



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 07:32 PM UTC

PDB ID : 7ALB / pdb_00007alb
Title : human GCH-GFRP stimulatory complex 7-deaza-GTP bound
Authors : Ebenhoch, R.; Nar, H.
Deposited on : 2020-10-06
Resolution : 1.98 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

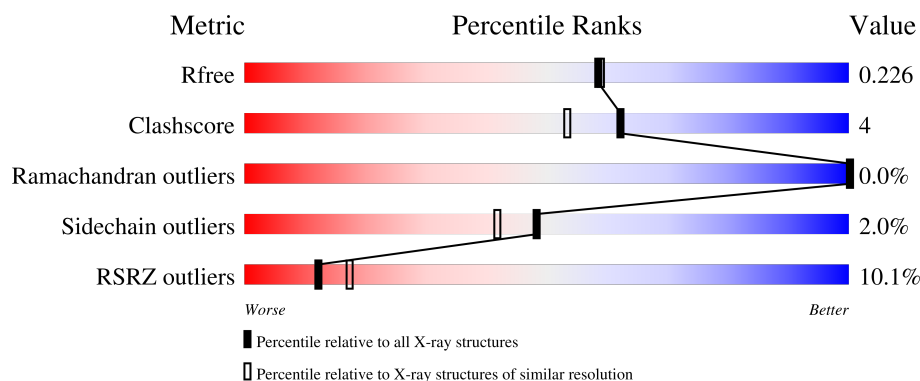
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.98 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	1506 (1.98-1.98)
Clashscore	190562	1534 (1.98-1.98)
Ramachandran outliers	187476	1518 (1.98-1.98)
Sidechain outliers	187428	1518 (1.98-1.98)
RSRZ outliers	180081	1506 (1.98-1.98)

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	16% 78% 13% 8%
1	B	209	7% 78% 11% 11%
1	C	209	11% 76% 15% 9%
1	D	209	5% 81% 11% 8%
1	E	209	11% 80% 11% 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	
2	l	87	
2	m	87	
2	n	87	
2	o	87	
2	p	87	
2	q	87	
2	r	87	
2	s	87	
2	t	87	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 45674 atoms, of which 340 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	187	Total	C	N	O	S	0	0	0
			1473	932	257	273	11			
1	C	190	Total	C	N	O	S	0	0	0
			1497	945	260	281	11			
1	D	192	Total	C	N	O	S	0	1	0
			1523	961	266	284	12			
1	E	192	Total	C	N	O	S	0	0	0
			1515	956	265	283	11			
1	F	189	Total	C	N	O	S	0	1	0
			1496	946	261	277	12			
1	G	189	Total	C	N	O	S	0	0	0
			1488	941	260	276	11			
1	H	190	Total	C	N	O	S	0	0	0
			1498	947	263	277	11			
1	I	190	Total	C	N	O	S	0	0	0
			1497	945	260	281	11			
1	J	190	Total	C	N	O	S	0	0	0
			1498	947	263	277	11			
1	K	192	Total	C	N	O	S	0	0	0
			1515	956	265	283	11			
1	L	187	Total	C	N	O	S	0	0	0
			1473	932	257	273	11			
1	M	190	Total	C	N	O	S	0	0	0
			1497	945	260	281	11			
1	N	190	Total	C	N	O	S	0	0	0
			1497	946	261	279	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	188	Total	C	N	O	S	0	0	0
			1480	937	259	273	11			
1	S	190	Total	C	N	O	S	0	0	0
			1497	945	260	281	11			
1	T	192	Total	C	N	O	S	0	0	0
			1511	954	265	281	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	83	Total	C	N	O	S	0	0	0
			670	424	118	123	5			
2	c	84	Total	C	N	O	S	0	0	0
			678	429	119	124	6			
2	d	83	Total	C	N	O	S	0	0	0
			669	424	118	121	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	83	Total	C	N	O	S	0	0	0
			669	424	118	121	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	83	Total	C	N	O	S	0	0	0
			669	424	118	121	6			
2	m	84	Total	C	N	O	S	0	0	0
			678	429	119	124	6			
2	n	83	Total	C	N	O	S	0	0	0
			669	424	118	121	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	83	Total	C	N	O	S	0	0	0
			669	424	118	121	6			
2	q	84	Total	C	N	O	S	0	0	0
			678	429	119	124	6			
2	r	84	Total	C	N	O	S	0	0	0
			678	429	119	124	6			
2	s	83	Total	C	N	O	S	0	0	0
			669	424	118	121	6			
2	t	84	Total	C	N	O	S	0	0	0
			678	429	119	124	6			

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).

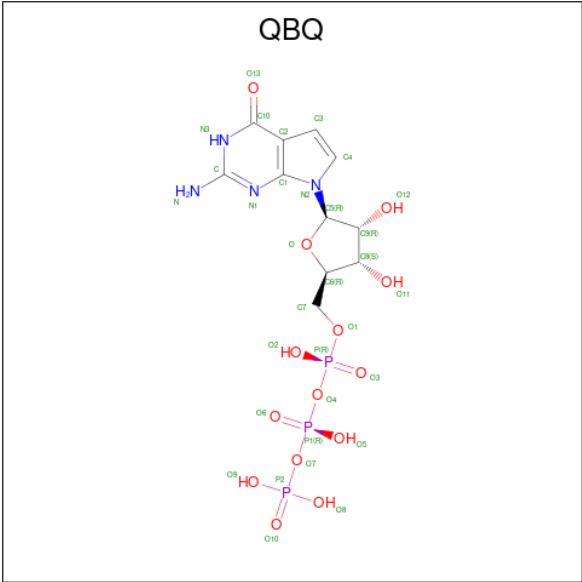
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Zn 1 1	0	0
3	B	1	Total Zn 1 1	0	0
3	C	1	Total Zn 1 1	0	0

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

- 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).



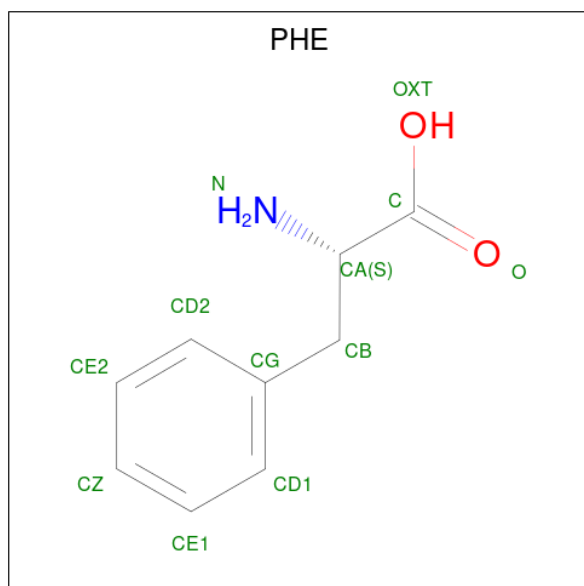
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	H	N	O	P	17	0
			49	11	17	4	14	3		
4	B	1	Total	C	H	N	O	P	17	0
			49	11	17	4	14	3		
4	C	1	Total	C	H	N	O	P	17	0
			49	11	17	4	14	3		
4	D	1	Total	C	H	N	O	P	17	0
			49	11	17	4	14	3		
4	E	1	Total	C	H	N	O	P	17	0
			49	11	17	4	14	3		
4	F	1	Total	C	H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

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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 PHENYLALANINE (CCD ID: PHE) (formula: $C_9H_{11}NO_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	a	1	Total	C	N	O	0	0
			12	9	1	2		
5	b	1	Total	C	N	O	0	0
			12	9	1	2		
5	c	1	Total	C	N	O	0	0
			12	9	1	2		
5	d	1	Total	C	N	O	0	0
			12	9	1	2		
5	e	1	Total	C	N	O	0	0
			12	9	1	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	f	1	Total	C	N	O	0	0
			12	9	1	2		
5	f	1	Total	C	N	O	0	0
			12	9	1	2		
5	g	1	Total	C	N	O	0	0
			12	9	1	2		
5	h	1	Total	C	N	O	0	0
			12	9	1	2		
5	i	1	Total	C	N	O	0	0
			12	9	1	2		
5	k	1	Total	C	N	O	0	0
			12	9	1	2		
5	l	1	Total	C	N	O	0	0
			12	9	1	2		
5	m	1	Total	C	N	O	0	0
			12	9	1	2		
5	n	1	Total	C	N	O	0	0
			12	9	1	2		
5	o	1	Total	C	N	O	0	0
			12	9	1	2		
5	p	1	Total	C	N	O	0	0
			12	9	1	2		
5	q	1	Total	C	N	O	0	0
			12	9	1	2		
5	r	1	Total	C	N	O	0	0
			12	9	1	2		
5	s	1	Total	C	N	O	0	0
			12	9	1	2		
5	t	1	Total	C	N	O	0	0
			12	9	1	2		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	19	Total	O	0	0
			19	19		
6	B	15	Total	O	0	0
			15	15		
6	C	33	Total	O	0	0
			33	33		
6	D	40	Total	O	0	0
			40	40		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	E	28	Total O 28 28	0	0
6	F	26	Total O 26 26	0	0
6	G	48	Total O 48 48	0	0
6	H	32	Total O 32 32	0	0
6	I	24	Total O 24 24	0	0
6	J	8	Total O 8 8	0	0
6	K	29	Total O 29 29	0	0
6	L	22	Total O 22 22	0	0
6	M	29	Total O 29 29	0	0
6	N	33	Total O 33 33	0	0
6	O	25	Total O 25 25	0	0
6	P	40	Total O 40 40	0	0
6	Q	33	Total O 33 33	0	0
6	R	24	Total O 24 24	0	0
6	S	23	Total O 23 23	0	0
6	T	28	Total O 28 28	0	0
6	a	12	Total O 12 12	0	0
6	b	9	Total O 9 9	0	0
6	c	20	Total O 20 20	0	0
6	d	18	Total O 18 18	0	0
6	e	19	Total O 19 19	0	0

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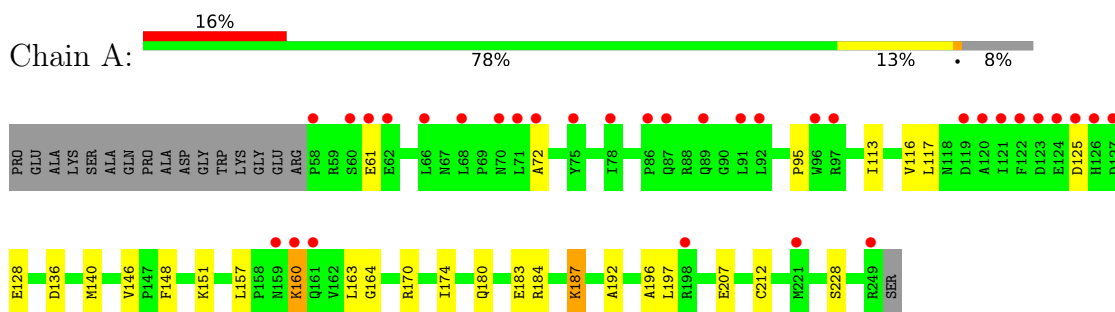
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	f	23	Total 23	O 23	0	0
6	g	26	Total 26	O 26	0	0
6	h	28	Total 28	O 28	0	0
6	i	14	Total 14	O 14	0	0
6	j	4	Total 4	O 4	0	0
6	k	14	Total 14	O 14	0	0
6	l	16	Total 16	O 16	0	0
6	m	14	Total 14	O 14	0	0
6	n	18	Total 18	O 18	0	0
6	o	21	Total 21	O 21	0	0
6	p	22	Total 22	O 22	0	0
6	q	24	Total 24	O 24	0	0
6	r	25	Total 25	O 25	0	0
6	s	25	Total 25	O 25	0	0
6	t	19	Total 19	O 19	0	0

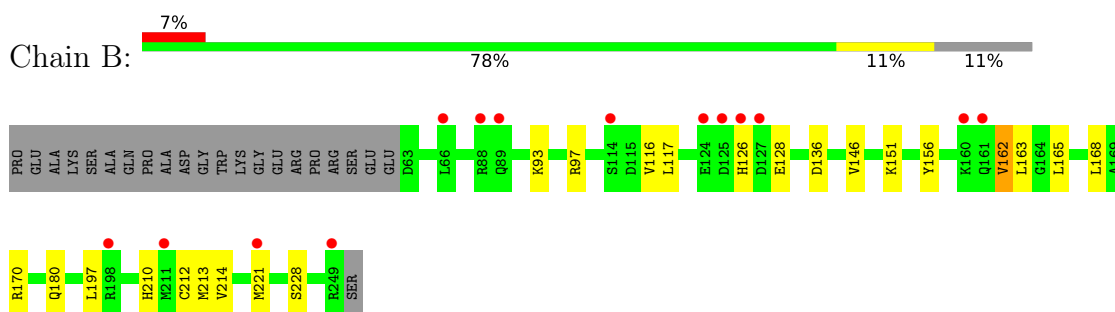
3 Residue-property plots [i](#)

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.

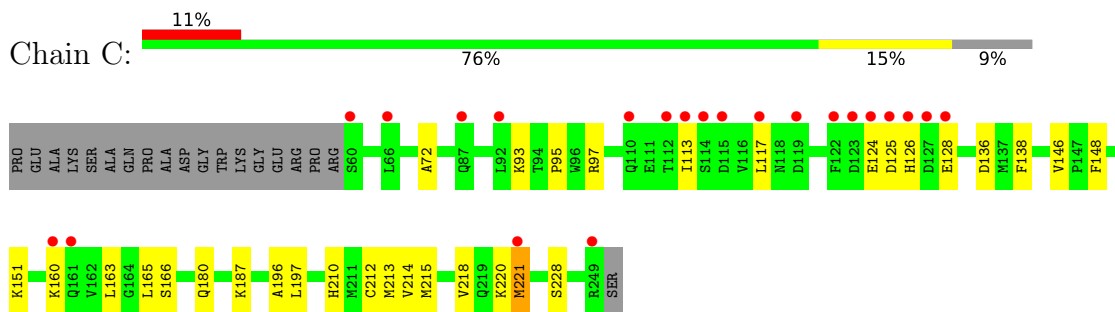
- Molecule 1: GTP cyclohydrolase 1



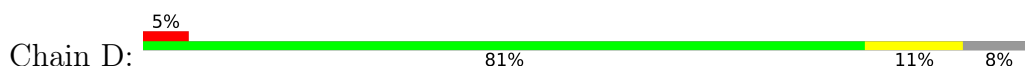
- Molecule 1: GTP cyclohydrolase 1

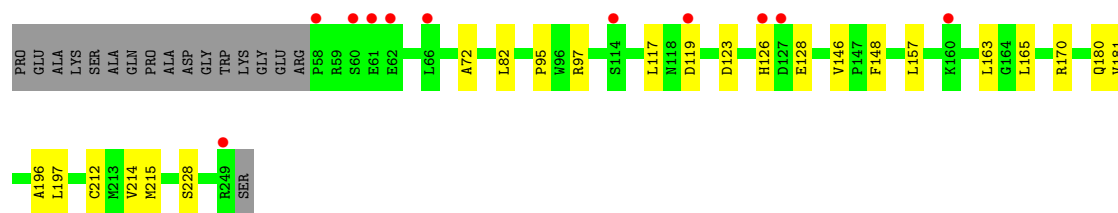


- Molecule 1: GTP cyclohydrolase 1

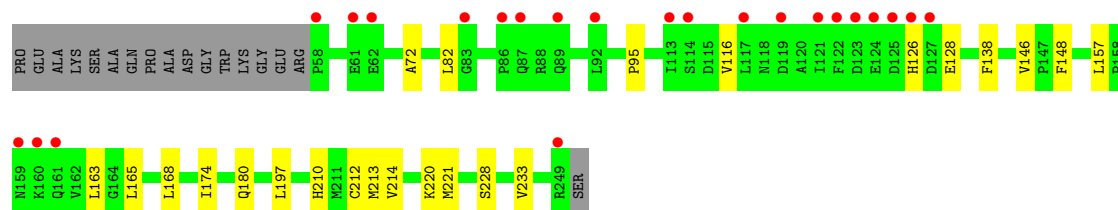
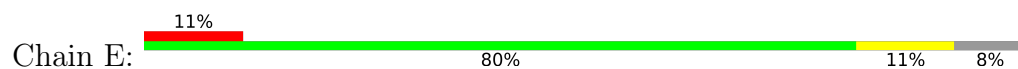


- Molecule 1: GTP cyclohydrolase 1

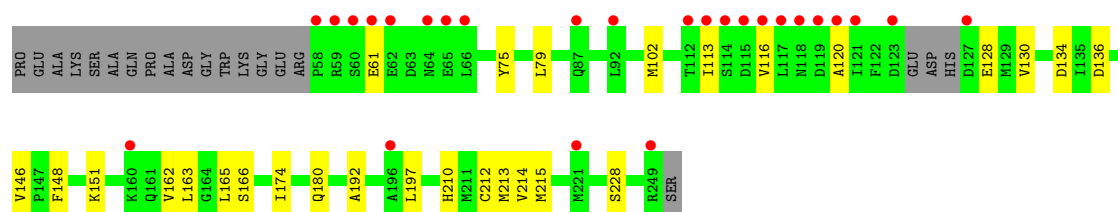
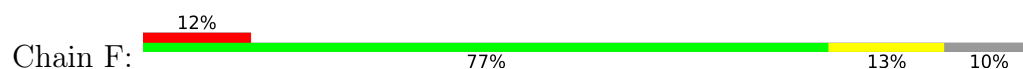




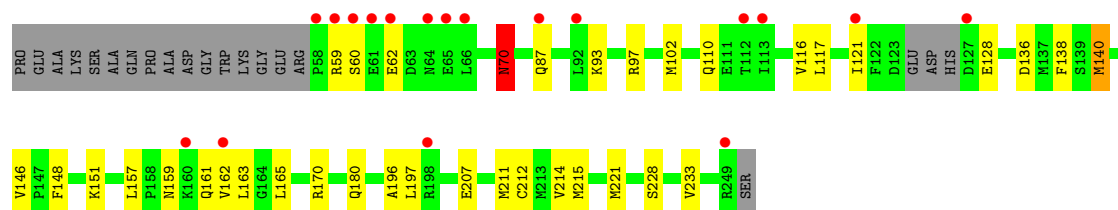
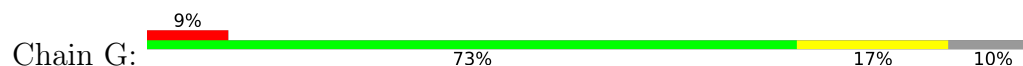
• Molecule 1: GTP cyclohydrolase 1



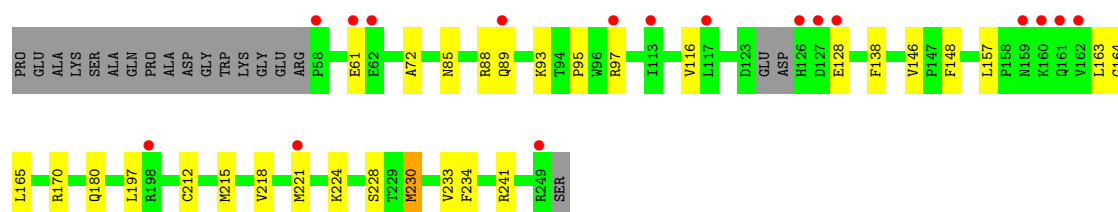
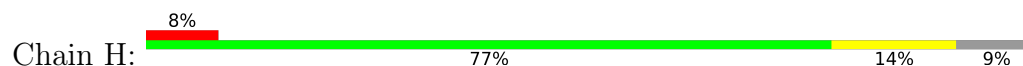
• Molecule 1: GTP cyclohydrolase 1



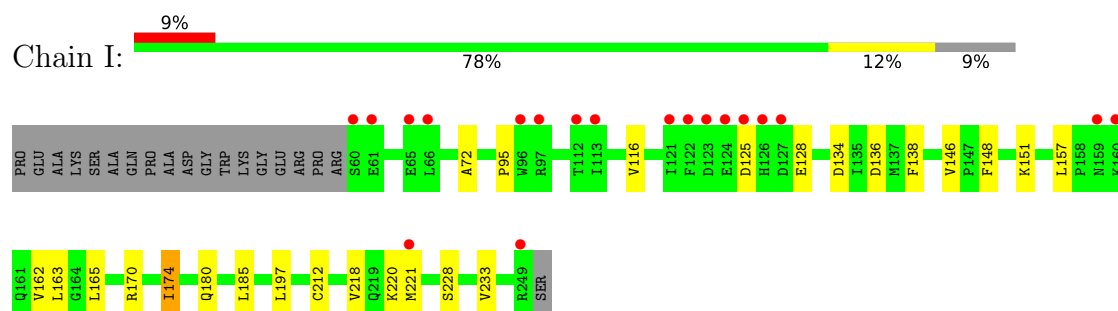
• Molecule 1: GTP cyclohydrolase 1



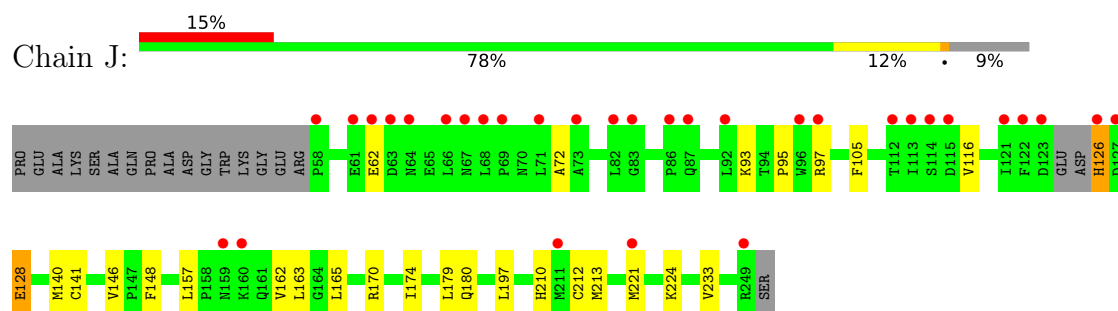
• Molecule 1: GTP cyclohydrolase 1



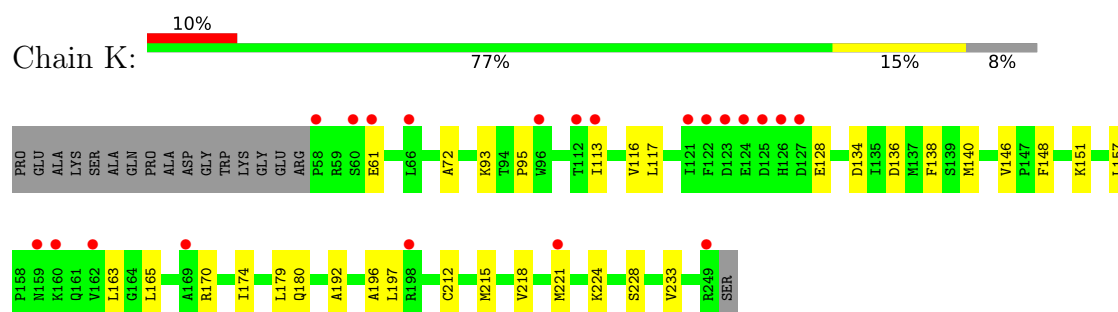
- Molecule 1: GTP cyclohydrolase 1



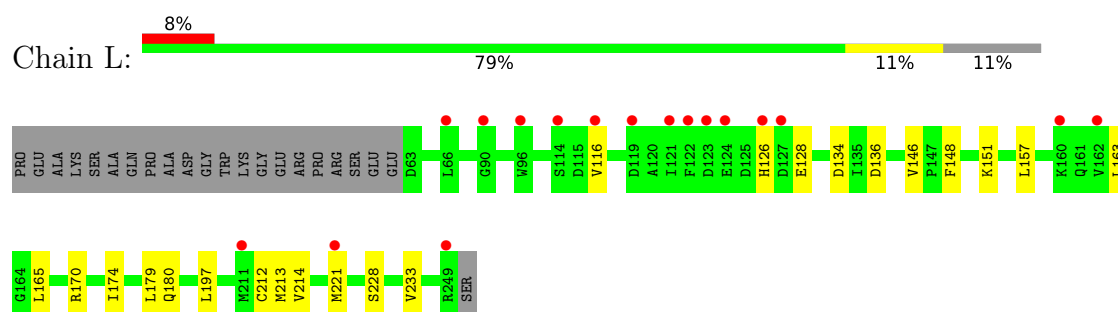
- Molecule 1: GTP cyclohydrolase 1



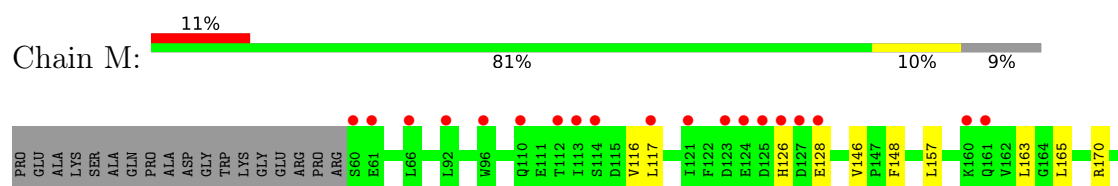
- Molecule 1: GTP cyclohydrolase 1



- Molecule 1: GTP cyclohydrolase 1

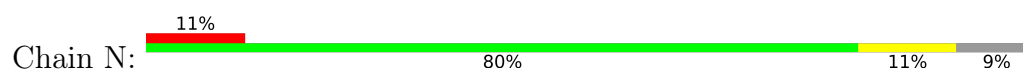


- Molecule 1: GTP cyclohydrolase 1

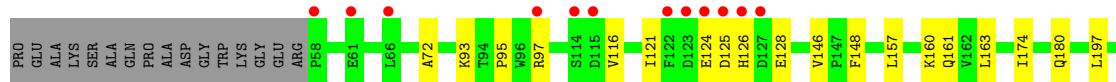
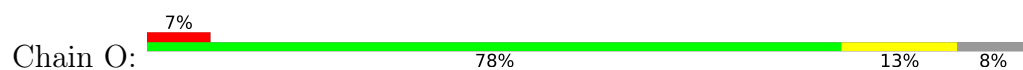




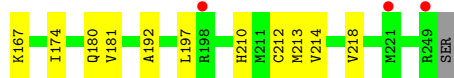
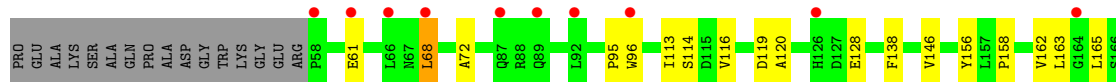
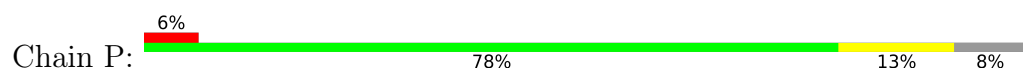
- Molecule 1: GTP cyclohydrolase 1



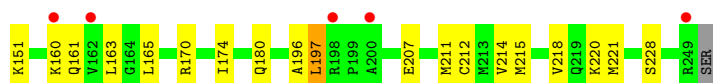
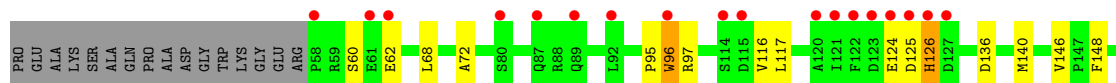
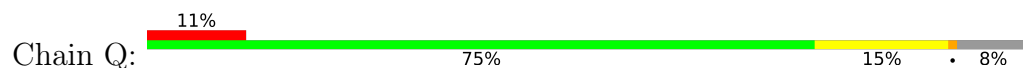
- Molecule 1: GTP cyclohydrolase 1



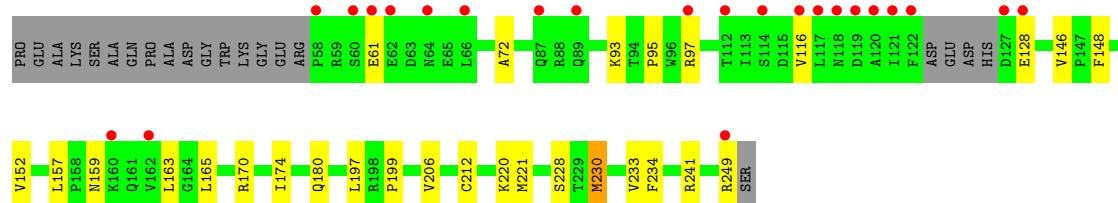
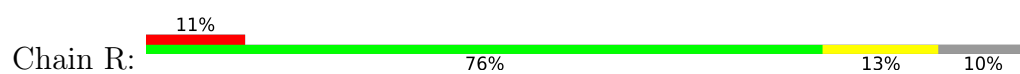
- Molecule 1: GTP cyclohydrolase 1



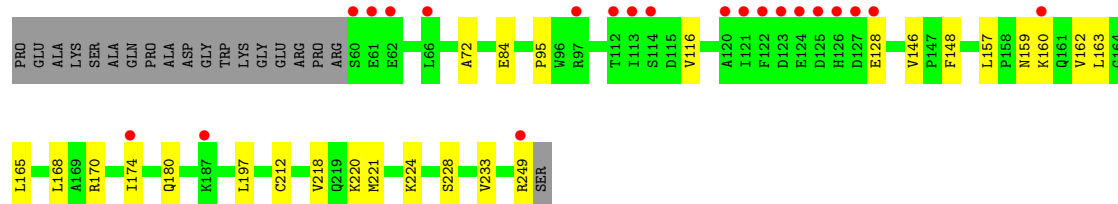
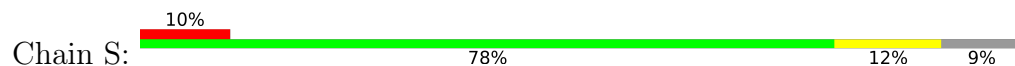
- Molecule 1: GTP cyclohydrolase 1



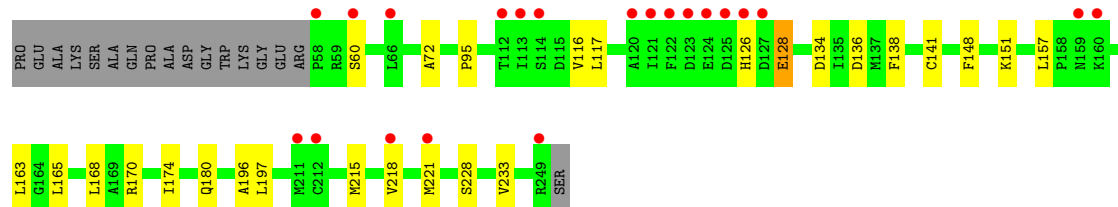
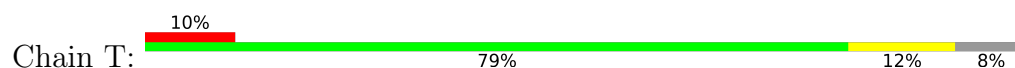
- Molecule 1: GTP cyclohydrolase 1



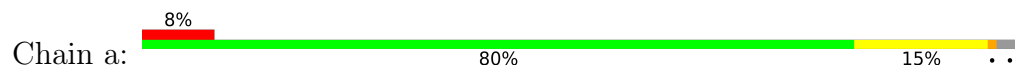
- Molecule 1: GTP cyclohydrolase 1



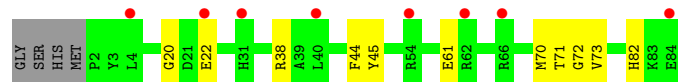
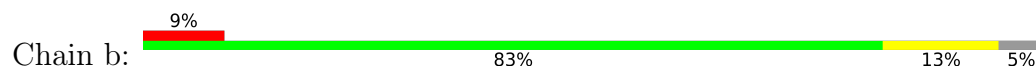
- Molecule 1: GTP cyclohydrolase 1



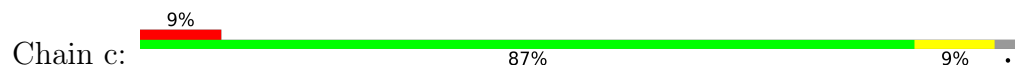
- Molecule 2: GTP cyclohydrolase 1 feedback regulatory protein

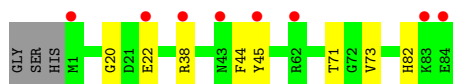


- Molecule 2: GTP cyclohydrolase 1 feedback regulatory protein

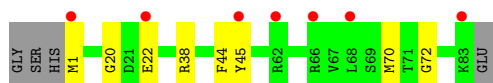
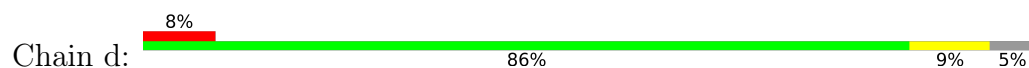


- Molecule 2: GTP cyclohydrolase 1 feedback regulatory protein

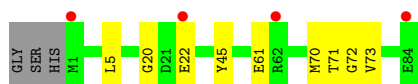
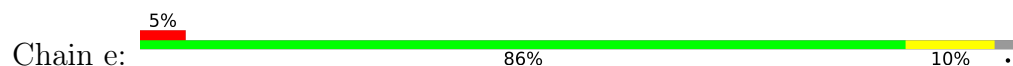




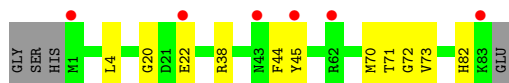
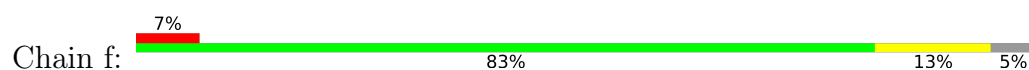
- Molecule 2: GTP cyclohydrolase 1 feedback regulatory protein



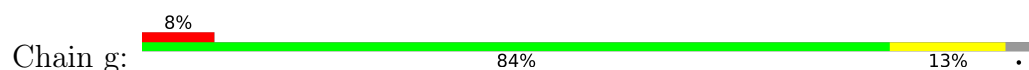
- Molecule 2: GTP cyclohydrolase 1 feedback regulatory protein



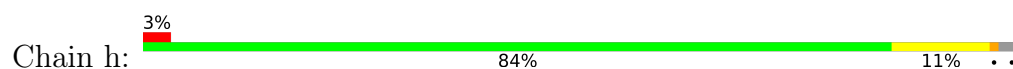
- Molecule 2: GTP cyclohydrolase 1 feedback regulatory protein



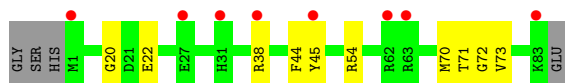
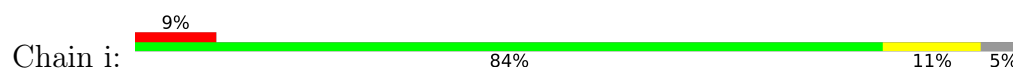
- Molecule 2: GTP cyclohydrolase 1 feedback regulatory protein



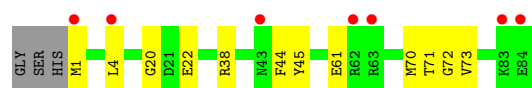
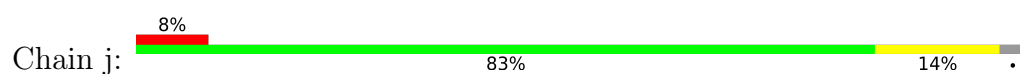
- Molecule 2: GTP cyclohydrolase 1 feedback regulatory protein



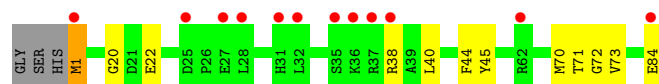
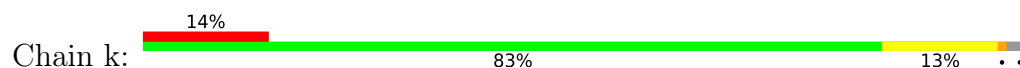
- Molecule 2: GTP cyclohydrolase 1 feedback regulatory protein



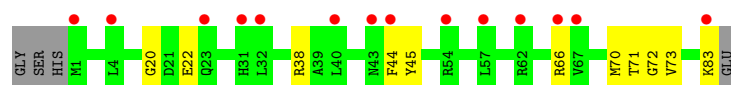
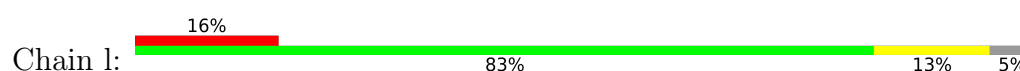
- Molecule 2: GTP cyclohydrolase 1 feedback regulatory protein



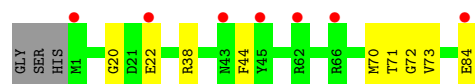
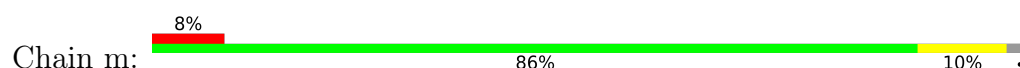
- Molecule 2: GTP cyclohydrolase 1 feedback regulatory protein



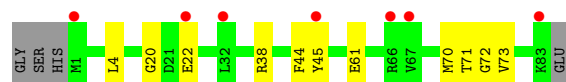
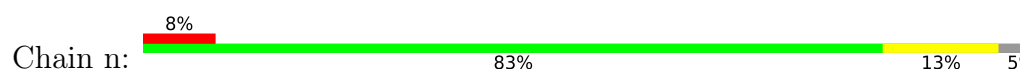
- Molecule 2: GTP cyclohydrolase 1 feedback regulatory protein



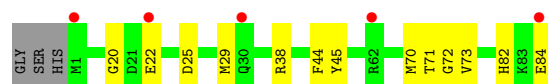
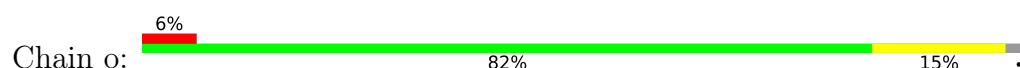
- Molecule 2: GTP cyclohydrolase 1 feedback regulatory protein



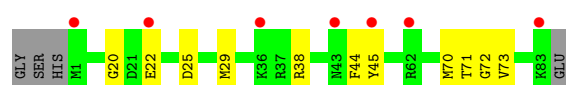
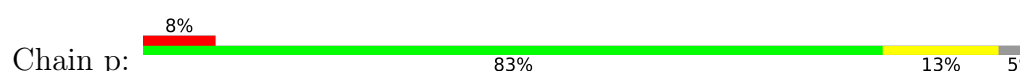
- Molecule 2: GTP cyclohydrolase 1 feedback regulatory protein



- Molecule 2: GTP cyclohydrolase 1 feedback regulatory protein

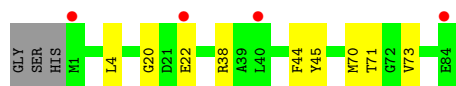


- Molecule 2: GTP cyclohydrolase 1 feedback regulatory protein



- Molecule 2: GTP cyclohydrolase 1 feedback regulatory protein

Chain q:  5% 86% 10% .



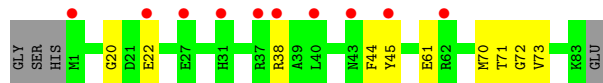
- Molecule 2: GTP cyclohydrolase 1 feedback regulatory protein

Chain r:  5% 86% 10% .



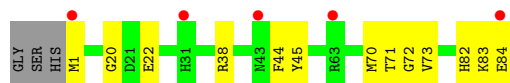
- Molecule 2: GTP cyclohydrolase 1 feedback regulatory protein

Chain s:  11% 84% 11% 5%



- Molecule 2: GTP cyclohydrolase 1 feedback regulatory protein

Chain t:  6% 82% 15% .



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	160.66Å 116.14Å 177.32Å 90.00° 94.94° 90.00°	Depositor
Resolution (Å)	160.06 – 1.98 160.06 – 1.98	Depositor EDS
% Data completeness (in resolution range)	72.5 (160.06-1.98) 72.5 (160.06-1.98)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.89 (at 1.98Å)	Xtriage
Refinement program	BUSTER 2.11.7 (18-SEP-2020)	Depositor
R, R_{free}	0.206 , 0.225 0.208 , 0.226	Depositor DCC
R_{free} test set	3700 reflections (1.13%)	wwPDB-VP
Wilson B-factor (Å ²)	27.4	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 40.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	45674	wwPDB-VP
Average B, all atoms (Å ²)	33.0	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 45.44 % 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 1.3204e-04. 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: 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	0.76	1/1540 (0.1%)	1.01	2/2079 (0.1%)
1	B	0.73	0/1497	1.02	1/2022 (0.0%)
1	C	0.78	0/1521	1.03	4/2054 (0.2%)
1	D	0.75	0/1548	1.01	2/2089 (0.1%)
1	E	0.75	0/1540	1.01	4/2079 (0.2%)
1	F	0.78	0/1519	1.04	3/2048 (0.1%)
1	G	0.81	1/1511 (0.1%)	1.04	3/2038 (0.1%)
1	H	0.82	1/1522 (0.1%)	1.02	2/2053 (0.1%)
1	I	0.76	0/1521	1.05	8/2054 (0.4%)
1	J	0.75	0/1522	1.02	3/2053 (0.1%)
1	K	0.77	1/1540 (0.1%)	1.01	3/2079 (0.1%)
1	L	0.79	1/1497 (0.1%)	1.03	2/2022 (0.1%)
1	M	0.76	0/1521	1.02	5/2054 (0.2%)
1	N	0.74	0/1520	1.05	5/2050 (0.2%)
1	O	0.74	0/1540	1.03	5/2079 (0.2%)
1	P	0.80	0/1540	1.03	1/2079 (0.0%)
1	Q	0.77	1/1540 (0.1%)	1.04	4/2079 (0.2%)
1	R	0.80	1/1503 (0.1%)	1.01	4/2027 (0.2%)
1	S	0.74	0/1521	1.03	4/2054 (0.2%)
1	T	0.77	0/1536	1.00	2/2074 (0.1%)
2	a	0.64	0/692	0.89	1/934 (0.1%)
2	b	0.62	0/684	0.90	1/923 (0.1%)
2	c	0.62	0/692	0.90	1/934 (0.1%)
2	d	0.63	0/683	0.89	1/922 (0.1%)
2	e	0.65	0/692	0.91	1/934 (0.1%)
2	f	0.66	0/683	0.91	1/922 (0.1%)
2	g	0.66	0/692	0.90	1/934 (0.1%)
2	h	0.65	0/692	0.90	1/934 (0.1%)
2	i	0.66	0/683	0.90	1/922 (0.1%)
2	j	0.63	0/692	0.89	1/934 (0.1%)
2	k	0.61	0/692	0.90	1/934 (0.1%)
2	l	0.60	0/683	0.89	1/922 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	m	0.59	0/692	0.88	1/934 (0.1%)
2	n	0.62	0/683	0.90	1/922 (0.1%)
2	o	0.66	0/692	0.90	1/934 (0.1%)
2	p	0.65	0/683	0.91	1/922 (0.1%)
2	q	0.66	0/692	0.91	1/934 (0.1%)
2	r	0.65	0/692	0.92	0/934
2	s	0.68	0/683	0.92	1/922 (0.1%)
2	t	0.65	0/692	0.94	3/934 (0.3%)
All	All	0.73	7/44268 (0.0%)	0.99	88/59751 (0.1%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	230	MET	SD-CE	-11.89	1.49	1.79
1	R	230	MET	SD-CE	-11.65	1.50	1.79
1	K	140	MET	SD-CE	-7.38	1.61	1.79
1	Q	140	MET	SD-CE	-7.07	1.61	1.79
1	G	140	MET	SD-CE	-6.48	1.63	1.79
1	L	213	MET	SD-CE	-5.71	1.65	1.79
1	A	140	MET	SD-CE	-5.46	1.65	1.79

All (88) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S	180	GLN	N-CA-C	8.24	120.48	108.86
1	R	180	GLN	N-CA-C	8.17	120.38	108.86
1	P	180	GLN	N-CA-C	8.15	120.36	108.86
1	O	180	GLN	N-CA-C	7.56	119.52	108.86
1	K	180	GLN	N-CA-C	7.55	119.51	108.86
1	I	180	GLN	N-CA-C	7.55	119.50	108.86
1	A	180	GLN	N-CA-C	7.40	119.29	108.86
1	H	180	GLN	N-CA-C	7.34	119.21	108.86
1	M	180	GLN	N-CA-C	7.22	119.04	108.86
1	E	180	GLN	N-CA-C	7.21	119.03	108.86
1	D	180	GLN	N-CA-C	7.11	118.89	108.86
1	B	180	GLN	N-CA-C	7.10	118.87	108.86
1	G	180	GLN	N-CA-C	7.08	118.84	108.86
1	T	180	GLN	N-CA-C	7.06	118.82	108.86
1	A	148	PHE	CA-CB-CG	7.02	120.82	113.80
1	C	180	GLN	N-CA-C	7.00	118.72	108.86
1	F	180	GLN	N-CA-C	6.84	118.51	108.86
1	L	180	GLN	N-CA-C	6.73	118.35	108.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	180	GLN	N-CA-C	6.58	118.13	108.86
1	N	148	PHE	CA-CB-CG	6.39	120.19	113.80
1	H	148	PHE	CA-CB-CG	6.26	120.06	113.80
1	R	148	PHE	CA-CB-CG	6.19	119.99	113.80
1	J	180	GLN	N-CA-C	6.12	118.26	109.14
1	L	148	PHE	CA-CB-CG	6.08	119.88	113.80
1	C	148	PHE	CA-CB-CG	6.08	119.88	113.80
1	K	148	PHE	CA-CB-CG	6.04	119.84	113.80
1	F	120	ALA	N-CA-C	5.99	119.87	111.30
1	Q	148	PHE	CA-CB-CG	5.98	119.78	113.80
1	J	148	PHE	CA-CB-CG	5.94	119.74	113.80
1	Q	220	LYS	CA-C-N	5.92	128.49	120.38
1	Q	220	LYS	C-N-CA	5.92	128.49	120.38
1	E	148	PHE	CA-CB-CG	5.85	119.65	113.80
1	S	148	PHE	CA-CB-CG	5.85	119.65	113.80
1	F	148	PHE	CA-CB-CG	5.83	119.63	113.80
1	M	148	PHE	CA-CB-CG	5.80	119.60	113.80
1	O	148	PHE	CA-CB-CG	5.78	119.58	113.80
1	G	148	PHE	CA-CB-CG	5.76	119.56	113.80
2	i	20	GLY	N-CA-C	5.73	119.12	110.18
1	I	148	PHE	CA-CB-CG	5.71	119.51	113.80
2	s	20	GLY	N-CA-C	5.60	118.91	110.18
1	N	220	LYS	CA-C-N	5.56	128.00	120.38
1	N	220	LYS	C-N-CA	5.56	128.00	120.38
1	M	214	VAL	N-CA-CB	5.55	116.19	111.64
2	j	20	GLY	N-CA-C	5.50	118.76	110.18
2	c	20	GLY	N-CA-C	5.48	118.58	110.42
1	M	220	LYS	CA-C-N	5.42	127.81	120.38
1	M	220	LYS	C-N-CA	5.42	127.81	120.38
1	I	125	ASP	N-CA-C	-5.40	107.25	112.97
1	T	148	PHE	CA-CB-CG	5.38	119.18	113.80
1	N	180	GLN	N-CA-C	5.38	117.15	109.14
2	p	20	GLY	N-CA-C	5.34	118.51	110.18
2	n	20	GLY	N-CA-C	5.34	118.51	110.18
2	h	20	GLY	N-CA-C	5.32	118.47	110.18
2	a	20	GLY	N-CA-C	5.30	118.45	110.18
2	t	20	GLY	N-CA-C	5.28	118.41	110.18
2	l	20	GLY	N-CA-C	5.28	118.41	110.18
1	O	125	ASP	N-CA-C	-5.25	103.38	110.68
2	t	83	LYS	CA-C-N	5.21	131.07	121.70
2	t	83	LYS	C-N-CA	5.21	131.07	121.70
1	D	148	PHE	CA-CB-CG	5.18	118.98	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S	220	LYS	CA-C-N	5.18	127.48	120.38
1	S	220	LYS	C-N-CA	5.18	127.48	120.38
2	e	20	GLY	N-CA-C	5.16	118.22	110.18
1	K	179	LEU	N-CA-C	-5.15	101.36	109.25
2	k	20	GLY	N-CA-C	5.14	118.20	110.18
2	g	20	GLY	N-CA-C	5.14	118.20	110.18
2	q	20	GLY	N-CA-C	5.13	118.19	110.18
1	E	220	LYS	CA-C-N	5.11	127.39	120.38
1	E	220	LYS	C-N-CA	5.11	127.39	120.38
1	I	220	LYS	CA-C-N	5.11	127.39	120.38
1	I	220	LYS	C-N-CA	5.11	127.39	120.38
1	O	220	LYS	CA-C-N	5.11	127.38	120.38
1	O	220	LYS	C-N-CA	5.11	127.38	120.38
1	J	179	LEU	N-CA-C	-5.10	101.44	109.25
2	m	20	GLY	N-CA-C	5.10	118.02	110.42
1	G	70	ASN	CA-CB-CG	5.09	117.69	112.60
2	f	20	GLY	N-CA-C	5.09	118.11	110.18
1	I	174	ILE	CB-CA-C	-5.08	105.47	111.97
1	C	220	LYS	CA-C-N	5.07	127.33	120.38
1	C	220	LYS	C-N-CA	5.07	127.33	120.38
1	R	220	LYS	CA-C-N	5.06	127.31	120.38
1	R	220	LYS	C-N-CA	5.06	127.31	120.38
1	N	179	LEU	N-CA-C	-5.05	101.53	109.25
2	o	20	GLY	N-CA-C	5.04	118.05	110.18
2	b	20	GLY	N-CA-C	5.03	118.03	110.18
2	d	20	GLY	N-CA-C	5.03	118.03	110.18
1	I	185	LEU	CA-C-N	5.02	126.97	120.44
1	I	185	LEU	C-N-CA	5.02	126.97	120.44

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1515	0	1539	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1473	0	1501	16	0
1	C	1497	0	1518	20	0
1	D	1523	0	1547	13	0
1	E	1515	0	1539	14	0
1	F	1496	0	1529	14	0
1	G	1488	0	1521	20	0
1	H	1498	0	1528	21	0
1	I	1497	0	1518	13	0
1	J	1498	0	1528	15	0
1	K	1515	0	1539	24	0
1	L	1473	0	1501	13	0
1	M	1497	0	1518	12	0
1	N	1497	0	1527	12	0
1	O	1515	0	1539	12	0
1	P	1515	0	1539	18	0
1	Q	1515	0	1539	19	0
1	R	1480	0	1517	21	0
1	S	1497	0	1518	16	0
1	T	1511	0	1535	16	0
2	a	678	0	680	10	0
2	b	670	0	669	8	0
2	c	678	0	680	5	0
2	d	669	0	674	4	0
2	e	678	0	680	6	0
2	f	669	0	674	7	0
2	g	678	0	680	6	0
2	h	678	0	680	7	0
2	i	669	0	674	8	0
2	j	678	0	680	8	0
2	k	678	0	680	8	0
2	l	669	0	674	6	0
2	m	678	0	680	5	0
2	n	669	0	674	7	0
2	o	678	0	680	9	0
2	p	669	0	674	7	0
2	q	678	0	680	5	0
2	r	678	0	680	6	0
2	s	669	0	674	7	0
2	t	678	0	680	7	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	1	0	0	0	0
3	E	1	0	0	0	0
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	0	0
4	B	32	17	0	1	0
4	C	32	17	0	2	0
4	D	32	17	0	1	0
4	E	32	17	0	1	0
4	F	32	17	0	1	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	1	0
4	N	32	17	0	0	0
4	O	32	17	0	0	0
4	P	32	17	0	1	0
4	Q	32	17	0	1	0
4	R	32	17	0	1	0
4	S	32	17	0	1	0
4	T	32	17	0	1	0
5	a	12	0	8	0	0
5	b	12	0	8	0	0
5	c	12	0	8	0	0
5	d	12	0	8	0	0
5	e	12	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	f	24	0	16	0	0
5	g	12	0	8	0	0
5	h	12	0	8	0	0
5	i	12	0	8	0	0
5	k	12	0	8	0	0
5	l	12	0	8	0	0
5	m	12	0	8	0	0
5	n	12	0	8	0	0
5	o	12	0	8	0	0
5	p	12	0	8	0	0
5	q	12	0	8	0	0
5	r	12	0	8	0	0
5	s	12	0	8	0	0
5	t	12	0	8	0	0
6	A	19	0	0	0	0
6	B	15	0	0	0	0
6	C	33	0	0	0	0
6	D	40	0	0	0	0
6	E	28	0	0	0	0
6	F	26	0	0	1	0
6	G	48	0	0	0	0
6	H	32	0	0	1	0
6	I	24	0	0	0	0
6	J	8	0	0	0	0
6	K	29	0	0	0	0
6	L	22	0	0	0	0
6	M	29	0	0	0	0
6	N	33	0	0	0	0
6	O	25	0	0	0	0
6	P	40	0	0	0	0
6	Q	33	0	0	0	0
6	R	24	0	0	0	0
6	S	23	0	0	0	0
6	T	28	0	0	0	0
6	a	12	0	0	0	0
6	b	9	0	0	0	0
6	c	20	0	0	0	0
6	d	18	0	0	0	0
6	e	19	0	0	0	0
6	f	23	0	0	0	0
6	g	26	0	0	0	0
6	h	28	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	i	14	0	0	0	0
6	j	4	0	0	0	0
6	k	14	0	0	0	0
6	l	16	0	0	0	0
6	m	14	0	0	0	0
6	n	18	0	0	0	0
6	o	21	0	0	0	0
6	p	22	0	0	0	0
6	q	24	0	0	1	0
6	r	25	0	0	0	0
6	s	25	0	0	0	0
6	t	19	0	0	0	0
All	All	45334	340	44247	365	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 4.

All (365) 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:R:230:MET:HE3	1:R:234:PHE:HB3	1.34	1.03
1:H:230:MET:HE3	1:H:234:PHE:HB3	1.43	0.99
1:Q:211:MET:HB3	1:Q:215:MET:HE2	1.51	0.92
1:P:116:VAL:HG21	1:P:174:ILE:HD11	1.56	0.86
1:G:60:SER:OG	1:G:62:GLU:HG2	1.75	0.85
1:G:211:MET:HB3	1:G:215:MET:HE2	1.59	0.85
1:K:93:LYS:HE3	1:P:119:ASP:OD1	1.79	0.82
1:E:163:LEU:HB2	1:E:197:LEU:HD11	1.64	0.78
1:D:228:SER:O	1:E:128:GLU:HB3	1.84	0.77
1:B:163:LEU:HB2	1:B:197:LEU:HD11	1.67	0.77
1:T:163:LEU:HB2	1:T:197:LEU:HD11	1.67	0.76
1:Q:60:SER:OG	1:Q:62:GLU:HG2	1.85	0.75
1:N:228:SER:O	1:O:128:GLU:HB3	1.88	0.74
1:G:163:LEU:HB2	1:G:197:LEU:HD11	1.67	0.74
1:A:163:LEU:HB2	1:A:197:LEU:HD11	1.70	0.73
1:C:136:ASP:OD1	1:C:151:LYS:HE2	1.89	0.73
2:p:22:GLU:HG2	2:p:45:TYR:HB2	1.72	0.72
1:I:228:SER:O	1:J:128:GLU:HB2	1.89	0.72
1:M:228:SER:O	1:N:128:GLU:HB3	1.90	0.72
1:K:93:LYS:CE	1:P:119:ASP:OD1	2.38	0.71
1:H:163:LEU:HB2	1:H:197:LEU:HD11	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:163:LEU:HB2	1:P:197:LEU:HD11	1.72	0.70
1:C:228:SER:O	1:D:128:GLU:HB3	1.93	0.69
1:S:163:LEU:HB2	1:S:197:LEU:HD11	1.74	0.69
1:O:124:GLU:HG2	1:O:126:HIS:HB2	1.75	0.68
1:Q:228:SER:O	1:R:128:GLU:HB3	1.92	0.68
1:K:128:GLU:HB3	1:O:228:SER:O	1.93	0.68
1:Q:68:LEU:CD2	1:Q:96:TRP:HE1	2.07	0.68
1:M:163:LEU:HB2	1:M:197:LEU:HD11	1.75	0.68
1:K:228:SER:O	1:L:128:GLU:HB2	1.94	0.67
1:A:128:GLU:HB3	1:E:228:SER:O	1.94	0.67
1:K:117:LEU:HD21	1:K:196:ALA:HB1	1.76	0.67
1:D:82:LEU:HD21	1:G:102:MET:HG3	1.76	0.67
1:H:228:SER:O	1:I:128:GLU:HB3	1.95	0.67
1:I:163:LEU:HB2	1:I:197:LEU:HD11	1.76	0.67
1:G:228:SER:O	1:H:128:GLU:HB3	1.96	0.66
1:G:117:LEU:HD21	1:G:196:ALA:HB1	1.79	0.65
1:A:228:SER:O	1:B:128:GLU:HB2	1.97	0.65
1:L:163:LEU:HB2	1:L:197:LEU:HD11	1.79	0.63
1:C:125:ASP:HA	1:C:160:LYS:HE3	1.80	0.63
1:L:228:SER:O	1:M:128:GLU:HB3	1.97	0.63
1:B:228:SER:O	1:C:128:GLU:HB3	1.99	0.63
1:G:146:VAL:HB	1:G:212:CYS:SG	2.38	0.63
1:J:163:LEU:HB2	1:J:197:LEU:HD11	1.79	0.63
1:H:230:MET:HE2	1:H:241:ARG:HG3	1.79	0.63
1:H:224:LYS:HE2	1:I:134:ASP:OD2	2.00	0.62
1:C:210:HIS:HB2	1:C:213:MET:HE2	1.81	0.62
1:C:117:LEU:HD21	1:C:196:ALA:HB1	1.81	0.61
1:R:230:MET:CE	1:R:234:PHE:HB3	2.22	0.61
2:a:22:GLU:HG2	2:a:45:TYR:HB2	1.82	0.61
1:A:117:LEU:HD21	1:A:196:ALA:HB1	1.83	0.61
1:C:163:LEU:HB2	1:C:197:LEU:HD11	1.81	0.61
2:h:22:GLU:HG2	2:h:45:TYR:HB2	1.81	0.61
2:i:22:GLU:HG2	2:i:45:TYR:HB2	1.83	0.61
1:F:228:SER:O	1:G:128:GLU:HB3	2.01	0.61
1:J:146:VAL:HB	1:J:212:CYS:SG	2.42	0.60
1:P:128:GLU:HB2	1:T:228:SER:O	2.01	0.60
2:r:22:GLU:HG2	2:r:45:TYR:HB2	1.82	0.60
2:f:71:THR:HG22	2:j:70:MET:HE3	1.84	0.60
1:A:116:VAL:HG11	1:A:174:ILE:HD11	1.84	0.60
1:M:117:LEU:HD21	1:M:196:ALA:HB1	1.84	0.60
1:O:163:LEU:HB2	1:O:197:LEU:HD11	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:230:MET:HE2	1:R:241:ARG:HG3	1.83	0.60
2:q:22:GLU:HG2	2:q:45:TYR:HB2	1.84	0.60
1:P:210:HIS:HB2	1:P:213:MET:HE2	1.84	0.59
2:s:22:GLU:HG2	2:s:45:TYR:HB2	1.84	0.59
1:S:224:LYS:HE2	1:T:134:ASP:OD2	2.02	0.59
2:c:22:GLU:HG2	2:c:45:TYR:HB2	1.85	0.59
2:k:71:THR:HG22	2:o:70:MET:HE3	1.84	0.59
2:b:22:GLU:HG2	2:b:45:TYR:HB2	1.84	0.59
2:d:22:GLU:HG2	2:d:45:TYR:HB2	1.84	0.59
1:K:138:PHE:HB3	1:T:215:MET:HE3	1.85	0.58
1:T:117:LEU:HD22	1:T:163:LEU:HD11	1.84	0.58
2:j:22:GLU:HG2	2:j:45:TYR:HB2	1.83	0.58
1:Q:117:LEU:HD21	1:Q:196:ALA:HB1	1.85	0.58
2:g:22:GLU:HG2	2:g:45:TYR:HB2	1.85	0.58
1:Q:68:LEU:HD21	1:Q:96:TRP:HE1	1.68	0.58
2:f:22:GLU:HG2	2:f:45:TYR:HB2	1.85	0.58
2:o:82:HIS:ND1	2:o:84:GLU:OE1	2.30	0.58
2:k:22:GLU:HG2	2:k:45:TYR:HB2	1.85	0.58
1:D:146:VAL:HB	1:D:212:CYS:SG	2.44	0.57
1:C:146:VAL:HB	1:C:212:CYS:SG	2.45	0.57
1:P:146:VAL:HB	1:P:212:CYS:SG	2.44	0.57
1:R:146:VAL:HB	1:R:212:CYS:SG	2.44	0.57
2:l:22:GLU:HG2	2:l:45:TYR:HB2	1.86	0.57
2:n:22:GLU:HG2	2:n:45:TYR:HB2	1.86	0.57
1:A:146:VAL:HB	1:A:212:CYS:SG	2.45	0.57
1:R:228:SER:O	1:S:128:GLU:HB3	2.05	0.57
2:t:22:GLU:HG2	2:t:45:TYR:HB2	1.85	0.57
1:F:163:LEU:HB2	1:F:197:LEU:HD11	1.87	0.57
1:L:146:VAL:HB	1:L:212:CYS:SG	2.45	0.57
2:o:22:GLU:HG2	2:o:45:TYR:HB2	1.87	0.57
1:F:146:VAL:HB	1:F:212:CYS:SG	2.45	0.56
1:N:163:LEU:HB2	1:N:197:LEU:HD11	1.85	0.56
1:B:146:VAL:HB	1:B:212:CYS:SG	2.44	0.56
1:E:146:VAL:HB	1:E:212:CYS:SG	2.46	0.56
2:a:71:THR:HG22	2:e:70:MET:HE3	1.87	0.56
1:A:187:LYS:HD2	1:B:126:HIS:HB2	1.87	0.56
1:I:146:VAL:HB	1:I:212:CYS:SG	2.45	0.56
1:L:116:VAL:HG21	1:L:174:ILE:HG12	1.88	0.56
1:R:163:LEU:HB2	1:R:197:LEU:HD11	1.88	0.56
1:E:210:HIS:HB2	1:E:213:MET:HE2	1.87	0.55
2:a:70:MET:HE3	2:b:71:THR:HG22	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:n:70:MET:HE3	2:o:71:THR:HG22	1.88	0.55
1:O:210:HIS:HB2	1:O:213:MET:HE2	1.89	0.55
1:J:210:HIS:HB2	1:J:213:MET:HE2	1.89	0.55
1:K:116:VAL:HG11	1:K:174:ILE:HD11	1.90	0.54
1:D:163:LEU:HB2	1:D:197:LEU:HD11	1.89	0.54
1:K:224:LYS:HE2	1:L:134:ASP:OD2	2.08	0.54
1:S:116:VAL:HG13	1:S:170:ARG:HB3	1.89	0.54
1:R:116:VAL:HG13	1:R:170:ARG:HB3	1.90	0.54
1:H:116:VAL:HG13	1:H:170:ARG:HB3	1.88	0.54
1:H:230:MET:HE2	1:H:241:ARG:CG	2.38	0.54
1:A:125:ASP:HA	1:A:160:LYS:HE3	1.90	0.53
1:Q:116:VAL:HG11	1:Q:174:ILE:HD11	1.90	0.53
1:S:146:VAL:HB	1:S:212:CYS:SG	2.47	0.53
2:s:61:GLU:OE1	2:t:82:HIS:NE2	2.36	0.53
1:R:230:MET:HE1	1:R:234:PHE:HD2	1.74	0.53
1:H:146:VAL:HB	1:H:212:CYS:SG	2.48	0.53
2:l:72:GLY:HA3	2:m:73:VAL:HB	1.90	0.53
1:K:163:LEU:HB2	1:K:197:LEU:HD21	1.90	0.53
1:I:116:VAL:HG21	1:I:174:ILE:HG12	1.91	0.53
1:P:120:ALA:HB1	1:P:167:LYS:HG3	1.90	0.53
2:b:72:GLY:HA3	2:c:73:VAL:HB	1.91	0.53
1:K:134:ASP:OD2	1:O:224:LYS:HE2	2.09	0.53
1:Q:146:VAL:HB	1:Q:212:CYS:SG	2.49	0.52
1:Q:124:GLU:HG3	1:Q:126:HIS:H	1.74	0.52
1:R:159:ASN:HB2	1:R:199:PRO:HA	1.91	0.52
1:F:134:ASP:OD2	1:J:224:LYS:HE2	2.08	0.52
1:K:146:VAL:HB	1:K:212:CYS:SG	2.49	0.52
1:P:113:ILE:HD12	1:P:192:ALA:HB1	1.91	0.52
1:P:156:TYR:CE2	1:P:158:PRO:HG3	2.45	0.52
1:R:249:ARG:CZ	1:S:249:ARG:HH22	2.23	0.51
1:S:157:LEU:HD12	1:S:233:VAL:HG21	1.93	0.51
2:i:70:MET:HE3	2:j:71:THR:HG22	1.91	0.51
1:G:59:ARG:HB3	1:G:110:GLN:HG2	1.93	0.51
1:R:230:MET:HE2	1:R:241:ARG:CG	2.40	0.51
2:n:61:GLU:OE1	2:o:82:HIS:NE2	2.43	0.51
2:e:22:GLU:HG2	2:e:45:TYR:HB2	1.92	0.51
2:r:70:MET:HE3	2:s:71:THR:HG22	1.93	0.51
1:D:123:ASP:H	1:H:89:GLN:HE22	1.57	0.51
1:E:82:LEU:HD21	1:F:102:MET:HG3	1.92	0.51
1:G:60:SER:HG	1:G:62:GLU:HG2	1.74	0.51
1:M:210:HIS:HB2	1:M:213:MET:HE2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:116:VAL:CG1	1:N:170:ARG:HB3	2.41	0.50
2:a:82:HIS:NE2	2:e:61:GLU:OE1	2.44	0.50
1:I:157:LEU:HD12	1:I:233:VAL:HG21	1.94	0.50
1:A:183:GLU:O	1:A:187:LYS:HG3	2.11	0.50
1:F:210:HIS:HB2	1:F:213:MET:HE2	1.92	0.50
1:K:116:VAL:HG21	1:K:174:ILE:HG12	1.93	0.50
1:D:117:LEU:HD21	1:D:196:ALA:HB1	1.93	0.50
1:B:126:HIS:CE1	2:a:40:LEU:HD11	2.47	0.50
1:G:116:VAL:HG13	1:G:170:ARG:HB3	1.93	0.50
1:E:116:VAL:HG11	1:E:174:ILE:HD11	1.92	0.50
1:P:68:LEU:HG	1:P:96:TRP:CZ2	2.46	0.50
1:J:105:PHE:CD2	1:J:140:MET:HE3	2.46	0.49
1:G:157:LEU:HD12	1:G:233:VAL:HG21	1.94	0.49
1:M:116:VAL:HG13	1:M:170:ARG:HB3	1.93	0.49
1:G:70:ASN:H	1:G:70:ASN:HD22	1.58	0.49
1:J:116:VAL:HG11	1:J:174:ILE:HD11	1.94	0.49
1:H:157:LEU:HD12	1:H:233:VAL:HG21	1.93	0.49
1:A:116:VAL:HG21	1:A:174:ILE:HG12	1.95	0.49
6:q:212:HOH:O	2:r:18:MET:HB3	2.13	0.49
1:O:146:VAL:HB	1:O:212:CYS:SG	2.53	0.48
1:R:165:LEU:HG	4:R:302:QBQ:C	2.43	0.48
2:p:71:THR:HG22	2:t:70:MET:HE3	1.95	0.48
2:h:70:MET:HE3	2:i:71:THR:HG22	1.93	0.48
2:f:73:VAL:HB	2:j:72:GLY:HA3	1.94	0.48
1:E:165:LEU:HG	4:E:302:QBQ:C	2.43	0.48
1:L:165:LEU:HG	4:L:1101:QBQ:C	2.44	0.48
2:p:72:GLY:HA3	2:q:73:VAL:HB	1.95	0.48
1:S:116:VAL:HG21	1:S:174:ILE:HG12	1.96	0.48
2:a:72:GLY:HA3	2:b:73:VAL:HB	1.94	0.48
2:m:70:MET:HE3	2:n:71:THR:HG22	1.96	0.48
2:q:70:MET:HE3	2:r:71:THR:HG22	1.94	0.48
1:B:156:TYR:OH	1:B:162:VAL:HG22	2.14	0.48
1:D:97:ARG:HE	1:D:97:ARG:HB2	1.48	0.48
1:I:165:LEU:HG	4:I:302:QBQ:C	2.43	0.47
1:J:165:LEU:HG	4:J:302:QBQ:C	2.44	0.47
2:i:54:ARG:NH2	2:j:1:MET:HE3	2.29	0.47
2:i:72:GLY:HA3	2:j:73:VAL:HB	1.97	0.47
2:l:70:MET:HE3	2:m:71:THR:HG22	1.94	0.47
1:B:165:LEU:HG	4:B:302:QBQ:C	2.44	0.47
2:s:70:MET:HE3	2:t:71:THR:HG22	1.97	0.47
2:p:38:ARG:HG3	2:p:44:PHE:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:210:HIS:HB2	1:B:213:MET:HE2	1.95	0.47
1:C:165:LEU:HG	4:C:302:QBQ:C	2.44	0.47
1:H:230:MET:HE1	1:H:234:PHE:HD2	1.80	0.47
1:K:113:ILE:HD12	1:K:192:ALA:HB1	1.95	0.47
1:Q:228:SER:O	1:R:128:GLU:CB	2.60	0.47
1:T:117:LEU:HD11	1:T:196:ALA:HB1	1.96	0.47
1:C:125:ASP:CA	1:C:160:LYS:HE3	2.44	0.47
1:K:93:LYS:NZ	1:P:119:ASP:OD1	2.48	0.47
1:K:165:LEU:HG	4:K:302:QBQ:C	2.45	0.47
1:N:159:ASN:O	1:N:160:LYS:HB2	2.14	0.47
2:s:72:GLY:HA3	2:t:73:VAL:HB	1.96	0.47
1:C:113:ILE:HD11	1:C:196:ALA:HB2	1.97	0.47
1:N:93:LYS:HB2	1:N:97:ARG:CZ	2.44	0.47
1:T:165:LEU:HG	4:T:302:QBQ:C	2.45	0.47
2:f:72:GLY:HA3	2:g:73:VAL:HB	1.96	0.47
1:G:165:LEU:HG	4:G:302:QBQ:C	2.44	0.47
1:C:124:GLU:C	1:C:126:HIS:H	2.23	0.47
1:L:126:HIS:CE1	2:k:40:LEU:HD11	2.49	0.47
2:b:38:ARG:HG3	2:b:44:PHE:O	2.15	0.47
2:g:70:MET:HE3	2:h:71:THR:HG22	1.97	0.47
1:Q:136:ASP:OD1	1:Q:151:LYS:HE2	2.15	0.46
1:N:163:LEU:HB2	1:N:197:LEU:HD21	1.96	0.46
1:A:113:ILE:HD12	1:A:192:ALA:HB1	1.98	0.46
1:H:93:LYS:HB2	1:H:97:ARG:CZ	2.45	0.46
1:M:165:LEU:HG	4:M:1101:QBQ:C	2.45	0.46
1:O:116:VAL:HG11	1:O:174:ILE:HD11	1.98	0.46
2:p:70:MET:HE3	2:q:71:THR:HG22	1.96	0.46
2:t:38:ARG:HG3	2:t:44:PHE:O	2.16	0.46
1:J:116:VAL:HG21	1:J:174:ILE:HG12	1.97	0.46
1:Q:163:LEU:HD13	1:Q:197:LEU:HD11	1.96	0.46
1:A:184:ARG:HA	1:A:187:LYS:HE3	1.97	0.46
2:k:70:MET:HE3	2:l:71:THR:HG22	1.98	0.46
2:n:72:GLY:HA3	2:o:73:VAL:HB	1.97	0.46
2:b:70:MET:HE3	2:c:71:THR:HG22	1.98	0.46
1:F:116:VAL:HG21	1:F:174:ILE:HD11	1.97	0.46
1:K:163:LEU:HB2	1:K:197:LEU:HD11	1.98	0.46
2:a:61:GLU:OE1	2:b:82:HIS:NE2	2.44	0.46
1:A:116:VAL:HG13	1:A:170:ARG:HB3	1.97	0.46
1:E:126:HIS:NE2	1:E:128:GLU:HB2	2.31	0.46
1:H:230:MET:CE	1:H:234:PHE:HB3	2.30	0.46
1:L:179:LEU:HD12	1:S:84:GLU:HG3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:j:38:ARG:HG3	2:j:44:PHE:O	2.16	0.46
1:J:157:LEU:HD12	1:J:233:VAL:HG21	1.98	0.46
1:E:82:LEU:HD11	1:F:102:MET:HE3	1.98	0.45
1:O:215:MET:HG2	1:P:138:PHE:HB3	1.99	0.45
1:R:163:LEU:HB2	1:R:197:LEU:HD21	1.98	0.45
1:H:85:ASN:O	1:H:88:ARG:HG2	2.16	0.45
2:m:38:ARG:HG3	2:m:44:PHE:O	2.16	0.45
1:G:121:ILE:CG2	1:G:161:GLN:HB3	2.46	0.45
1:Q:165:LEU:HG	4:Q:302:QBQ:C	2.46	0.45
1:P:72:ALA:O	1:P:95:PRO:HB3	2.16	0.45
1:S:72:ALA:O	1:S:95:PRO:HB3	2.16	0.45
1:C:166:SER:OG	4:C:302:QBQ:O10	2.26	0.45
2:n:38:ARG:HG3	2:n:44:PHE:O	2.17	0.45
1:B:117:LEU:HD22	1:B:163:LEU:HD11	1.98	0.45
1:F:113:ILE:HD12	1:F:192:ALA:HB1	1.99	0.45
1:P:116:VAL:CG2	1:P:174:ILE:HD11	2.38	0.45
1:S:159:ASN:O	1:S:160:LYS:HB2	2.17	0.45
2:d:38:ARG:HG3	2:d:44:PHE:O	2.17	0.45
2:h:72:GLY:HA3	2:i:73:VAL:HB	1.99	0.45
2:k:38:ARG:HG3	2:k:44:PHE:O	2.16	0.45
1:H:165:LEU:HG	4:H:302:QBQ:C	2.47	0.45
1:R:116:VAL:HG21	1:R:174:ILE:HG12	1.99	0.45
2:r:72:GLY:HA3	2:s:73:VAL:HB	1.99	0.45
2:a:38:ARG:HG3	2:a:44:PHE:O	2.17	0.45
1:K:163:LEU:CB	1:K:197:LEU:HD11	2.46	0.44
2:i:38:ARG:HG3	2:i:44:PHE:O	2.16	0.44
1:B:163:LEU:HD23	1:B:168:LEU:CD2	2.47	0.44
1:R:157:LEU:HD12	1:R:233:VAL:HG21	1.99	0.44
2:d:70:MET:HE3	2:e:71:THR:HG22	1.99	0.44
1:H:218:VAL:CG1	1:I:170:ARG:HG2	2.47	0.44
2:c:38:ARG:HG3	2:c:44:PHE:O	2.18	0.44
2:p:73:VAL:HB	2:t:72:GLY:HA3	1.99	0.44
1:C:93:LYS:HB2	1:C:97:ARG:CZ	2.47	0.44
1:C:221:MET:HG2	6:H:429:HOH:O	2.16	0.44
2:r:38:ARG:HG3	2:r:44:PHE:O	2.17	0.44
1:B:136:ASP:OD1	1:B:151:LYS:HE2	2.18	0.44
1:G:102:MET:HE1	1:G:140:MET:CE	2.48	0.44
2:l:38:ARG:HG3	2:l:44:PHE:O	2.17	0.44
1:M:163:LEU:HB2	1:M:197:LEU:HD21	2.00	0.44
2:g:72:GLY:HA3	2:h:73:VAL:HB	2.00	0.44
1:H:163:LEU:HD12	1:H:164:GLY:H	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:72:ALA:O	1:K:95:PRO:HB3	2.17	0.44
1:E:163:LEU:HD23	1:E:168:LEU:CD2	2.48	0.44
1:E:138:PHE:HB3	1:F:215:MET:HG2	2.00	0.43
2:k:73:VAL:HB	2:o:72:GLY:HA3	1.99	0.43
2:m:72:GLY:HA3	2:n:73:VAL:HB	2.00	0.43
1:K:215:MET:HG2	1:T:138:PHE:HB3	2.01	0.43
1:S:218:VAL:CG1	1:T:170:ARG:HG2	2.48	0.43
1:C:160:LYS:HA	1:C:160:LYS:HD3	1.80	0.43
1:G:136:ASP:OD1	1:G:151:LYS:HE2	2.18	0.43
1:P:163:LEU:HG	1:P:167:LYS:HB2	2.01	0.43
2:d:72:GLY:HA3	2:e:73:VAL:HB	2.01	0.43
2:k:72:GLY:HA3	2:l:73:VAL:HB	2.00	0.43
1:K:116:VAL:HG13	1:K:170:ARG:HB3	2.00	0.43
1:O:93:LYS:HB2	1:O:97:ARG:CZ	2.49	0.43
1:A:72:ALA:O	1:A:95:PRO:HB3	2.19	0.43
1:C:138:PHE:HB3	1:H:215:MET:HG2	2.00	0.43
1:J:93:LYS:HB2	1:J:97:ARG:CZ	2.48	0.43
1:Q:72:ALA:O	1:Q:95:PRO:HB3	2.18	0.43
1:S:165:LEU:HG	4:S:302:QBQ:C	2.48	0.43
2:h:38:ARG:HG3	2:h:44:PHE:O	2.18	0.43
1:A:163:LEU:HD12	1:A:164:GLY:H	1.83	0.43
1:R:93:LYS:HB2	1:R:97:ARG:CZ	2.49	0.43
2:o:38:ARG:HG3	2:o:44:PHE:O	2.19	0.43
1:G:93:LYS:HB2	1:G:97:ARG:CZ	2.48	0.43
1:L:116:VAL:HG13	1:L:170:ARG:HB3	2.01	0.43
2:g:38:ARG:HG3	2:g:44:PHE:O	2.19	0.43
6:h:221:HOH:O	2:i:22:GLU:HG3	2.18	0.43
2:s:38:ARG:HG3	2:s:44:PHE:O	2.18	0.43
1:A:136:ASP:OD1	1:A:151:LYS:HE2	2.18	0.42
1:E:157:LEU:HD12	1:E:233:VAL:HG21	2.01	0.42
1:T:116:VAL:HG11	1:T:174:ILE:HD11	2.01	0.42
2:f:82:HIS:NE2	2:j:61:GLU:OE1	2.49	0.42
1:P:218:VAL:CG1	1:Q:170:ARG:HG2	2.49	0.42
1:T:136:ASP:OD1	1:T:151:LYS:HE2	2.19	0.42
1:F:165:LEU:HG	4:F:302:QBQ:C	2.48	0.42
1:M:163:LEU:CB	1:M:197:LEU:HD11	2.48	0.42
1:N:159:ASN:HB2	1:N:199:PRO:HA	2.02	0.42
1:M:146:VAL:HB	1:M:212:CYS:SG	2.60	0.42
1:P:165:LEU:HG	4:P:302:QBQ:C	2.49	0.42
1:Q:163:LEU:HB2	1:Q:197:LEU:HD11	2.02	0.42
1:Q:218:VAL:CG1	1:R:170:ARG:HG3	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:72:ALA:O	1:D:95:PRO:HB3	2.20	0.42
1:H:72:ALA:O	1:H:95:PRO:HB3	2.20	0.42
1:N:146:VAL:HB	1:N:212:CYS:SG	2.59	0.42
1:R:72:ALA:O	1:R:95:PRO:HB3	2.20	0.42
2:b:61:GLU:OE1	2:c:82:HIS:NE2	2.51	0.42
2:f:38:ARG:HG3	2:f:44:PHE:O	2.19	0.42
1:I:218:VAL:CG1	1:J:170:ARG:HG2	2.50	0.42
1:M:126:HIS:NE2	1:M:128:GLU:HB2	2.35	0.42
2:k:1:MET:HE3	2:k:1:MET:HB3	1.87	0.42
1:C:72:ALA:O	1:C:95:PRO:HB3	2.20	0.42
1:I:72:ALA:O	1:I:95:PRO:HB3	2.20	0.42
1:K:157:LEU:HD12	1:K:233:VAL:HG21	2.01	0.42
1:K:218:VAL:CG1	1:L:170:ARG:HG2	2.49	0.42
2:f:70:MET:HE3	2:g:71:THR:HG22	2.01	0.42
2:q:38:ARG:HG3	2:q:44:PHE:O	2.20	0.42
1:K:117:LEU:HD21	1:K:196:ALA:CB	2.47	0.42
1:M:157:LEU:HD12	1:M:233:VAL:HG21	2.01	0.42
1:N:143:HIS:ND1	1:Q:97:ARG:NH2	2.68	0.42
1:A:187:LYS:CD	1:B:126:HIS:HB2	2.51	0.41
1:J:72:ALA:O	1:J:95:PRO:HB3	2.21	0.41
1:S:228:SER:O	1:T:128:GLU:HB2	2.20	0.41
2:a:66:ARG:HD3	2:a:84:GLU:HG3	2.02	0.41
2:a:73:VAL:HB	2:e:72:GLY:HA3	2.01	0.41
1:J:116:VAL:HG13	1:J:170:ARG:HB3	2.02	0.41
1:B:93:LYS:HB2	1:B:97:ARG:CZ	2.50	0.41
1:E:72:ALA:O	1:E:95:PRO:HB3	2.20	0.41
1:S:163:LEU:HD23	1:S:168:LEU:CD2	2.50	0.41
1:B:221:MET:SD	1:I:138:PHE:HZ	2.43	0.41
1:J:126:HIS:ND1	1:J:128:GLU:OE2	2.53	0.41
1:S:170:ARG:HG2	1:S:170:ARG:HH11	1.85	0.41
1:T:72:ALA:O	1:T:95:PRO:HB3	2.21	0.41
1:T:163:LEU:HD23	1:T:168:LEU:CD2	2.50	0.41
1:F:75:TYR:O	1:F:79:LEU:HG	2.21	0.41
1:K:136:ASP:OD1	1:K:151:LYS:HE2	2.21	0.41
1:Q:116:VAL:HG21	1:Q:174:ILE:HG12	2.02	0.41
1:B:116:VAL:HG13	1:B:170:ARG:HB3	2.01	0.41
1:C:218:VAL:CG1	1:D:170:ARG:HG2	2.51	0.41
1:F:130:VAL:HG11	6:F:405:HOH:O	2.20	0.41
1:G:102:MET:HE1	1:G:140:MET:HE2	2.02	0.41
1:N:72:ALA:O	1:N:95:PRO:HB3	2.21	0.41
1:T:157:LEU:HD12	1:T:233:VAL:HG21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:116:VAL:HG13	1:N:170:ARG:HB3	2.03	0.41
1:I:136:ASP:OD1	1:I:151:LYS:HE2	2.21	0.40
1:O:121:ILE:HG23	1:O:161:GLN:HB3	2.02	0.40
1:R:152:VAL:HG22	1:R:206:VAL:HG22	2.03	0.40
1:C:215:MET:HE3	1:H:138:PHE:HB3	2.04	0.40
2:p:25:ASP:O	2:p:29:MET:HG2	2.21	0.40
1:D:165:LEU:HG	4:D:302:QBP:C	2.52	0.40
1:D:215:MET:HG2	1:G:138:PHE:HB3	2.03	0.40
1:F:136:ASP:OD1	1:F:151:LYS:HE2	2.21	0.40
1:L:157:LEU:HD12	1:L:233:VAL:HG21	2.03	0.40
1:T:157:LEU:HD23	1:T:157:LEU:HA	1.94	0.40
2:h:82:HIS:ND1	2:h:84:GLU:OE1	2.55	0.40
2:o:25:ASP:O	2:o:29:MET:HG2	2.22	0.40
1:O:72:ALA:O	1:O:95:PRO:HB3	2.22	0.40
1:D:126:HIS:NE2	1:D:128:GLU:HB2	2.36	0.40
1:L:136:ASP:OD1	1:L:151:LYS:HE2	2.21	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	185/209 (88%)	183 (99%)	2 (1%)	0	100	100
1	C	188/209 (90%)	185 (98%)	3 (2%)	0	100	100
1	D	191/209 (91%)	187 (98%)	4 (2%)	0	100	100
1	E	190/209 (91%)	187 (98%)	3 (2%)	0	100	100
1	F	186/209 (89%)	182 (98%)	4 (2%)	0	100	100
1	G	185/209 (88%)	184 (100%)	1 (0%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	186/209 (89%)	184 (99%)	2 (1%)	0	100	100
1	I	188/209 (90%)	185 (98%)	3 (2%)	0	100	100
1	J	186/209 (89%)	183 (98%)	3 (2%)	0	100	100
1	K	190/209 (91%)	188 (99%)	2 (1%)	0	100	100
1	L	185/209 (88%)	184 (100%)	1 (0%)	0	100	100
1	M	188/209 (90%)	183 (97%)	5 (3%)	0	100	100
1	N	186/209 (89%)	184 (99%)	1 (0%)	1 (0%)	24	14
1	O	190/209 (91%)	189 (100%)	1 (0%)	0	100	100
1	P	190/209 (91%)	187 (98%)	3 (2%)	0	100	100
1	Q	190/209 (91%)	188 (99%)	2 (1%)	0	100	100
1	R	184/209 (88%)	181 (98%)	3 (2%)	0	100	100
1	S	188/209 (90%)	185 (98%)	3 (2%)	0	100	100
1	T	190/209 (91%)	189 (100%)	1 (0%)	0	100	100
2	a	82/87 (94%)	80 (98%)	2 (2%)	0	100	100
2	b	81/87 (93%)	79 (98%)	2 (2%)	0	100	100
2	c	82/87 (94%)	80 (98%)	2 (2%)	0	100	100
2	d	81/87 (93%)	79 (98%)	2 (2%)	0	100	100
2	e	82/87 (94%)	80 (98%)	2 (2%)	0	100	100
2	f	81/87 (93%)	79 (98%)	2 (2%)	0	100	100
2	g	82/87 (94%)	80 (98%)	2 (2%)	0	100	100
2	h	82/87 (94%)	80 (98%)	2 (2%)	0	100	100
2	i	81/87 (93%)	79 (98%)	2 (2%)	0	100	100
2	j	82/87 (94%)	80 (98%)	2 (2%)	0	100	100
2	k	82/87 (94%)	80 (98%)	2 (2%)	0	100	100
2	l	81/87 (93%)	79 (98%)	2 (2%)	0	100	100
2	m	82/87 (94%)	80 (98%)	2 (2%)	0	100	100
2	n	81/87 (93%)	79 (98%)	2 (2%)	0	100	100
2	o	82/87 (94%)	80 (98%)	2 (2%)	0	100	100
2	p	81/87 (93%)	79 (98%)	2 (2%)	0	100	100
2	q	82/87 (94%)	80 (98%)	2 (2%)	0	100	100
2	r	82/87 (94%)	80 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	s	81/87 (93%)	79 (98%)	2 (2%)	0	100	100
2	t	82/87 (94%)	80 (98%)	2 (2%)	0	100	100
All	All	5388/5920 (91%)	5297 (98%)	90 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	N	160	LYS

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	27
1	B	164/181 (91%)	162 (99%)	2 (1%)	63	58
1	C	167/181 (92%)	164 (98%)	3 (2%)	51	46
1	D	170/181 (94%)	166 (98%)	4 (2%)	43	35
1	E	169/181 (93%)	167 (99%)	2 (1%)	63	58
1	F	167/181 (92%)	162 (97%)	5 (3%)	36	27
1	G	166/181 (92%)	159 (96%)	7 (4%)	26	15
1	H	167/181 (92%)	165 (99%)	2 (1%)	63	58
1	I	167/181 (92%)	165 (99%)	2 (1%)	63	58
1	J	167/181 (92%)	161 (96%)	6 (4%)	31	20
1	K	169/181 (93%)	167 (99%)	2 (1%)	63	58
1	L	164/181 (91%)	162 (99%)	2 (1%)	63	58
1	M	167/181 (92%)	165 (99%)	2 (1%)	63	58
1	N	167/181 (92%)	164 (98%)	3 (2%)	51	46
1	O	169/181 (93%)	165 (98%)	4 (2%)	43	35
1	P	169/181 (93%)	163 (96%)	6 (4%)	31	20

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Q	169/181 (93%)	160 (95%)	9 (5%)	20	9
1	R	165/181 (91%)	163 (99%)	2 (1%)	63	58
1	S	167/181 (92%)	165 (99%)	2 (1%)	63	58
1	T	168/181 (93%)	162 (96%)	6 (4%)	31	20
2	a	75/77 (97%)	74 (99%)	1 (1%)	61	57
2	b	74/77 (96%)	74 (100%)	0	100	100
2	c	75/77 (97%)	75 (100%)	0	100	100
2	d	74/77 (96%)	73 (99%)	1 (1%)	59	54
2	e	75/77 (97%)	74 (99%)	1 (1%)	61	57
2	f	74/77 (96%)	73 (99%)	1 (1%)	59	54
2	g	75/77 (97%)	73 (97%)	2 (3%)	39	31
2	h	75/77 (97%)	74 (99%)	1 (1%)	61	57
2	i	74/77 (96%)	74 (100%)	0	100	100
2	j	75/77 (97%)	74 (99%)	1 (1%)	61	57
2	k	75/77 (97%)	73 (97%)	2 (3%)	39	31
2	l	74/77 (96%)	72 (97%)	2 (3%)	39	31
2	m	75/77 (97%)	73 (97%)	2 (3%)	39	31
2	n	74/77 (96%)	73 (99%)	1 (1%)	59	54
2	o	75/77 (97%)	75 (100%)	0	100	100
2	p	74/77 (96%)	74 (100%)	0	100	100
2	q	75/77 (97%)	74 (99%)	1 (1%)	61	57
2	r	75/77 (97%)	74 (99%)	1 (1%)	61	57
2	s	74/77 (96%)	74 (100%)	0	100	100
2	t	75/77 (97%)	73 (97%)	2 (3%)	39	31
All	All	4839/5160 (94%)	4744 (98%)	95 (2%)	48	42

All (95) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61	GLU
1	A	157	LEU
1	A	160	LYS
1	A	187	LYS
1	A	207	GLU

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Mol	Chain	Res	Type
1	B	162	VAL
1	B	214	VAL
1	C	187	LYS
1	C	214	VAL
1	C	221	MET
1	D	119	ASP
1	D	157	LEU
1	D	181	VAL
1	D	214	VAL
1	E	214	VAL
1	E	221	MET
1	F	61	GLU
1	F	128	GLU
1	F	162	VAL
1	F	166	SER
1	F	214	VAL
1	G	70	ASN
1	G	87	GLN
1	G	159	ASN
1	G	162	VAL
1	G	207	GLU
1	G	214	VAL
1	G	221	MET
1	H	61	GLU
1	H	221	MET
1	I	162	VAL
1	I	221	MET
1	J	62	GLU
1	J	126	HIS
1	J	128	GLU
1	J	141	CYS
1	J	162	VAL
1	J	221	MET
1	K	61	GLU
1	K	221	MET
1	L	214	VAL
1	L	221	MET
1	M	214	VAL
1	M	221	MET
1	N	117	LEU
1	N	214	VAL
1	N	221	MET

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Mol	Chain	Res	Type
1	O	157	LEU
1	O	160	LYS
1	O	214	VAL
1	O	221	MET
1	P	61	GLU
1	P	68	LEU
1	P	114	SER
1	P	162	VAL
1	P	181	VAL
1	P	214	VAL
1	Q	96	TRP
1	Q	125	ASP
1	Q	126	HIS
1	Q	160	LYS
1	Q	161	GLN
1	Q	197	LEU
1	Q	207	GLU
1	Q	214	VAL
1	Q	221	MET
1	R	61	GLU
1	R	221	MET
1	S	162	VAL
1	S	221	MET
1	T	60	SER
1	T	126	HIS
1	T	128	GLU
1	T	141	CYS
1	T	218	VAL
1	T	221	MET
2	a	84	GLU
2	d	1	MET
2	e	5	LEU
2	f	4	LEU
2	g	4	LEU
2	g	31	HIS
2	h	84	GLU
2	j	4	LEU
2	k	1	MET
2	k	84	GLU
2	l	66	ARG
2	l	83	LYS
2	m	22	GLU

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Mol	Chain	Res	Type
2	m	84	GLU
2	n	4	LEU
2	q	4	LEU
2	r	84	GLU
2	t	1	MET
2	t	84	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	ASN
1	B	64	ASN
1	B	70	ASN
1	B	89	GLN
1	B	110	GLN
1	B	161	GLN
1	C	70	ASN
1	D	70	ASN
1	D	143	HIS
1	D	161	GLN
1	E	70	ASN
1	E	143	HIS
1	F	70	ASN
1	G	64	ASN
1	G	70	ASN
1	H	70	ASN
1	H	89	GLN
1	I	64	ASN
1	I	70	ASN
1	I	110	GLN
1	J	70	ASN
1	K	70	ASN
1	L	64	ASN
1	L	70	ASN
1	L	110	GLN
1	L	126	HIS
1	M	70	ASN
1	M	159	ASN
1	N	70	ASN
1	O	70	ASN
1	P	70	ASN
1	P	126	HIS

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Mol	Chain	Res	Type
1	Q	70	ASN
1	Q	126	HIS
1	R	70	ASN
1	S	64	ASN
1	S	70	ASN
1	S	110	GLN
1	S	143	HIS
1	T	67	ASN
1	T	70	ASN
1	T	159	ASN
1	T	180	GLN
1	T	188	GLN
2	k	75	GLN
2	q	31	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 60 ligands modelled in this entry, 20 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	F	302	-	33,34,34	1.03	2 (6%)	47,54,54	0.89	2 (4%)
4	QBQ	R	302	-	33,34,34	1.14	3 (9%)	47,54,54	0.83	1 (2%)
5	PHE	c	101	-	11,12,12	0.62	0	11,15,15	0.25	0
5	PHE	i	101	-	11,12,12	0.69	0	11,15,15	0.39	0
4	QBQ	E	302	-	33,34,34	1.22	3 (9%)	47,54,54	0.88	2 (4%)
5	PHE	o	101	-	11,12,12	0.75	1 (9%)	11,15,15	0.50	0
4	QBQ	L	1101	-	33,34,34	1.35	6 (18%)	47,54,54	0.95	3 (6%)
4	QBQ	I	302	-	33,34,34	1.09	3 (9%)	47,54,54	0.89	3 (6%)
5	PHE	f	101	-	11,12,12	0.72	0	11,15,15	0.34	0
5	PHE	l	101	-	11,12,12	0.67	0	11,15,15	0.45	0
5	PHE	e	101	-	11,12,12	0.69	0	11,15,15	0.38	0
4	QBQ	Q	302	-	33,34,34	1.10	4 (12%)	47,54,54	0.90	1 (2%)
4	QBQ	T	302	-	33,34,34	1.25	3 (9%)	47,54,54	0.86	1 (2%)
5	PHE	n	101	-	11,12,12	0.73	0	11,15,15	0.37	0
4	QBQ	P	302	-	33,34,34	0.99	2 (6%)	47,54,54	0.81	1 (2%)
4	QBQ	C	302	-	33,34,34	1.16	4 (12%)	47,54,54	0.92	2 (4%)
4	QBQ	M	1101	-	33,34,34	1.20	4 (12%)	47,54,54	0.80	1 (2%)
4	QBQ	D	302	-	33,34,34	1.36	7 (21%)	47,54,54	0.91	3 (6%)
5	PHE	s	101	-	11,12,12	0.70	0	11,15,15	0.29	0
4	QBQ	B	302	-	33,34,34	1.16	4 (12%)	47,54,54	0.93	3 (6%)
4	QBQ	N	1101	-	33,34,34	1.10	3 (9%)	47,54,54	0.74	0
5	PHE	h	101	-	11,12,12	0.73	0	11,15,15	0.29	0
5	PHE	m	101	-	11,12,12	0.69	0	11,15,15	0.25	0
4	QBQ	K	302	-	33,34,34	1.15	3 (9%)	47,54,54	0.89	1 (2%)
5	PHE	b	101	-	11,12,12	0.66	0	11,15,15	0.32	0
5	PHE	f	102	-	11,12,12	0.81	0	11,15,15	0.14	0
4	QBQ	S	302	-	33,34,34	1.17	3 (9%)	47,54,54	0.85	2 (4%)
5	PHE	p	101	-	11,12,12	0.61	0	11,15,15	0.26	0
5	PHE	a	101	-	11,12,12	0.67	0	11,15,15	0.27	0
5	PHE	k	101	-	11,12,12	0.77	0	11,15,15	0.37	0
5	PHE	q	101	-	11,12,12	0.92	1 (9%)	11,15,15	0.75	1 (9%)
5	PHE	r	101	-	11,12,12	0.65	0	11,15,15	0.31	0
4	QBQ	J	302	-	33,34,34	1.23	3 (9%)	47,54,54	0.89	2 (4%)
5	PHE	g	101	-	11,12,12	0.72	0	11,15,15	0.31	0
4	QBQ	O	302	-	33,34,34	0.54	0	47,54,54	0.87	2 (4%)
4	QBQ	G	302	-	33,34,34	1.17	3 (9%)	47,54,54	0.88	1 (2%)
4	QBQ	A	302	-	33,34,34	1.17	3 (9%)	47,54,54	0.84	1 (2%)
5	PHE	t	101	-	11,12,12	0.65	0	11,15,15	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	QBQ	H	302	-	33,34,34	1.24	5 (15%)	47,54,54	0.88	1 (2%)
5	PHE	d	101	-	11,12,12	0.68	0	11,15,15	0.39	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	F	302	-	-	5/22/38/38	0/3/3/3
4	QBQ	R	302	-	-	4/22/38/38	0/3/3/3
5	PHE	c	101	-	-	0/8/8/8	0/1/1/1
5	PHE	i	101	-	-	0/8/8/8	0/1/1/1
4	QBQ	E	302	-	-	6/22/38/38	0/3/3/3
5	PHE	o	101	-	-	0/8/8/8	0/1/1/1
4	QBQ	L	1101	-	-	4/22/38/38	0/3/3/3
4	QBQ	I	302	-	-	2/22/38/38	0/3/3/3
5	PHE	f	101	-	-	0/8/8/8	0/1/1/1
5	PHE	l	101	-	-	0/8/8/8	0/1/1/1
5	PHE	e	101	-	-	0/8/8/8	0/1/1/1
4	QBQ	Q	302	-	-	3/22/38/38	0/3/3/3
4	QBQ	T	302	-	-	4/22/38/38	0/3/3/3
5	PHE	n	101	-	-	0/8/8/8	0/1/1/1
4	QBQ	P	302	-	-	8/22/38/38	0/3/3/3
4	QBQ	C	302	-	-	1/22/38/38	0/3/3/3
4	QBQ	M	1101	-	-	2/22/38/38	0/3/3/3
4	QBQ	D	302	-	-	3/22/38/38	0/3/3/3
5	PHE	s	101	-	-	0/8/8/8	0/1/1/1
4	QBQ	B	302	-	-	3/22/38/38	0/3/3/3
4	QBQ	N	1101	-	-	5/22/38/38	0/3/3/3
5	PHE	h	101	-	-	0/8/8/8	0/1/1/1
5	PHE	m	101	-	-	0/8/8/8	0/1/1/1
4	QBQ	K	302	-	-	2/22/38/38	0/3/3/3
5	PHE	b	101	-	-	0/8/8/8	0/1/1/1
5	PHE	f	102	-	-	0/8/8/8	0/1/1/1
4	QBQ	S	302	-	-	5/22/38/38	0/3/3/3
5	PHE	p	101	-	-	1/8/8/8	0/1/1/1
5	PHE	a	101	-	-	0/8/8/8	0/1/1/1
5	PHE	k	101	-	-	0/8/8/8	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PHE	q	101	-	-	1/8/8/8	0/1/1/1
5	PHE	r	101	-	-	0/8/8/8	0/1/1/1
4	QBQ	J	302	-	-	4/22/38/38	0/3/3/3
5	PHE	g	101	-	-	0/8/8/8	0/1/1/1
4	QBQ	O	302	-	-	3/22/38/38	0/3/3/3
4	QBQ	G	302	-	-	3/22/38/38	0/3/3/3
4	QBQ	A	302	-	-	3/22/38/38	0/3/3/3
5	PHE	t	101	-	-	1/8/8/8	0/1/1/1
4	QBQ	H	302	-	-	3/22/38/38	0/3/3/3
5	PHE	d	101	-	-	0/8/8/8	0/1/1/1

All (70) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	T	302	QBQ	P2-O8	-4.59	1.37	1.54
4	J	302	QBQ	P2-O8	-4.51	1.38	1.54
4	L	1101	QBQ	P2-O8	-4.32	1.38	1.54
4	D	302	QBQ	P2-O8	-4.22	1.39	1.54
4	E	302	QBQ	P2-O8	-4.14	1.39	1.54
4	M	1101	QBQ	P2-O8	-4.07	1.39	1.54
4	S	302	QBQ	P2-O8	-4.05	1.39	1.54
4	N	1101	QBQ	P2-O8	-4.02	1.39	1.54
4	K	302	QBQ	P2-O8	-3.97	1.40	1.54
4	G	302	QBQ	P2-O8	-3.89	1.40	1.54
4	R	302	QBQ	P2-O8	-3.82	1.40	1.54
4	H	302	QBQ	P2-O8	-3.76	1.40	1.54
4	A	302	QBQ	P2-O8	-3.51	1.41	1.54
4	B	302	QBQ	P2-O8	-3.50	1.41	1.54
4	I	302	QBQ	P2-O8	-3.44	1.42	1.54
4	Q	302	QBQ	P2-O8	-3.43	1.42	1.54
4	C	302	QBQ	P2-O8	-3.28	1.42	1.54
4	F	302	QBQ	P2-O8	-3.04	1.43	1.54
4	P	302	QBQ	P2-O8	-3.04	1.43	1.54
4	L	1101	QBQ	P2-O10	-2.89	1.41	1.50
4	L	1101	QBQ	P-O2	-2.82	1.42	1.55
4	D	302	QBQ	P2-O10	-2.69	1.42	1.50
5	q	101	PHE	OXT-C	-2.66	1.22	1.30
4	P	302	QBQ	C2-C1	-2.58	1.38	1.45
4	J	302	QBQ	P2-O9	-2.51	1.45	1.54
4	R	302	QBQ	C2-C1	-2.48	1.38	1.45
4	A	302	QBQ	C2-C1	-2.45	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	1101	QBQ	C2-C1	-2.43	1.39	1.45
4	D	302	QBQ	P1-O5	-2.43	1.44	1.55
4	L	1101	QBQ	P2-O9	-2.41	1.45	1.54
4	B	302	QBQ	C2-C1	-2.37	1.39	1.45
4	C	302	QBQ	P1-O5	-2.36	1.44	1.55
4	K	302	QBQ	C2-C1	-2.35	1.39	1.45
4	Q	302	QBQ	C2-C1	-2.35	1.39	1.45
4	T	302	QBQ	C2-C1	-2.34	1.39	1.45
4	F	302	QBQ	C2-C1	-2.32	1.39	1.45
4	D	302	QBQ	C2-C1	-2.30	1.39	1.45
4	J	302	QBQ	C2-C1	-2.30	1.39	1.45
4	Q	302	QBQ	P1-O5	-2.30	1.44	1.55
4	G	302	QBQ	C2-C1	-2.29	1.39	1.45
4	H	302	QBQ	C2-C1	-2.29	1.39	1.45
4	C	302	QBQ	P2-O9	-2.29	1.46	1.54
4	E	302	QBQ	C2-C1	-2.27	1.39	1.45
4	H	302	QBQ	P1-O5	-2.27	1.44	1.55
4	C	302	QBQ	C2-C1	-2.27	1.39	1.45
4	N	1101	QBQ	C2-C1	-2.25	1.39	1.45
4	B	302	QBQ	P2-O9	-2.24	1.46	1.54
4	H	302	QBQ	P-O2	-2.22	1.45	1.55
4	E	302	QBQ	P1-O5	-2.21	1.45	1.55
4	T	302	QBQ	P2-O9	-2.21	1.46	1.54
4	G	302	QBQ	P-O2	-2.21	1.45	1.55
4	I	302	QBQ	C2-C1	-2.19	1.39	1.45
4	S	302	QBQ	C2-C1	-2.17	1.39	1.45
5	o	101	PHE	OXT-C	-2.17	1.23	1.30
4	B	302	QBQ	P-O3	-2.17	1.43	1.50
4	S	302	QBQ	P2-O9	-2.16	1.46	1.54
4	D	302	QBQ	P2-O9	-2.15	1.46	1.54
4	M	1101	QBQ	P-O2	-2.15	1.45	1.55
4	R	302	QBQ	P1-O5	-2.15	1.45	1.55
4	L	1101	QBQ	C2-C1	-2.14	1.39	1.45
4	D	302	QBQ	P1-O6	-2.12	1.43	1.50
4	M	1101	QBQ	P2-O9	-2.09	1.47	1.54
4	H	302	QBQ	P1-O6	-2.08	1.43	1.50
4	A	302	QBQ	P2-O9	-2.07	1.47	1.54
4	I	302	QBQ	P2-O9	-2.06	1.47	1.54
4	L	1101	QBQ	P-O3	-2.02	1.43	1.50
4	K	302	QBQ	P2-O9	-2.02	1.47	1.54
4	D	302	QBQ	P-O2	-2.02	1.46	1.55
4	N	1101	QBQ	P2-O9	-2.01	1.47	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	Q	302	QBQ	P2-O9	-2.00	1.47	1.54

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	O	302	QBQ	O-C5-N2	2.85	114.81	108.36
4	Q	302	QBQ	C6-O-C5	-2.52	103.90	109.47
4	G	302	QBQ	C10-C2-C1	-2.41	116.86	118.35
5	q	101	PHE	OXT-C-O	-2.41	118.61	124.08
4	L	1101	QBQ	O8-P2-O7	2.38	112.62	104.64
4	L	1101	QBQ	C10-C2-C1	-2.33	116.91	118.35
4	M	1101	QBQ	C6-O-C5	-2.25	104.50	109.47
4	D	302	QBQ	C10-C2-C1	-2.25	116.96	118.35
4	B	302	QBQ	C6-O-C5	-2.22	104.57	109.47
4	O	302	QBQ	C9-C5-N2	2.21	119.41	113.25
4	C	302	QBQ	C10-C2-C1	-2.21	116.98	118.35
4	D	302	QBQ	O8-P2-O7	2.20	112.02	104.64
4	F	302	QBQ	C10-C2-C1	-2.19	116.99	118.35
4	R	302	QBQ	C10-C2-C1	-2.19	116.99	118.35
4	A	302	QBQ	C6-O-C5	-2.19	104.63	109.47
4	D	302	QBQ	C6-O-C5	-2.19	104.64	109.47
4	E	302	QBQ	O8-P2-O7	2.17	111.92	104.64
4	B	302	QBQ	C10-C2-C1	-2.16	117.01	118.35
4	P	302	QBQ	C6-O-C5	-2.16	104.70	109.47
4	L	1101	QBQ	C6-O-C5	-2.15	104.72	109.47
4	B	302	QBQ	O8-P2-O7	2.15	111.84	104.64
4	F	302	QBQ	C6-O-C5	-2.14	104.73	109.47
4	I	302	QBQ	C10-C2-C1	-2.13	117.03	118.35
4	K	302	QBQ	C6-O-C5	-2.11	104.80	109.47
4	I	302	QBQ	C6-O-C5	-2.11	104.81	109.47
4	E	302	QBQ	C10-C2-C1	-2.11	117.05	118.35
4	S	302	QBQ	O8-P2-O7	2.09	111.65	104.64
4	I	302	QBQ	O8-P2-O7	2.06	111.54	104.64
4	H	302	QBQ	C6-O-C5	-2.05	104.95	109.47
4	C	302	QBQ	C6-O-C5	-2.04	104.96	109.47
4	S	302	QBQ	C6-O-C5	-2.04	104.96	109.47
4	J	302	QBQ	C10-C2-C1	-2.04	117.09	118.35
4	T	302	QBQ	C10-C2-C1	-2.04	117.09	118.35
4	J	302	QBQ	C6-O-C5	-2.02	105.00	109.47

There are no chirality outliers.

All (76) 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	D	302	QBQ	P1-O7-P2-O8
4	E	302	QBQ	C7-O1-P-O4
4	F	302	QBQ	P1-O7-P2-O8
4	G	302	QBQ	P1-O7-P2-O8
4	H	302	QBQ	P1-O7-P2-O8
4	I	302	QBQ	P1-O7-P2-O8
4	J	302	QBQ	P1-O7-P2-O8
4	K	302	QBQ	P1-O7-P2-O9
4	M	1101	QBQ	P1-O7-P2-O8
4	O	302	QBQ	P1-O7-P2-O9
4	P	302	QBQ	P1-O7-P2-O8
4	P	302	QBQ	C7-O1-P-O3
4	P	302	QBQ	C7-O1-P-O4
4	Q	302	QBQ	P1-O7-P2-O8
4	T	302	QBQ	P1-O7-P2-O9
4	E	302	QBQ	P1-O7-P2-O10
4	S	302	QBQ	P1-O4-P-O3
4	T	302	QBQ	P1-O4-P-O3
4	A	302	QBQ	P1-O7-P2-O10
4	S	302	QBQ	P1-O7-P2-O10
4	E	302	QBQ	P1-O7-P2-O8
4	N	1101	QBQ	P1-O7-P2-O9
4	R	302	QBQ	P1-O4-P-O2
4	P	302	QBQ	C7-O1-P-O2
4	R	302	QBQ	C7-O1-P-O3
4	S	302	QBQ	C7-O1-P-O3
4	T	302	QBQ	C7-O1-P-O3
4	L	1101	QBQ	P1-O7-P2-O10
4	L	1101	QBQ	P1-O4-P-O3
4	L	1101	QBQ	P1-O4-P-O2
4	O	302	QBQ	P1-O4-P-O3
4	O	302	QBQ	P1-O4-P-O2
4	P	302	QBQ	P1-O4-P-O3
4	P	302	QBQ	P1-O4-P-O2
4	P	302	QBQ	O-C6-C7-O1
4	B	302	QBQ	P1-O7-P2-O10
4	G	302	QBQ	P1-O7-P2-O10
4	H	302	QBQ	P1-O7-P2-O10
4	I	302	QBQ	P1-O7-P2-O10
4	E	302	QBQ	P1-O4-P-O2
4	F	302	QBQ	P1-O4-P-O3

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Mol	Chain	Res	Type	Atoms
4	C	302	QBQ	P1-O7-P2-O10
4	D	302	QBQ	P1-O7-P2-O10
4	F	302	QBQ	P1-O7-P2-O10
4	J	302	QBQ	P1-O7-P2-O10
4	F	302	QBQ	P1-O7-P2-O9
4	J	302	QBQ	P1-O7-P2-O9
4	N	1101	QBQ	P1-O7-P2-O8
4	P	302	QBQ	P1-O7-P2-O9
4	R	302	QBQ	P1-O7-P2-O9
4	S	302	QBQ	P1-O7-P2-O8
4	E	302	QBQ	P1-O4-P-O3
4	F	302	QBQ	P1-O4-P-O2
4	N	1101	QBQ	P1-O4-P-O2
4	R	302	QBQ	P1-O4-P-O3
4	S	302	QBQ	P1-O4-P-O2
4	T	302	QBQ	P1-O4-P-O2
4	N	1101	QBQ	C9-C5-N2-C4
4	E	302	QBQ	O-C6-C7-O1
5	q	101	PHE	OXT-C-CA-N
4	A	302	QBQ	P1-O4-P-O2
4	B	302	QBQ	P1-O4-P-O2
4	D	302	QBQ	P1-O4-P-O2
4	J	302	QBQ	P1-O4-P-O2
4	K	302	QBQ	P1-O4-P-O2
4	Q	302	QBQ	P1-O4-P-O2
4	G	302	QBQ	O-C6-C7-O1
4	H	302	QBQ	O-C6-C7-O1
4	L	1101	QBQ	O-C6-C7-O1
4	M	1101	QBQ	O-C6-C7-O1
4	N	1101	QBQ	O-C6-C7-O1
4	Q	302	QBQ	O-C6-C7-O1
5	p	101	PHE	OXT-C-CA-N
5	t	101	PHE	OXT-C-CA-N

There are no ring outliers.

17 monomers are involved in 18 short contacts:

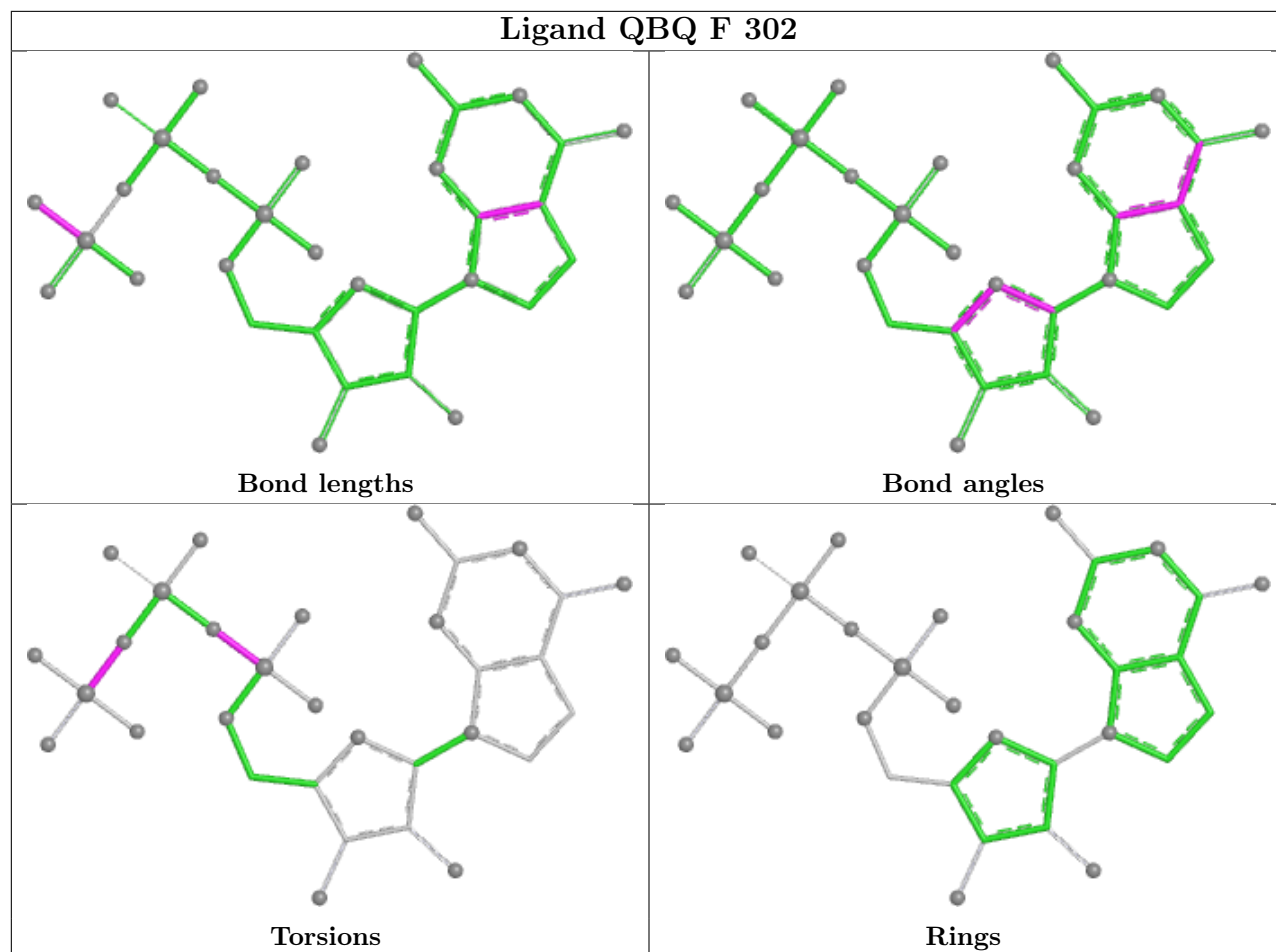
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	302	QBQ	1	0
4	R	302	QBQ	1	0
4	E	302	QBQ	1	0
4	L	1101	QBQ	1	0

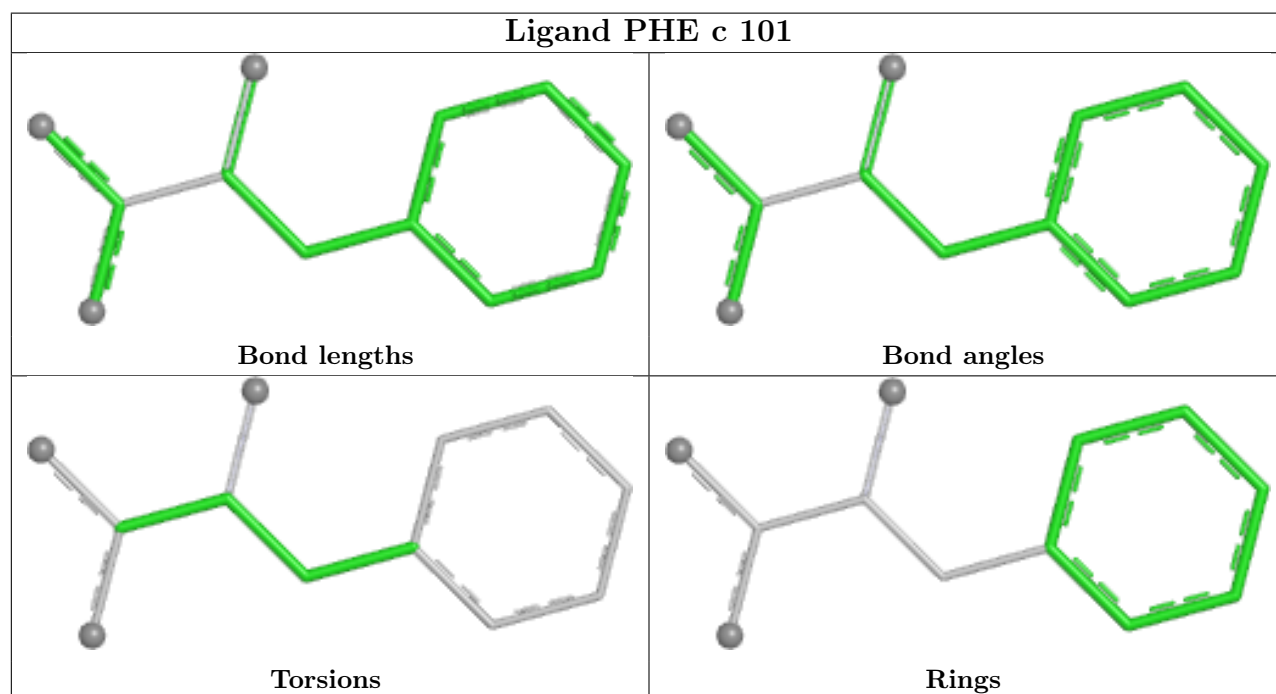
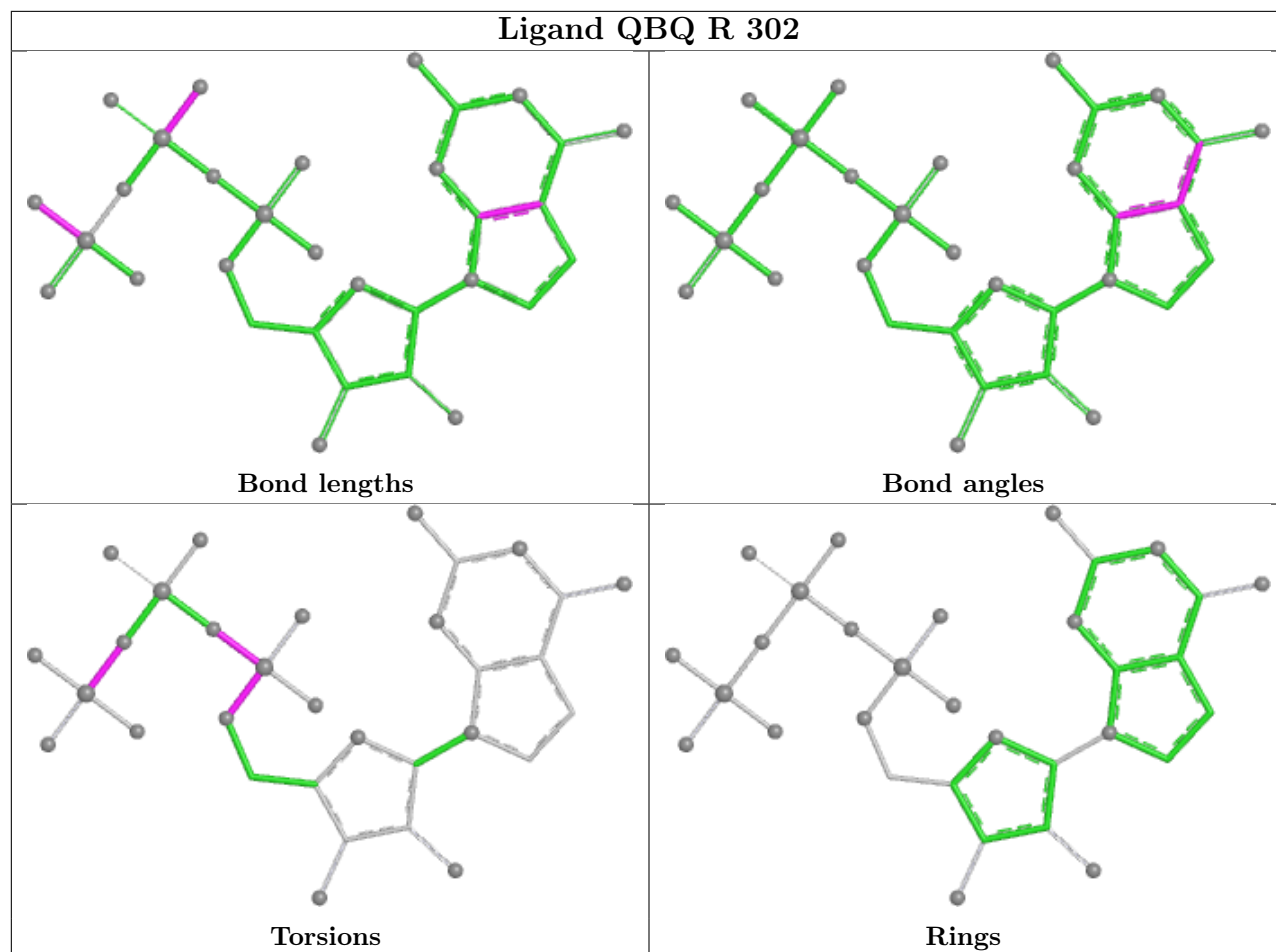
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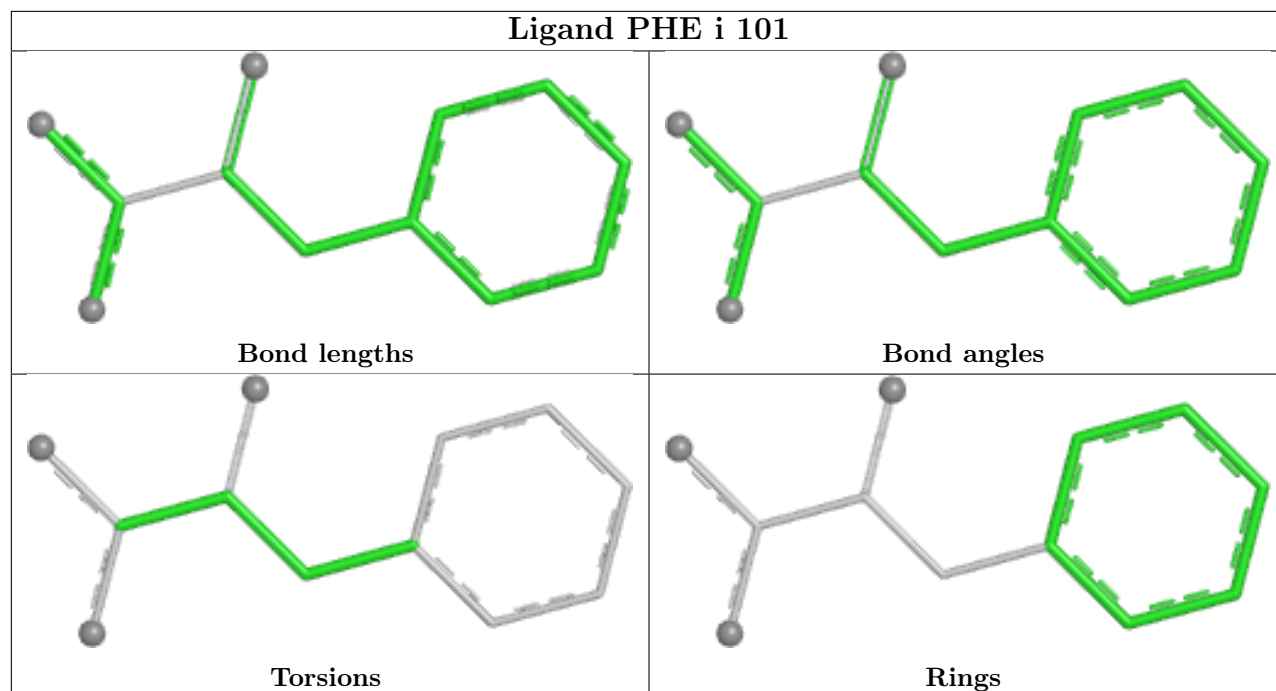
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	I	302	QBQ	1	0
4	Q	302	QBQ	1	0
4	T	302	QBQ	1	0
4	P	302	QBQ	1	0
4	C	302	QBQ	2	0
4	M	1101	QBQ	1	0
4	D	302	QBQ	1	0
4	B	302	QBQ	1	0
4	K	302	QBQ	1	0
4	S	302	QBQ	1	0
4	J	302	QBQ	1	0
4	G	302	QBQ	1	0
4	H	302	QBQ	1	0

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

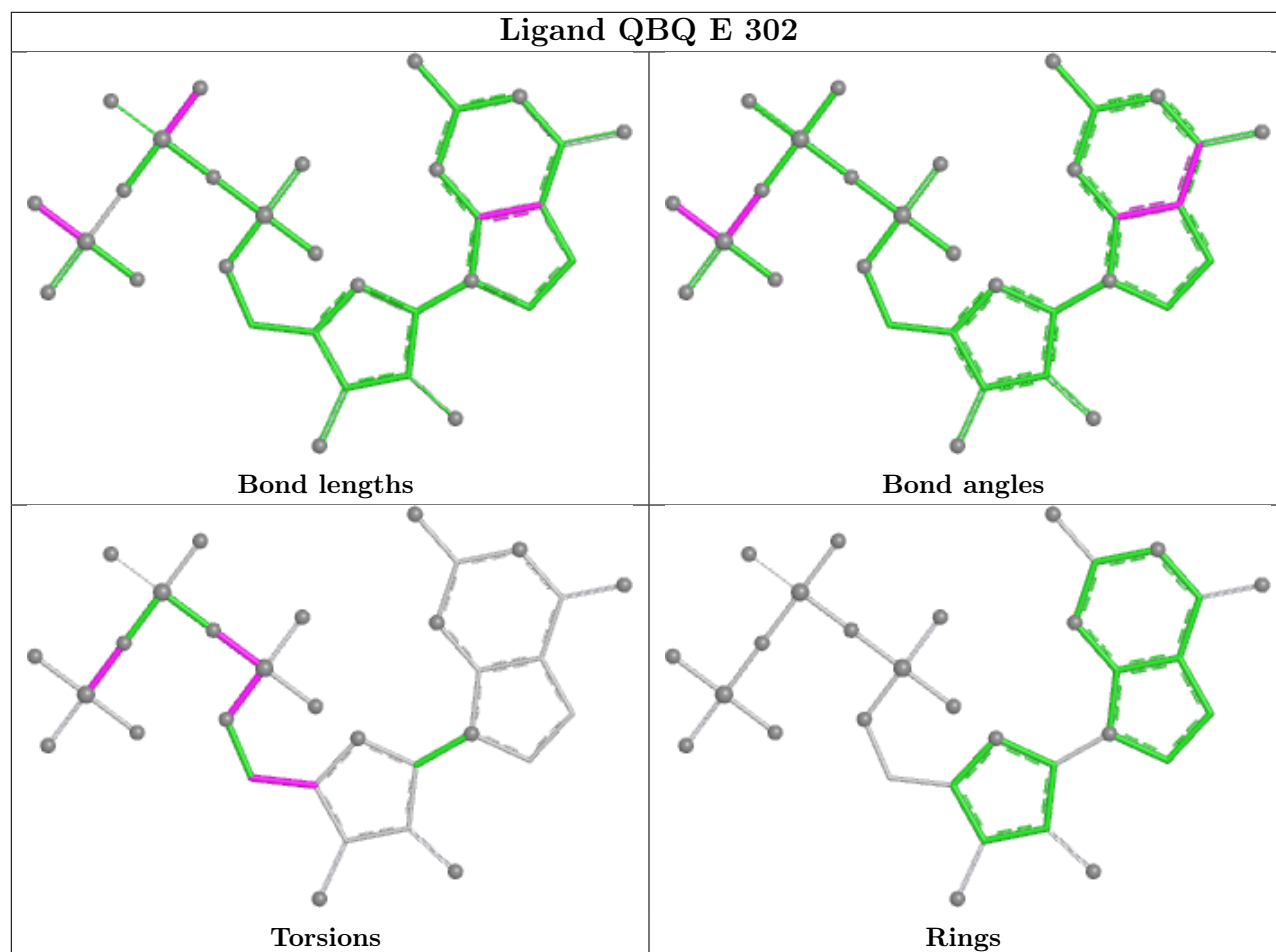




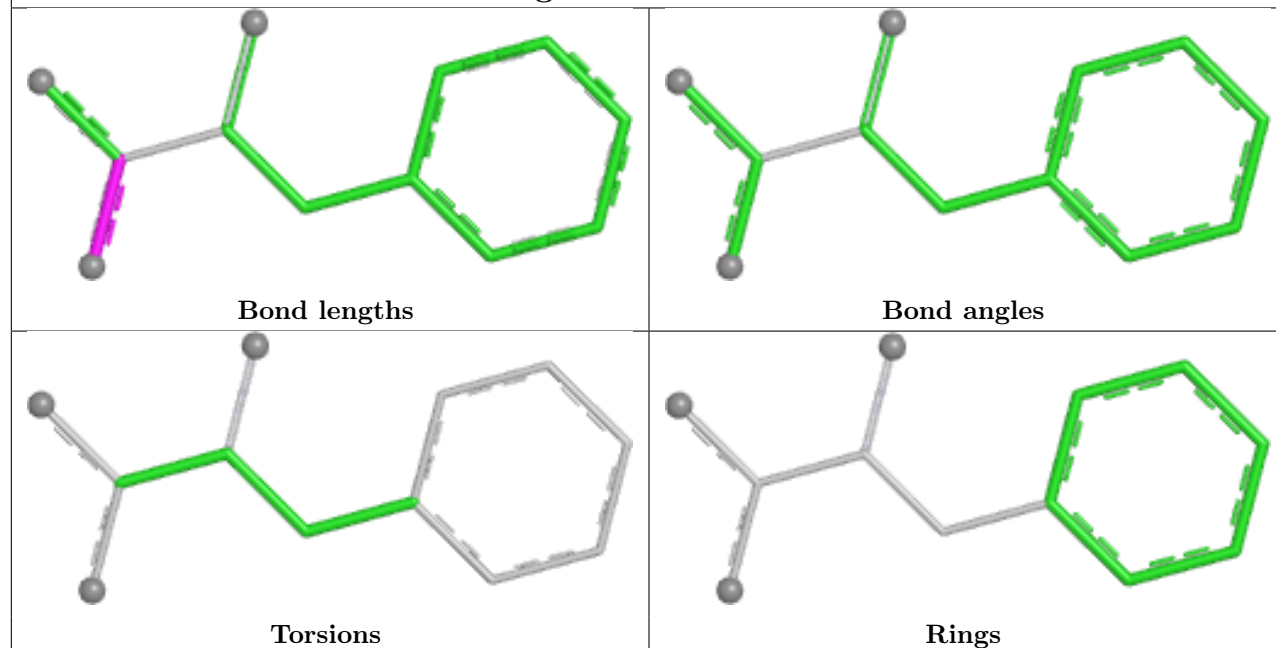
Ligand PHE i 101



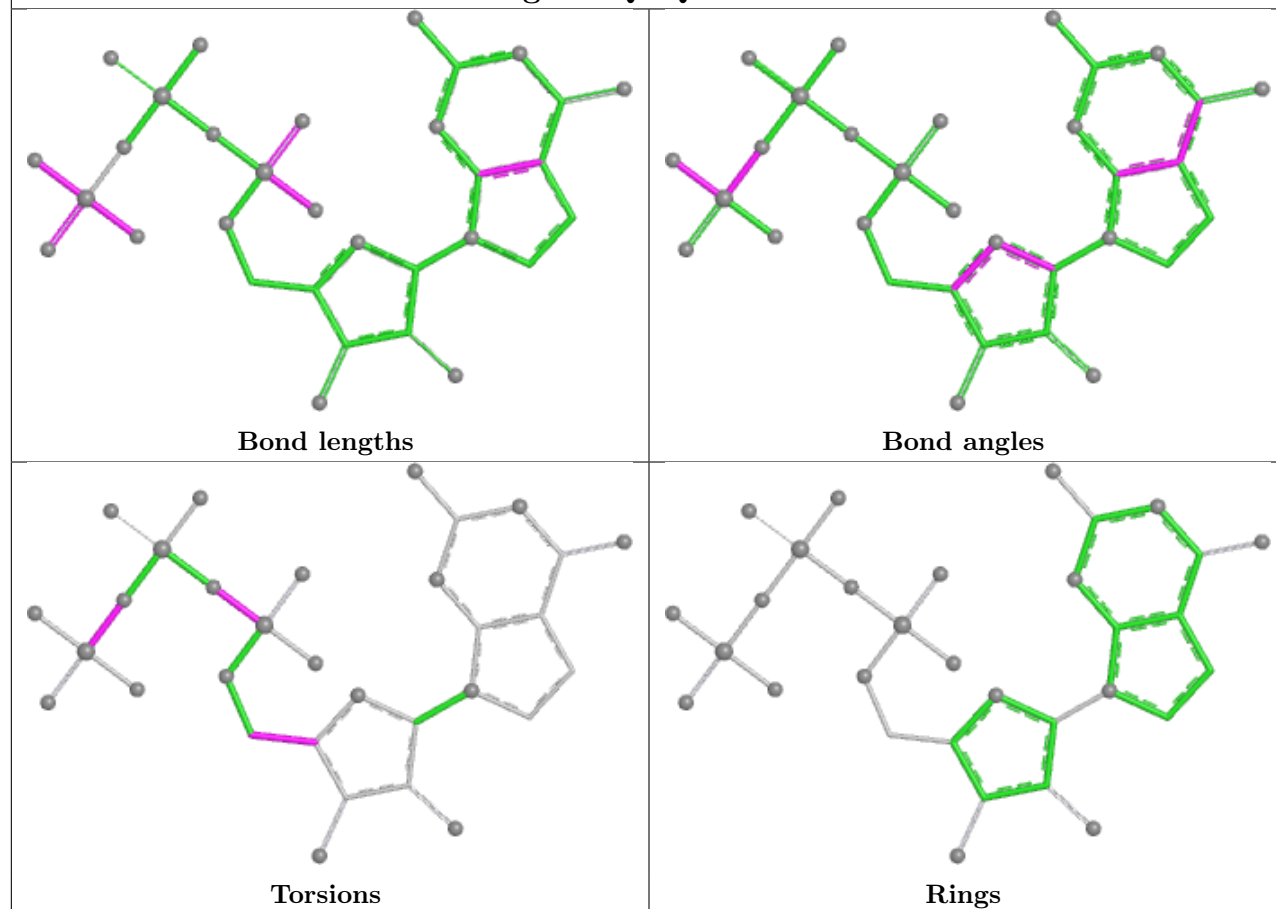
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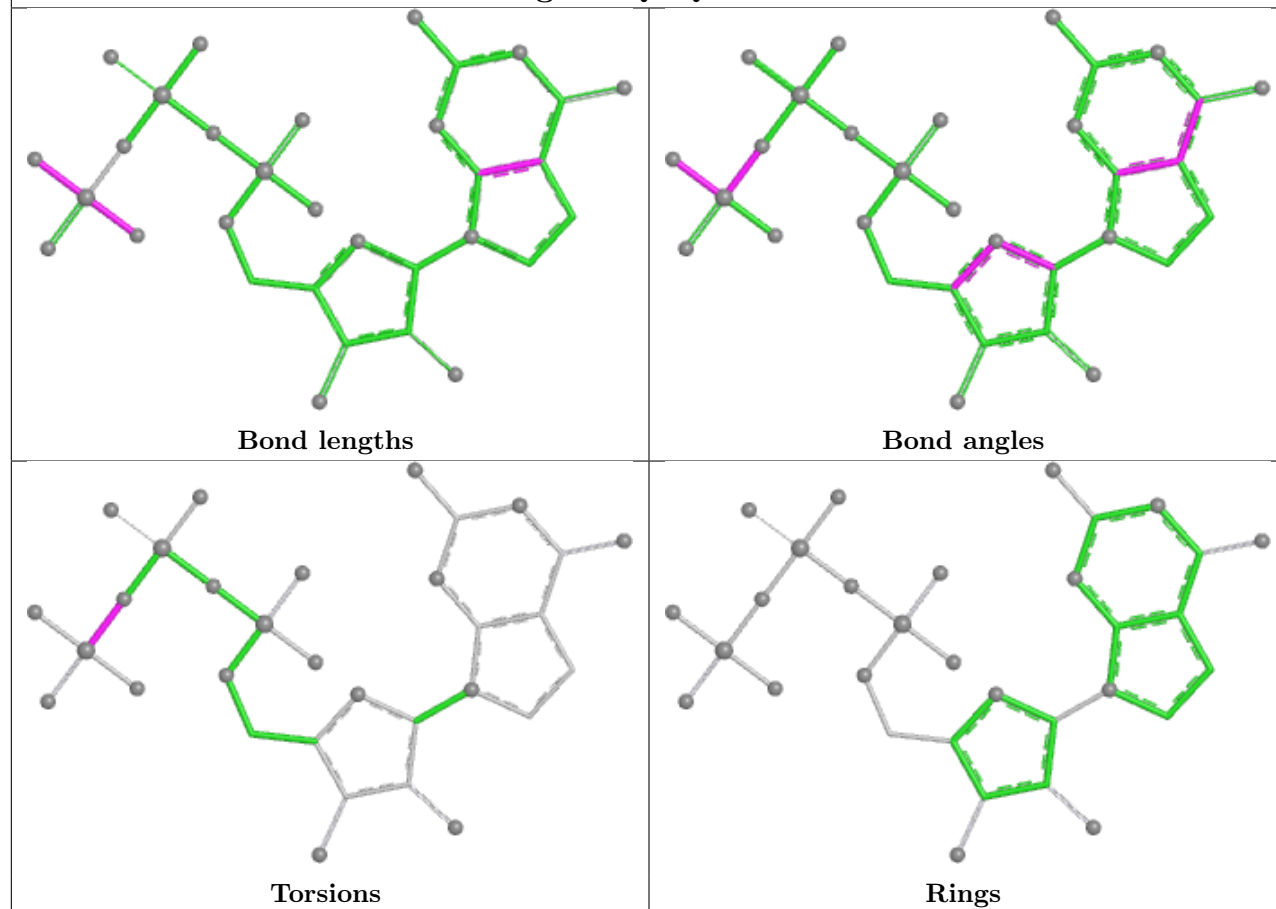
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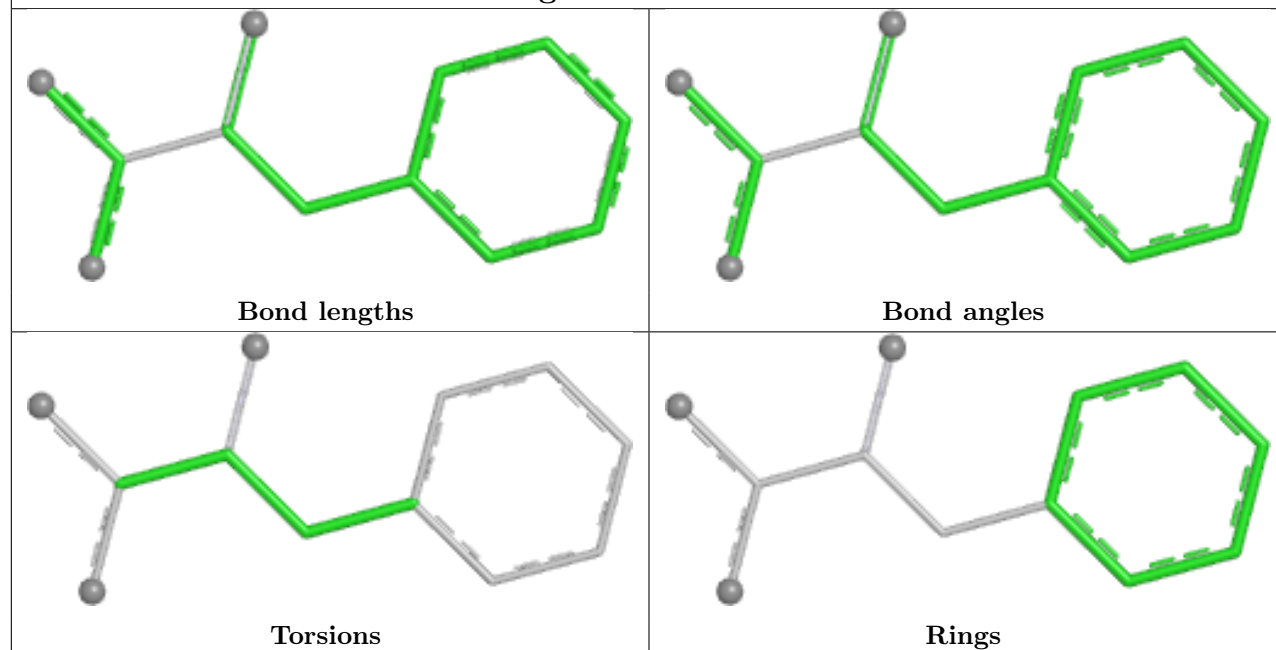
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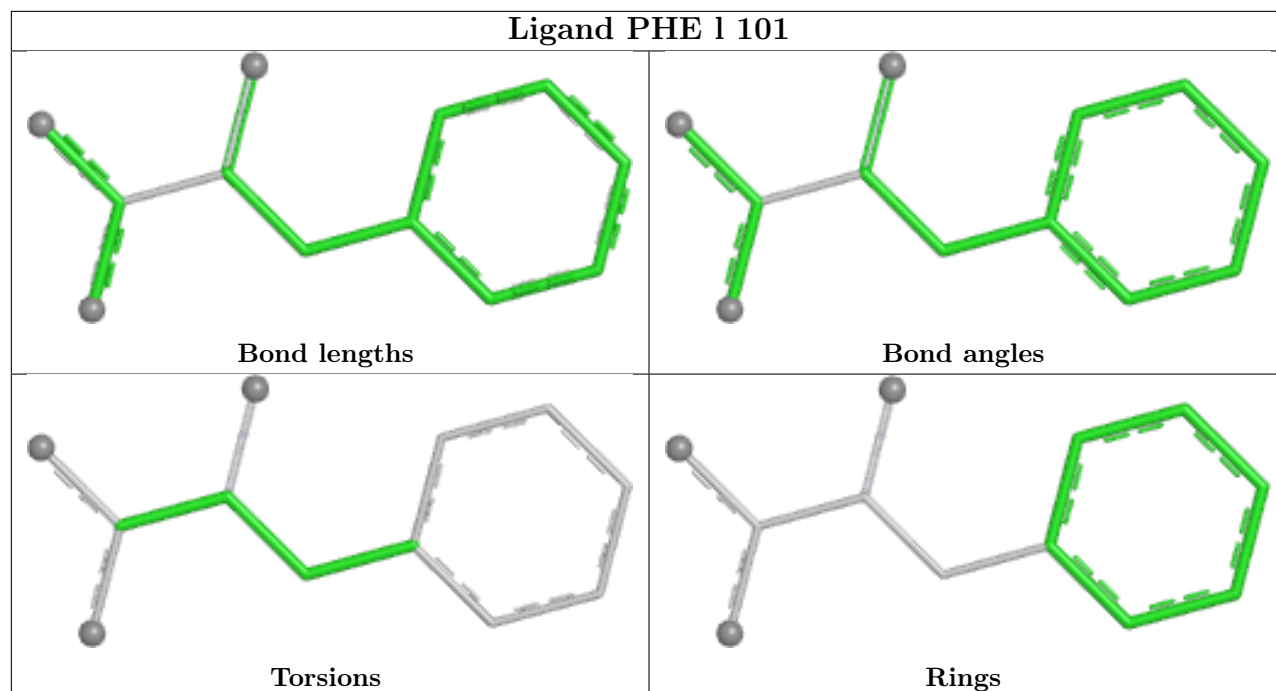
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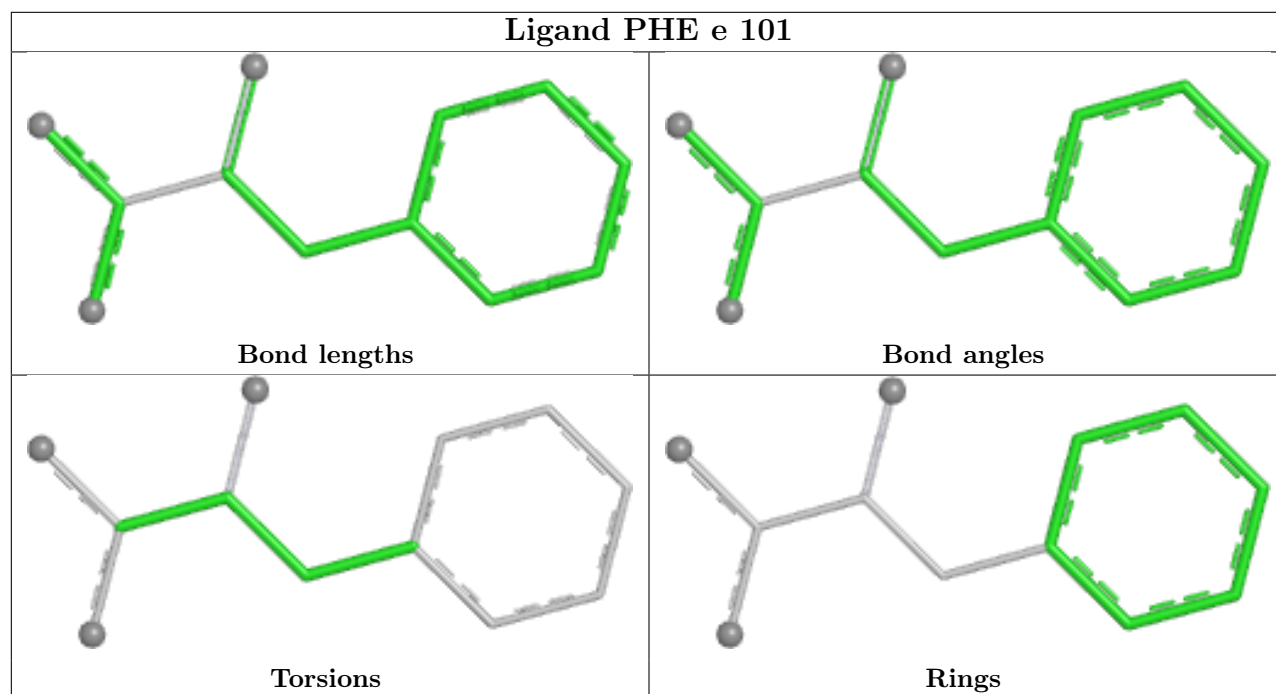
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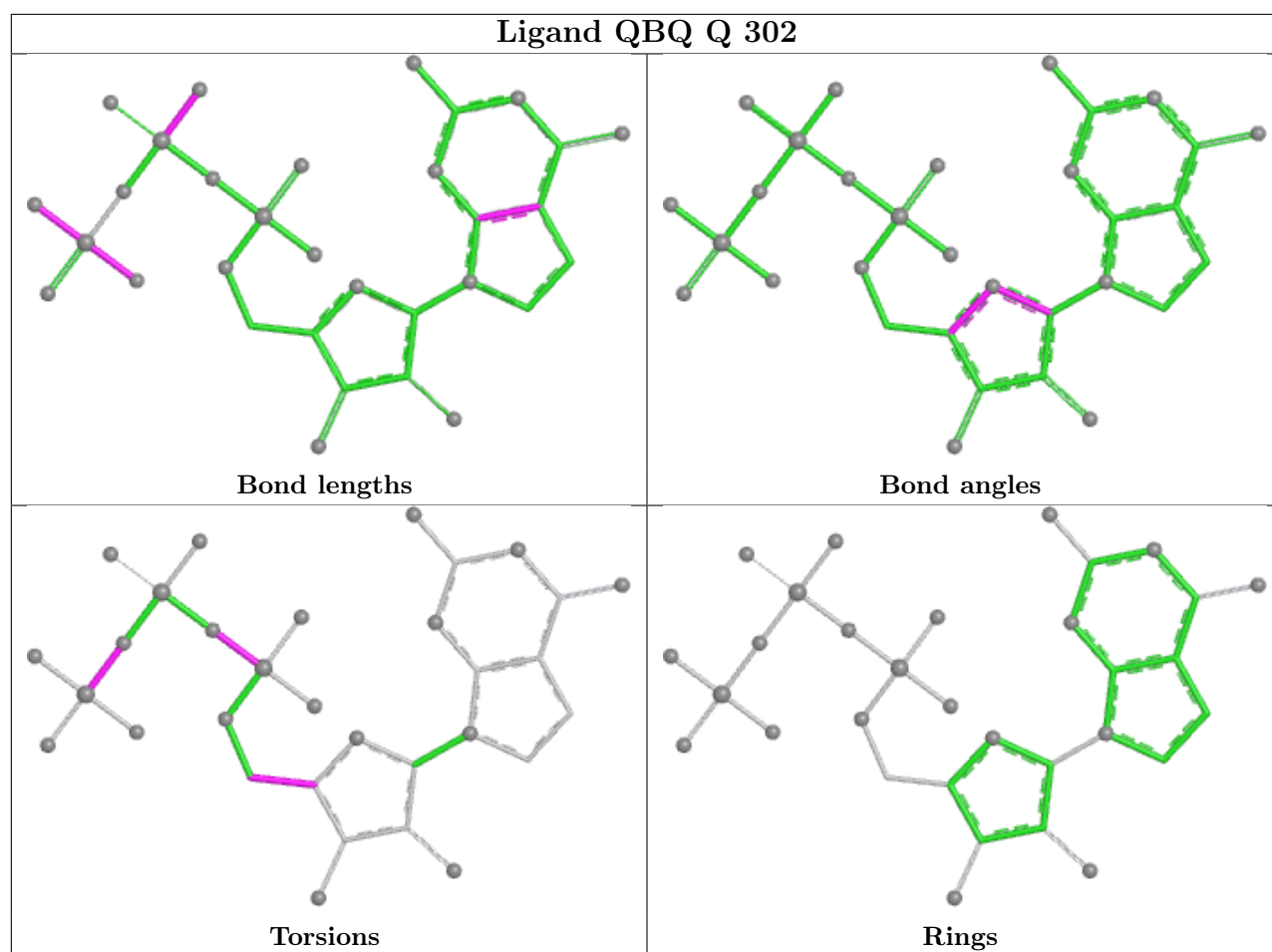


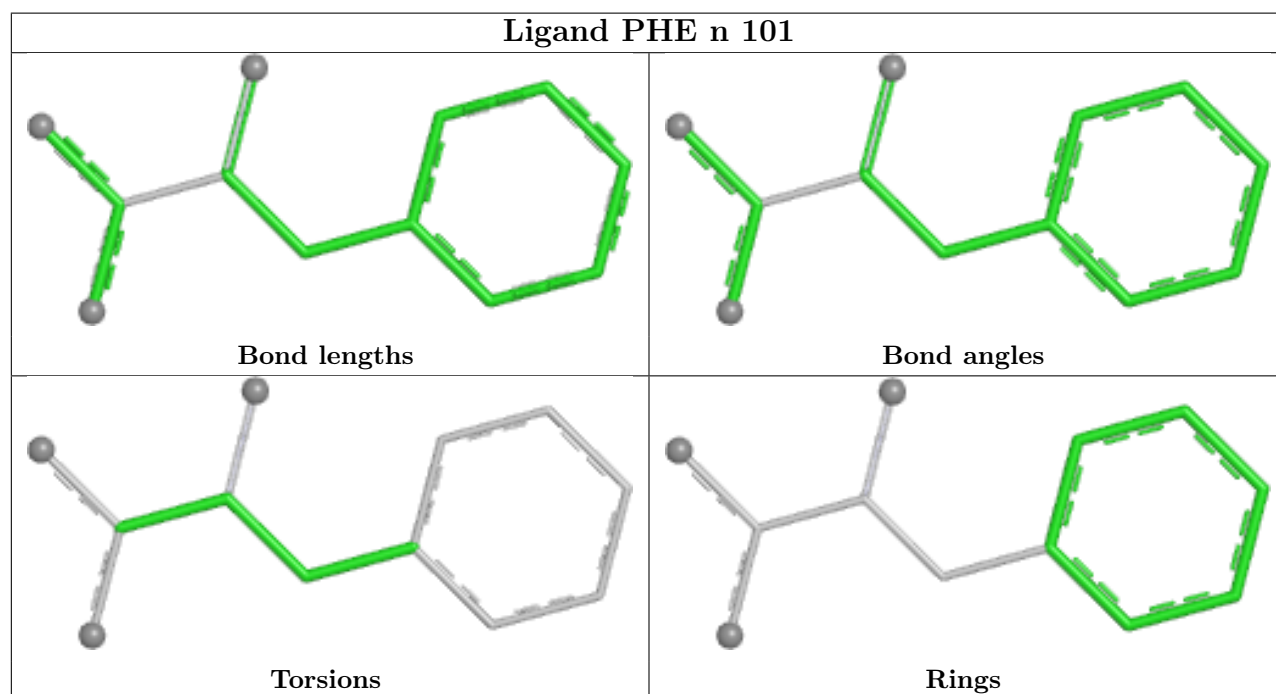
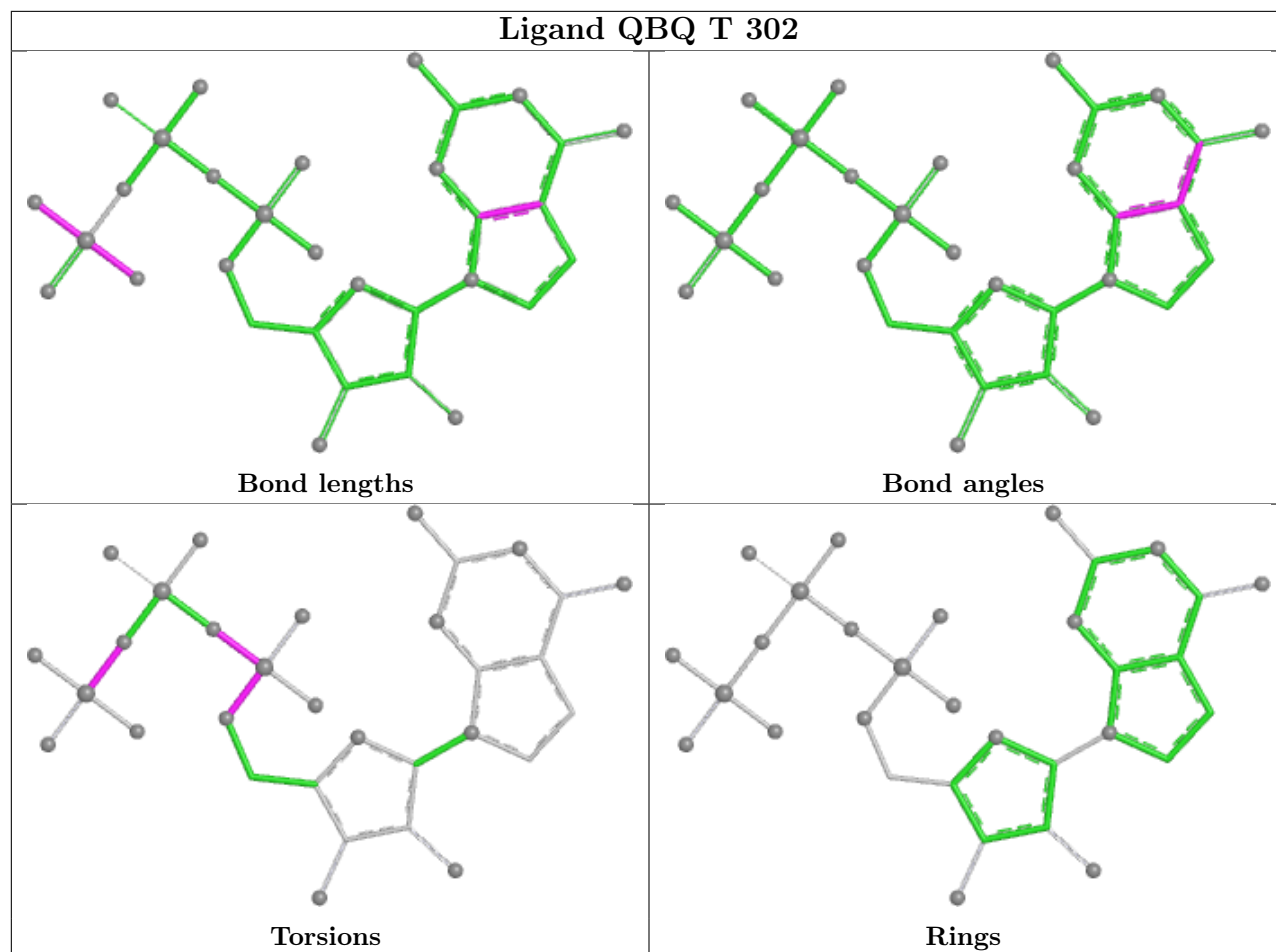
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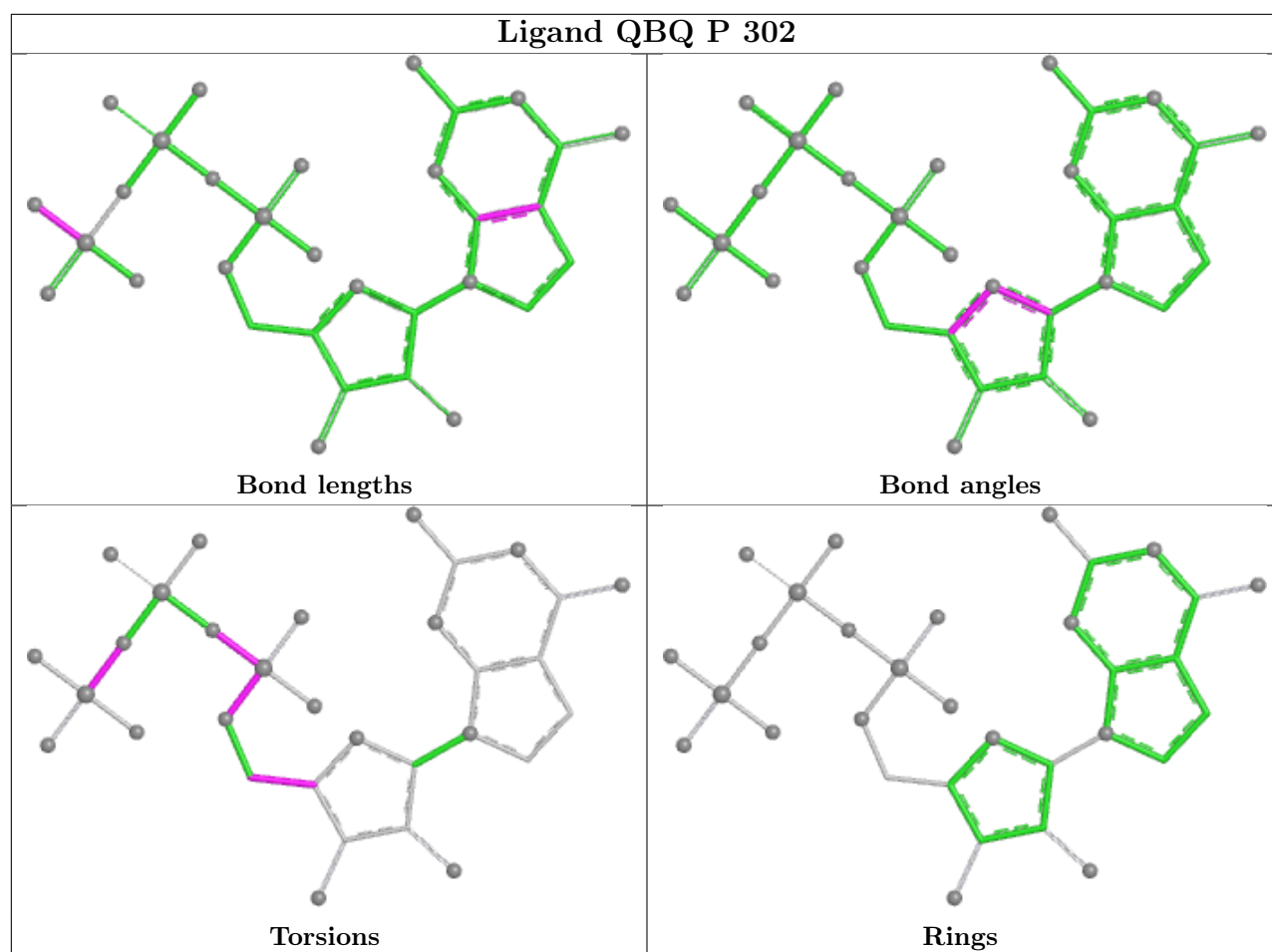


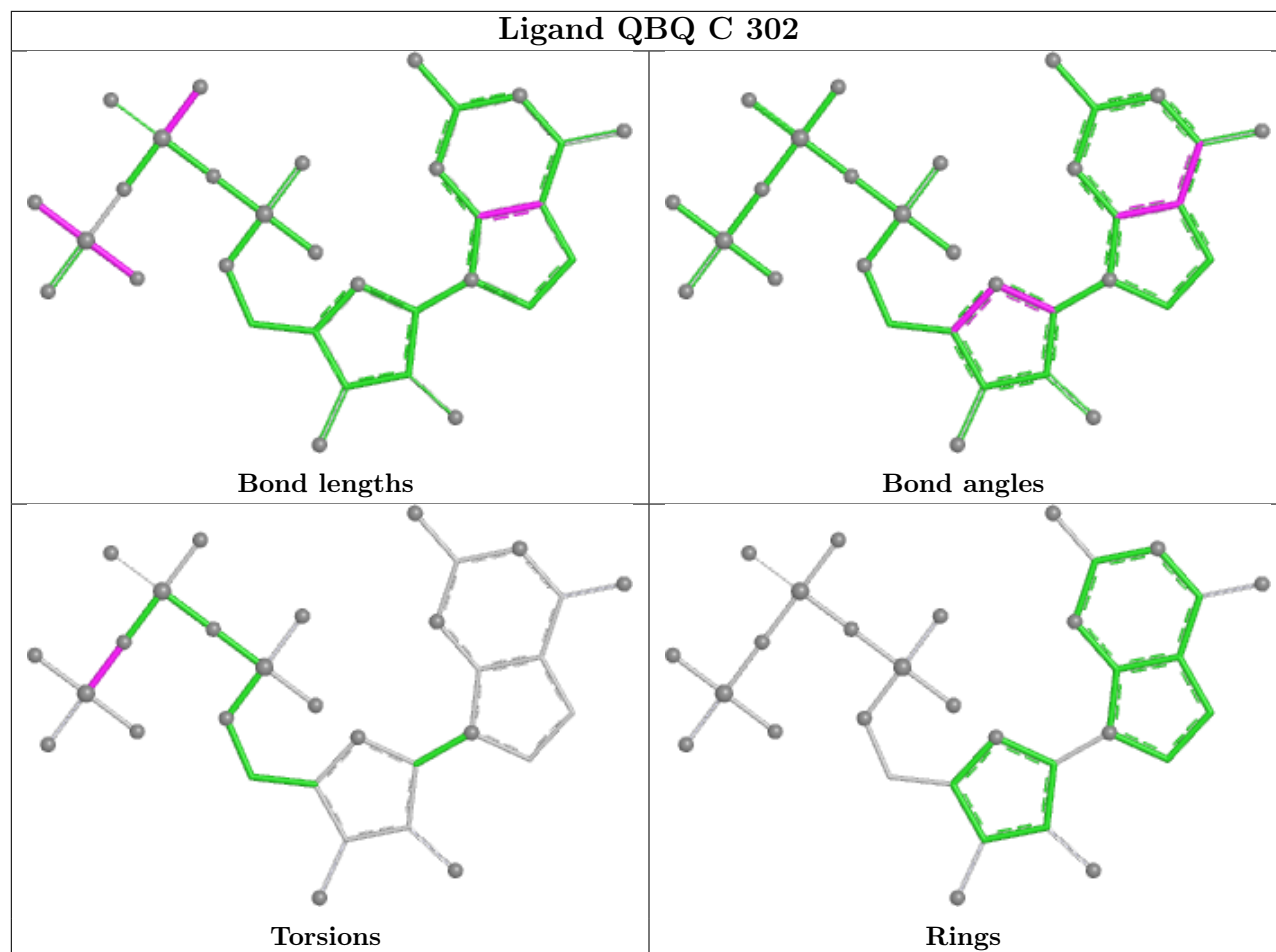
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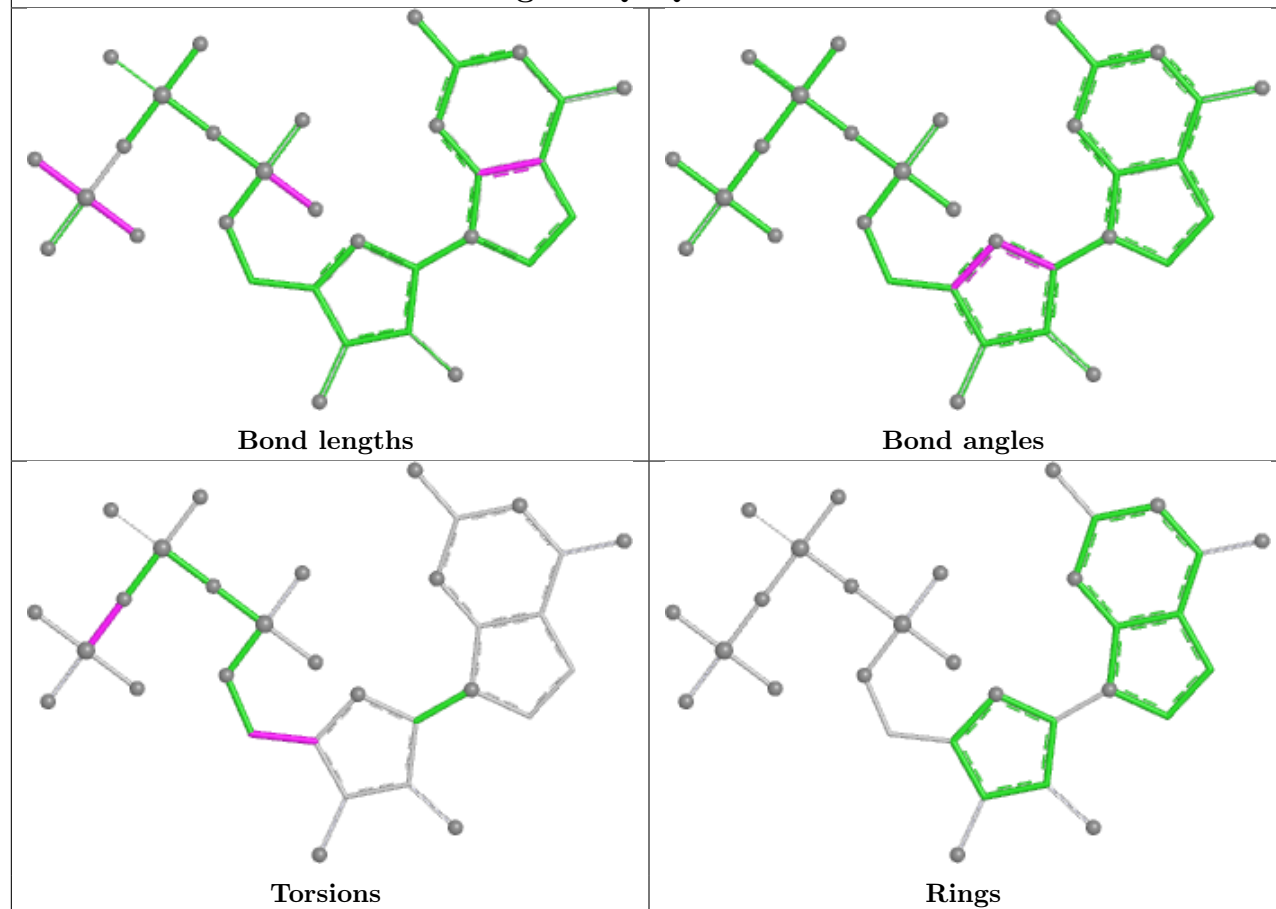


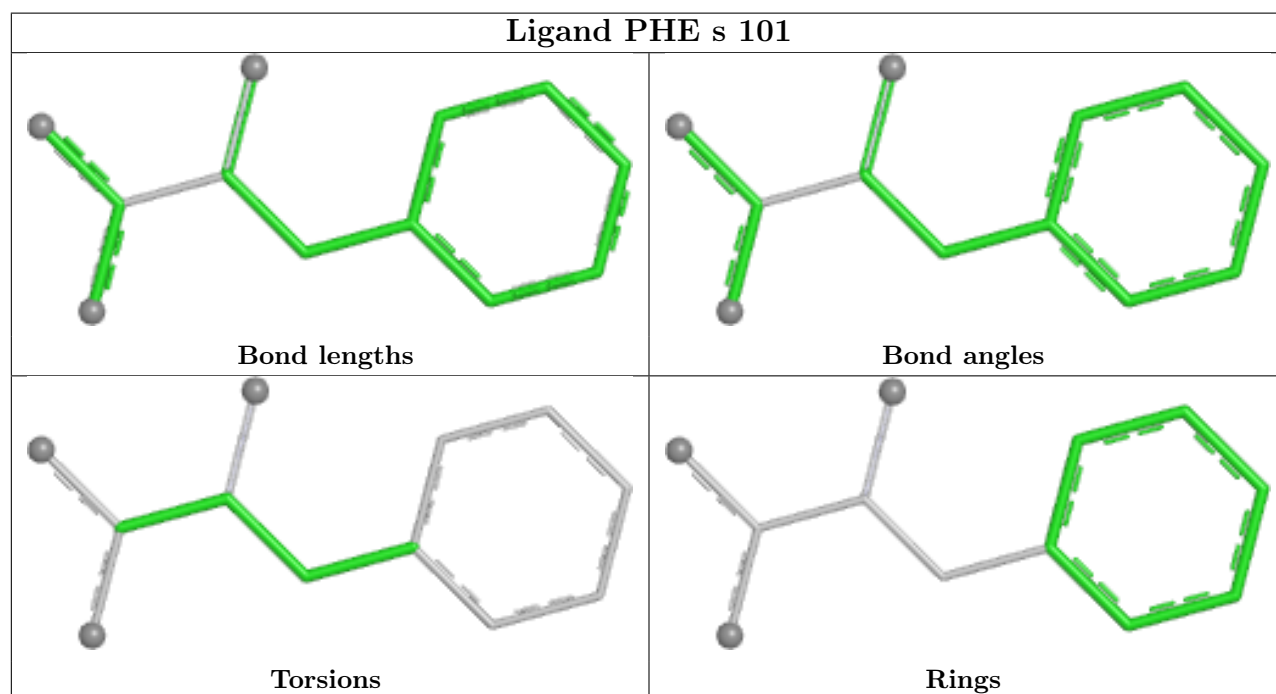
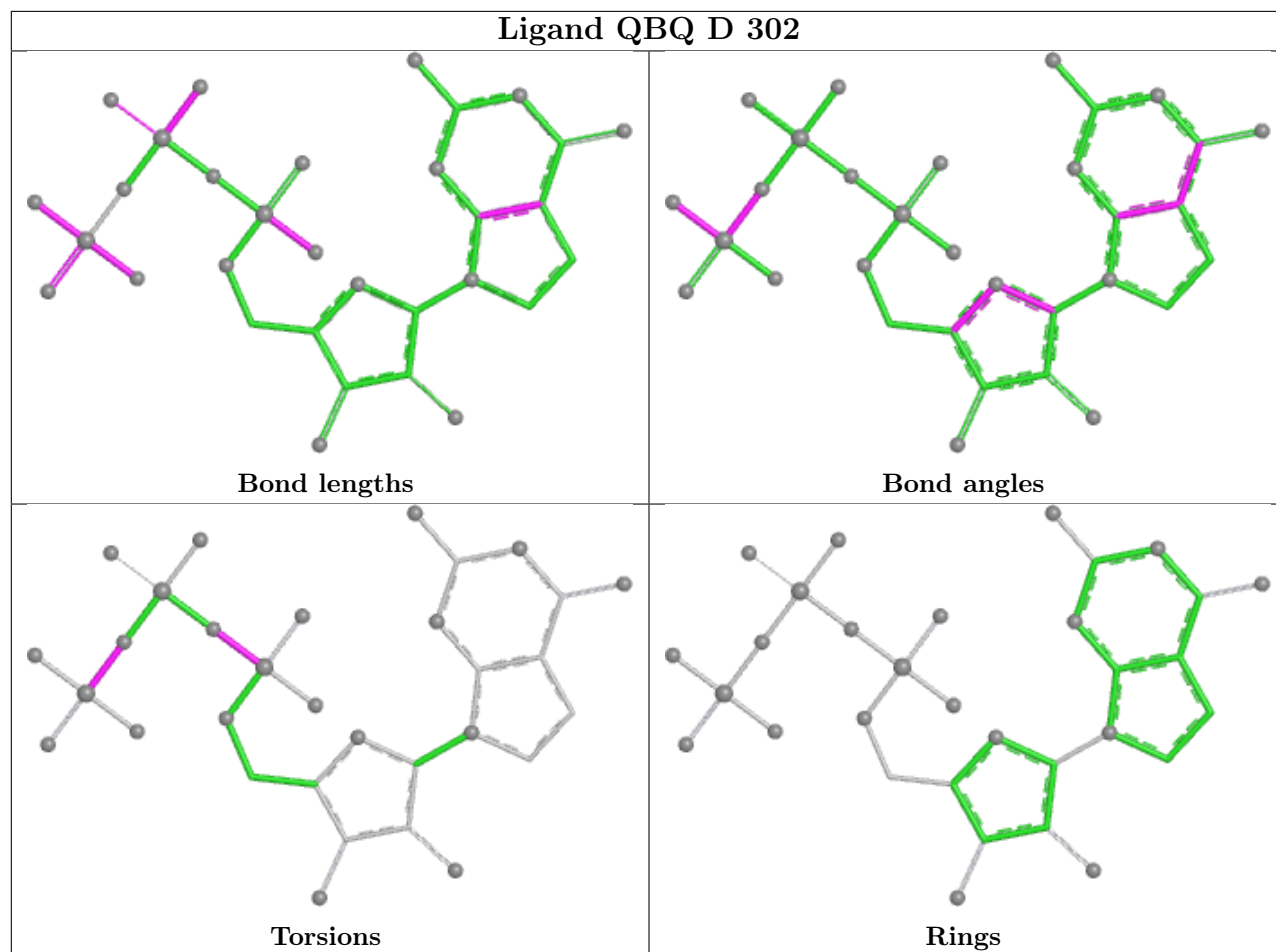


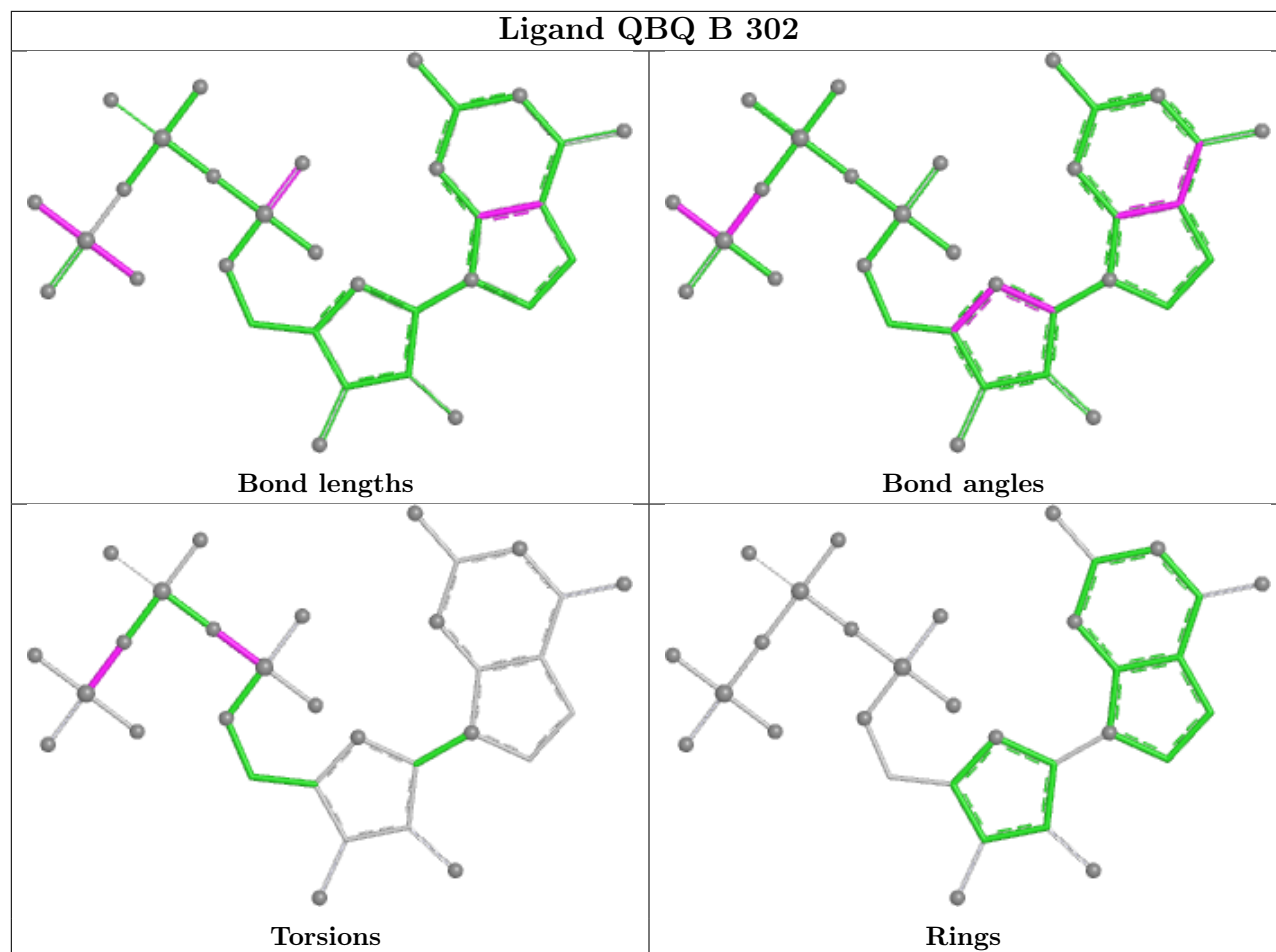




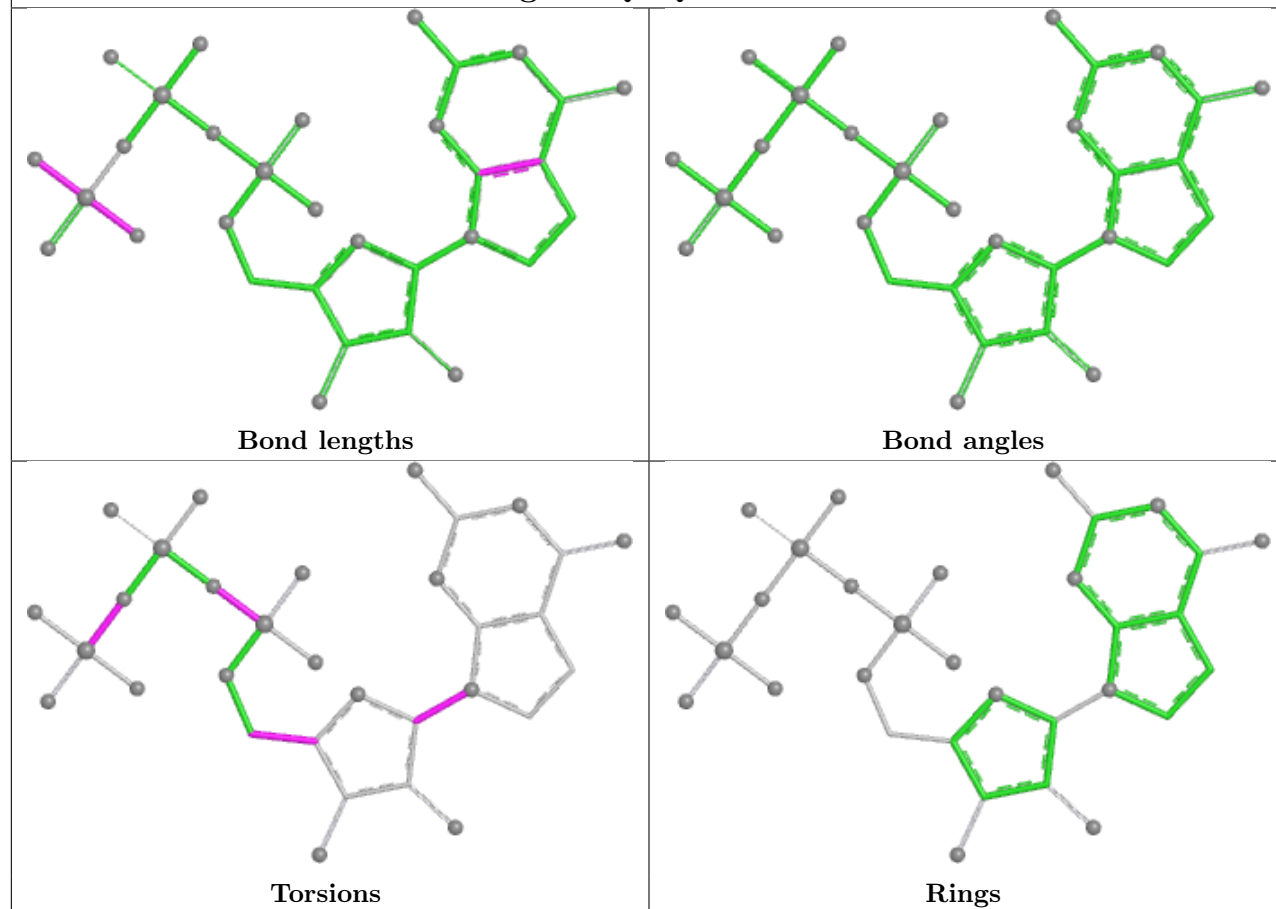
Ligand QBQ M 1101



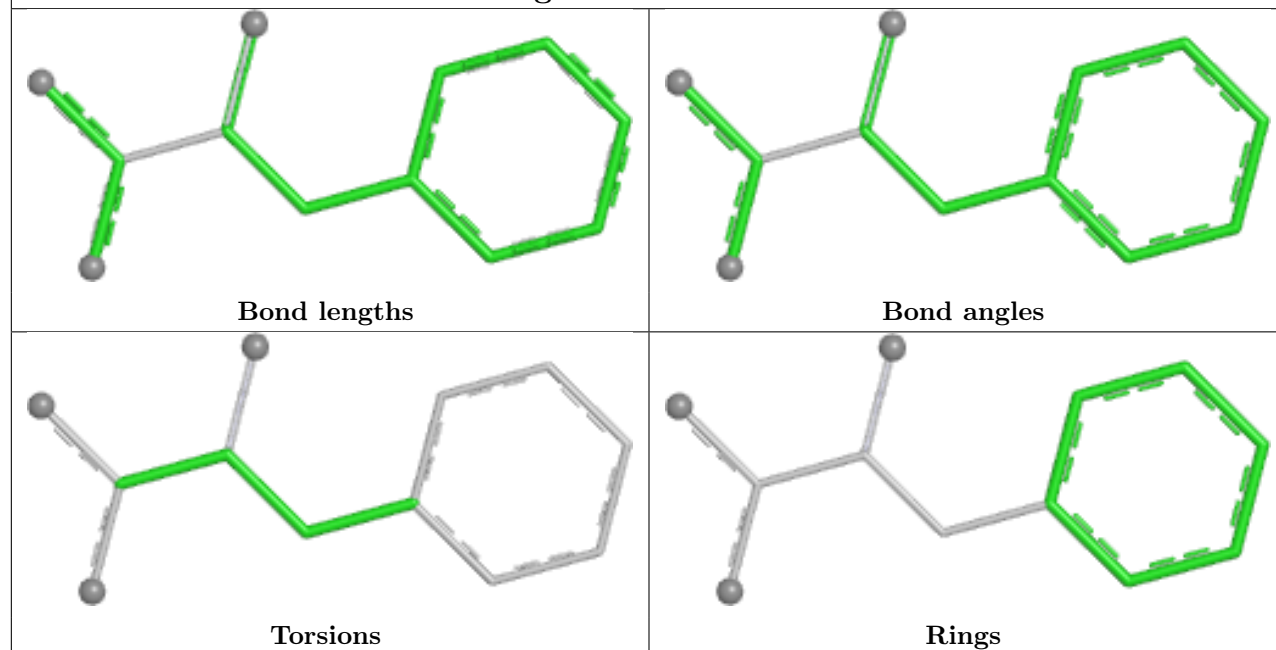


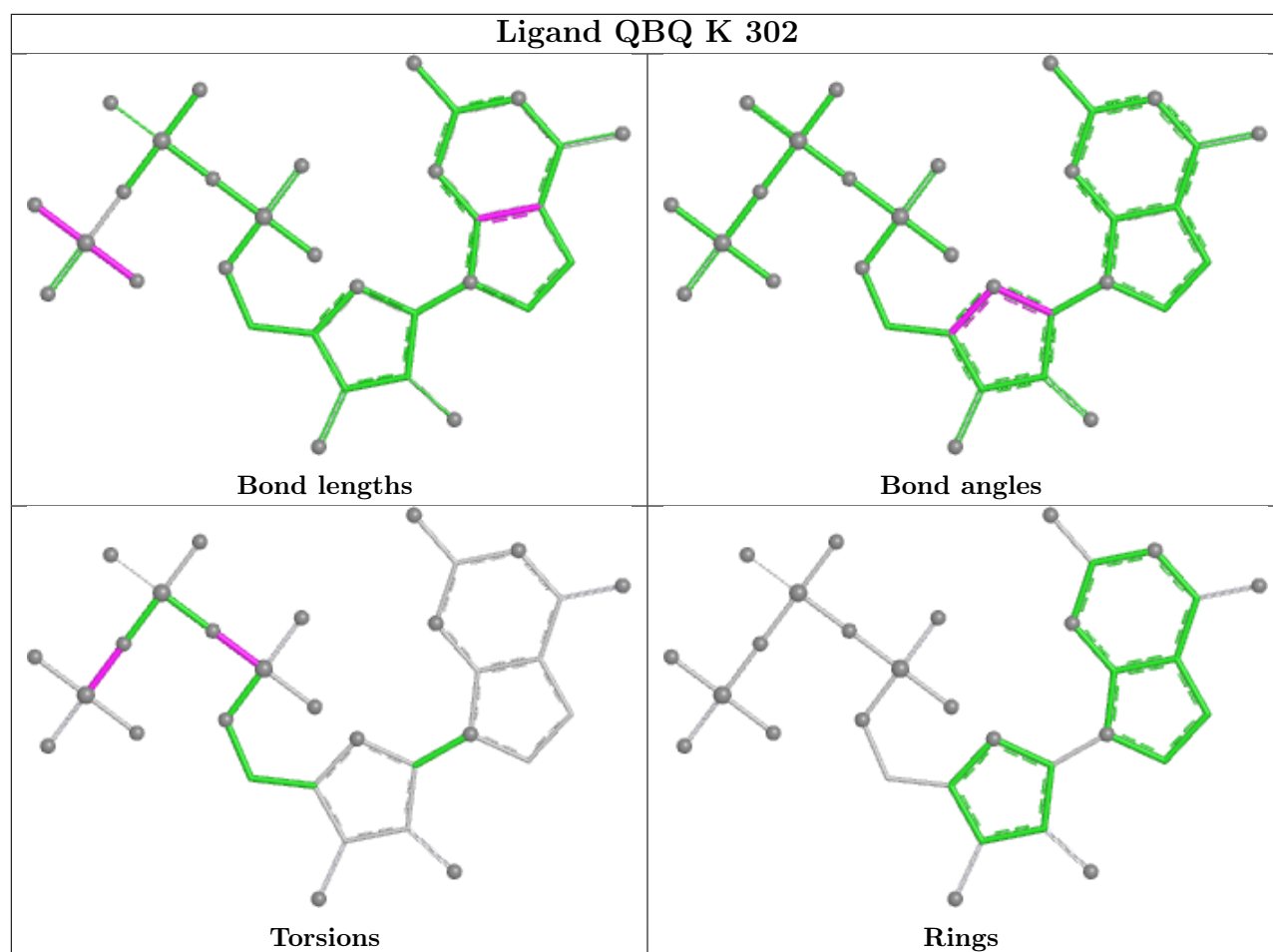
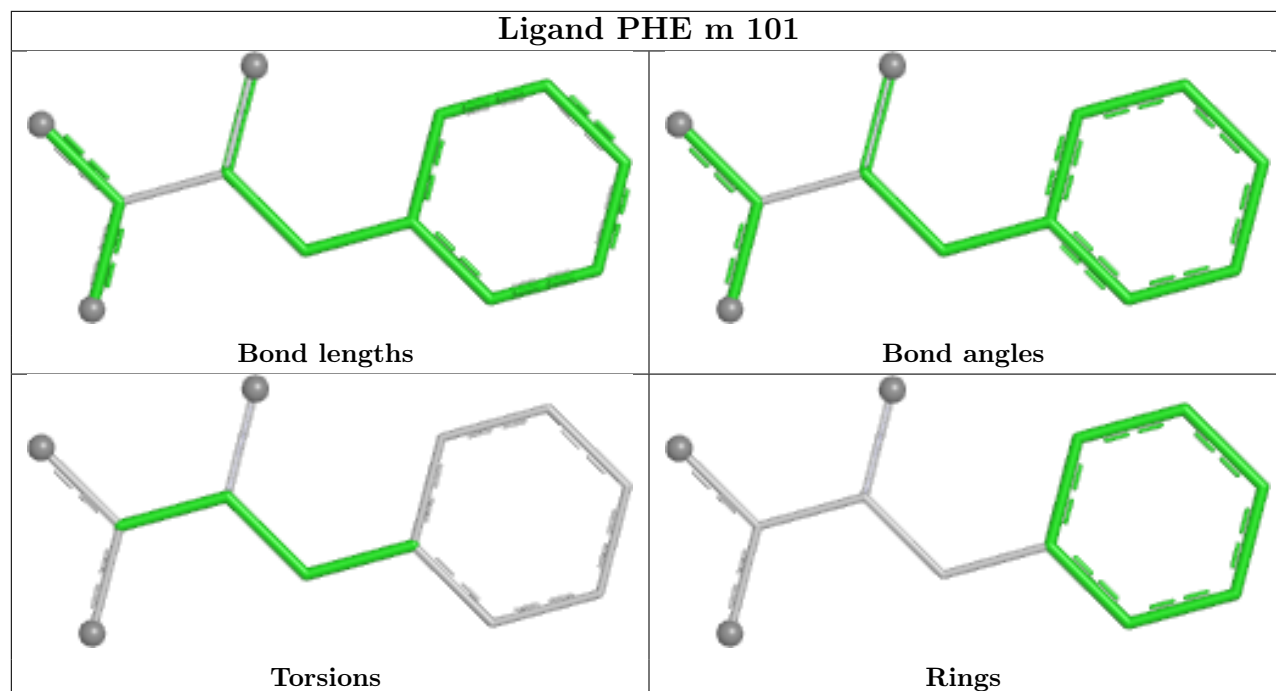


Ligand QBQ N 1101

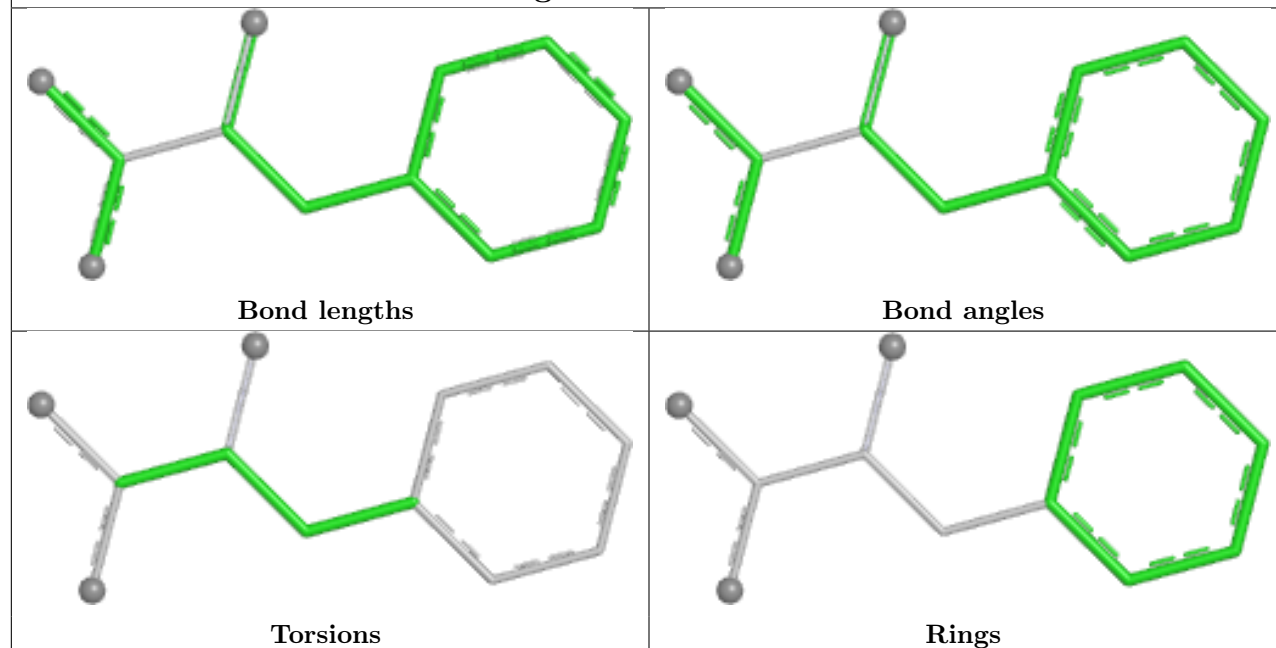


Ligand PHE h 101

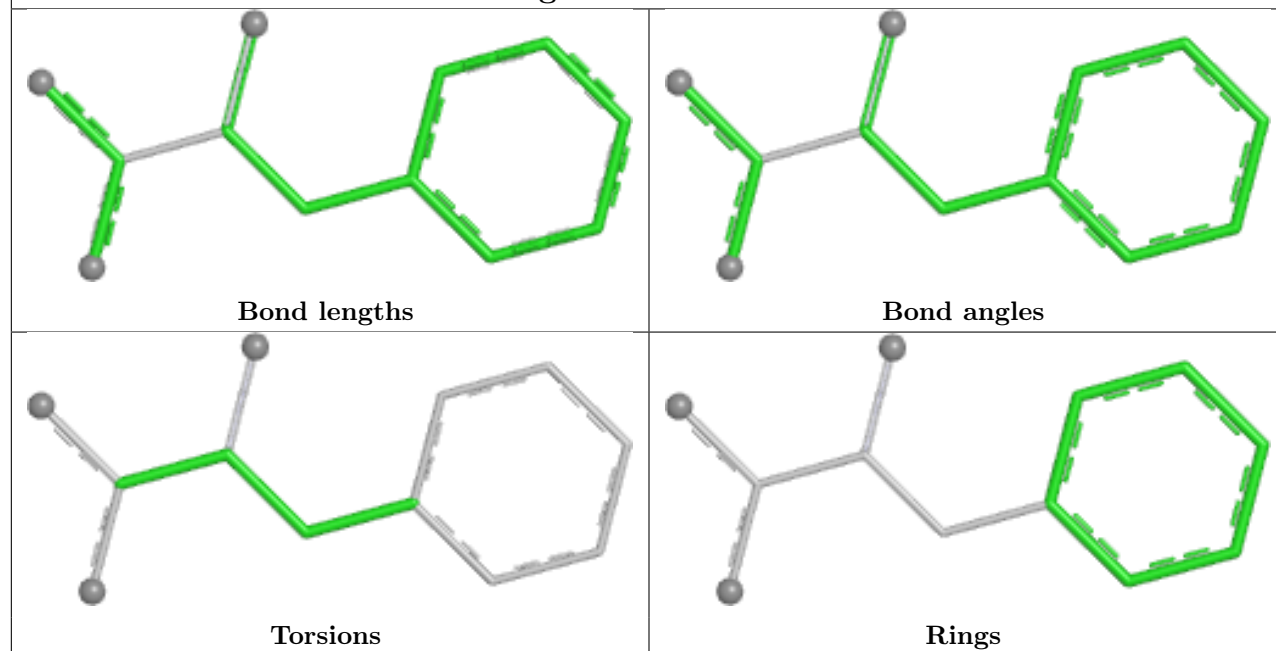




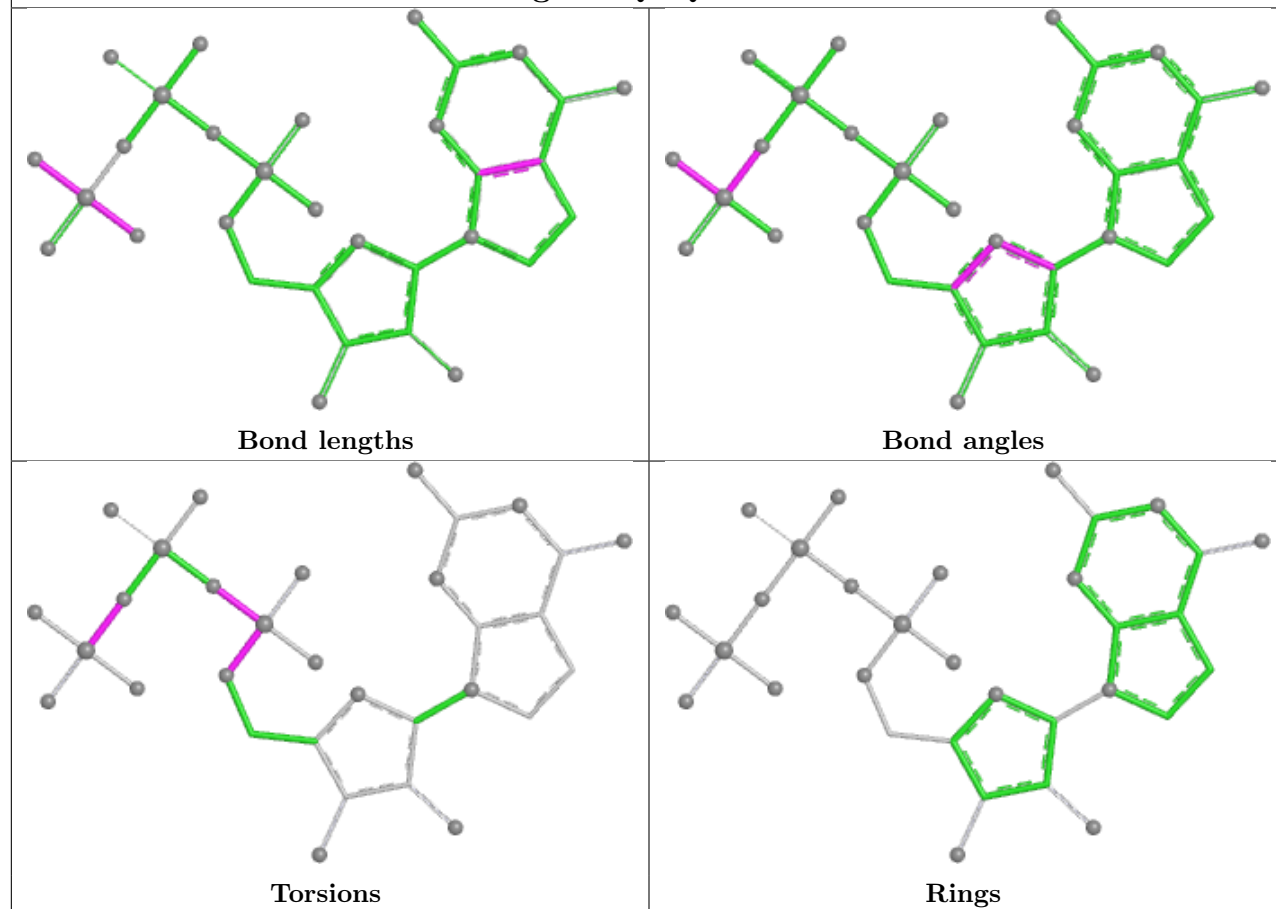
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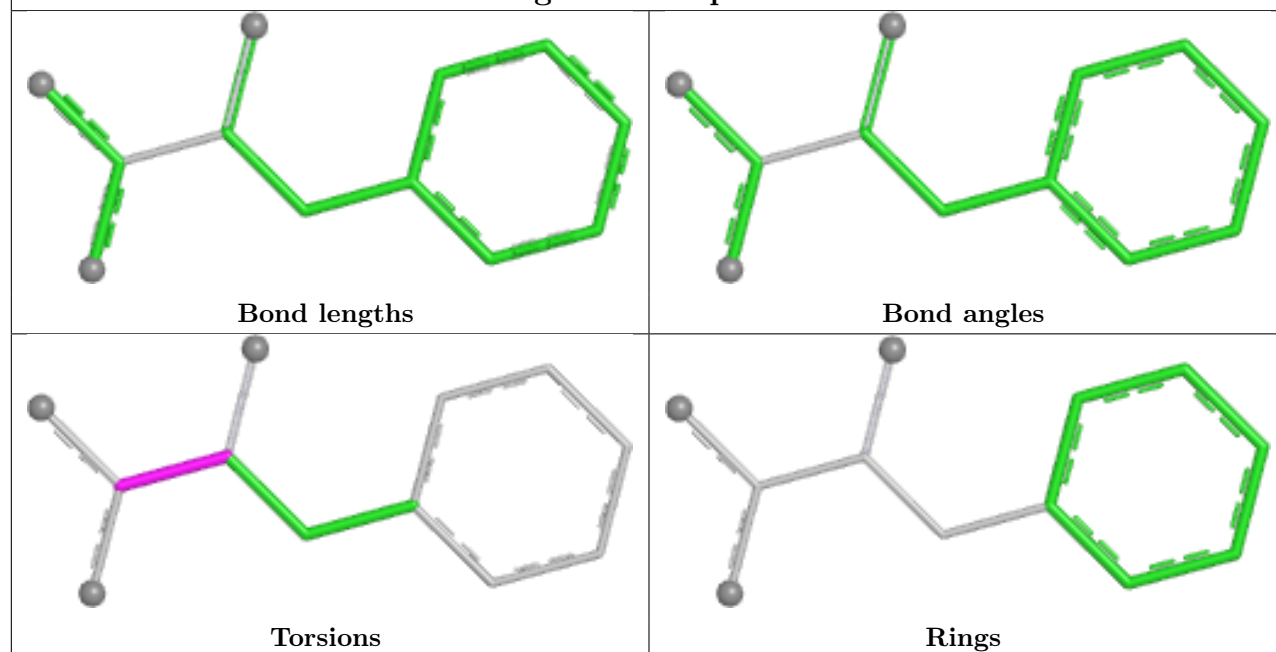
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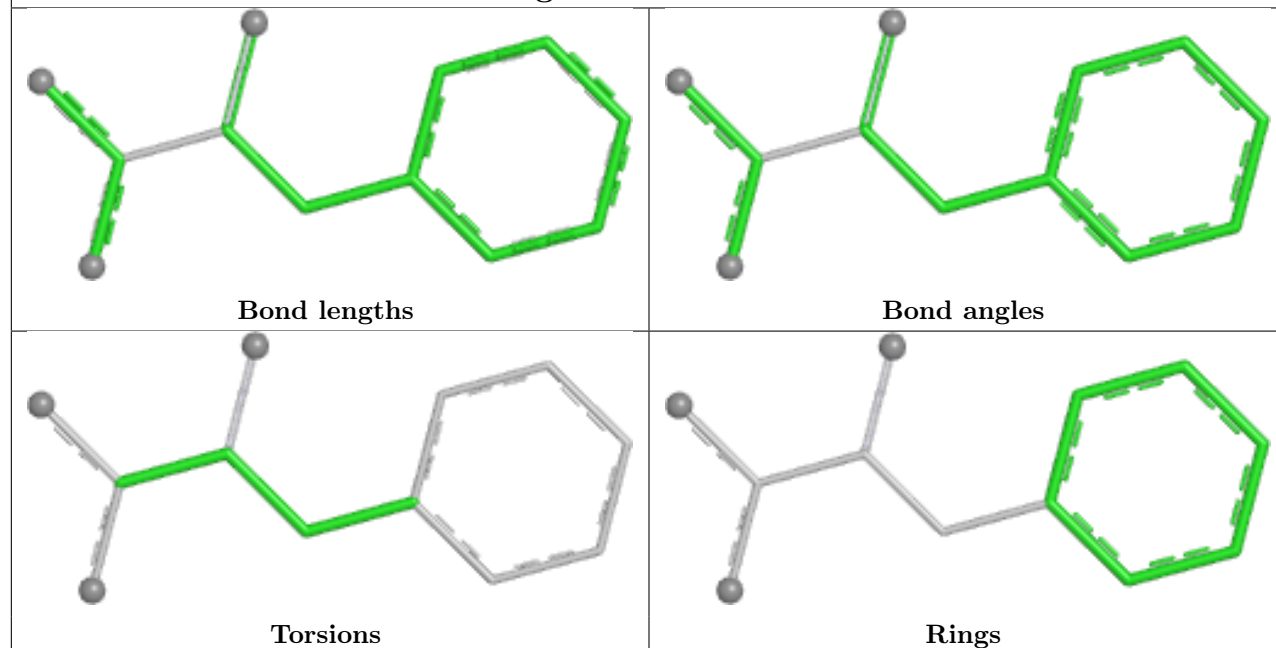
Ligand QBQ S 302



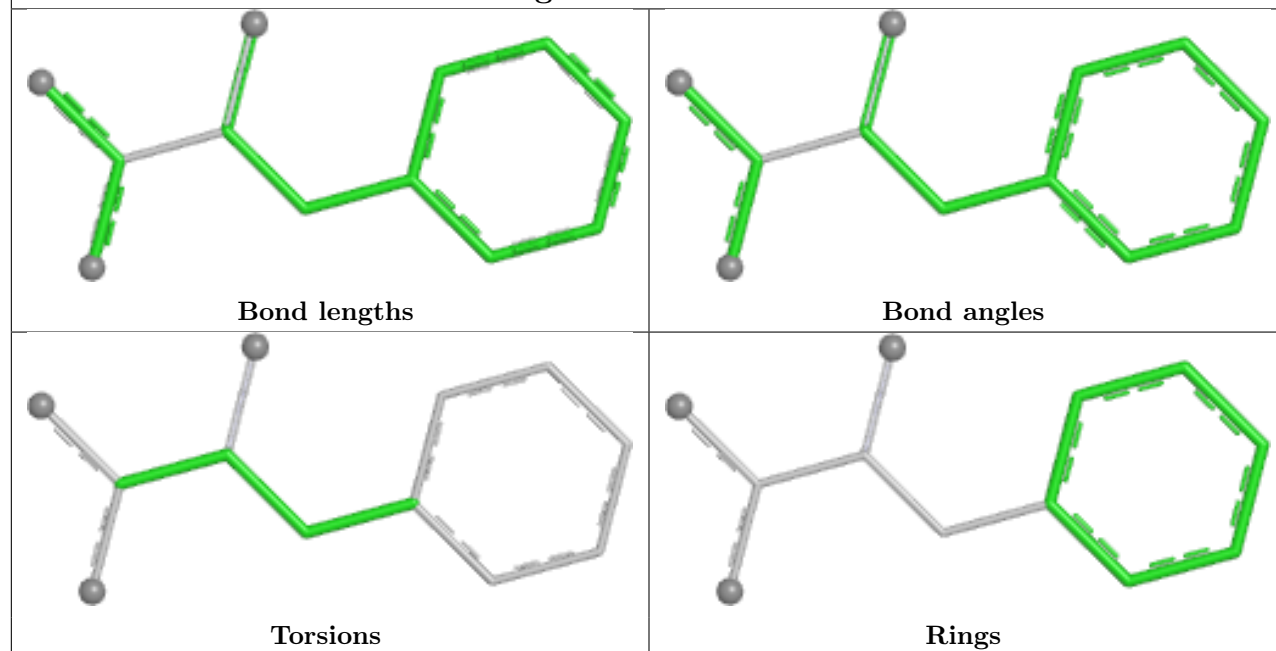
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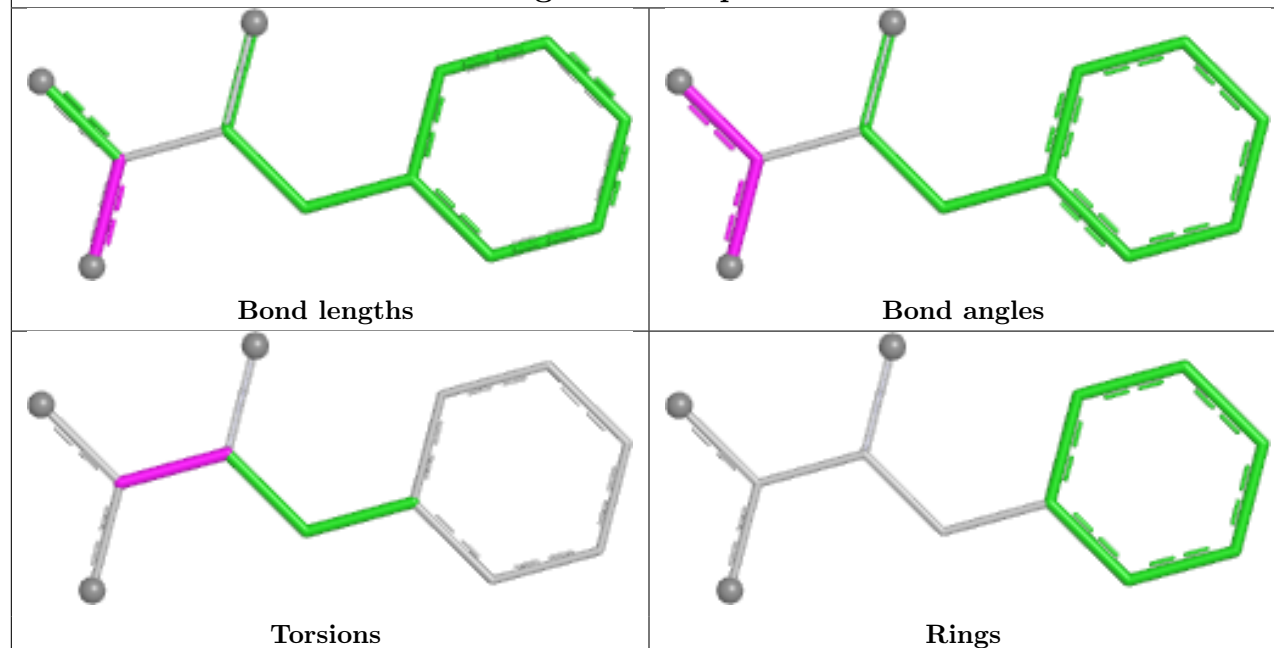
Ligand PHE a 101



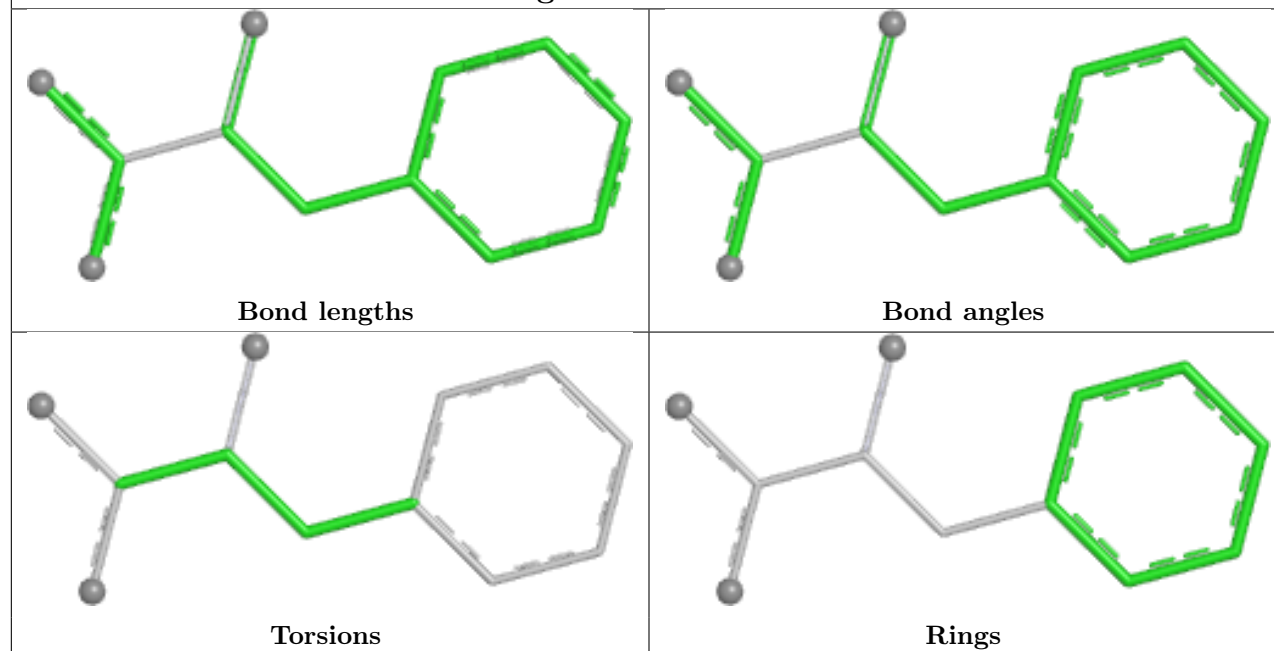
Ligand PHE k 101



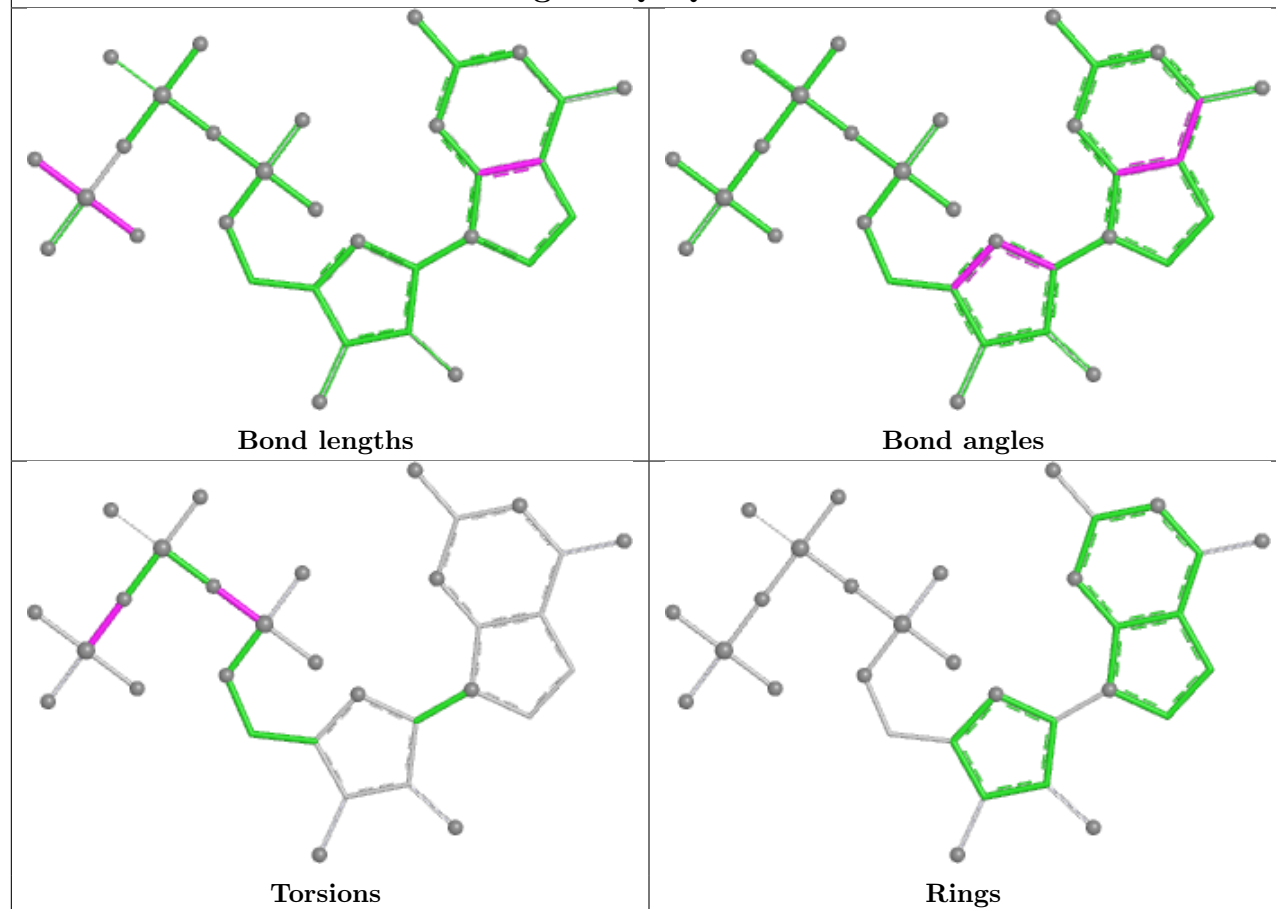
Ligand PHE q 101



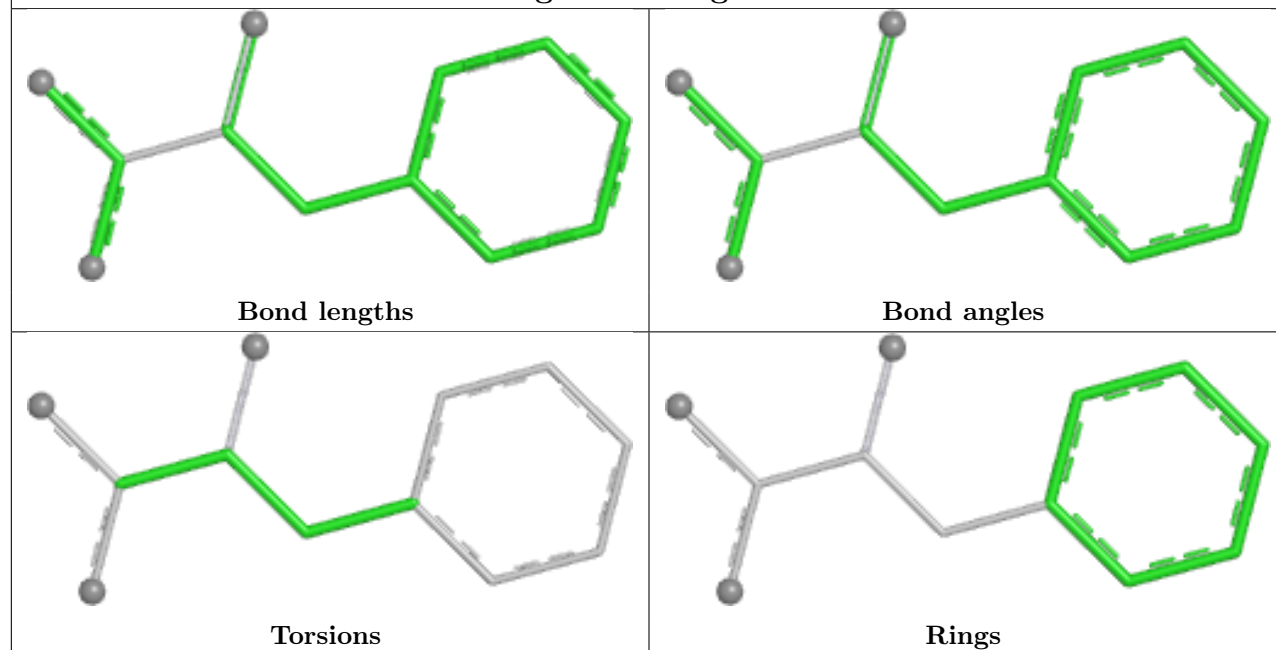
Ligand PHE r 101

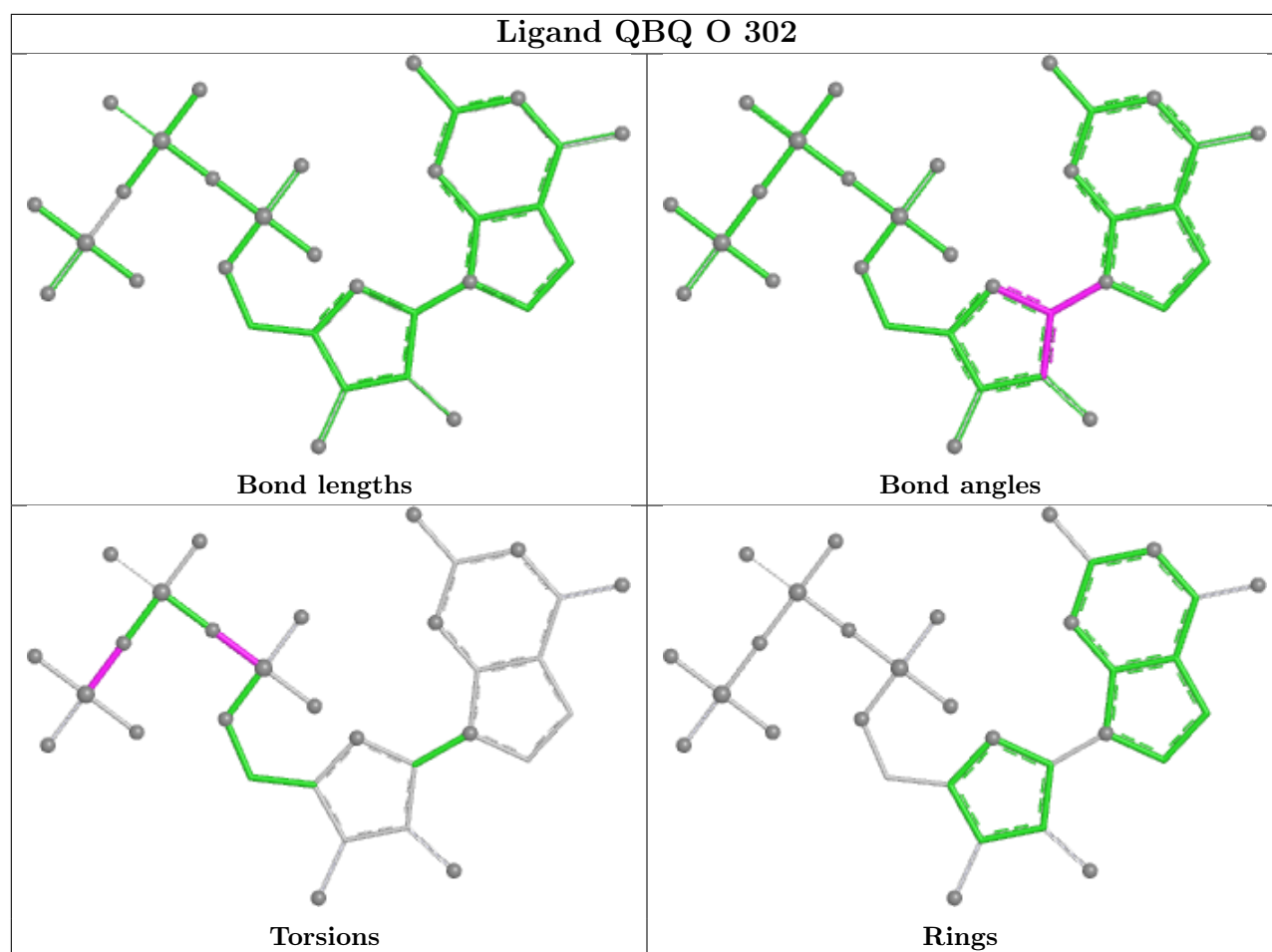


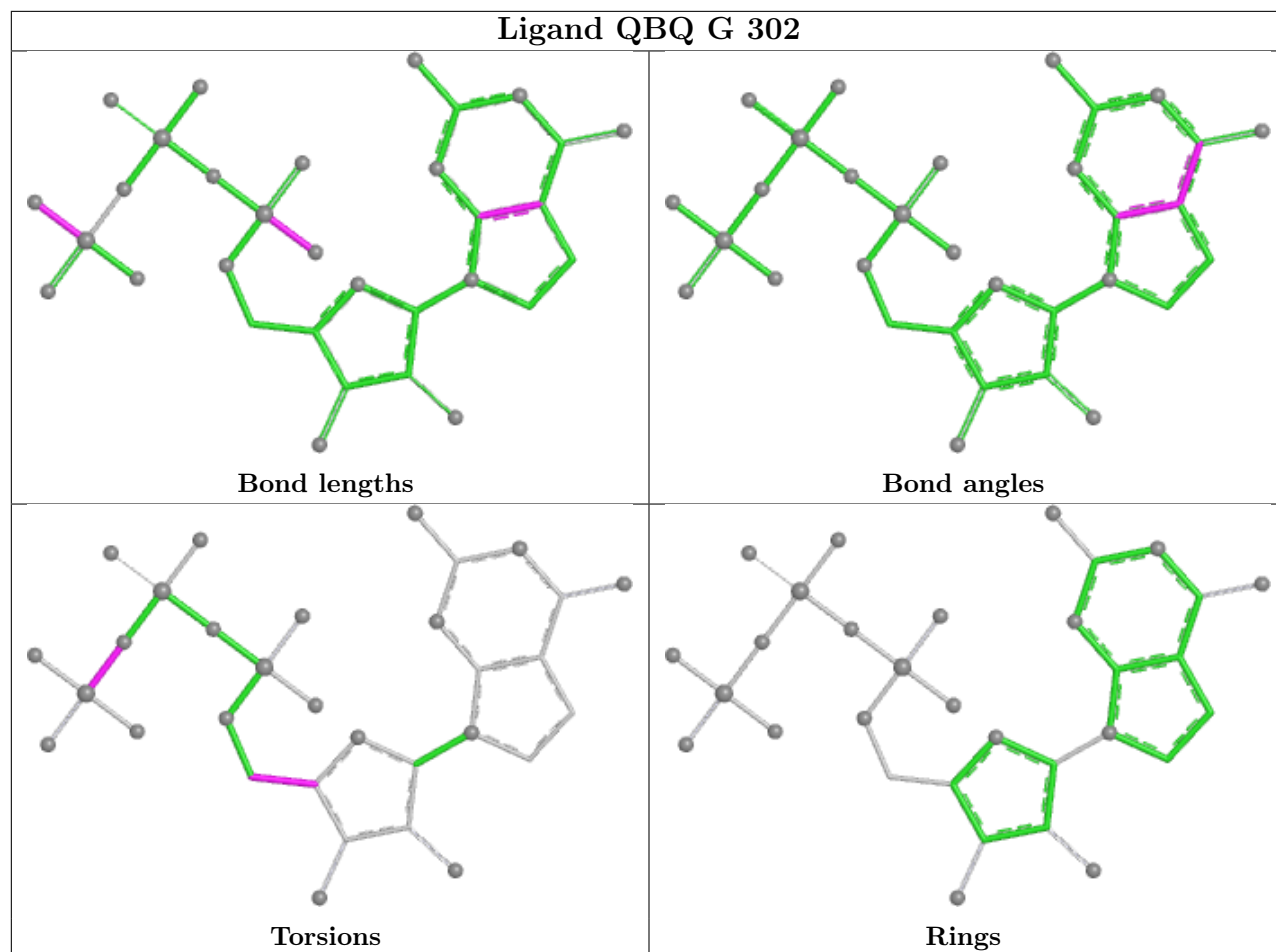
Ligand QBQ J 302

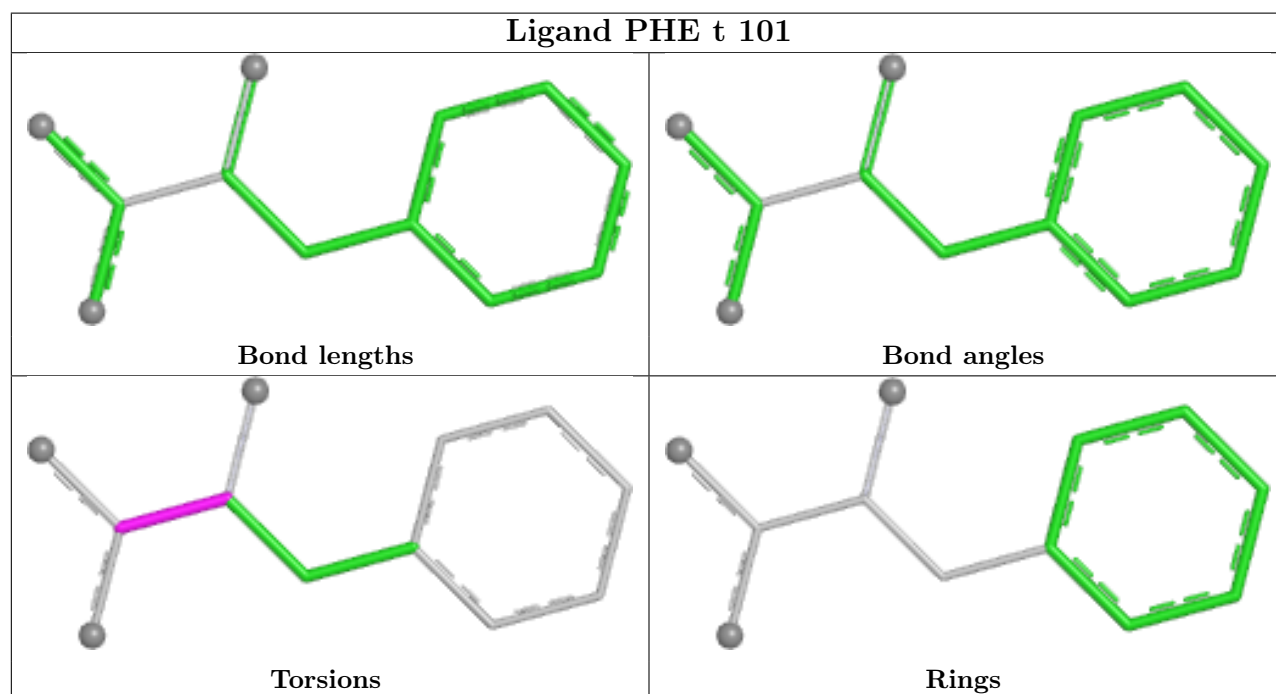
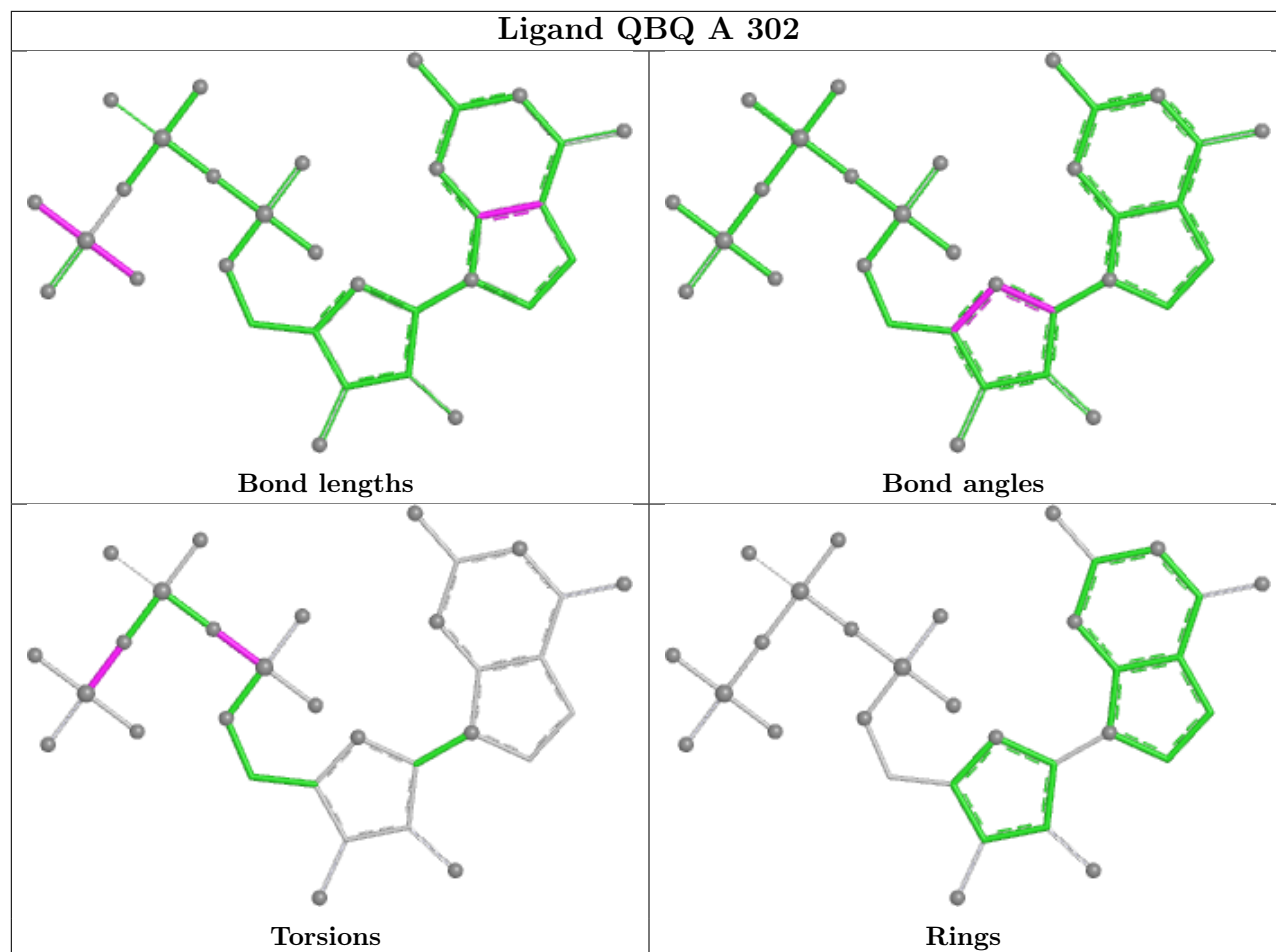


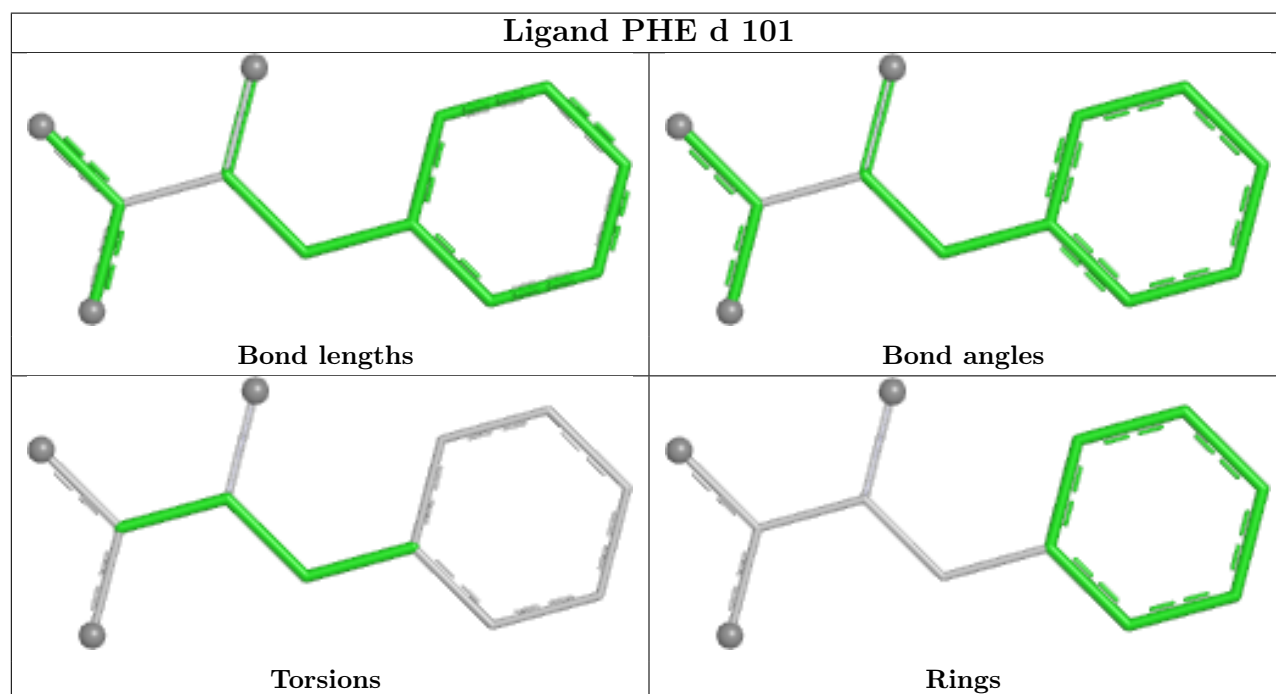
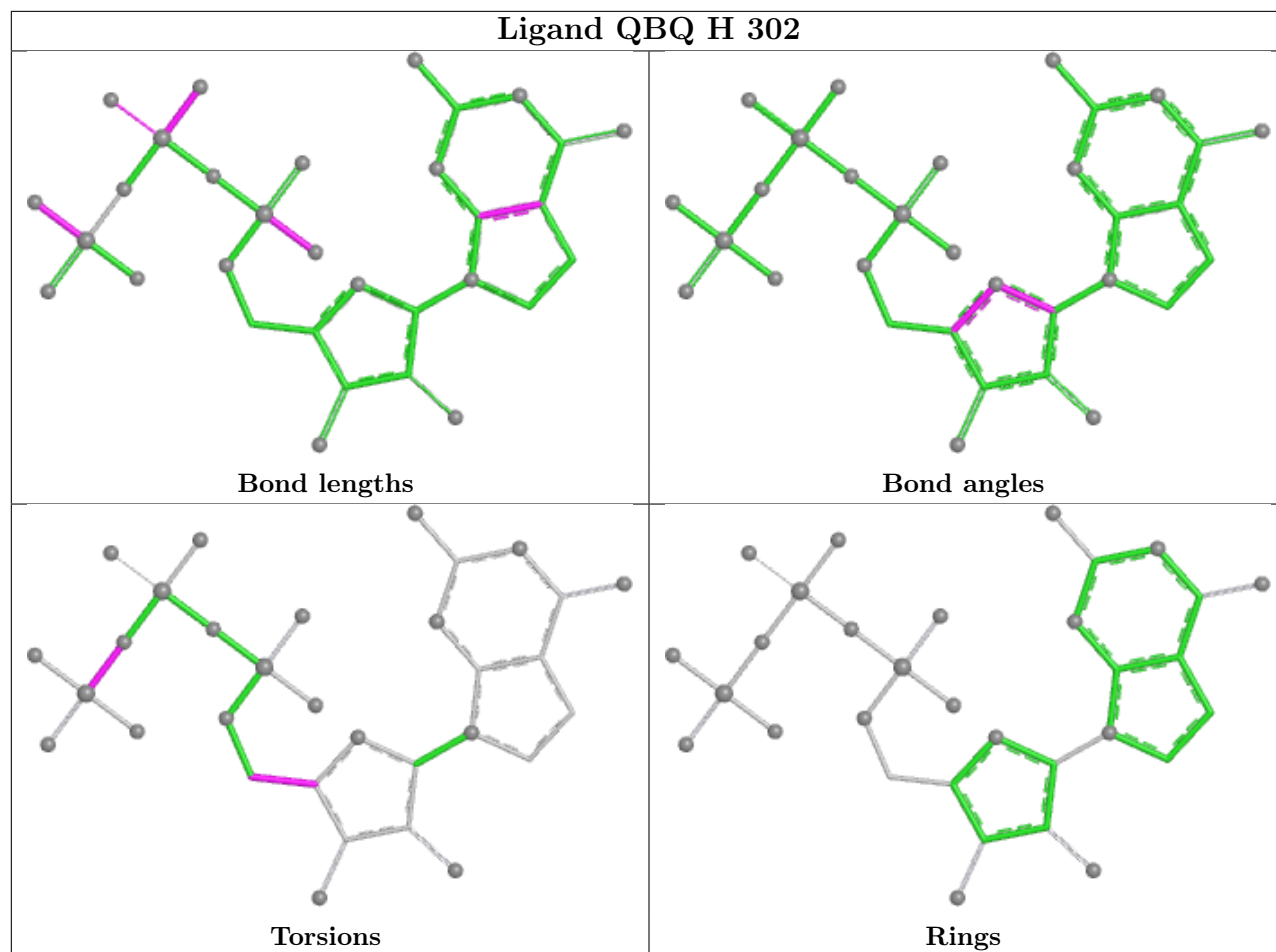
Ligand PHE g 101











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%)	0.79	33 (17%) 4 5	18, 30, 67, 80	0
1	B	187/209 (89%)	0.43	14 (7%) 20 27	19, 29, 52, 64	0
1	C	190/209 (90%)	0.45	22 (11%) 9 13	17, 27, 54, 70	0
1	D	192/209 (91%)	0.23	11 (5%) 29 38	15, 26, 47, 63	1 (0%)
1	E	192/209 (91%)	0.48	23 (11%) 9 12	15, 28, 57, 72	0
1	F	189/209 (90%)	0.53	26 (13%) 6 9	15, 28, 59, 83	1 (0%)
1	G	189/209 (90%)	0.35	18 (9%) 14 19	18, 26, 53, 79	0
1	H	190/209 (90%)	0.31	17 (8%) 15 22	17, 25, 51, 67	0
1	I	190/209 (90%)	0.49	19 (10%) 12 18	17, 28, 55, 73	0
1	J	190/209 (90%)	0.74	32 (16%) 4 5	18, 31, 63, 78	0
1	K	192/209 (91%)	0.46	21 (10%) 10 15	19, 28, 54, 75	0
1	L	187/209 (89%)	0.51	17 (9%) 15 20	20, 30, 52, 76	0
1	M	190/209 (90%)	0.59	22 (11%) 9 13	22, 32, 60, 74	0
1	N	190/209 (90%)	0.48	23 (12%) 8 12	20, 28, 56, 66	0
1	O	192/209 (91%)	0.36	15 (7%) 19 25	16, 28, 52, 72	0
1	P	192/209 (91%)	0.32	13 (6%) 23 31	15, 27, 43, 54	0
1	Q	192/209 (91%)	0.48	23 (11%) 9 12	18, 28, 54, 76	0
1	R	188/209 (89%)	0.66	23 (12%) 8 11	18, 30, 61, 73	0
1	S	190/209 (90%)	0.51	21 (11%) 10 14	18, 28, 60, 77	0
1	T	192/209 (91%)	0.54	21 (10%) 10 15	18, 27, 55, 77	0
2	a	84/87 (96%)	0.66	7 (8%) 17 24	23, 35, 53, 59	0
2	b	83/87 (95%)	0.80	8 (9%) 13 19	20, 39, 53, 65	0
2	c	84/87 (96%)	0.51	8 (9%) 14 19	22, 33, 49, 62	0
2	d	83/87 (95%)	0.61	7 (8%) 17 23	21, 36, 49, 55	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
2	e	84/87 (96%)	0.69	4 (4%) 35 45	22, 35, 55, 64	0
2	f	83/87 (95%)	0.70	6 (7%) 21 28	19, 39, 53, 59	0
2	g	84/87 (96%)	0.48	7 (8%) 17 24	20, 32, 46, 58	0
2	h	84/87 (96%)	0.25	3 (3%) 46 56	19, 30, 43, 62	0
2	i	83/87 (95%)	0.56	8 (9%) 13 19	20, 32, 48, 54	0
2	j	84/87 (96%)	0.59	7 (8%) 17 24	22, 35, 50, 62	0
2	k	84/87 (96%)	0.87	12 (14%) 6 8	25, 41, 61, 63	0
2	l	83/87 (95%)	0.98	14 (16%) 4 5	27, 44, 58, 61	0
2	m	84/87 (96%)	0.82	7 (8%) 17 24	24, 41, 56, 66	0
2	n	83/87 (95%)	0.80	7 (8%) 17 23	23, 39, 54, 58	0
2	o	84/87 (96%)	0.74	5 (5%) 27 36	23, 37, 53, 64	0
2	p	83/87 (95%)	0.73	7 (8%) 17 23	19, 36, 50, 55	0
2	q	84/87 (96%)	0.36	4 (4%) 35 45	20, 30, 46, 58	0
2	r	84/87 (96%)	0.39	4 (4%) 35 45	20, 31, 45, 50	0
2	s	83/87 (95%)	0.63	10 (12%) 9 12	20, 32, 51, 55	0
2	t	84/87 (96%)	0.45	5 (5%) 27 36	19, 33, 50, 64	0
All	All	5478/5920 (92%)	0.53	554 (10%) 12 17	15, 30, 55, 83	2 (0%)

All (554) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	T	125	ASP	8.0
1	I	125	ASP	7.4
1	R	122	PHE	6.1
1	B	126	HIS	6.0
1	R	121	ILE	5.8
1	R	160	LYS	5.7
1	L	124	GLU	5.7
1	Q	126	HIS	5.6
1	T	126	HIS	5.5
1	C	60	SER	5.4
1	M	60	SER	5.4
1	F	66	LEU	5.3
1	L	126	HIS	5.2
1	K	126	HIS	5.1
1	T	124	GLU	5.0

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Mol	Chain	Res	Type	RSRZ
1	Q	124	GLU	5.0
1	F	58	PRO	4.9
1	N	127	ASP	4.9
1	S	126	HIS	4.8
2	m	45	TYR	4.7
1	A	126	HIS	4.7
1	I	126	HIS	4.7
1	K	127	ASP	4.6
1	N	124	GLU	4.6
1	A	160	LYS	4.6
1	A	125	ASP	4.6
1	Q	121	ILE	4.5
2	p	22	GLU	4.5
1	T	122	PHE	4.5
1	G	92	LEU	4.4
1	C	126	HIS	4.4
1	E	126	HIS	4.4
2	h	84	GLU	4.4
1	F	92	LEU	4.3
1	J	58	PRO	4.3
1	K	125	ASP	4.3
1	T	123	ASP	4.3
1	A	60	SER	4.3
1	L	123	ASP	4.3
1	Q	96	TRP	4.3
2	m	1	MET	4.3
2	b	84	GLU	4.3
1	O	127	ASP	4.2
1	S	125	ASP	4.2
2	l	83	LYS	4.2
1	M	96	TRP	4.2
1	C	127	ASP	4.2
1	M	126	HIS	4.1
1	G	127	ASP	4.0
2	i	27	GLU	4.0
1	E	58	PRO	4.0
1	A	92	LEU	3.9
1	L	122	PHE	3.9
1	R	66	LEU	3.9
1	C	124	GLU	3.9
1	N	160	LYS	3.9
1	S	127	ASP	3.9

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Mol	Chain	Res	Type	RSRZ
2	p	83	LYS	3.9
2	c	1	MET	3.9
1	G	66	LEU	3.8
1	Q	122	PHE	3.8
1	A	96	TRP	3.8
1	C	160	LYS	3.8
1	R	162	VAL	3.8
1	S	124	GLU	3.7
1	R	120	ALA	3.7
2	g	31	HIS	3.7
1	S	62	GLU	3.7
2	s	22	GLU	3.7
1	T	112	THR	3.7
1	B	127	ASP	3.7
1	K	124	GLU	3.7
1	A	68	LEU	3.6
1	J	112	THR	3.6
1	E	127	ASP	3.6
1	L	160	LYS	3.6
1	H	127	ASP	3.6
1	J	127	ASP	3.6
1	N	119	ASP	3.6
1	C	110	GLN	3.6
1	M	110	GLN	3.6
1	A	58	PRO	3.6
1	J	87	GLN	3.5
1	A	221	MET	3.5
1	A	127	ASP	3.5
1	T	58	PRO	3.5
1	E	122	PHE	3.5
1	I	127	ASP	3.5
1	J	249	ARG	3.5
1	I	159	ASN	3.5
1	Q	120	ALA	3.5
1	O	249	ARG	3.5
1	J	160	LYS	3.5
1	R	114	SER	3.5
1	I	121	ILE	3.5
1	T	121	ILE	3.5
2	t	84	GLU	3.4
1	T	249	ARG	3.4
2	f	1	MET	3.4

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Mol	Chain	Res	Type	RSRZ
1	M	124	GLU	3.4
2	a	84	GLU	3.4
1	R	89	GLN	3.4
1	L	221	MET	3.4
2	o	1	MET	3.4
1	H	126	HIS	3.4
1	O	61	GLU	3.4
1	S	123	ASP	3.4
1	I	249	ARG	3.4
2	m	62	ARG	3.4
2	l	1	MET	3.4
1	F	118	ASN	3.4
1	L	66	LEU	3.4
2	j	1	MET	3.4
2	e	22	GLU	3.3
1	L	121	ILE	3.3
1	E	249	ARG	3.3
1	M	112	THR	3.3
1	Q	89	GLN	3.3
1	F	123	ASP	3.3
1	T	221	MET	3.3
1	O	124	GLU	3.3
2	c	84	GLU	3.3
2	j	84	GLU	3.3
1	C	123	ASP	3.3
1	I	123	ASP	3.3
2	k	62	ARG	3.3
1	C	113	ILE	3.3
1	E	124	GLU	3.3
1	M	113	ILE	3.3
1	T	211	MET	3.3
1	M	160	LYS	3.3
1	H	97	ARG	3.3
2	a	62	ARG	3.3
1	S	121	ILE	3.2
2	e	1	MET	3.2
1	J	126	HIS	3.2
1	A	78	ILE	3.2
1	J	121	ILE	3.2
1	R	249	ARG	3.2
1	I	160	LYS	3.2
2	l	40	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	60	SER	3.2
1	I	60	SER	3.2
1	P	249	ARG	3.2
1	Q	123	ASP	3.2
1	I	124	GLU	3.2
2	d	22	GLU	3.2
2	t	1	MET	3.1
1	A	66	LEU	3.1
1	B	249	ARG	3.1
1	F	249	ARG	3.1
2	o	22	GLU	3.1
1	Q	160	LYS	3.1
1	P	96	TRP	3.1
1	N	123	ASP	3.1
1	Q	127	ASP	3.1
1	S	160	LYS	3.1
1	T	212	CYS	3.1
1	O	126	HIS	3.1
1	E	121	ILE	3.1
1	F	121	ILE	3.1
1	M	66	LEU	3.1
2	s	27	GLU	3.1
1	J	68	LEU	3.0
2	s	45	TYR	3.0
1	I	97	ARG	3.0
1	F	61	GLU	3.0
1	R	112	THR	3.0
1	E	123	ASP	3.0
1	B	161	GLN	3.0
1	K	121	ILE	3.0
1	C	249	ARG	3.0
1	N	117	LEU	3.0
2	f	22	GLU	3.0
2	t	31	HIS	3.0
1	J	123	ASP	3.0
2	m	22	GLU	3.0
1	P	126	HIS	3.0
1	T	60	SER	3.0
1	T	114	SER	3.0
1	C	125	ASP	3.0
1	T	127	ASP	3.0
2	f	83	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
2	o	30	GLN	3.0
1	M	249	ARG	3.0
2	r	84	GLU	3.0
1	C	92	LEU	2.9
1	J	82	LEU	2.9
1	T	66	LEU	2.9
1	D	127	ASP	2.9
1	K	123	ASP	2.9
1	O	125	ASP	2.9
1	D	249	ARG	2.9
2	h	22	GLU	2.9
1	B	66	LEU	2.9
1	I	66	LEU	2.9
1	J	66	LEU	2.9
2	k	32	LEU	2.9
2	p	62	ARG	2.9
1	F	116	VAL	2.9
1	F	221[A]	MET	2.9
1	E	61	GLU	2.9
1	H	61	GLU	2.9
1	G	58	PRO	2.9
1	J	86	PRO	2.9
1	F	87	GLN	2.9
1	G	59	ARG	2.9
1	E	119	ASP	2.9
1	M	125	ASP	2.9
1	R	119	ASP	2.9
1	P	221	MET	2.9
2	q	1	MET	2.9
2	c	45	TYR	2.9
1	J	122	PHE	2.9
1	G	249	ARG	2.9
2	n	66	ARG	2.9
1	F	119	ASP	2.9
1	Q	125	ASP	2.9
1	R	127	ASP	2.9
1	I	113	ILE	2.9
1	L	249	ARG	2.8
1	A	124	GLU	2.8
1	M	128	GLU	2.8
1	O	123	ASP	2.8
2	i	1	MET	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	87	GLN	2.8
1	E	89	GLN	2.8
1	R	87	GLN	2.8
1	S	97	ARG	2.8
1	S	249	ARG	2.8
2	b	62	ARG	2.8
1	S	61	GLU	2.8
1	I	122	PHE	2.8
1	N	60	SER	2.8
1	F	64	ASN	2.8
1	A	71	LEU	2.8
1	A	121	ILE	2.8
1	A	249	ARG	2.8
1	N	66	LEU	2.8
2	j	83	LYS	2.8
1	J	61	GLU	2.8
1	Q	62	GLU	2.8
1	M	127	ASP	2.8
1	O	211	MET	2.8
1	B	160	LYS	2.8
2	c	83	LYS	2.8
1	C	117	LEU	2.8
1	I	96	TRP	2.8
2	p	1	MET	2.8
1	K	249	ARG	2.7
1	N	249	ARG	2.7
2	h	62	ARG	2.7
2	p	36	LYS	2.7
1	G	62	GLU	2.7
1	H	62	GLU	2.7
1	R	117	LEU	2.7
1	J	113	ILE	2.7
1	M	221	MET	2.7
1	Q	162	VAL	2.7
1	T	218	VAL	2.7
1	C	128	GLU	2.7
1	G	65	GLU	2.7
1	F	127	ASP	2.7
1	J	211	MET	2.7
2	g	1	MET	2.7
2	k	1	MET	2.7
1	A	86	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
2	g	2	PRO	2.7
1	Q	87	GLN	2.7
1	R	60	SER	2.7
1	A	70	ASN	2.7
1	B	124	GLU	2.7
1	M	61	GLU	2.7
1	L	96	TRP	2.7
2	g	45	TYR	2.7
2	i	45	TYR	2.7
2	f	62	ARG	2.7
1	G	60	SER	2.7
1	O	58	PRO	2.7
1	P	58	PRO	2.7
1	N	113	ILE	2.7
1	S	113	ILE	2.7
1	H	249	ARG	2.6
1	N	97	ARG	2.6
1	R	62	GLU	2.6
1	K	60	SER	2.6
2	i	83	LYS	2.6
1	J	71	LEU	2.6
2	q	40	LEU	2.6
1	D	126	HIS	2.6
2	s	31	HIS	2.6
1	I	221	MET	2.6
1	A	161	GLN	2.6
1	J	62	GLU	2.6
1	F	60	SER	2.6
1	A	122	PHE	2.6
1	N	61	GLU	2.6
2	a	22	GLU	2.6
1	N	58	PRO	2.6
1	N	122	PHE	2.6
1	J	221	MET	2.6
1	E	161	GLN	2.6
1	A	119	ASP	2.6
2	c	22	GLU	2.6
1	A	72	ALA	2.6
1	N	116	VAL	2.6
1	H	58	PRO	2.5
1	R	97	ARG	2.5
2	f	45	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	211	MET	2.5
1	D	160	LYS	2.5
1	N	121	ILE	2.5
1	L	114	SER	2.5
1	S	60	SER	2.5
1	J	115	ASP	2.5
2	t	63	ARG	2.5
1	A	89	GLN	2.5
1	C	112	THR	2.5
1	P	89	GLN	2.5
2	g	23	GLN	2.5
2	n	1	MET	2.5
1	L	127	ASP	2.5
1	F	160	LYS	2.5
1	L	90	GLY	2.5
1	M	117	LEU	2.5
1	P	66	LEU	2.5
2	k	28	LEU	2.5
2	s	40	LEU	2.5
1	M	161	GLN	2.5
1	N	87	GLN	2.5
1	R	61	GLU	2.5
1	S	128	GLU	2.5
1	K	221	MET	2.5
1	K	160	LYS	2.5
2	j	63	ARG	2.4
1	C	66	LEU	2.4
1	C	122	PHE	2.4
1	F	117	LEU	2.4
1	C	115	ASP	2.4
1	J	63	ASP	2.4
2	l	67	VAL	2.4
1	Q	249	ARG	2.4
2	m	66	ARG	2.4
1	G	64	ASN	2.4
1	N	159	ASN	2.4
1	G	61	GLU	2.4
1	H	161	GLN	2.4
1	I	61	GLU	2.4
1	P	61	GLU	2.4
1	E	92	LEU	2.4
1	J	92	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
2	d	83	LYS	2.4
2	n	83	LYS	2.4
2	b	54	ARG	2.4
2	j	62	ARG	2.4
1	K	58	PRO	2.4
2	j	43	ASN	2.4
2	s	43	ASN	2.4
1	B	221	MET	2.4
1	J	114	SER	2.4
1	S	114	SER	2.4
1	T	160	LYS	2.4
1	M	123	ASP	2.4
1	Q	115	ASP	2.4
2	k	25	ASP	2.4
1	E	113	ILE	2.4
1	F	59	ARG	2.4
1	G	113	ILE	2.4
1	G	121	ILE	2.4
2	e	62	ARG	2.4
2	i	63	ARG	2.4
2	k	37	ARG	2.4
2	s	62	ARG	2.4
1	A	62	GLU	2.4
1	F	62	GLU	2.4
1	H	128	GLU	2.4
1	R	128	GLU	2.4
2	e	84	GLU	2.4
2	q	84	GLU	2.4
1	J	69	PRO	2.4
1	N	161	GLN	2.4
1	R	118	ASN	2.4
2	a	1	MET	2.4
1	K	96	TRP	2.4
1	N	115	ASP	2.3
1	M	92	LEU	2.3
2	a	37	ARG	2.3
1	D	61	GLU	2.3
2	b	22	GLU	2.3
1	J	73	ALA	2.3
1	S	120	ALA	2.3
2	i	31	HIS	2.3
1	N	221	MET	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	114	SER	2.3
1	C	114	SER	2.3
1	O	114	SER	2.3
1	E	125	ASP	2.3
2	d	66	ARG	2.3
2	l	66	ARG	2.3
1	E	87	GLN	2.3
2	n	32	LEU	2.3
1	I	112	THR	2.3
1	S	122	PHE	2.3
1	A	120	ALA	2.3
1	F	120	ALA	2.3
1	L	211	MET	2.3
1	M	121	ILE	2.3
1	R	58	PRO	2.3
2	l	62	ARG	2.3
2	s	38	ARG	2.3
1	H	162	VAL	2.3
2	q	22	GLU	2.3
2	r	22	GLU	2.3
1	G	87	GLN	2.3
1	E	159	ASN	2.3
1	G	112	THR	2.3
1	H	221	MET	2.3
2	d	1	MET	2.3
2	n	45	TYR	2.3
2	a	83	LYS	2.3
1	A	97	ARG	2.3
1	G	198	ARG	2.3
1	N	114	SER	2.3
1	D	62	GLU	2.3
1	N	63	ASP	2.3
1	Q	61	GLU	2.3
2	g	84	GLU	2.3
2	o	84	GLU	2.3
1	G	160	LYS	2.3
1	H	160	LYS	2.3
2	b	40	LEU	2.3
1	K	198	ARG	2.2
1	O	97	ARG	2.2
1	A	75	TYR	2.2
1	I	65	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	P	164	GLY	2.2
1	Q	200	ALA	2.2
1	A	123	ASP	2.2
1	B	125	ASP	2.2
1	B	89	GLN	2.2
1	P	87	GLN	2.2
1	O	218	VAL	2.2
1	H	159	ASN	2.2
1	J	159	ASN	2.2
2	p	43	ASN	2.2
1	B	88	ARG	2.2
2	b	66	ARG	2.2
2	k	38	ARG	2.2
2	l	54	ARG	2.2
2	s	37	ARG	2.2
1	A	91	LEU	2.2
1	K	61	GLU	2.2
2	n	22	GLU	2.2
1	Q	80	SER	2.2
1	T	120	ALA	2.2
1	A	159	ASN	2.2
2	k	31	HIS	2.2
2	m	43	ASN	2.2
2	r	62	ARG	2.2
1	O	66	LEU	2.2
2	j	4	LEU	2.2
1	J	83	GLY	2.2
1	D	58	PRO	2.2
1	A	198	ARG	2.2
1	J	64	ASN	2.2
1	S	187	LYS	2.2
2	d	62	ARG	2.2
1	A	61	GLU	2.2
1	L	116	VAL	2.2
2	l	32	LEU	2.2
1	H	198	ARG	2.2
1	R	64	ASN	2.1
1	F	65	GLU	2.1
2	l	44	PHE	2.1
2	m	84	GLU	2.1
1	T	113	ILE	2.1
1	C	87	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	J	96	TRP	2.1
1	F	112	THR	2.1
1	F	115	ASP	2.1
1	K	112	THR	2.1
1	D	66	LEU	2.1
1	S	66	LEU	2.1
2	i	62	ARG	2.1
2	l	57	LEU	2.1
2	b	31	HIS	2.1
2	k	84	GLU	2.1
1	K	159	ASN	2.1
1	K	122	PHE	2.1
1	K	113	ILE	2.1
1	O	115	ASP	2.1
1	D	114	SER	2.1
2	k	35	SER	2.1
1	J	97	ARG	2.1
1	L	162	VAL	2.1
1	R	116	VAL	2.1
1	E	160	LYS	2.1
1	E	86	PRO	2.1
1	Q	92	LEU	2.1
2	f	43	ASN	2.1
2	g	4	LEU	2.1
2	l	43	ASN	2.1
1	F	196	ALA	2.1
1	C	119	ASP	2.1
1	F	113	ILE	2.1
2	p	45	TYR	2.1
1	B	198	ARG	2.1
1	M	198	ARG	2.1
1	Q	198	ARG	2.1
2	c	38	ARG	2.1
1	E	62	GLU	2.1
1	S	112	THR	2.1
1	K	162	VAL	2.1
1	T	159	ASN	2.1
2	c	43	ASN	2.1
2	n	67	VAL	2.1
2	r	43	ASN	2.1
2	t	43	ASN	2.1
1	C	161	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	H	89	GLN	2.1
1	E	117	LEU	2.1
1	H	117	LEU	2.1
1	K	66	LEU	2.1
2	d	68	LEU	2.1
1	K	169	ALA	2.1
2	c	62	ARG	2.1
2	k	27	GLU	2.0
1	E	114	SER	2.0
1	Q	114	SER	2.0
1	S	174	ILE	2.0
2	k	36	LYS	2.0
2	d	45	TYR	2.0
2	s	1	MET	2.0
2	l	31	HIS	2.0
1	J	67	ASN	2.0
1	G	162	VAL	2.0
1	Q	58	PRO	2.0
1	P	68	LEU	2.0
1	P	92	LEU	2.0
2	b	4	LEU	2.0
2	l	4	LEU	2.0
1	D	119	ASP	2.0
1	L	119	ASP	2.0
2	a	25	ASP	2.0
2	o	62	ARG	2.0
1	F	114	SER	2.0
1	M	114	SER	2.0
1	C	221	MET	2.0
1	H	113	ILE	2.0
1	O	122	PHE	2.0
1	E	83	GLY	2.0
2	l	23	GLN	2.0
1	P	198	ARG	2.0
2	i	38	ARG	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	QBQ	P	302	32/32	0.81	0.15	43,48,56,59	17
4	QBQ	F	302	32/32	0.91	0.10	31,38,49,55	17
4	QBQ	N	1101	32/32	0.93	0.09	32,37,44,48	17
5	PHE	l	101	12/12	0.93	0.07	24,25,27,28	0
5	PHE	m	101	12/12	0.93	0.08	22,23,24,24	0
4	QBQ	R	302	32/32	0.94	0.08	30,35,44,47	17
4	QBQ	L	1101	32/32	0.94	0.09	30,34,44,47	17
4	QBQ	Q	302	32/32	0.94	0.08	27,31,38,42	17
4	QBQ	E	302	32/32	0.95	0.07	25,31,40,45	17
4	QBQ	M	1101	32/32	0.95	0.08	31,35,44,47	17
4	QBQ	S	302	32/32	0.95	0.08	30,33,45,47	17
5	PHE	a	101	12/12	0.95	0.06	22,23,24,24	0
5	PHE	c	101	12/12	0.95	0.07	18,19,21,21	0
5	PHE	d	101	12/12	0.95	0.07	19,21,22,23	0
5	PHE	k	101	12/12	0.95	0.06	25,26,28,28	0
4	QBQ	G	302	32/32	0.95	0.07	25,31,41,47	17
4	QBQ	K	302	32/32	0.95	0.08	34,38,47,48	17
4	QBQ	C	302	32/32	0.96	0.07	27,32,43,46	17
5	PHE	b	101	12/12	0.96	0.06	20,20,22,22	0
4	QBQ	I	302	32/32	0.96	0.06	25,30,41,45	17
4	QBQ	D	302	32/32	0.96	0.06	21,24,30,35	17
5	PHE	e	101	12/12	0.96	0.06	21,22,23,23	0
5	PHE	f	101	12/12	0.96	0.06	19,21,21,22	0
5	PHE	f	102	12/12	0.96	0.06	18,20,20,21	0
5	PHE	g	101	12/12	0.96	0.06	18,20,20,21	0
3	ZN	T	301	1/1	0.96	0.06	34,34,34,34	0
4	QBQ	A	302	32/32	0.96	0.06	26,33,43,48	17
4	QBQ	T	302	32/32	0.96	0.07	27,33,43,46	17
5	PHE	n	101	12/12	0.96	0.06	21,22,22,23	0
3	ZN	E	301	1/1	0.97	0.05	34,34,34,34	0
4	QBQ	B	302	32/32	0.97	0.05	22,30,38,43	17
3	ZN	F	301	1/1	0.97	0.04	37,37,37,37	0

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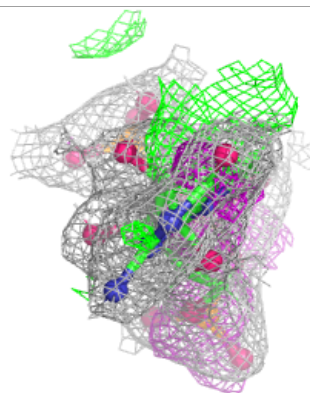
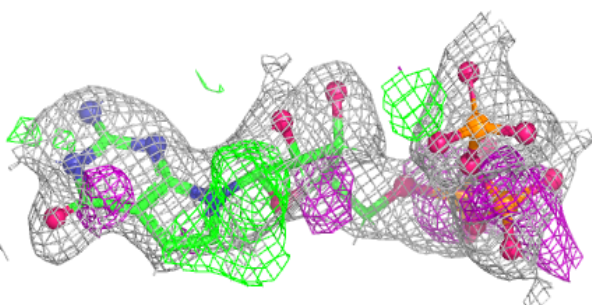
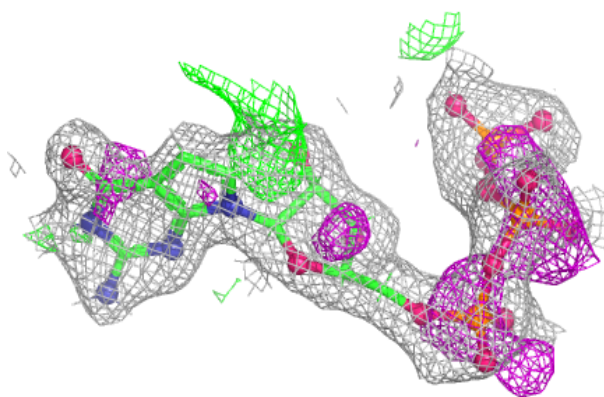
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ZN	J	301	1/1	0.97	0.05	37,37,37,37	0
4	QBQ	O	302	32/32	0.97	0.06	23,30,38,41	17
3	ZN	P	301	1/1	0.97	0.05	32,32,32,32	0
3	ZN	Q	301	1/1	0.97	0.03	32,32,32,32	0
5	PHE	h	101	12/12	0.97	0.06	18,19,21,21	0
5	PHE	i	101	12/12	0.97	0.06	19,21,23,24	0
3	ZN	R	301	1/1	0.97	0.04	36,36,36,36	0
4	QBQ	H	302	32/32	0.97	0.06	22,28,36,40	17
3	ZN	A	301	1/1	0.97	0.04	35,35,35,35	0
4	QBQ	J	302	32/32	0.97	0.06	28,34,46,52	17
5	PHE	o	101	12/12	0.97	0.06	22,22,24,24	0
5	PHE	p	101	12/12	0.97	0.05	19,20,21,22	0
5	PHE	q	101	12/12	0.97	0.05	20,21,22,23	0
5	PHE	r	101	12/12	0.97	0.05	19,21,21,21	0
5	PHE	s	101	12/12	0.97	0.05	18,19,19,20	0
5	PHE	t	101	12/12	0.97	0.05	17,18,19,19	0
3	ZN	B	301	1/1	0.98	0.03	34,34,34,34	0
3	ZN	C	301	1/1	0.98	0.04	30,30,30,30	0
3	ZN	H	301	1/1	0.98	0.03	30,30,30,30	0
3	ZN	S	301	1/1	0.98	0.03	35,35,35,35	0
3	ZN	D	301	1/1	0.98	0.03	34,34,34,34	0
3	ZN	K	301	1/1	0.98	0.04	31,31,31,31	0
3	ZN	L	1102	1/1	0.98	0.04	37,37,37,37	0
3	ZN	M	1102	1/1	0.98	0.04	40,40,40,40	0
3	ZN	O	301	1/1	0.98	0.04	35,35,35,35	0
3	ZN	I	301	1/1	0.99	0.03	35,35,35,35	0
3	ZN	N	1102	1/1	0.99	0.02	32,32,32,32	0
3	ZN	G	301	1/1	0.99	0.02	32,32,32,32	0

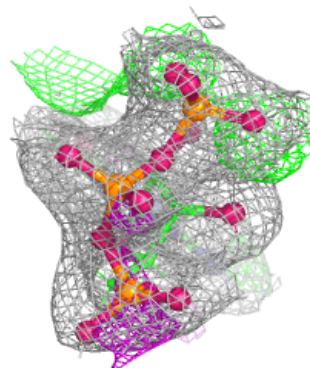
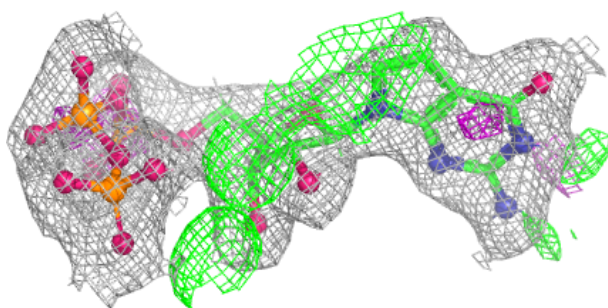
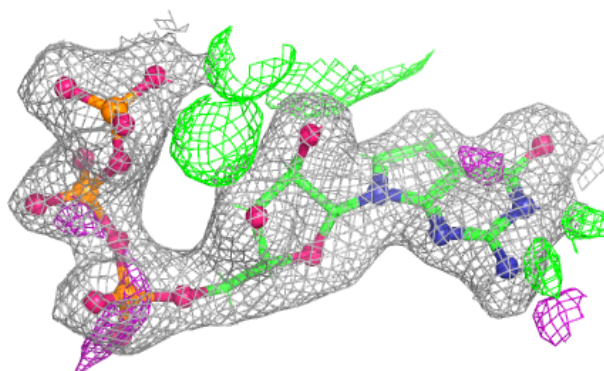
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around QBQ 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)

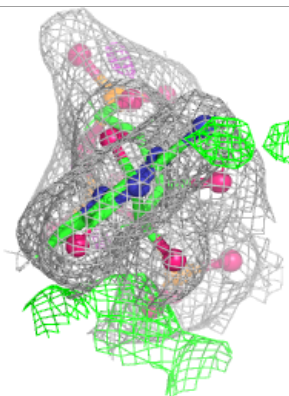
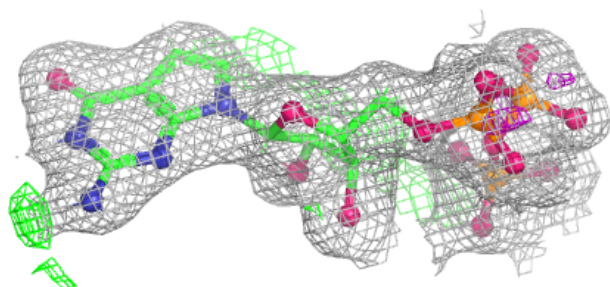
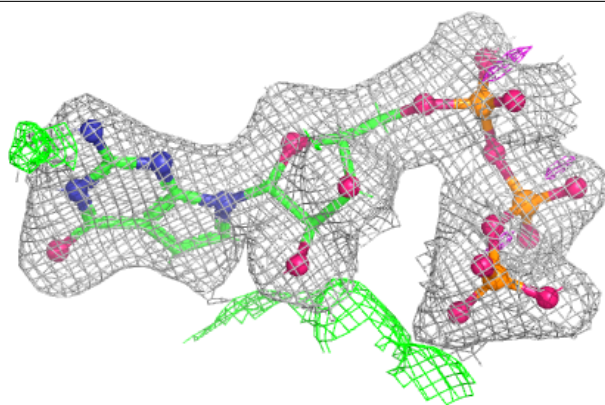
**Electron density around QBQ F 302:**

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

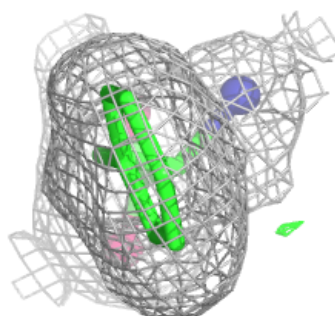
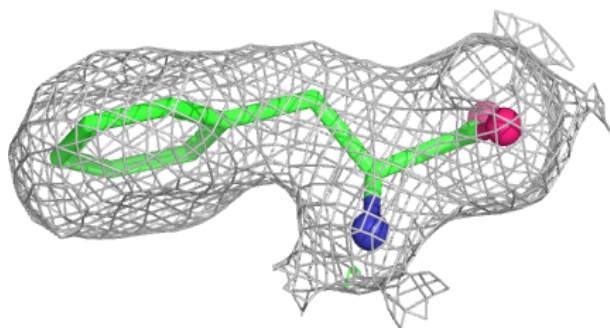
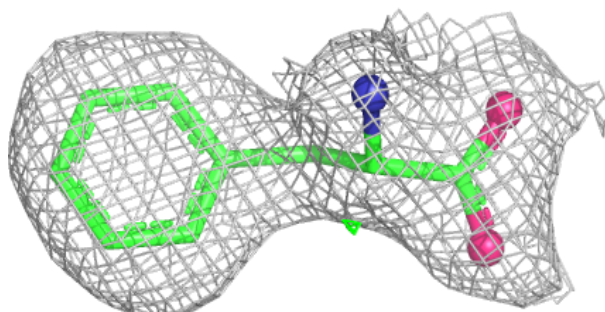


Electron density around QBQ N 1101:

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

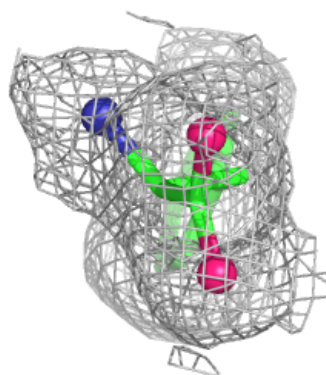
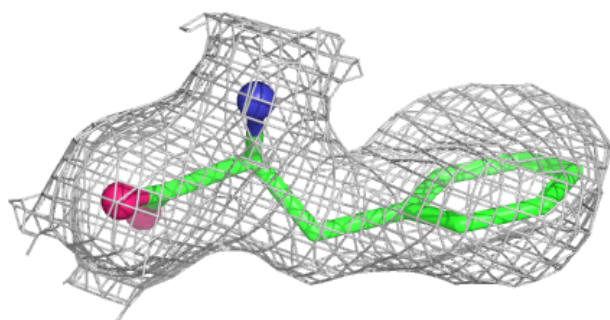
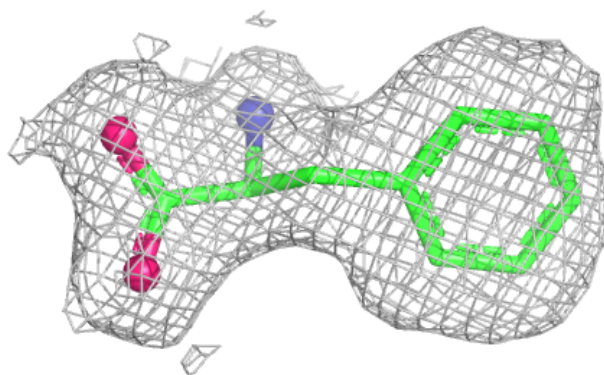
**Electron density around PHE 1 101:**

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

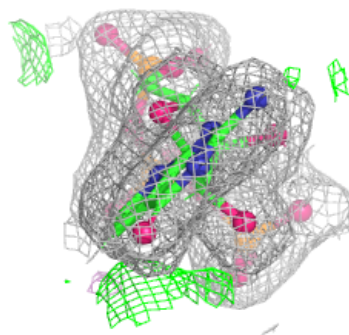
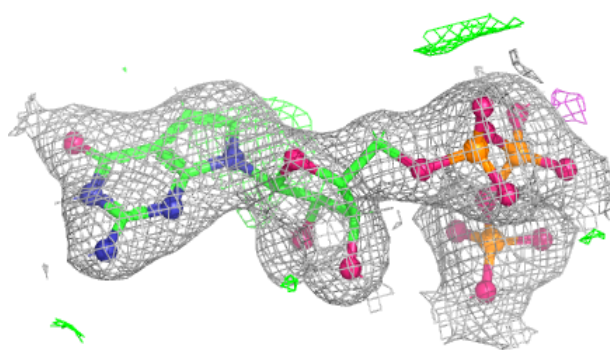
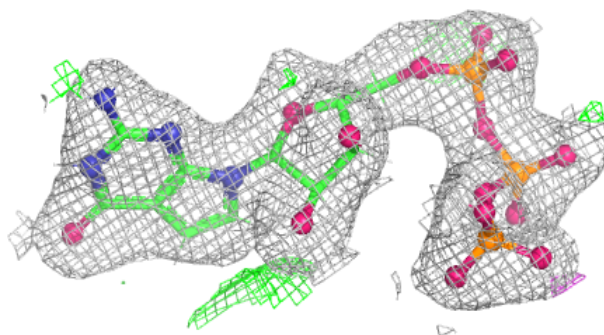


Electron density around PHE m 101:

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

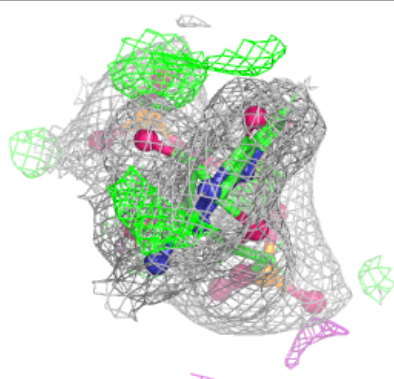
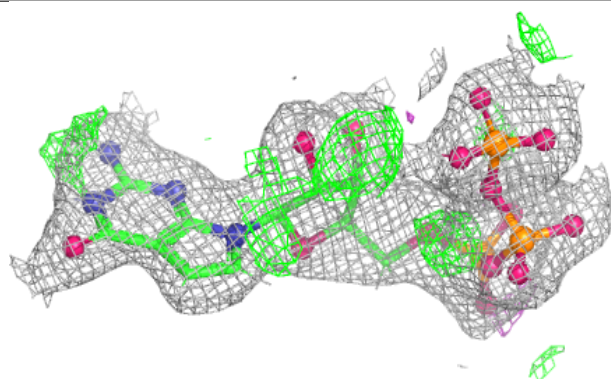
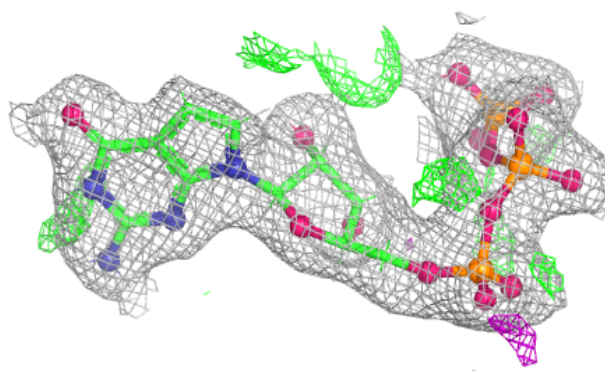
**Electron density around QBQ R 302:**

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

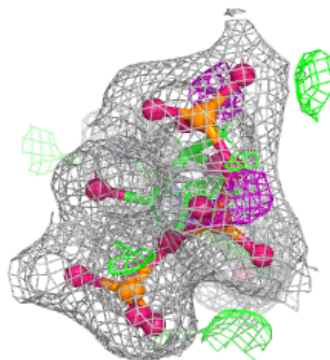
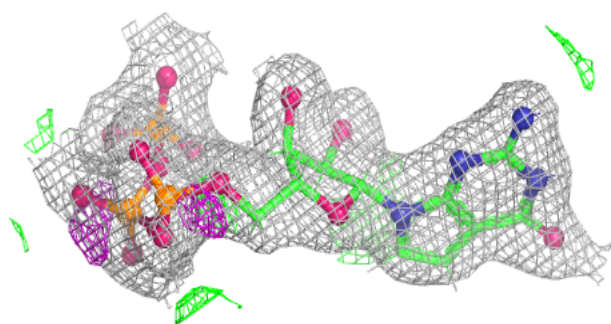
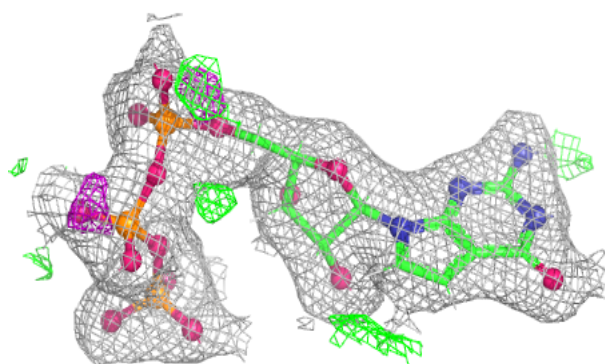


Electron density around QBQ L 1101:

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

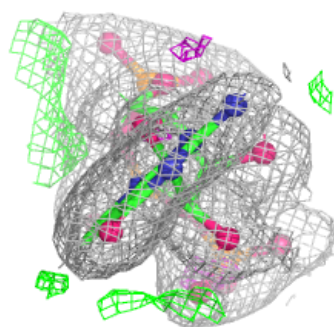
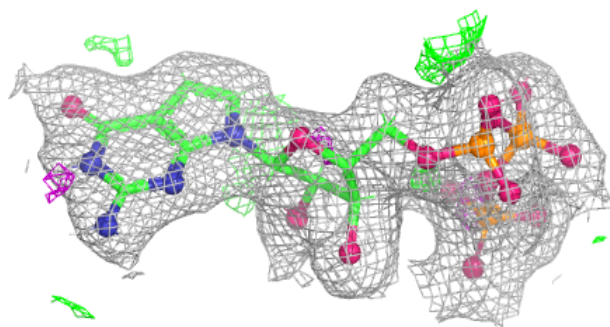
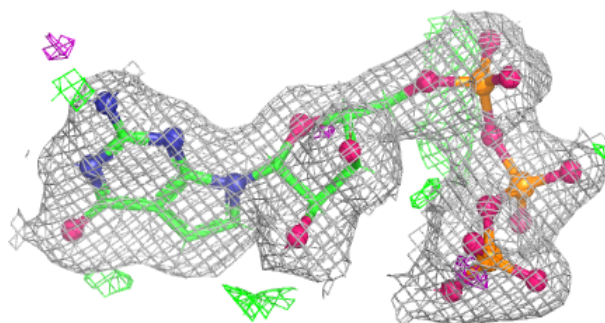
**Electron density around QBQ Q 302:**

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

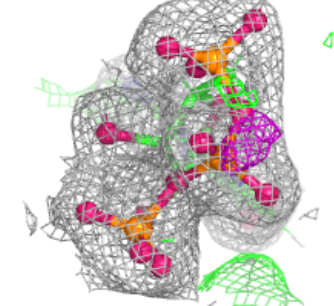
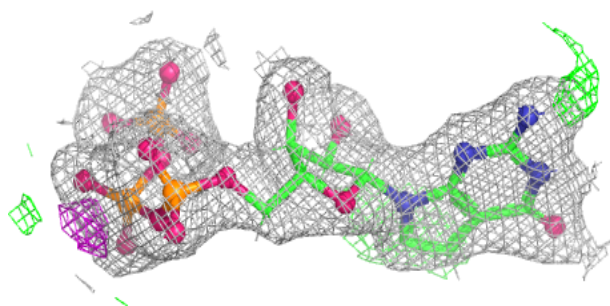
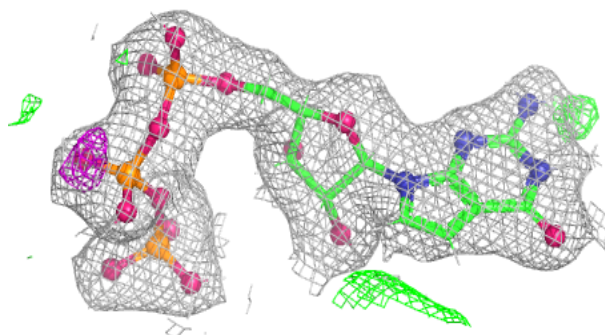


Electron density around QBQ E 302:

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

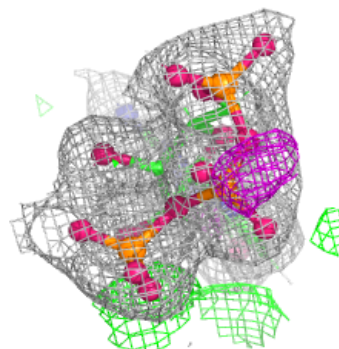
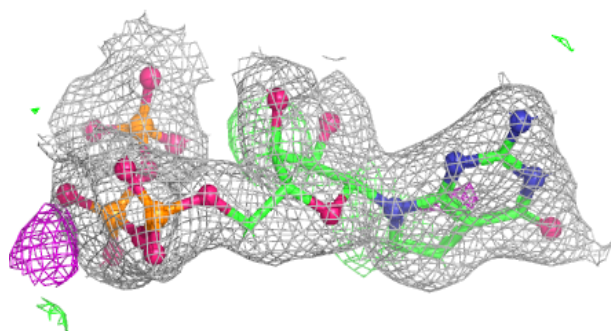
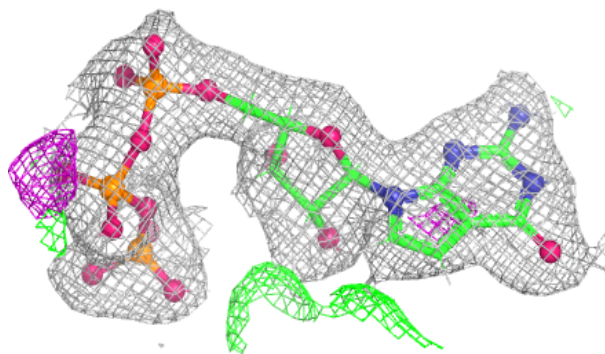
**Electron density around QBQ M 1101:**

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

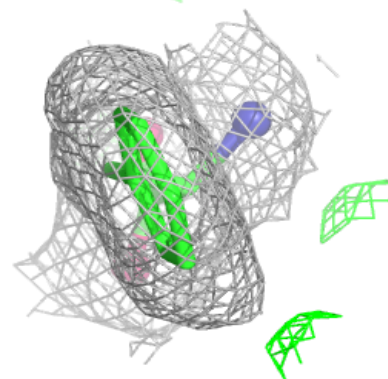
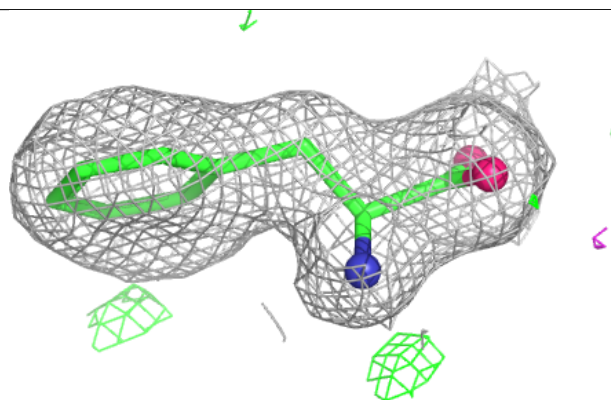
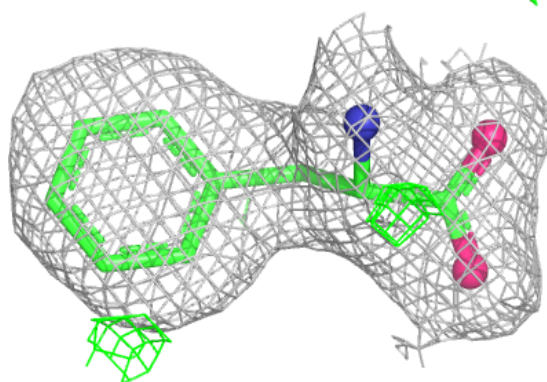


Electron density around QBQ S 302:

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

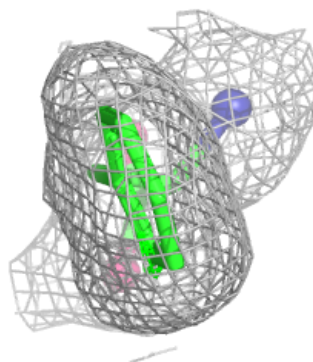
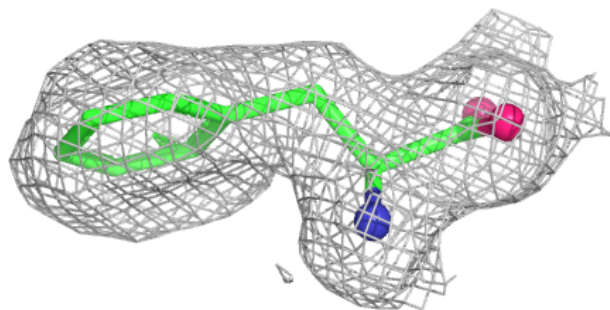
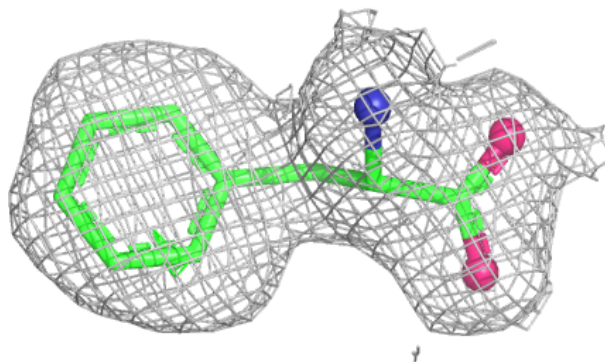
**Electron density around PHE a 101:**

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

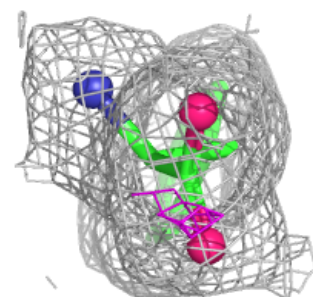
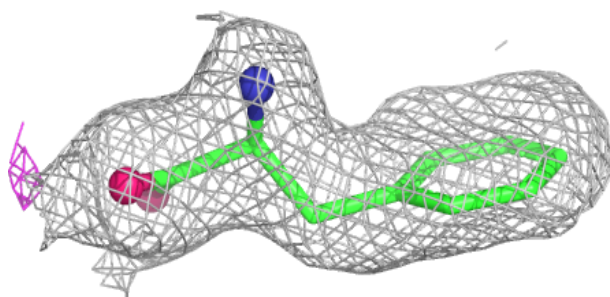
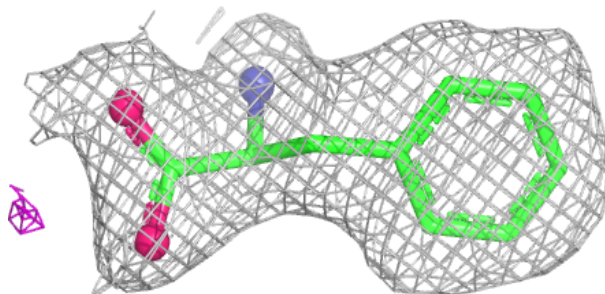


Electron density around PHE c 101:

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

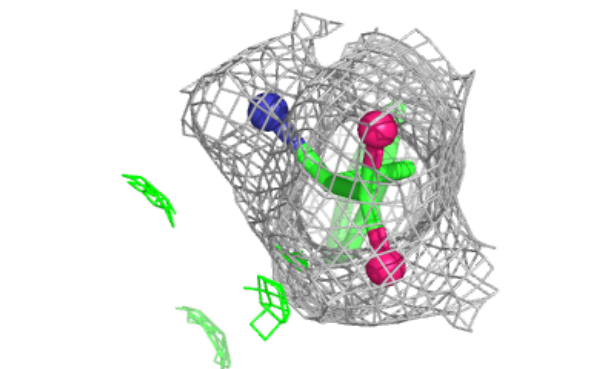
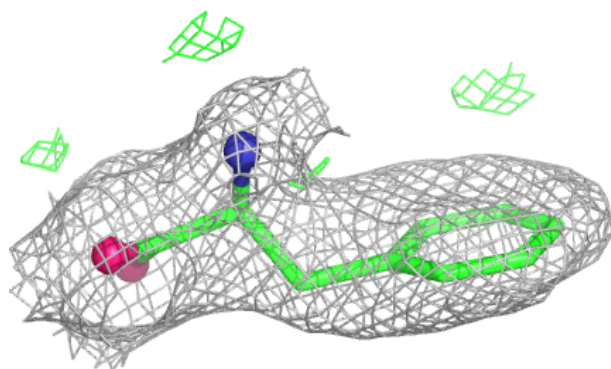
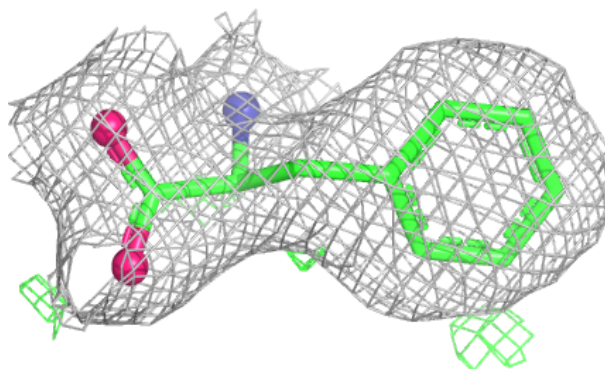
**Electron density around PHE d 101:**

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

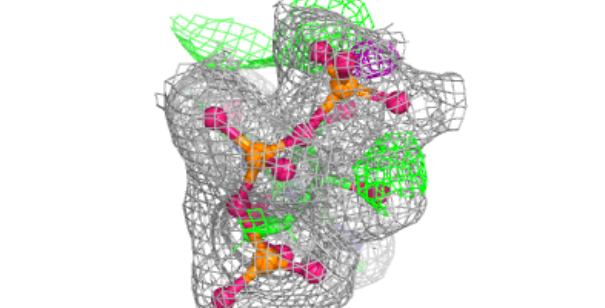
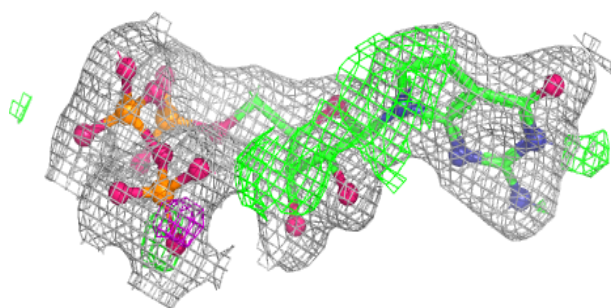
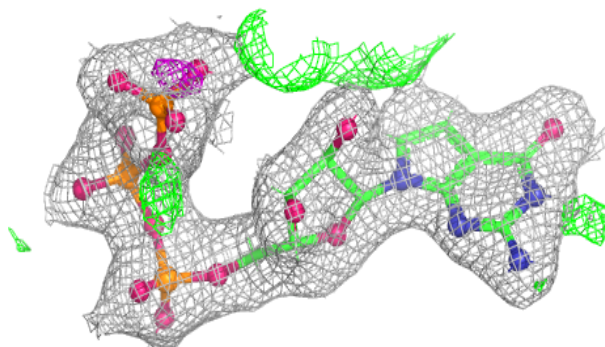


Electron density around PHE k 101:

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

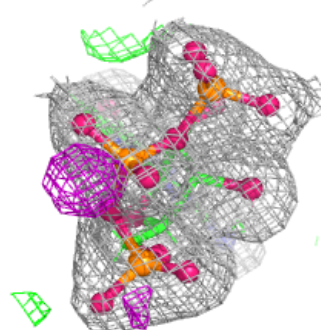
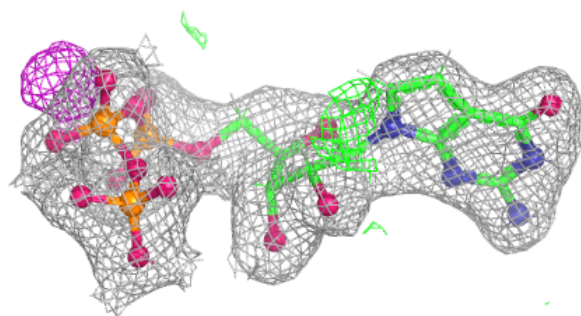
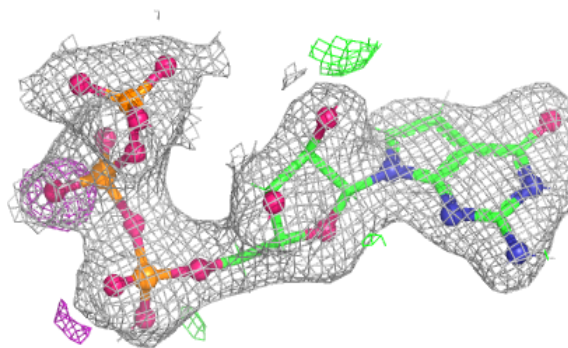
**Electron density around QBQ G 302:**

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

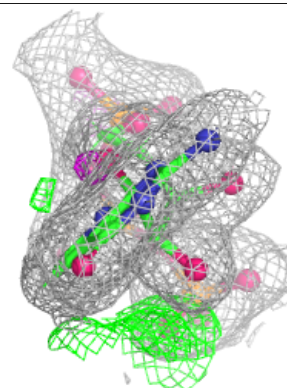
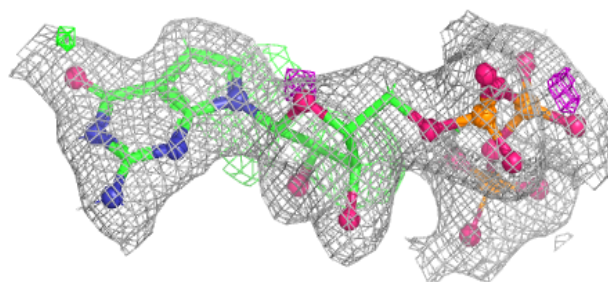
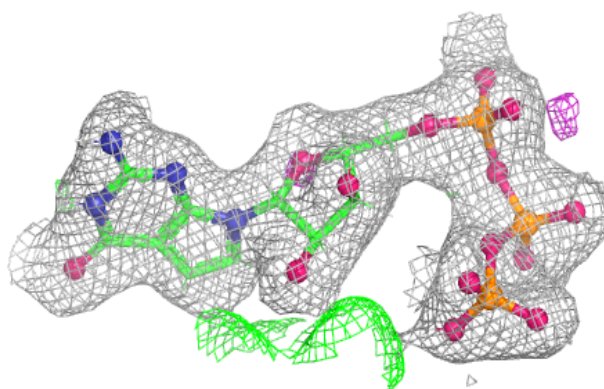


Electron density around QBQ K 302:

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

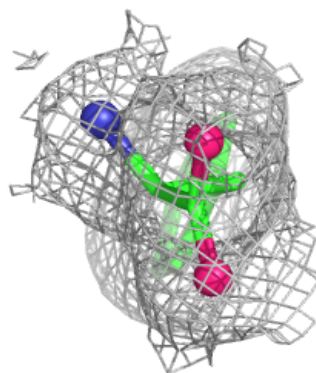
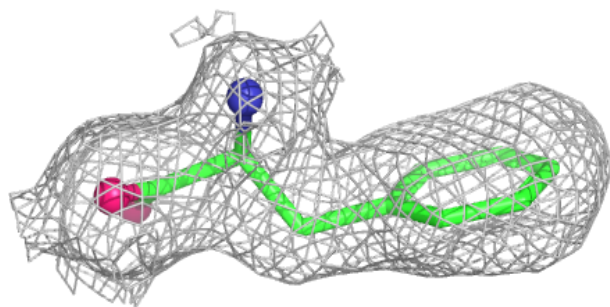
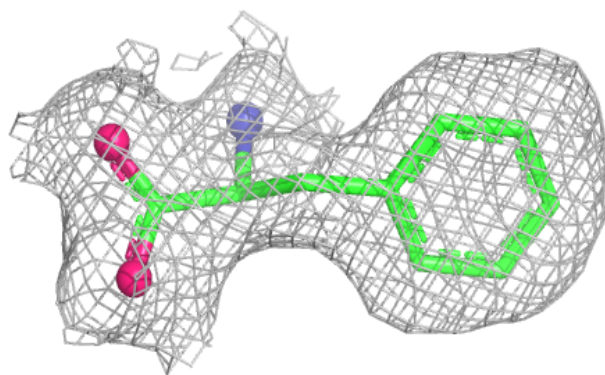
**Electron density around QBQ C 302:**

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

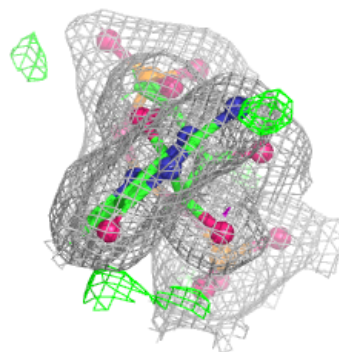
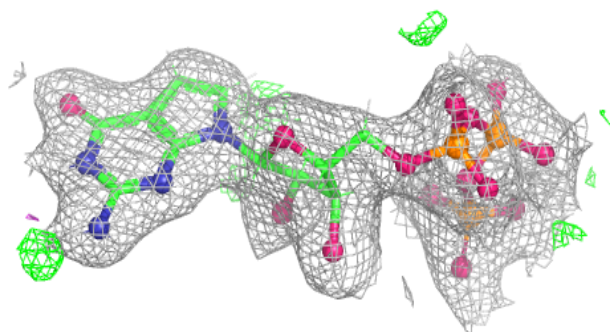
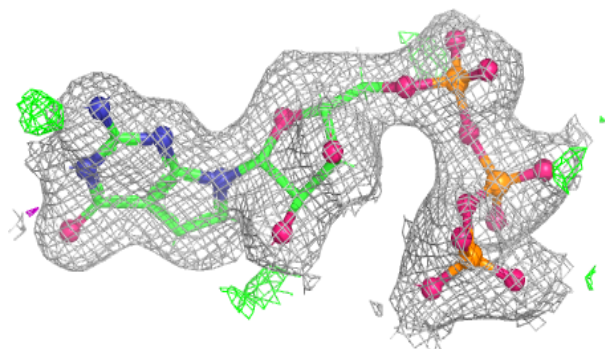


Electron density around PHE b 101:

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

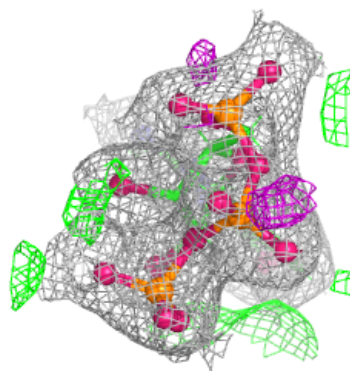
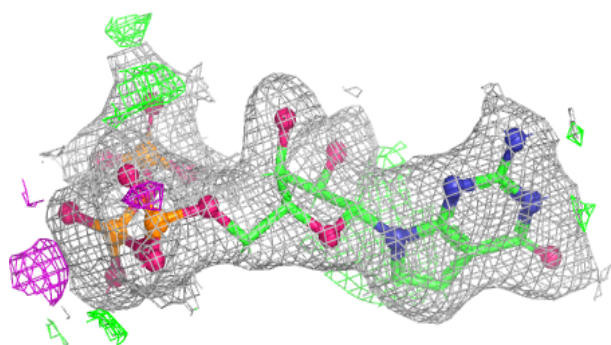
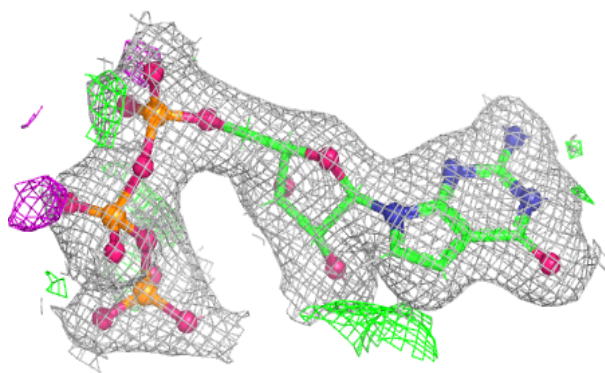
**Electron density around QBQ I 302:**

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

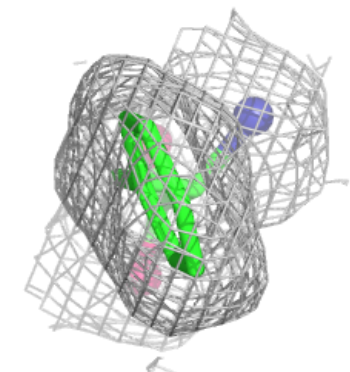
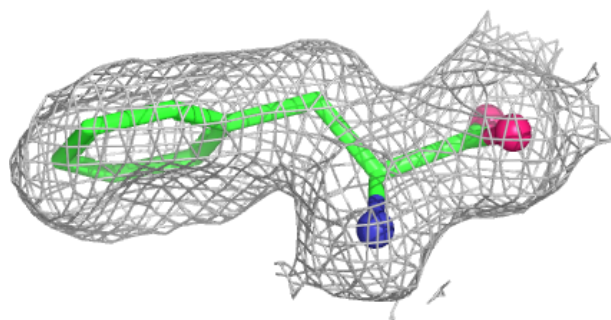
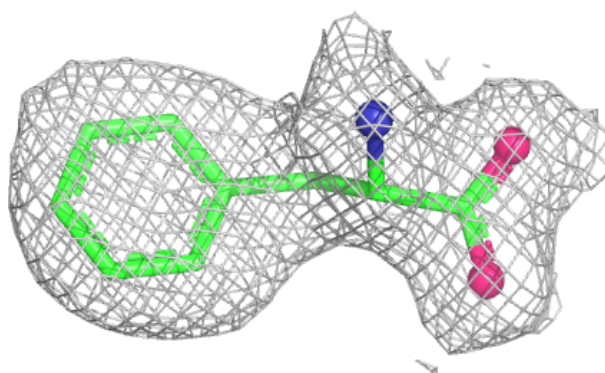


Electron density around QBQ D 302:

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

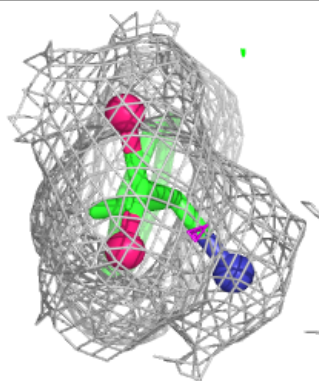
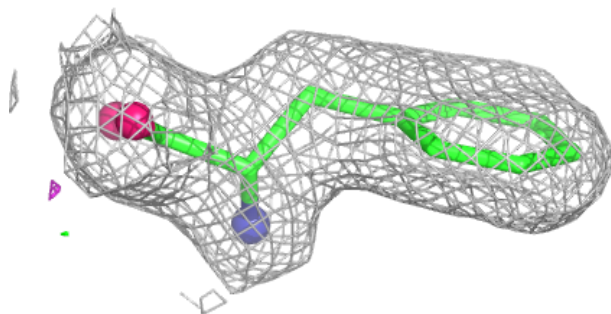
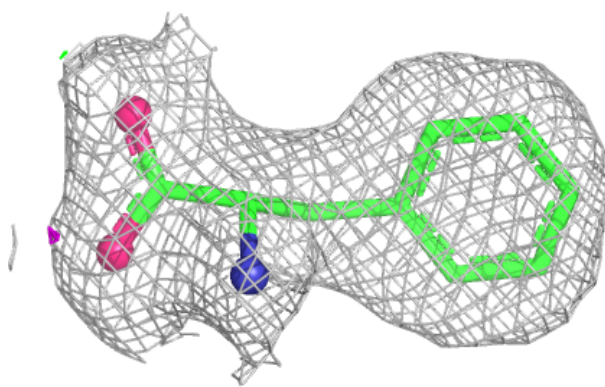
**Electron density around PHE e 101:**

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

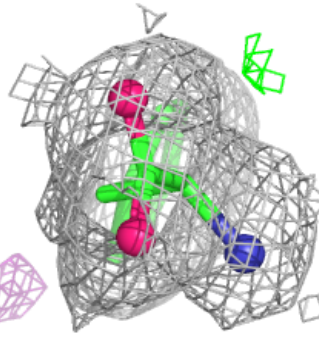
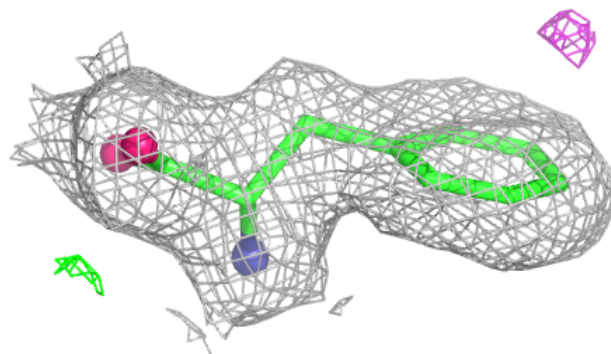
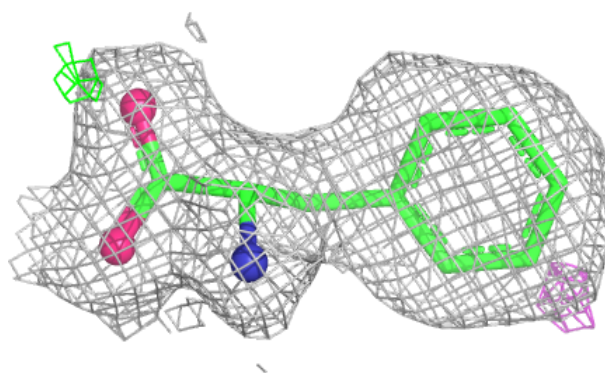


Electron density around PHE f 101:

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

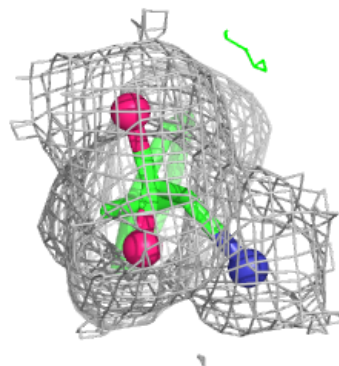
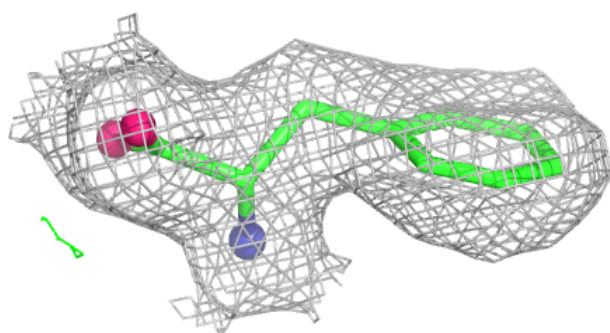
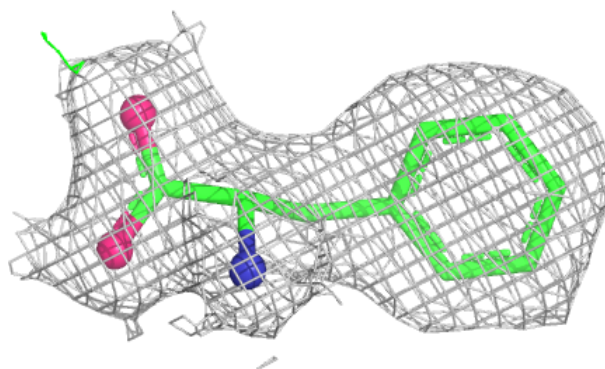
**Electron density around PHE f 102:**

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



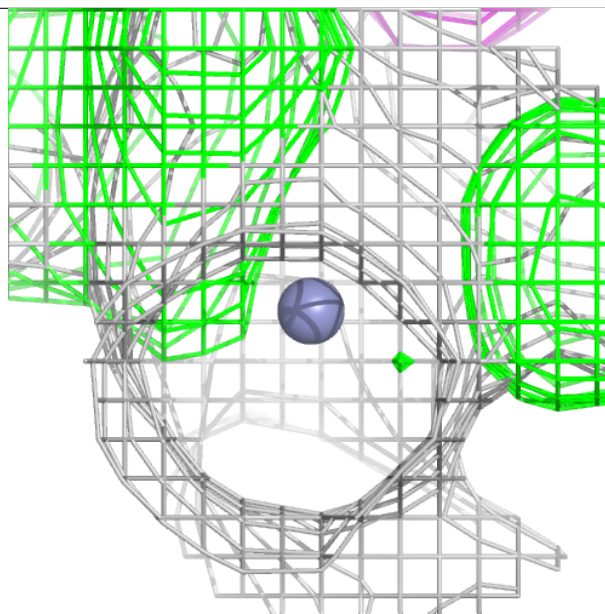
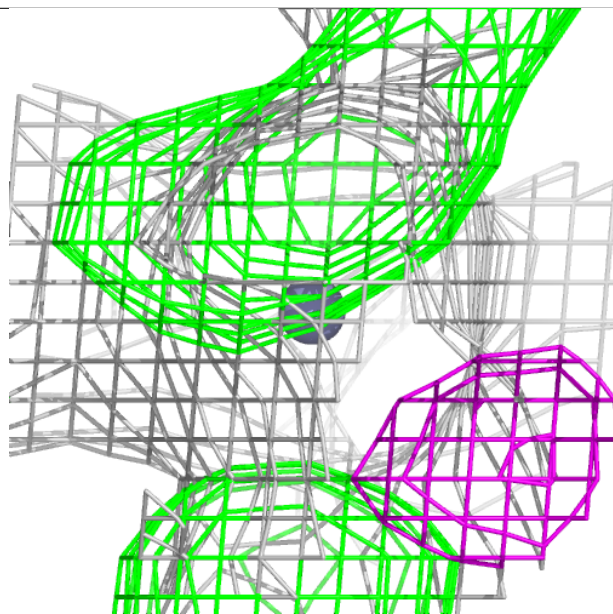
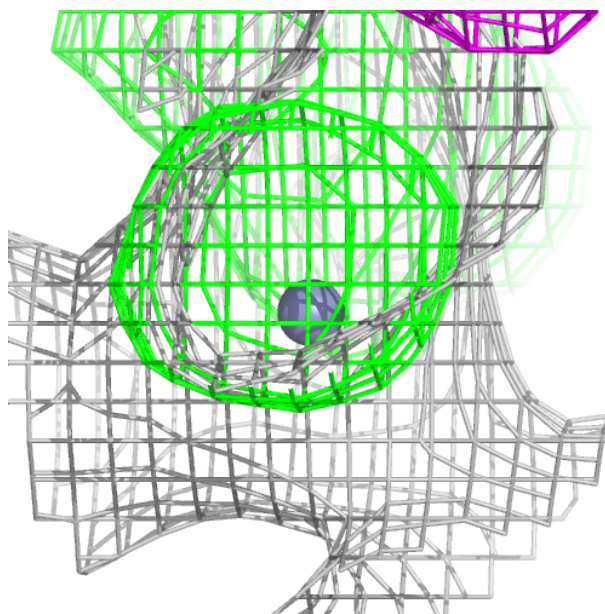
Electron density around PHE g 101:

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



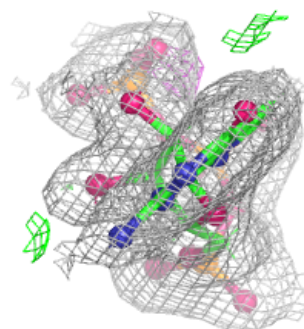
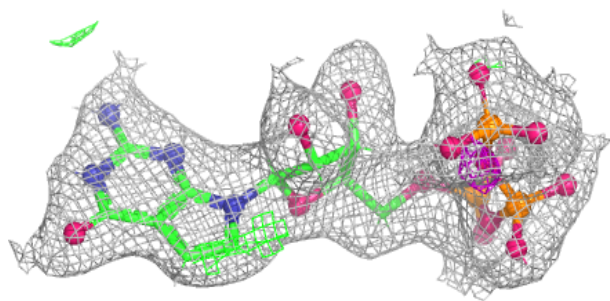
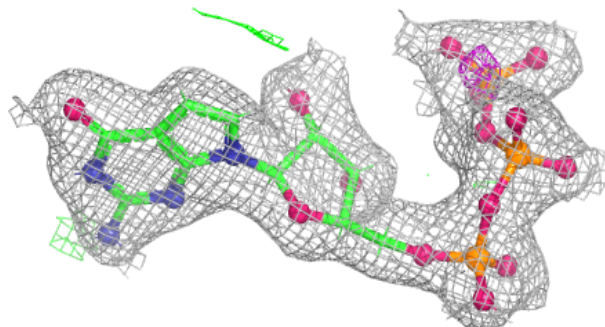
Electron density around ZN T 301:

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

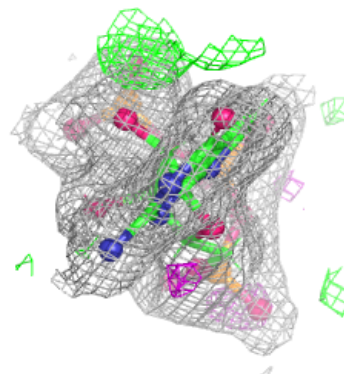
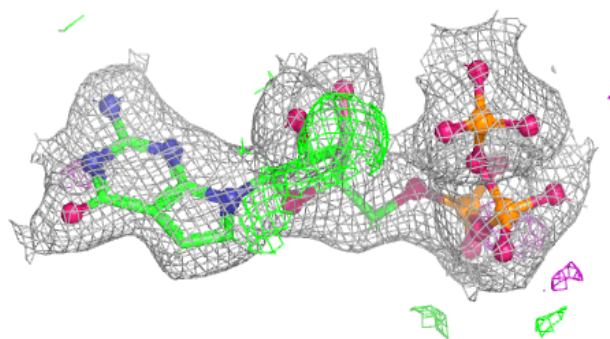
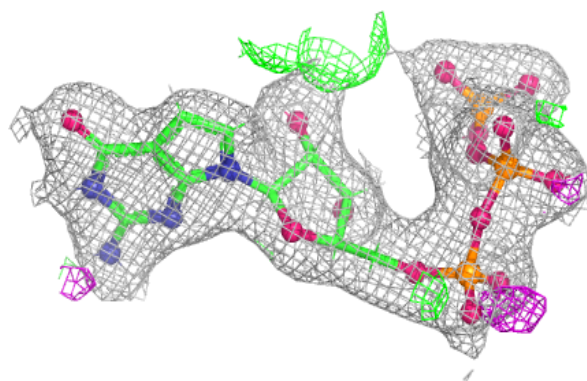


Electron density around QBQ A 302:

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

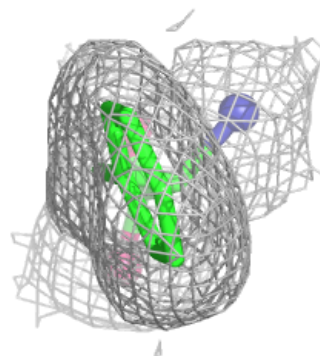
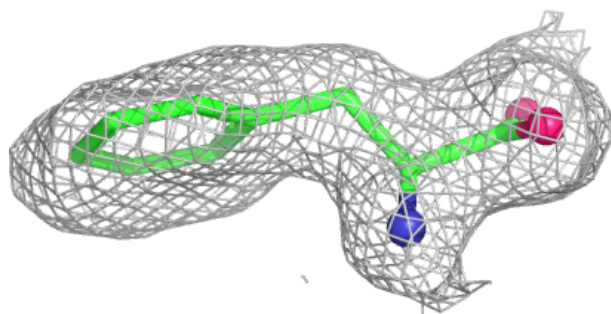
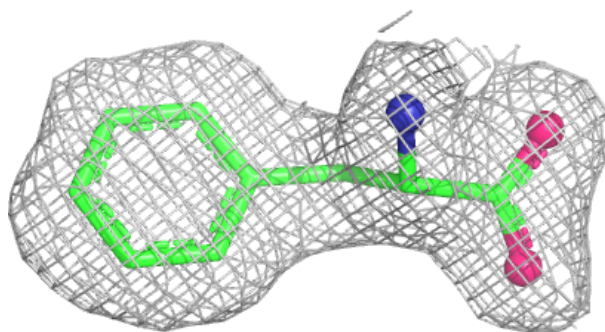
**Electron density around QBQ T 302:**

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



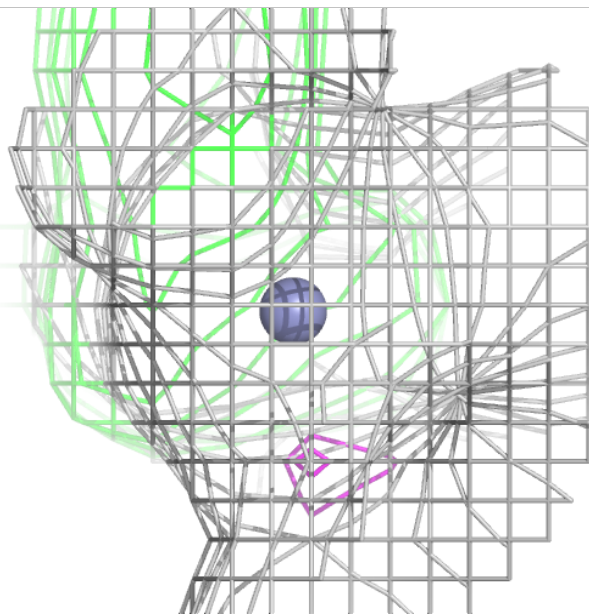
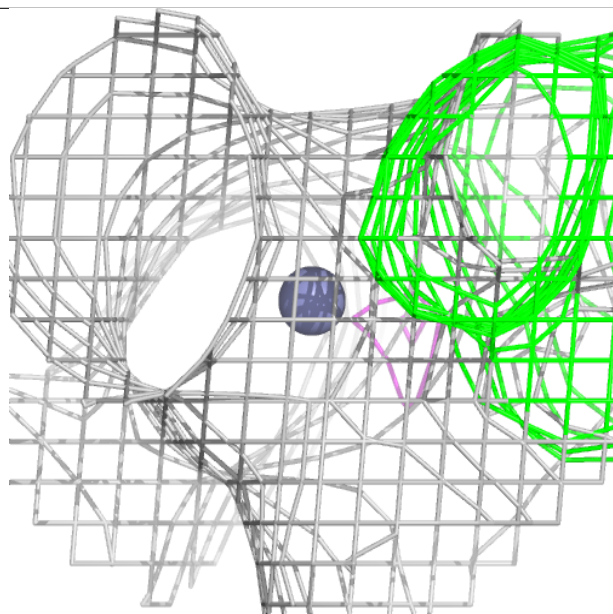
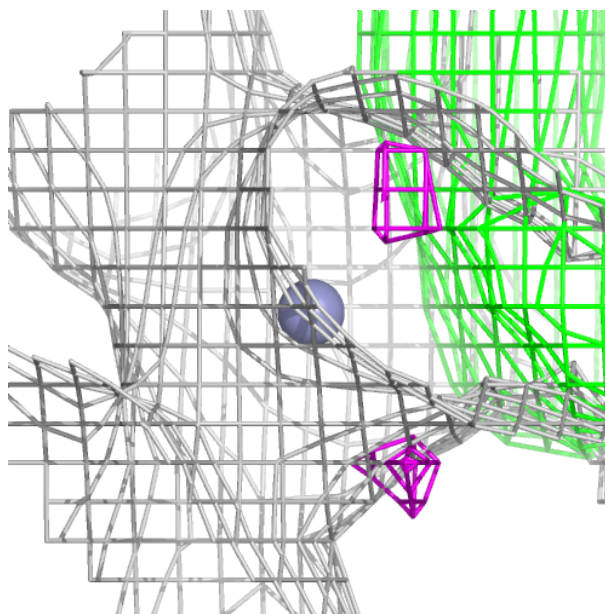
Electron density around PHE n 101:

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



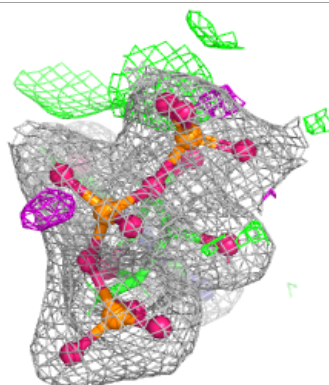
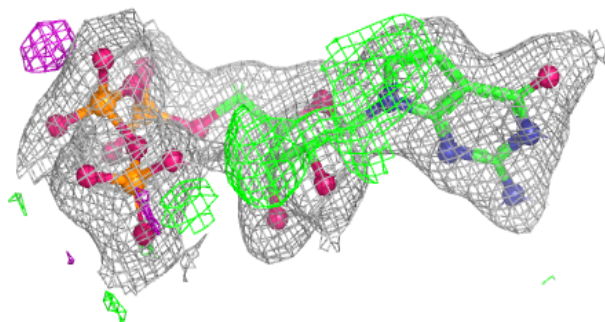
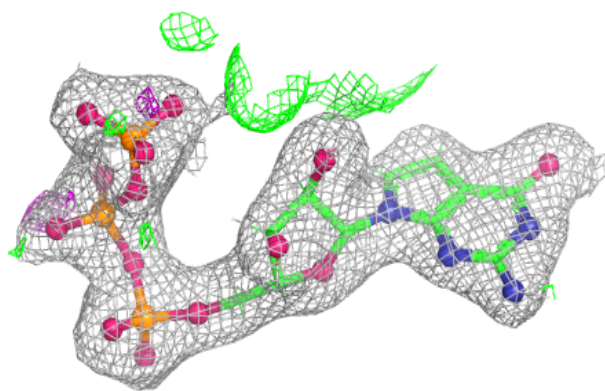
Electron density around ZN E 301:

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



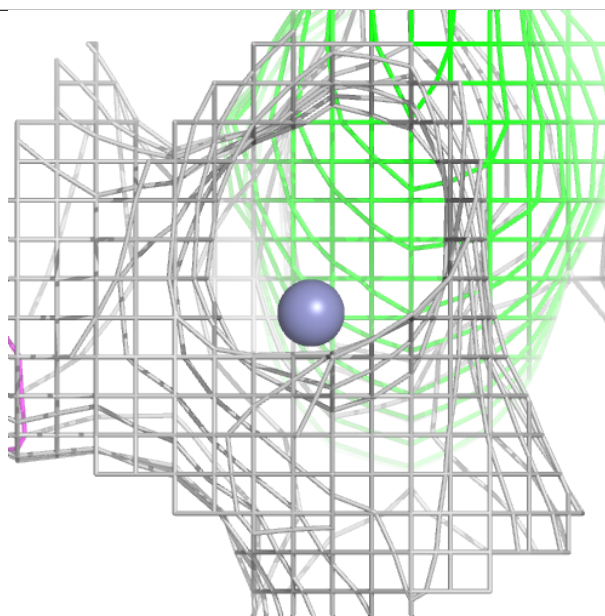
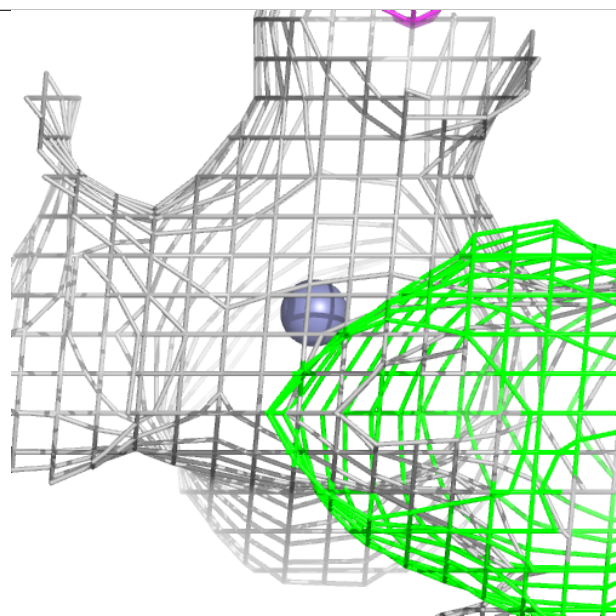
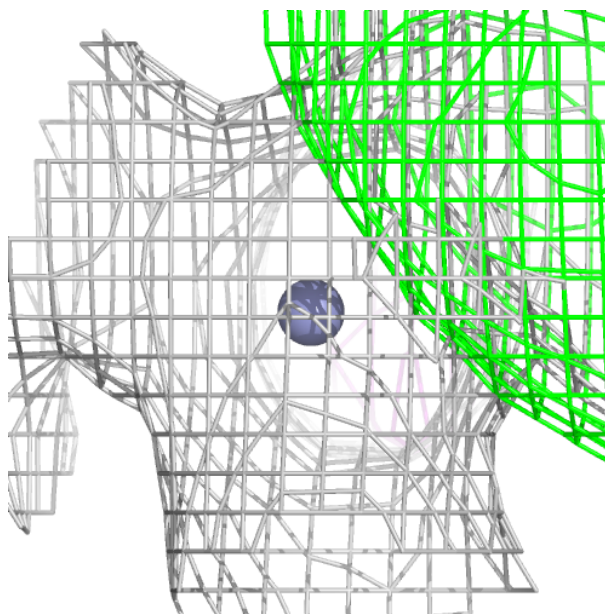
Electron density around QBQ B 302:

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



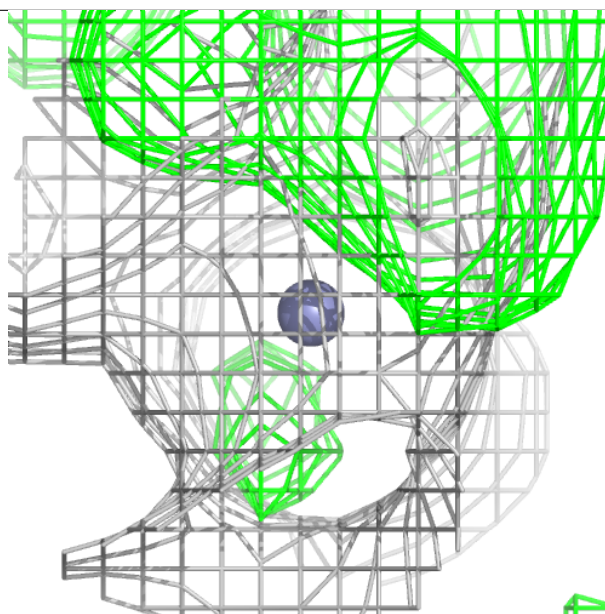
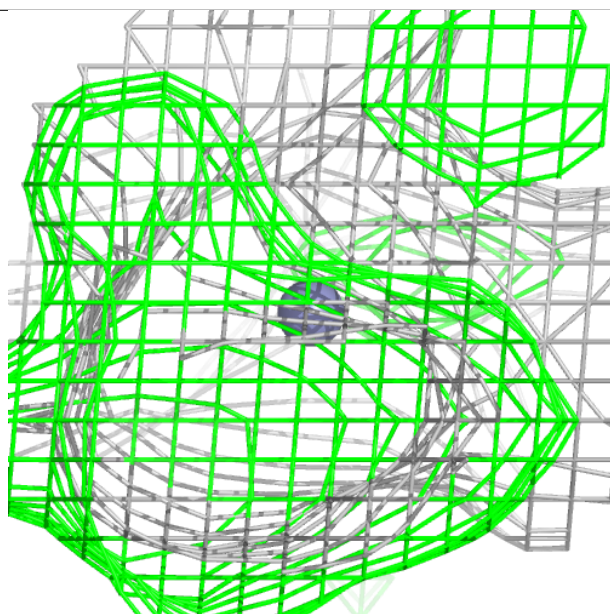
Electron density around ZN F 301:

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



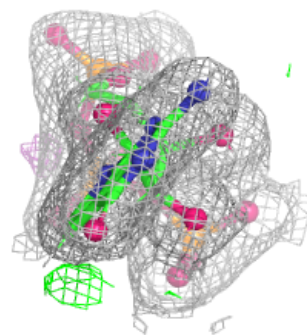
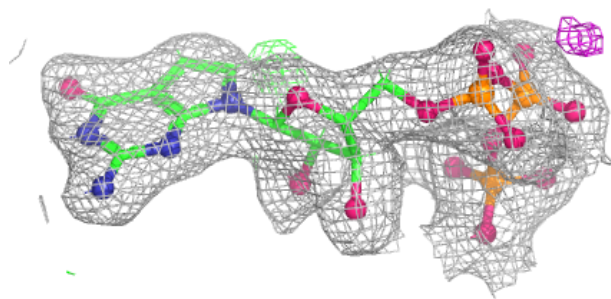
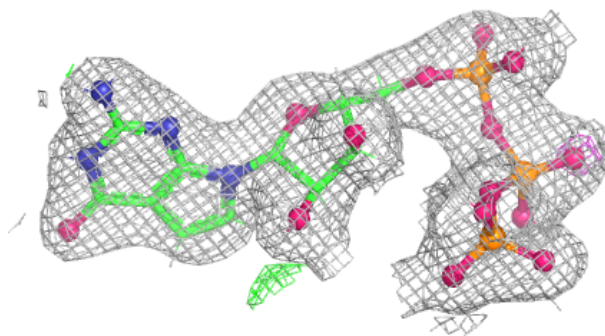
Electron density around ZN J 301:

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



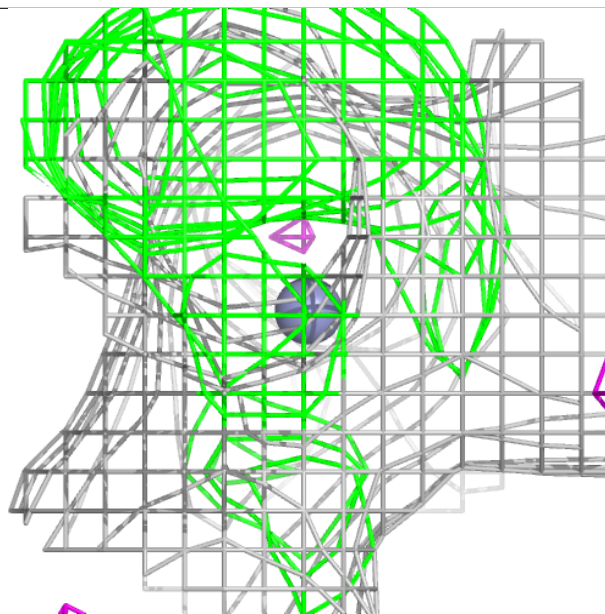
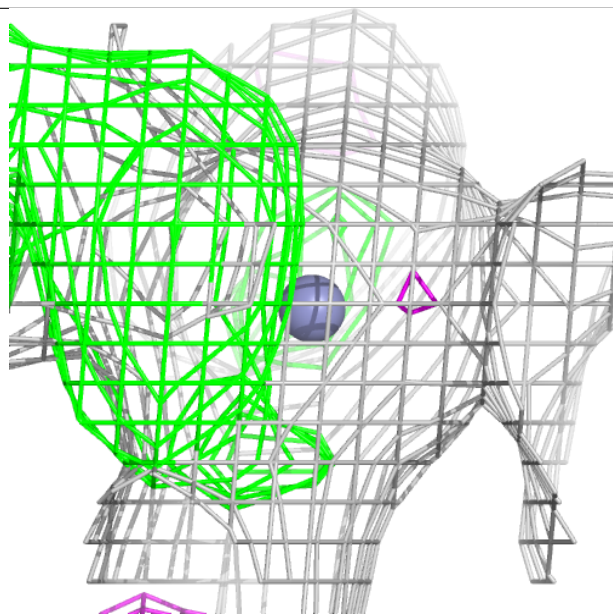
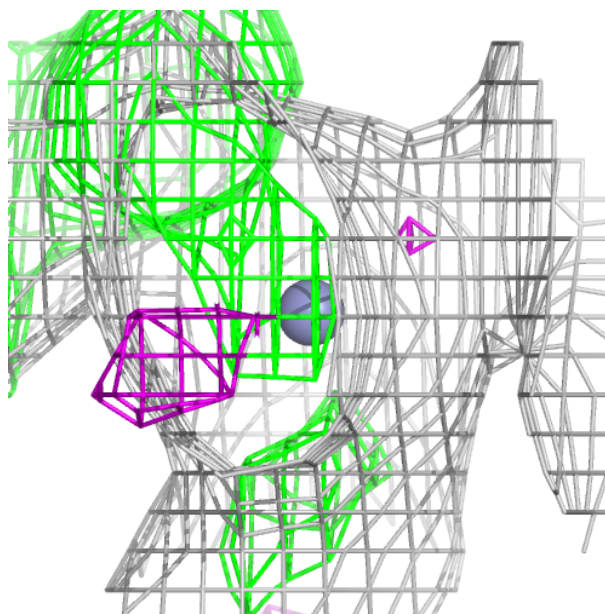
Electron density around QBQ O 302:

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



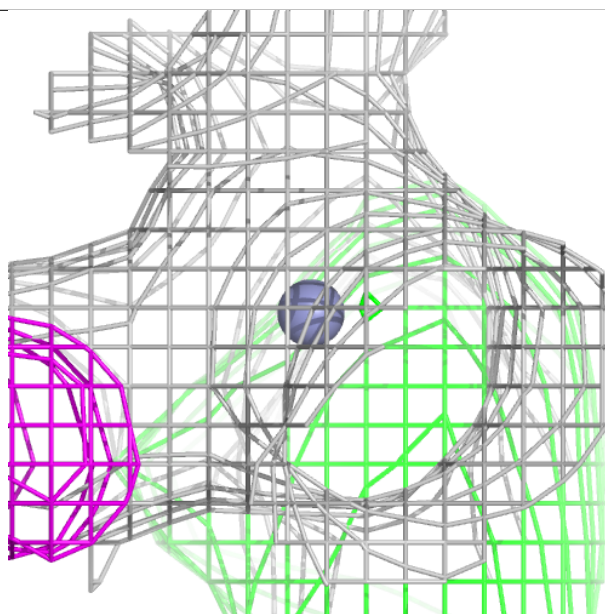
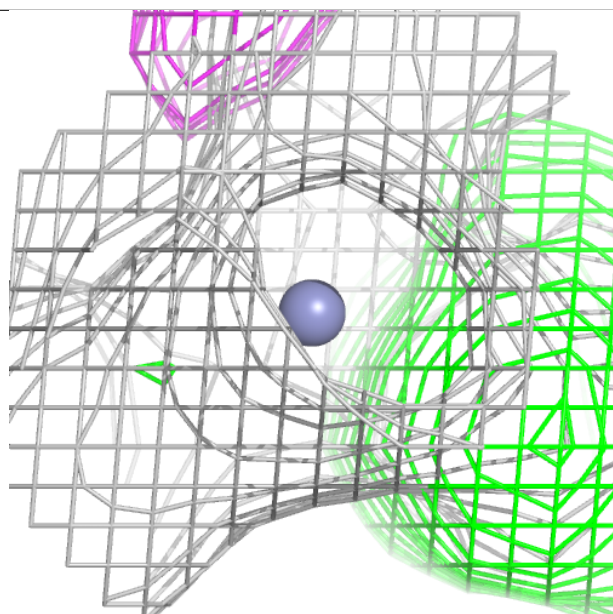
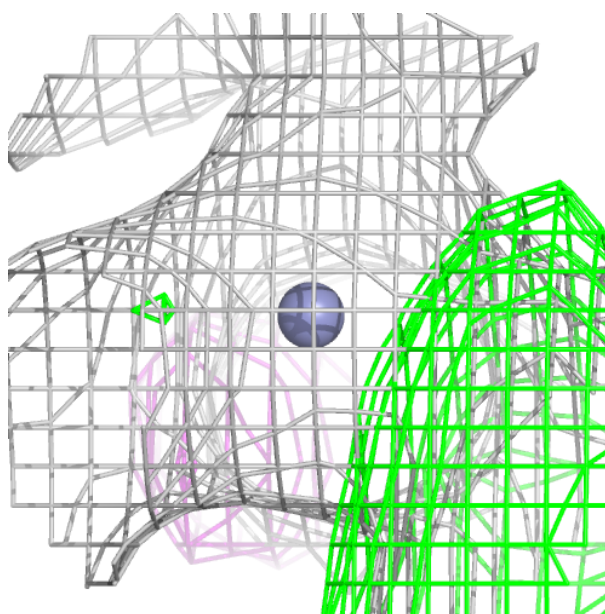
Electron density around ZN P 301:

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



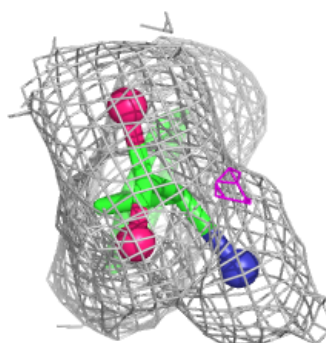
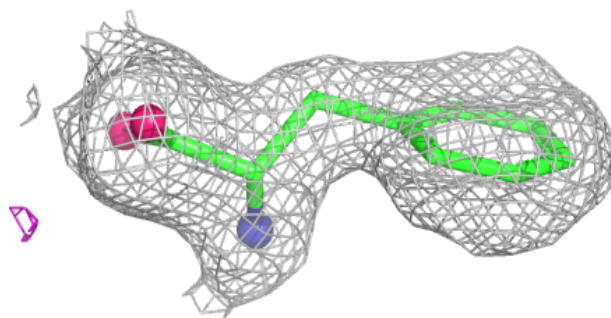
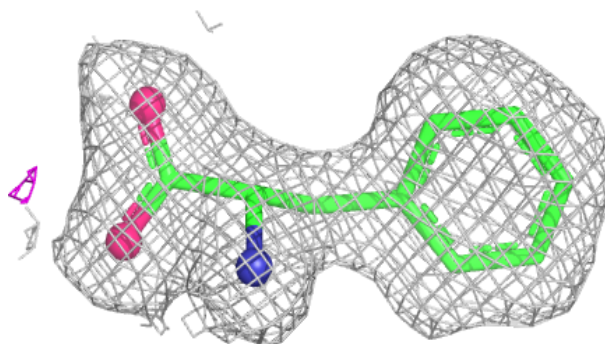
Electron density around ZN Q 301:

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

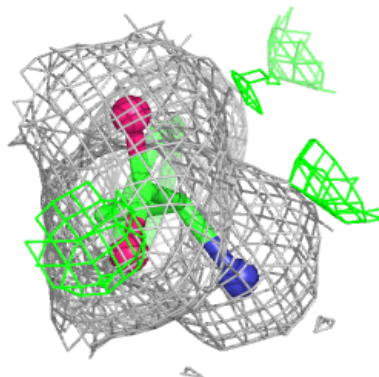
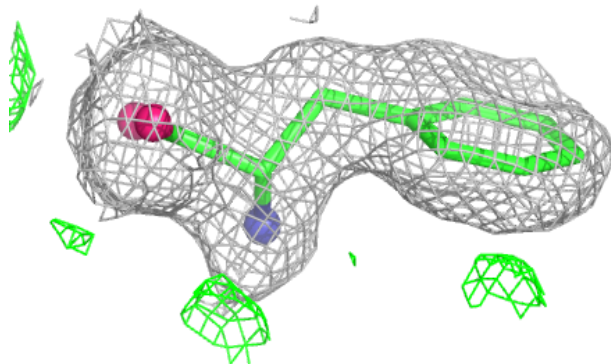
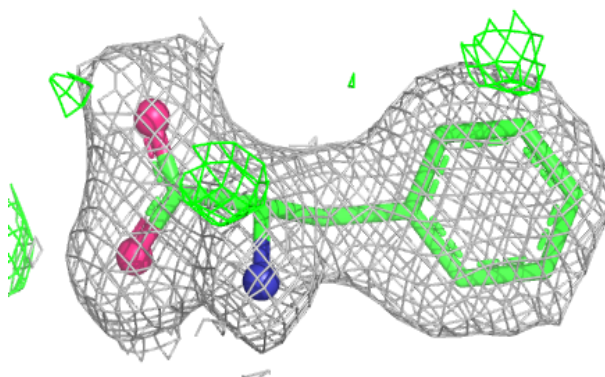


Electron density around PHE h 101:

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

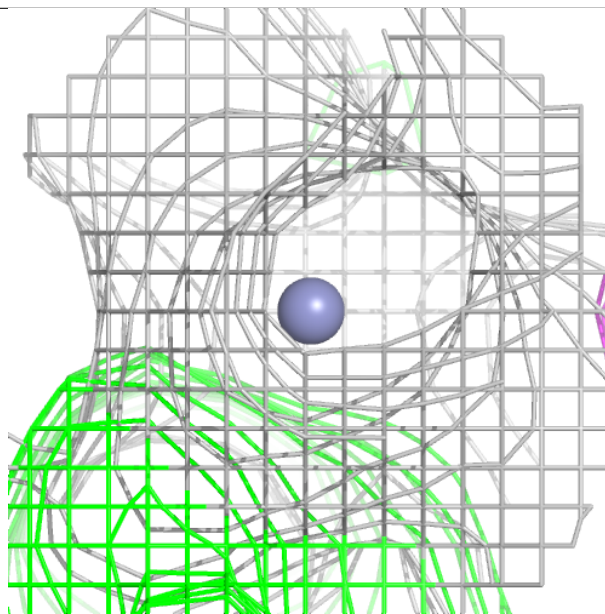
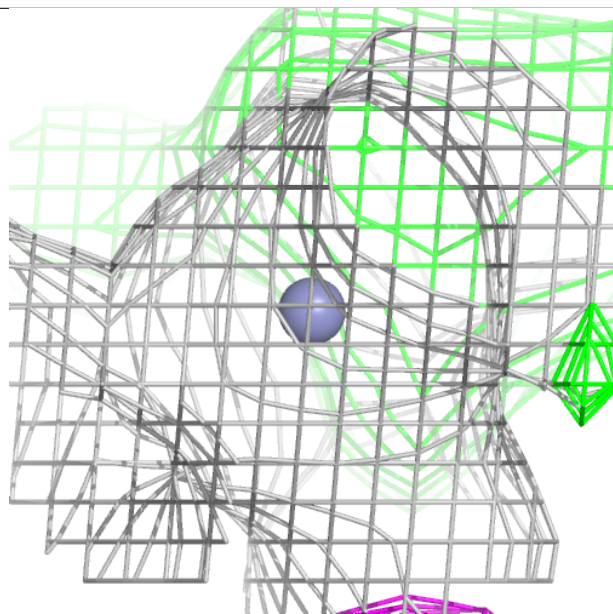
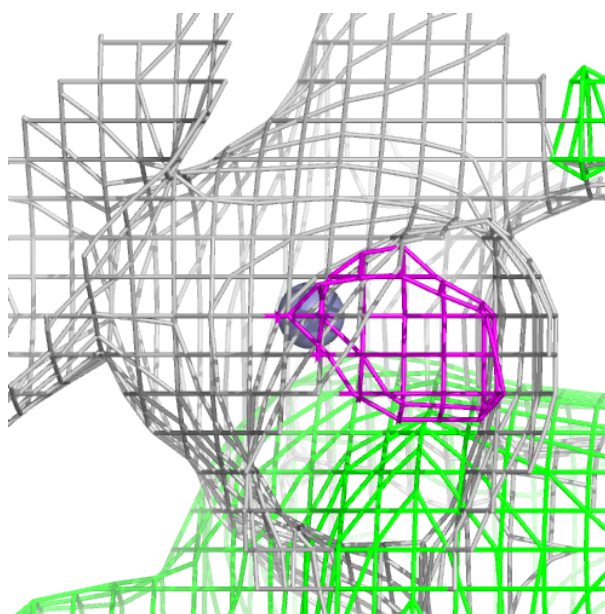
**Electron density around PHE i 101:**

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



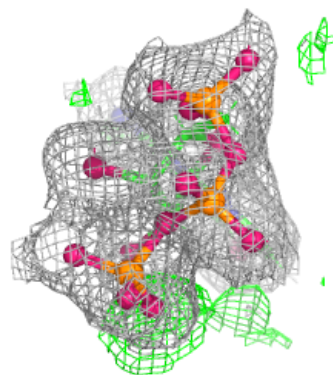
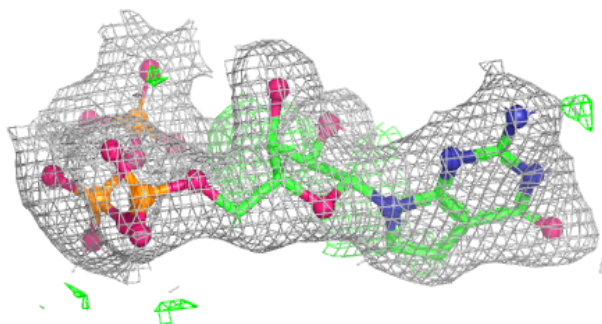
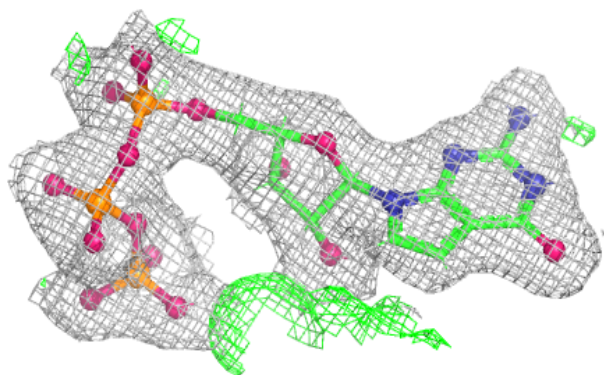
Electron density around ZN R 301:

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



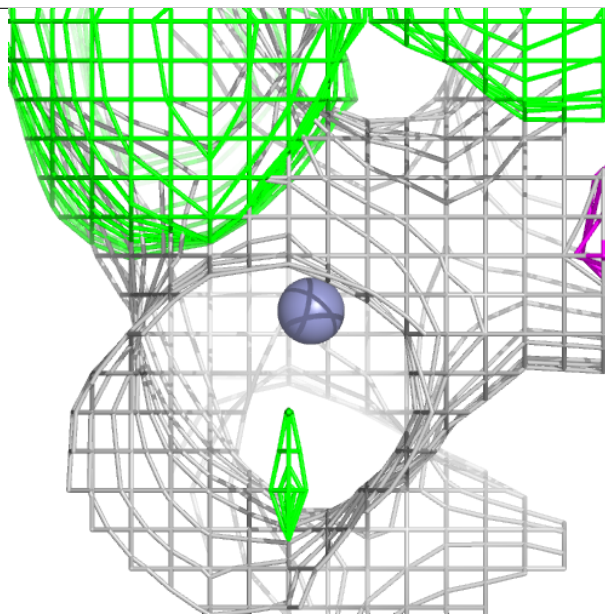
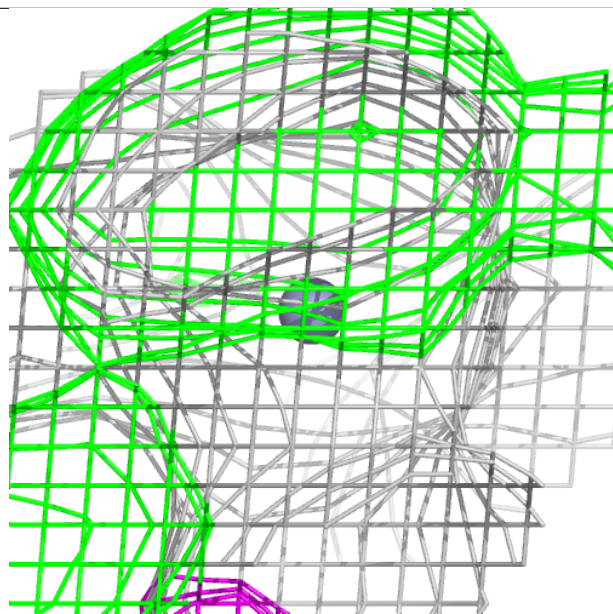
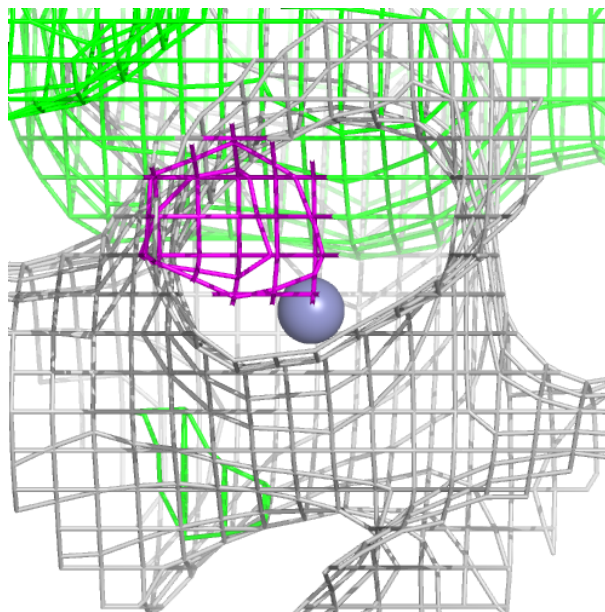
Electron density around QBQ H 302:

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



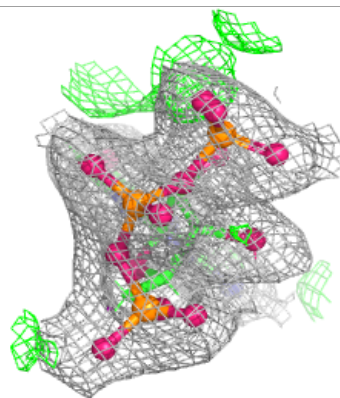
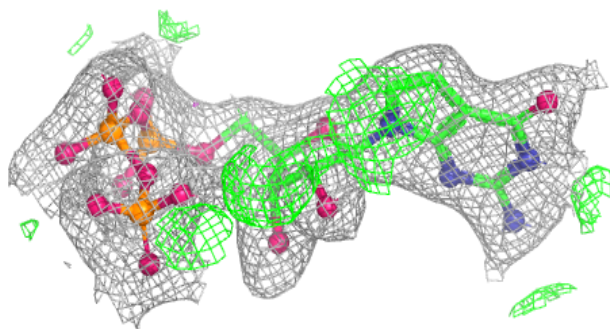
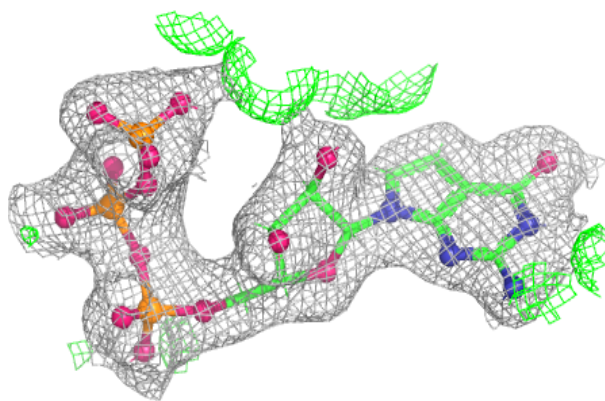
Electron density around ZN A 301:

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

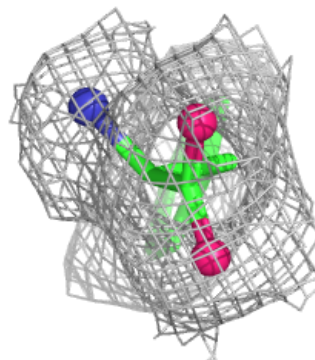
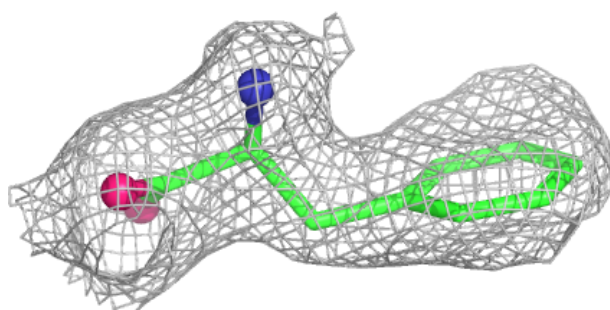
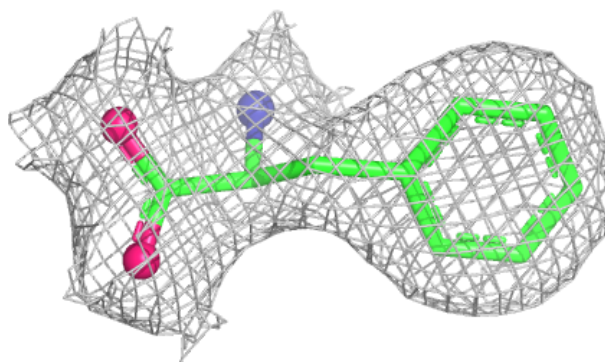


Electron density around QBQ J 302:

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

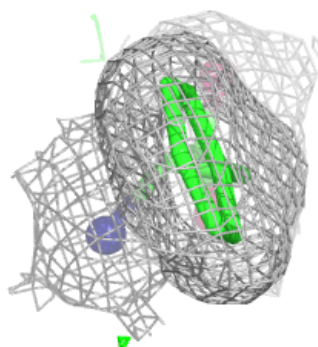
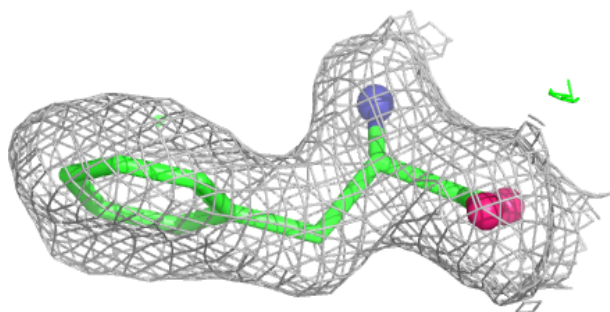
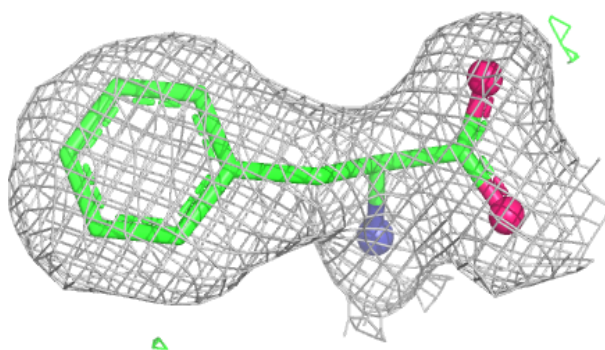
**Electron density around PHE o 101:**

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

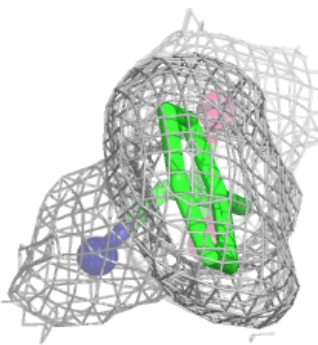
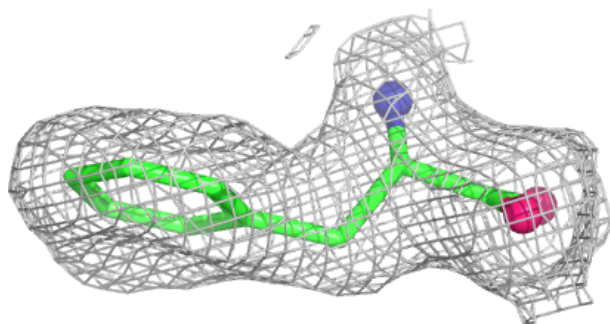
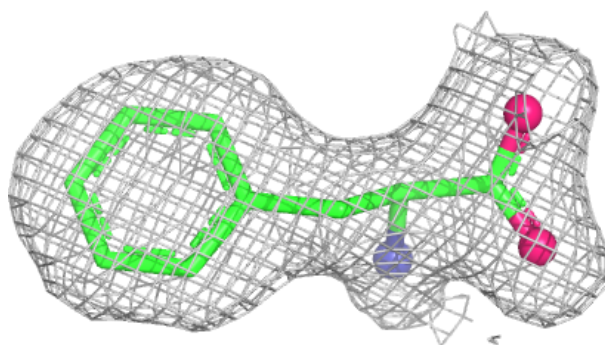


Electron density around PHE p 101:

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

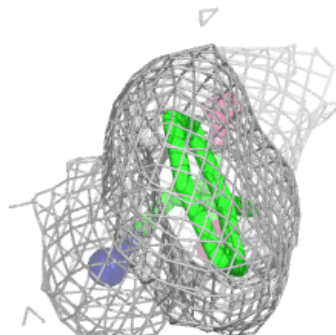
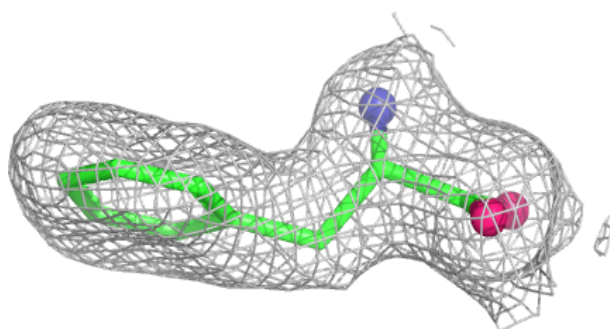
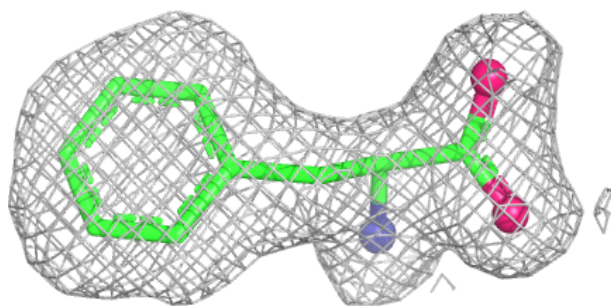
**Electron density around PHE q 101:**

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

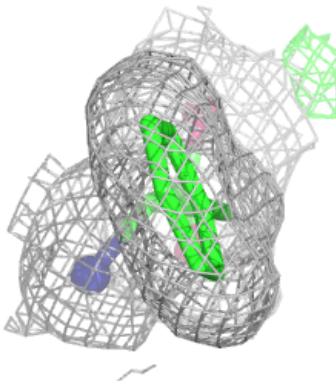
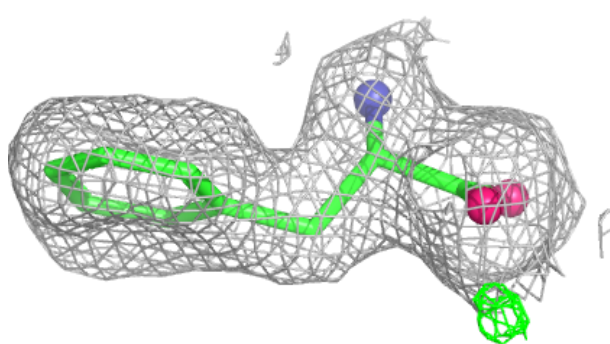
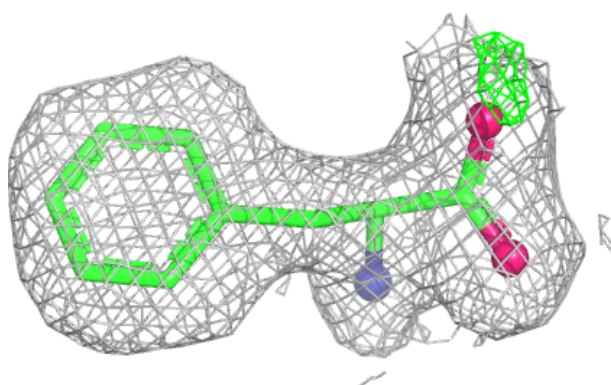


Electron density around PHE r 101:

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

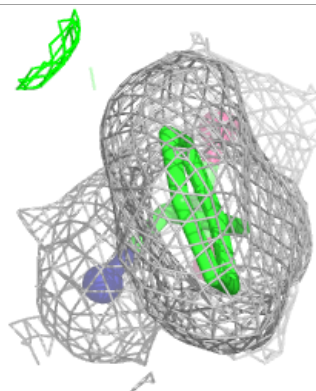
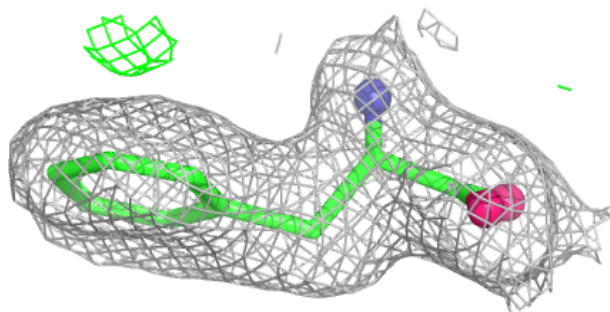
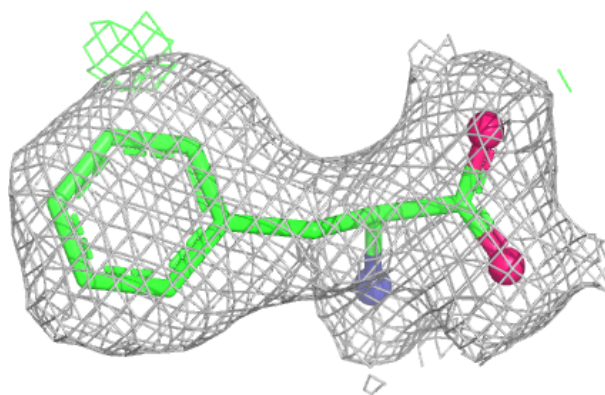
**Electron density around PHE s 101:**

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



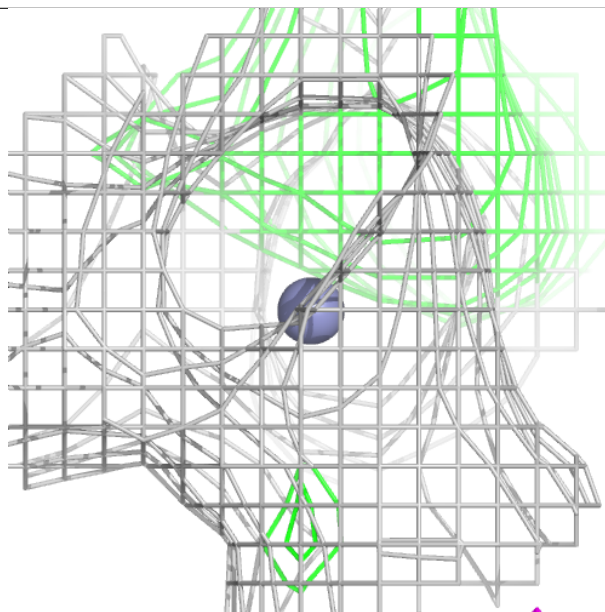
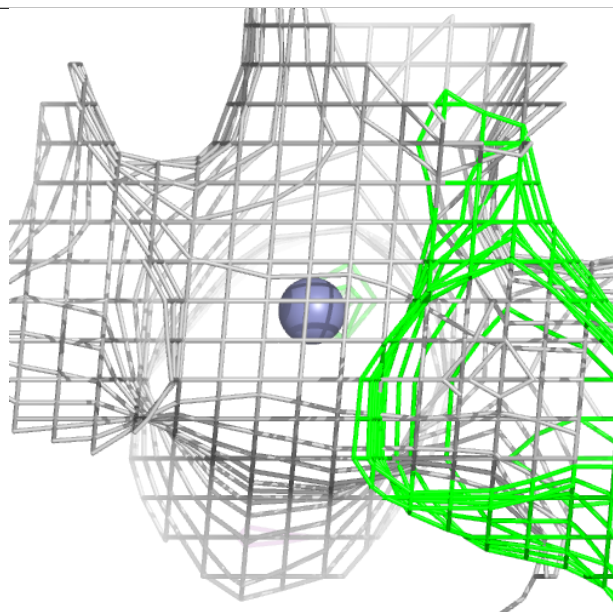
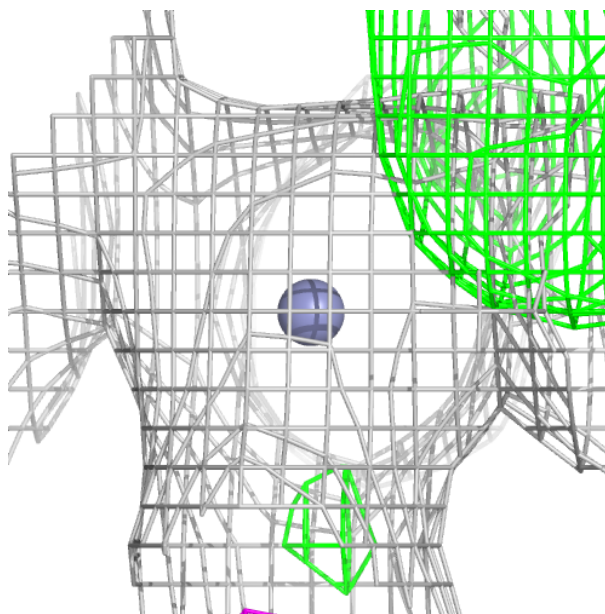
Electron density around PHE t 101:

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



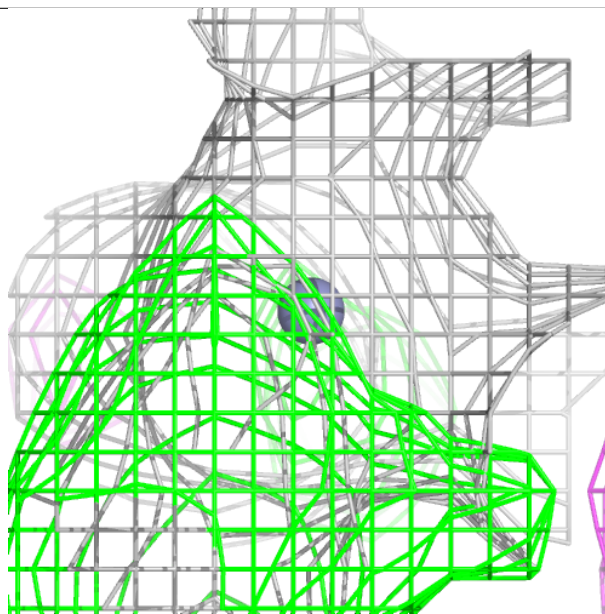
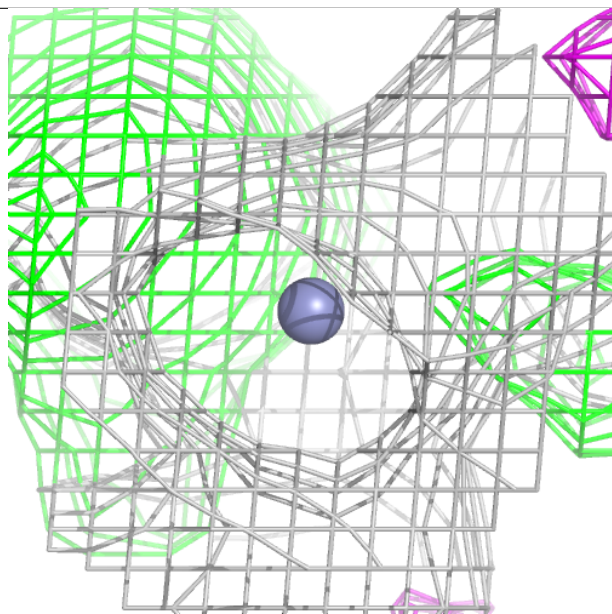
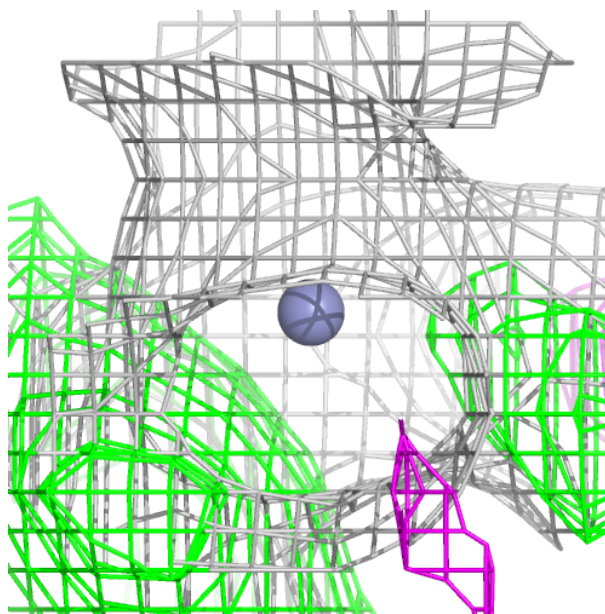
Electron density around ZN B 301:

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



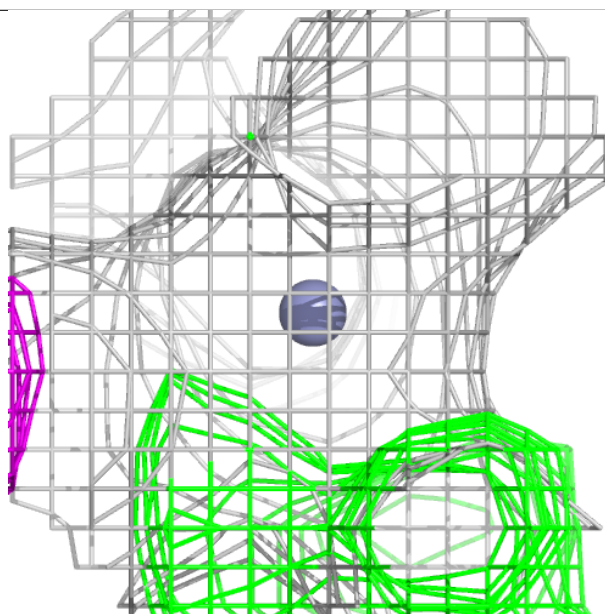
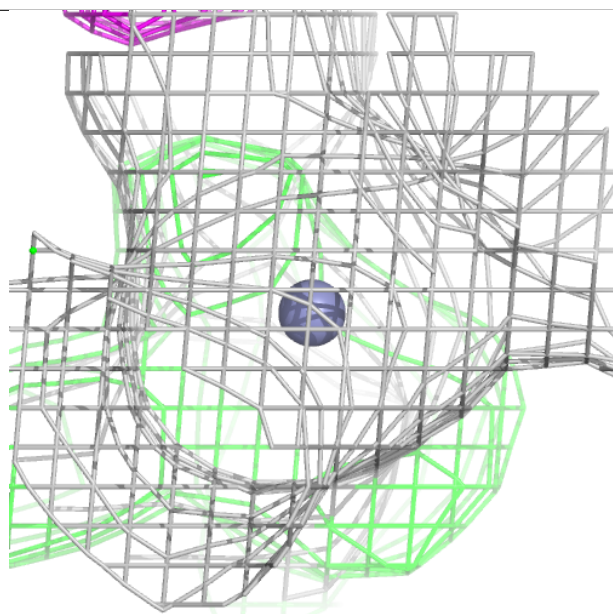
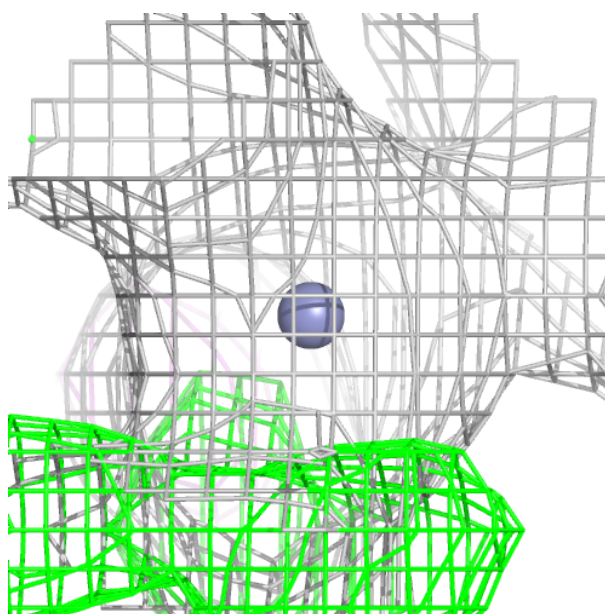
Electron density around ZN C 301:

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



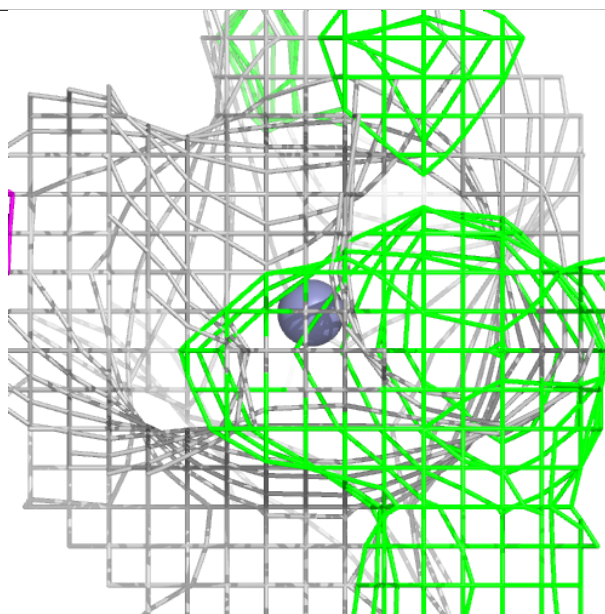
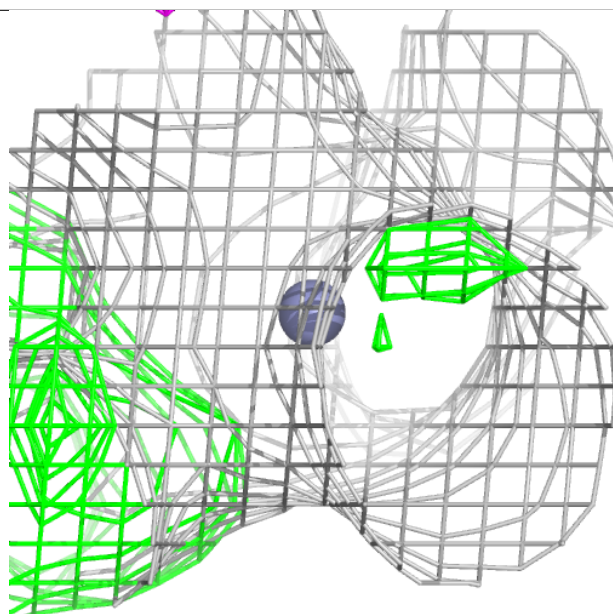
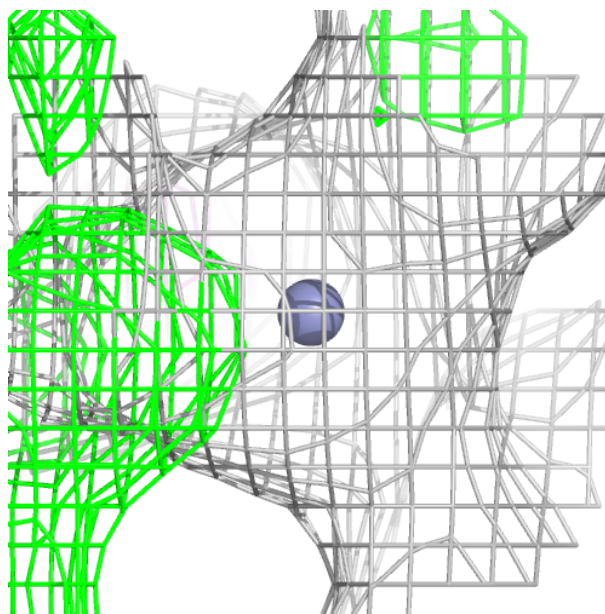
Electron density around ZN H 301:

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



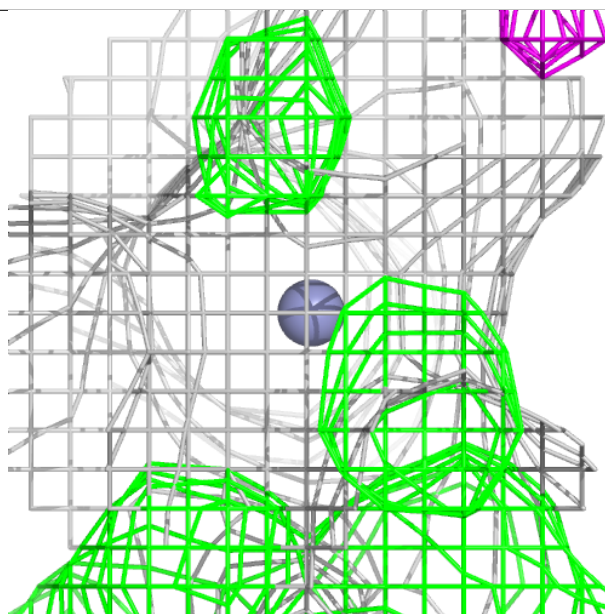
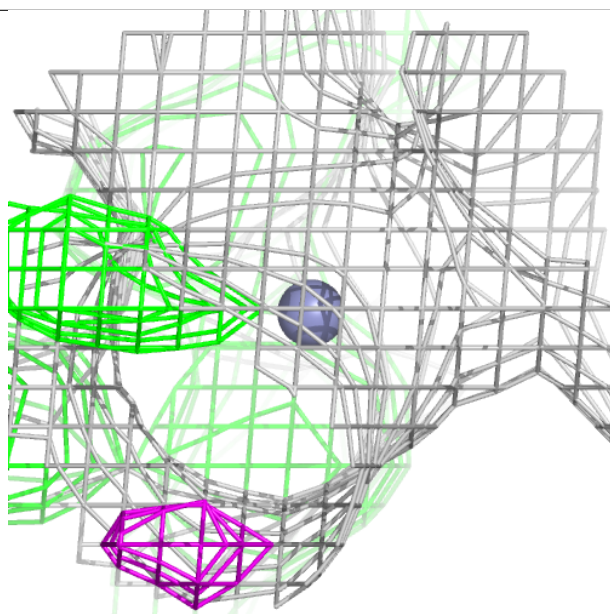
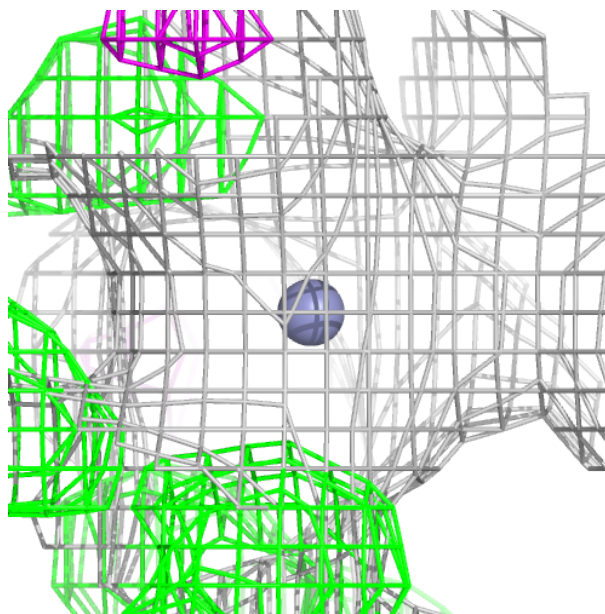
Electron density around ZN S 301:

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



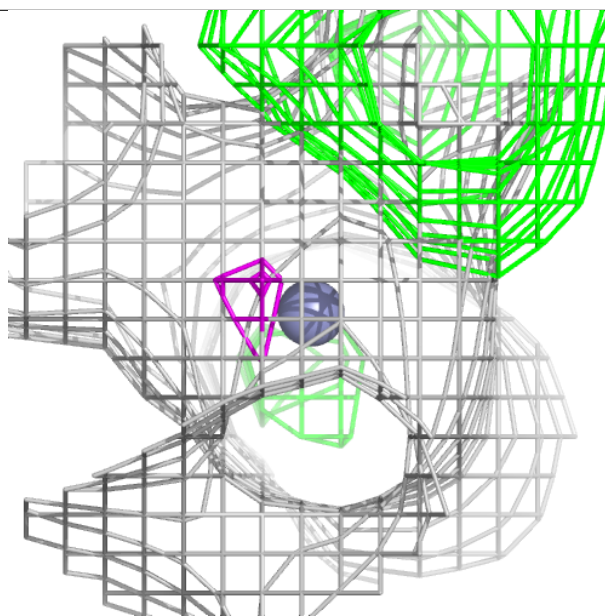
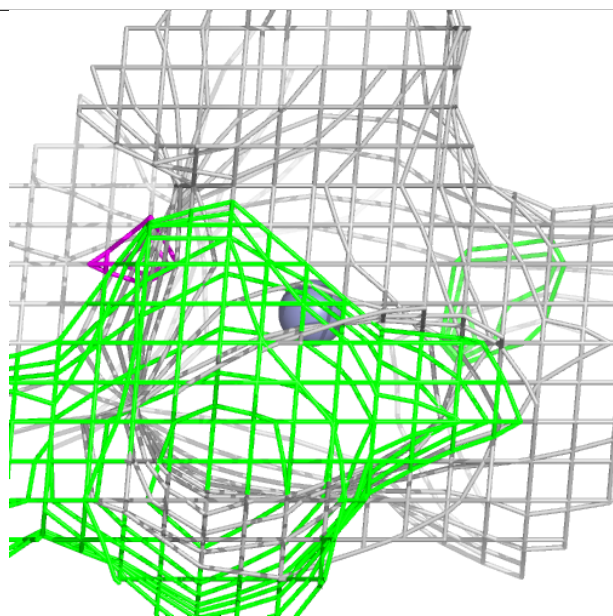
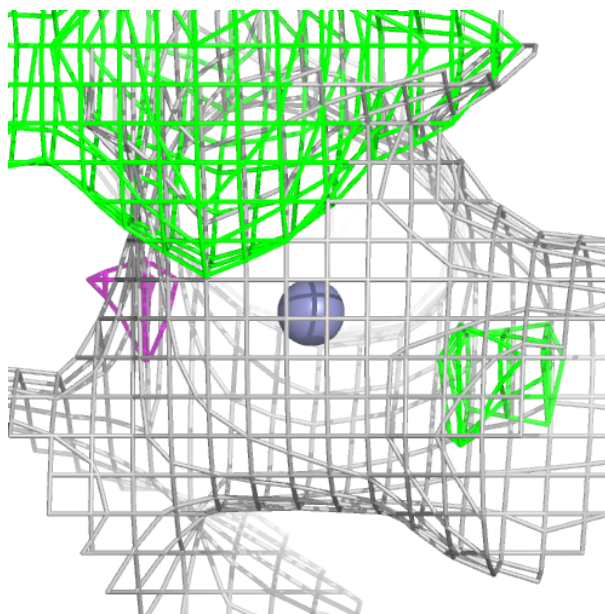
Electron density around ZN D 301:

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



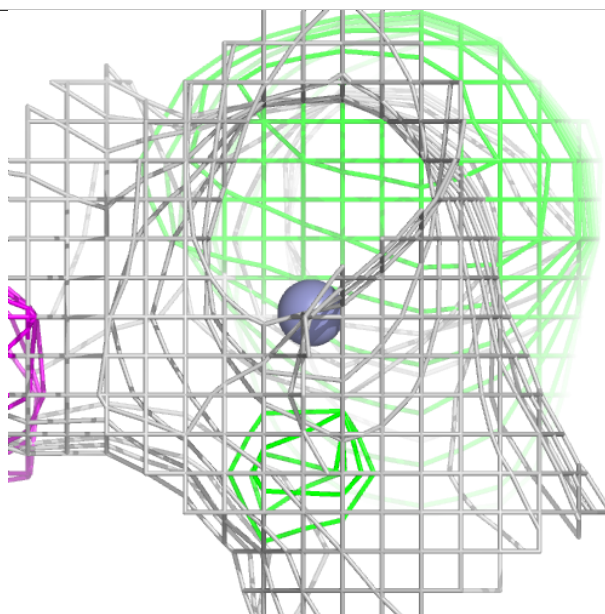
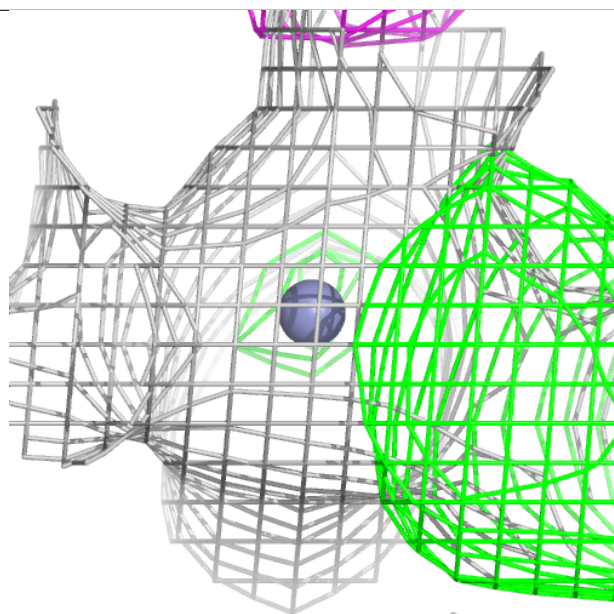
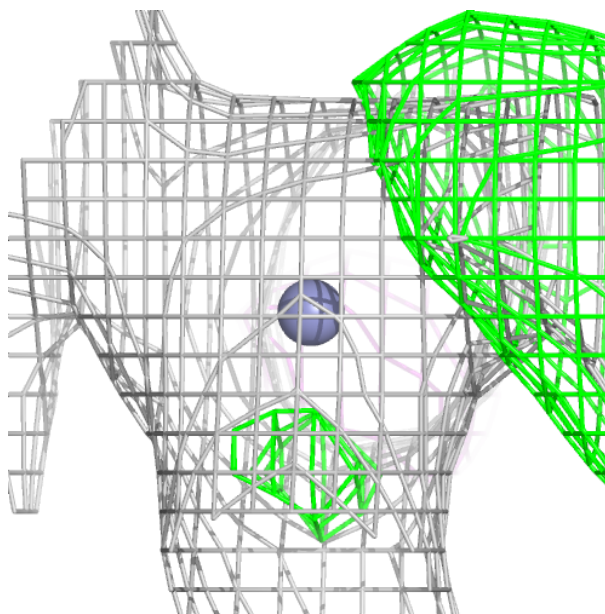
Electron density around ZN K 301:

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



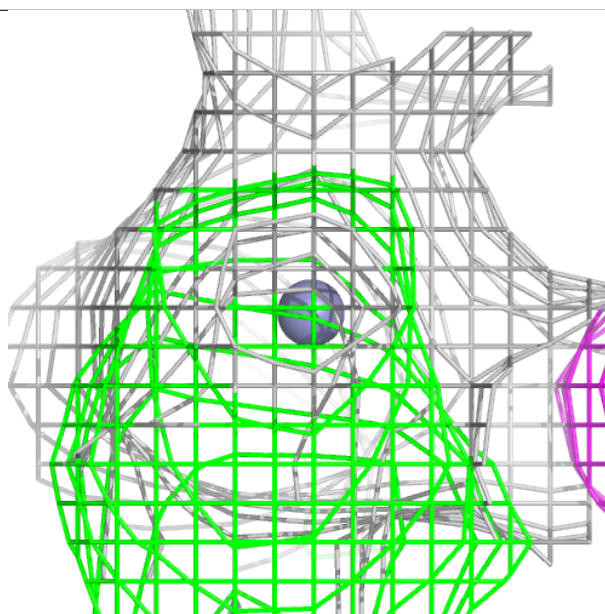
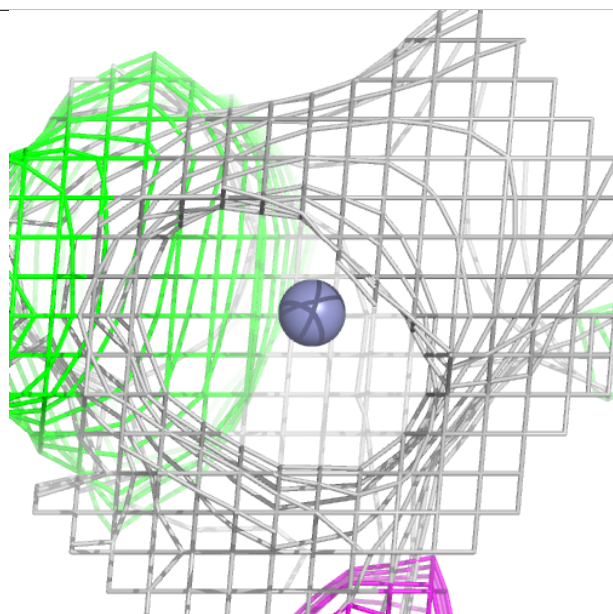
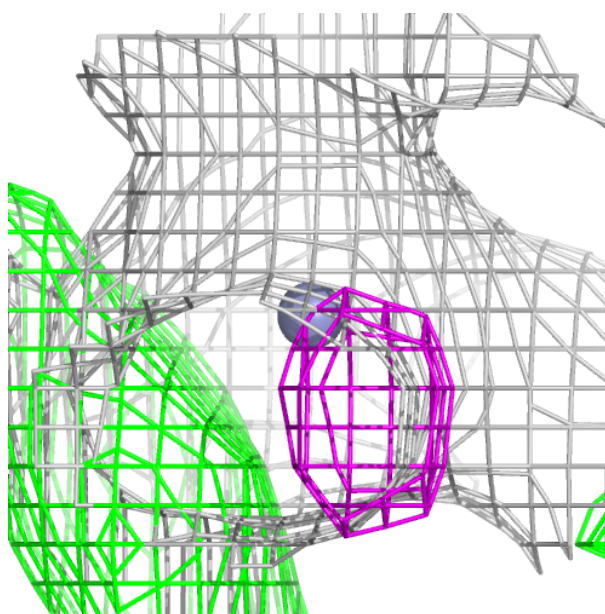
Electron density around ZN L 1102:

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



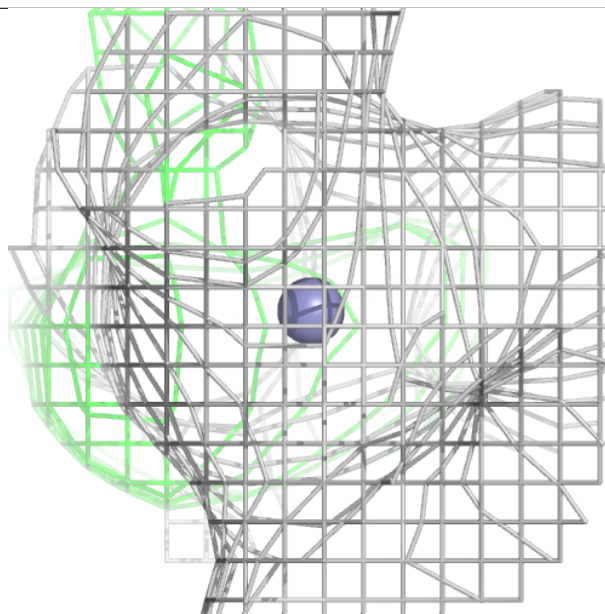
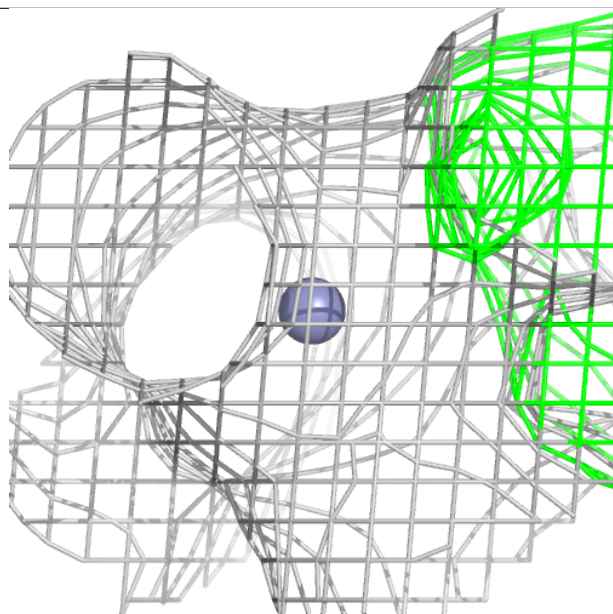
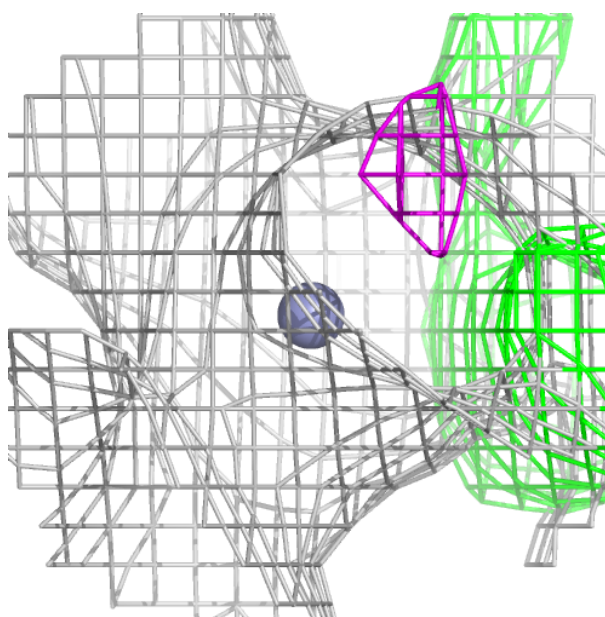
Electron density around ZN M 1102:

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



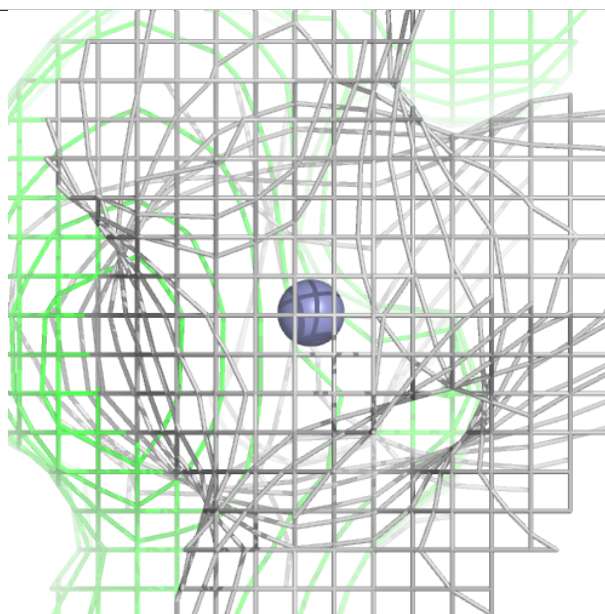
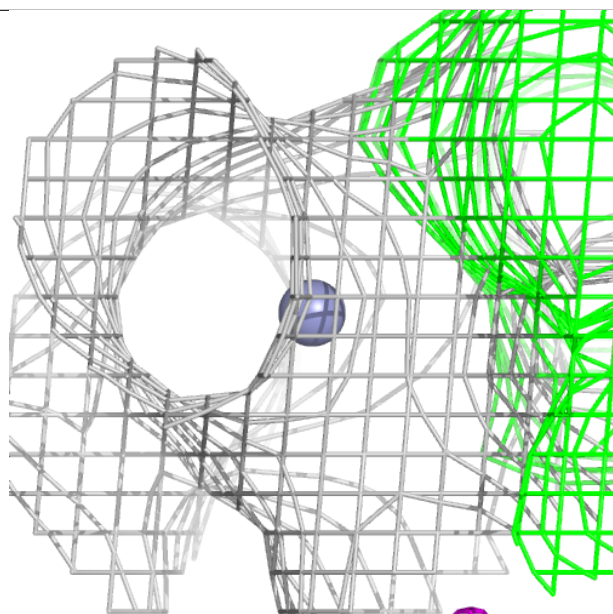
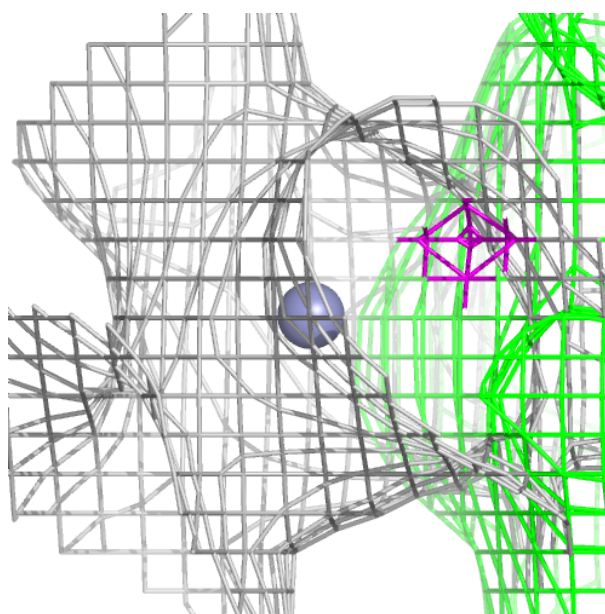
Electron density around ZN O 301:

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



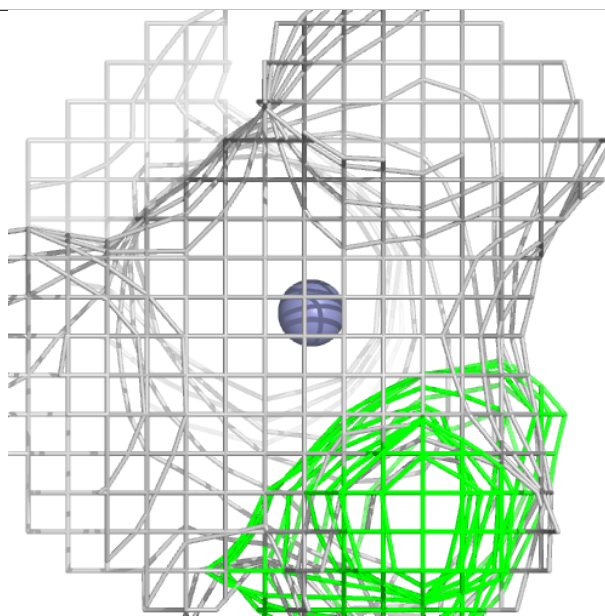
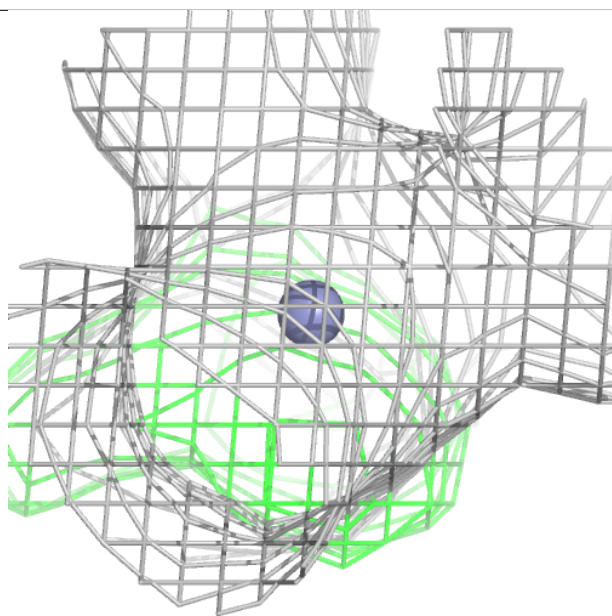
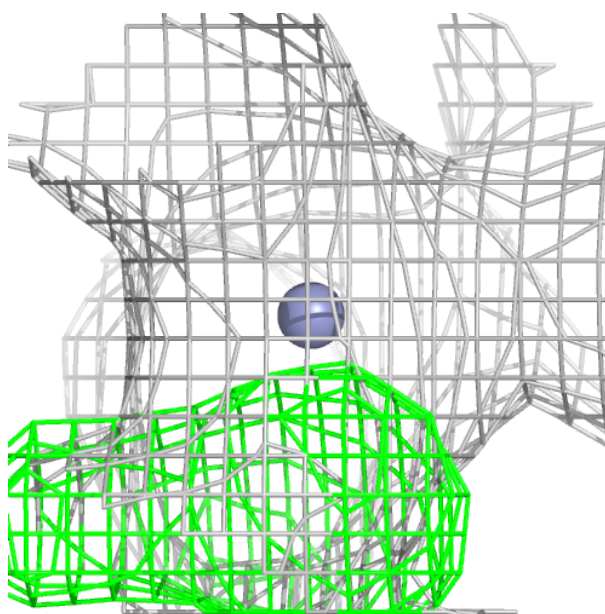
Electron density around ZN I 301:

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



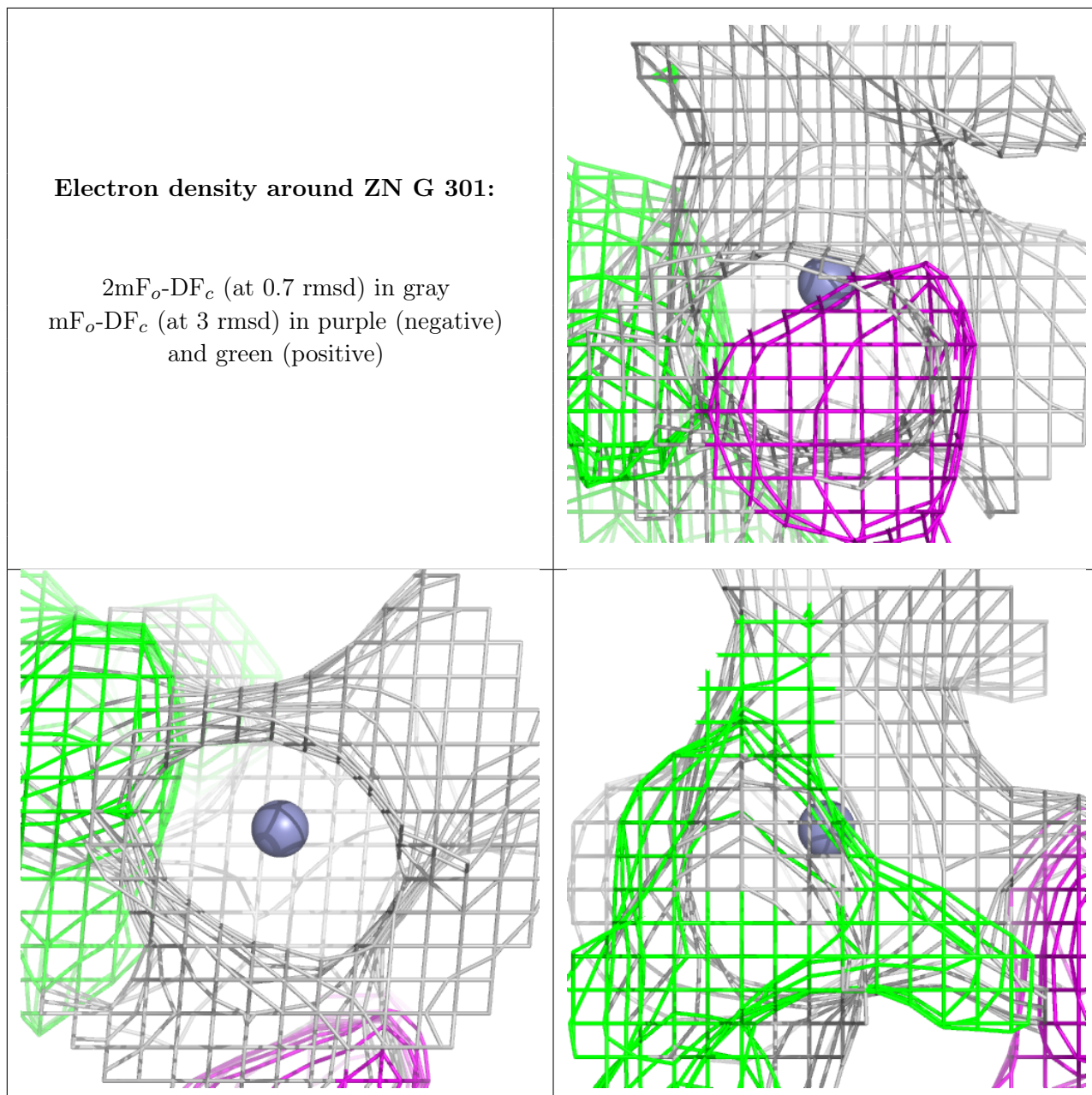
Electron density around ZN N 1102:

$2mF_o-DF_c$ (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)



6.5 Other polymers ⓘ

There are no such residues in this entry.