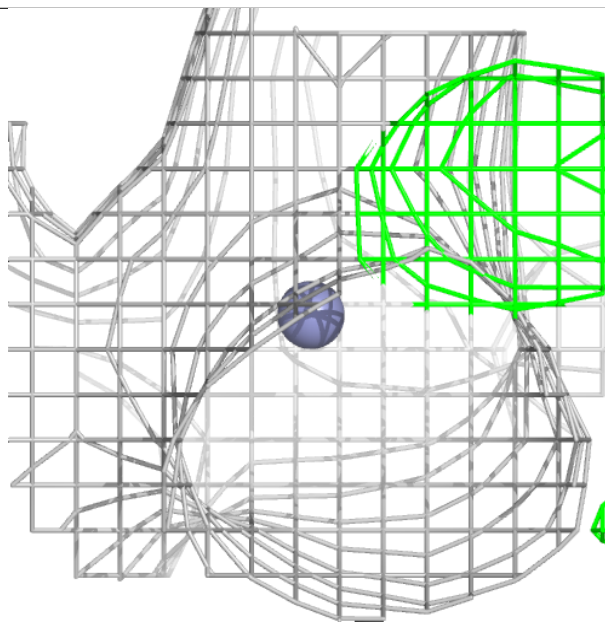
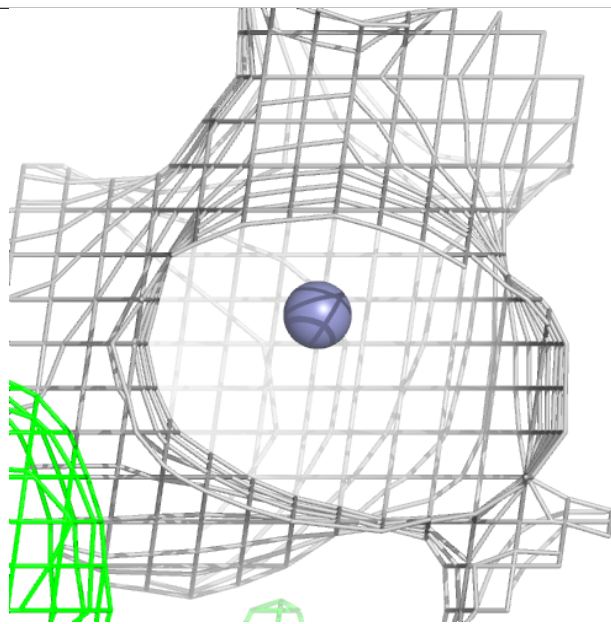
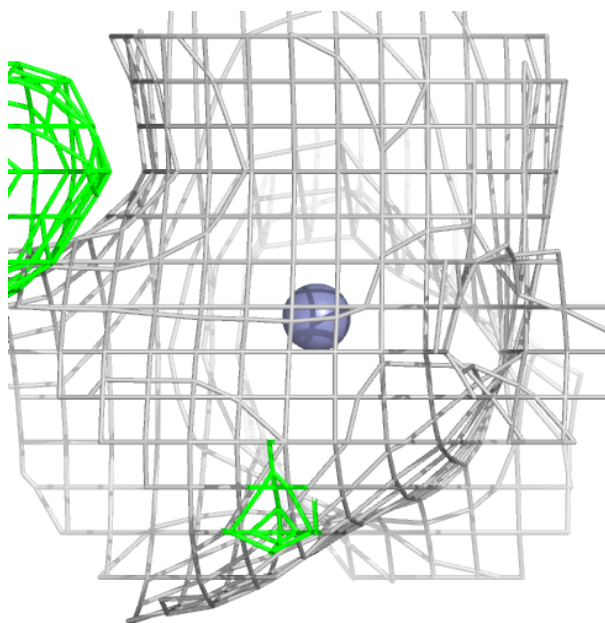
Electron density around ZN R 301:

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



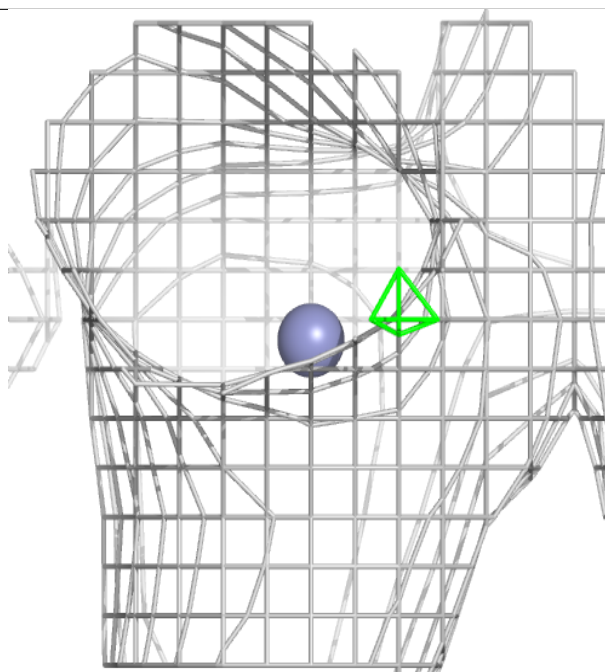
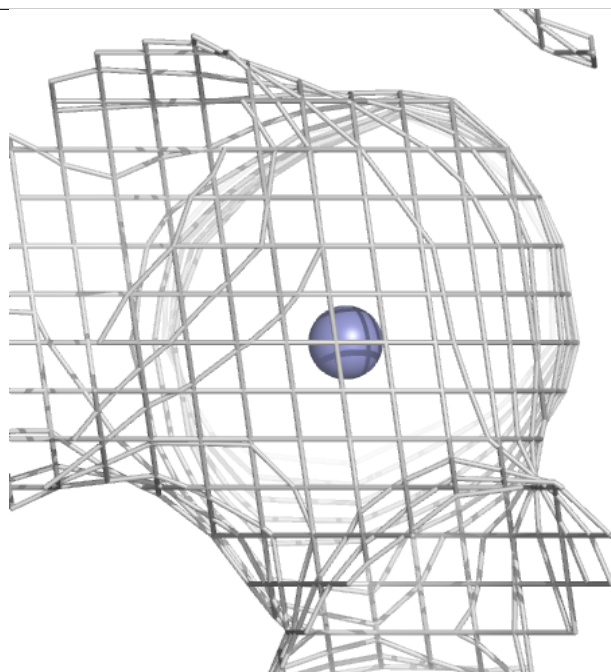
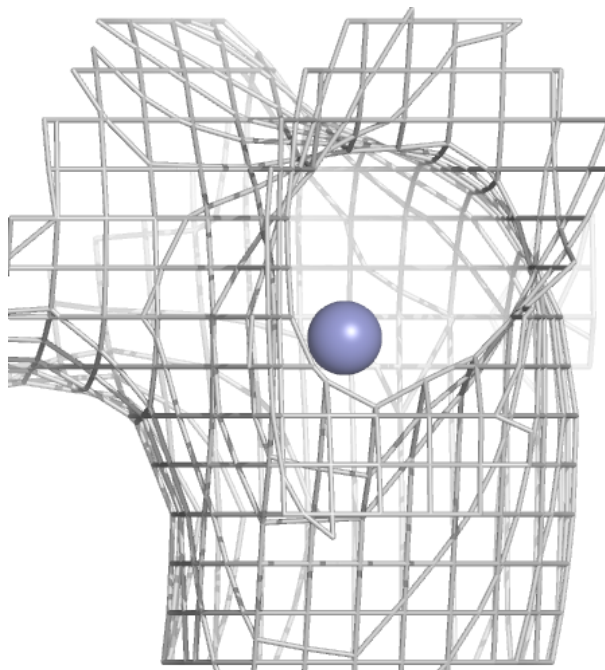
Electron density around ZN F 301:

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



Electron density around ZN B 301:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.