



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 1, 2021 – 11:17 AM EDT

PDB ID : 3K39
Title : Crystal Structure of B/Perth Neuraminidase D197E mutant in complex with Peramivir
Authors : Oakley, A.J.; McKimm-Breschkin, J.L.
Deposited on : 2009-10-02
Resolution : 2.54 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.23.2
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.2

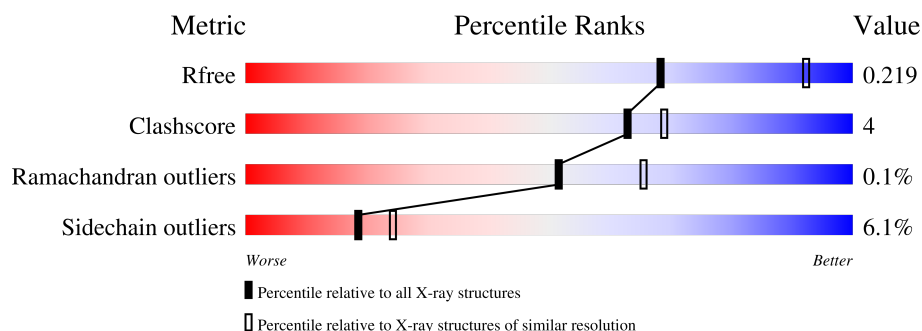
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.54 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.












Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	397	86% 10% ..
1	B	397	85% 12% ..
1	C	397	88% 8% ..
1	D	397	85% 11% ..
1	E	397	87% 9% ..
1	F	397	86% 10% ..
1	G	397	86% 10% ..

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Mol	Chain	Length	Quality of chain
1	H	397	 87%9% . .
1	I	397	 86%10% . .
1	J	397	 87%10% . .
1	K	397	 87%9% . .
1	L	397	 86%10% . .
1	M	397	 86%11% . .
1	N	397	 88%8% . .
1	O	397	 87%10% . .
1	P	397	 87%9% . .

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 49796 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

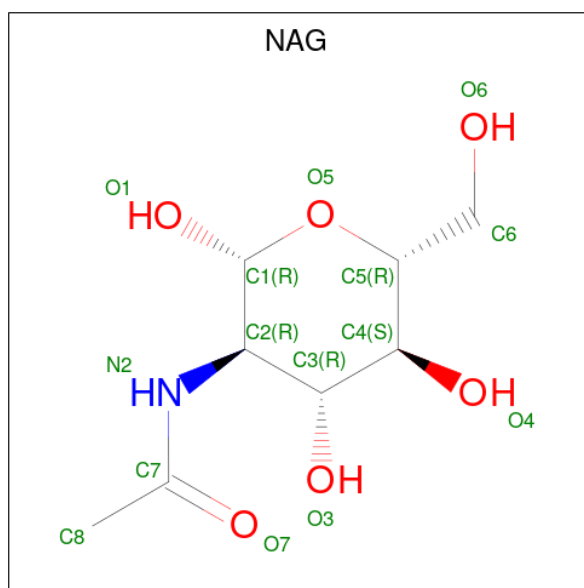
- Molecule 1 is a protein called Neuraminidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	389	Total	C	N	O	S	0	1	0
			3016	1892	522	573	29			
1	B	389	Total	C	N	O	S	0	1	0
			3016	1892	522	573	29			
1	C	389	Total	C	N	O	S	0	1	0
			3016	1892	522	573	29			
1	D	389	Total	C	N	O	S	0	1	0
			3016	1892	522	573	29			
1	E	389	Total	C	N	O	S	0	1	0
			3016	1892	522	573	29			
1	F	389	Total	C	N	O	S	0	1	0
			3016	1892	522	573	29			
1	G	389	Total	C	N	O	S	0	1	0
			3016	1892	522	573	29			
1	H	389	Total	C	N	O	S	0	1	0
			3016	1892	522	573	29			
1	I	389	Total	C	N	O	S	0	1	0
			3016	1892	522	573	29			
1	J	389	Total	C	N	O	S	0	1	0
			3016	1892	522	573	29			
1	K	389	Total	C	N	O	S	0	1	0
			3016	1892	522	573	29			
1	L	389	Total	C	N	O	S	0	1	0
			3016	1892	522	573	29			
1	M	389	Total	C	N	O	S	0	1	0
			3016	1892	522	573	29			
1	N	389	Total	C	N	O	S	0	1	0
			3016	1892	522	573	29			
1	O	389	Total	C	N	O	S	0	1	0
			3016	1892	522	573	29			
1	P	389	Total	C	N	O	S	0	1	0
			3016	1892	522	573	29			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	197	GLU	ASP	engineered mutation	UNP Q3S340
B	197	GLU	ASP	engineered mutation	UNP Q3S340
C	197	GLU	ASP	engineered mutation	UNP Q3S340
D	197	GLU	ASP	engineered mutation	UNP Q3S340
E	197	GLU	ASP	engineered mutation	UNP Q3S340
F	197	GLU	ASP	engineered mutation	UNP Q3S340
G	197	GLU	ASP	engineered mutation	UNP Q3S340
H	197	GLU	ASP	engineered mutation	UNP Q3S340
I	197	GLU	ASP	engineered mutation	UNP Q3S340
J	197	GLU	ASP	engineered mutation	UNP Q3S340
K	197	GLU	ASP	engineered mutation	UNP Q3S340
L	197	GLU	ASP	engineered mutation	UNP Q3S340
M	197	GLU	ASP	engineered mutation	UNP Q3S340
N	197	GLU	ASP	engineered mutation	UNP Q3S340
O	197	GLU	ASP	engineered mutation	UNP Q3S340
P	197	GLU	ASP	engineered mutation	UNP Q3S340

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	E	1	Total	C	N	O	0	0
			14	8	1	5		
2	F	1	Total	C	N	O	0	0
			14	8	1	5		
2	G	1	Total	C	N	O	0	0
			14	8	1	5		
2	H	1	Total	C	N	O	0	0
			14	8	1	5		
2	I	1	Total	C	N	O	0	0
			14	8	1	5		
2	J	1	Total	C	N	O	0	0
			14	8	1	5		
2	K	1	Total	C	N	O	0	0
			14	8	1	5		
2	L	1	Total	C	N	O	0	0
			14	8	1	5		
2	M	1	Total	C	N	O	0	0
			14	8	1	5		
2	N	1	Total	C	N	O	0	0
			14	8	1	5		
2	O	1	Total	C	N	O	0	0
			14	8	1	5		
2	P	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

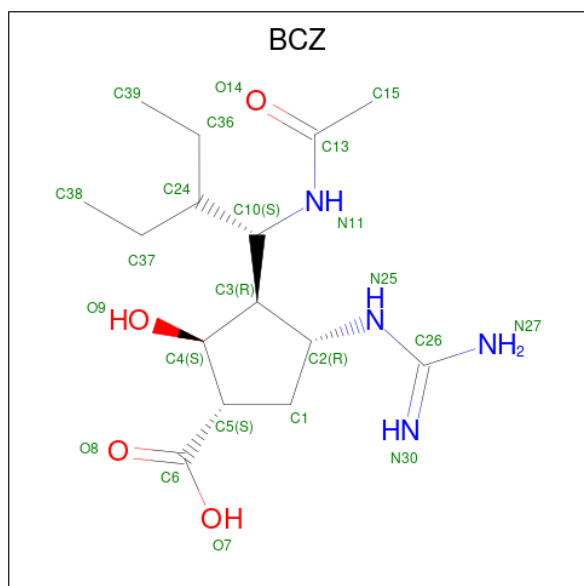
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ca	0	0
			1	1		
3	B	1	Total	Ca	0	0
			1	1		
3	C	1	Total	Ca	0	0
			1	1		
3	D	1	Total	Ca	0	0
			1	1		
3	E	1	Total	Ca	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	F	1	Total 1 Ca 1	0	0
3	G	1	Total 1 Ca 1	0	0
3	H	1	Total 1 Ca 1	0	0
3	I	1	Total 1 Ca 1	0	0
3	J	1	Total 1 Ca 1	0	0
3	K	1	Total 1 Ca 1	0	0
3	L	1	Total 1 Ca 1	0	0
3	M	1	Total 1 Ca 1	0	0
3	N	1	Total 1 Ca 1	0	0
3	O	1	Total 1 Ca 1	0	0
3	P	1	Total 1 Ca 1	0	0

- Molecule 4 is 3-(1-ACETYLAMINO-2-ETHYL-BUTYL)-4-GUANIDINO-2-HYDROXY-CYCLOPENTANECARBOXYLIC ACID (three-letter code: BCZ) (formula: $C_{15}H_{28}N_4O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total 23	C 15	N 4	O 4	0	0
4	B	1	Total 23	C 15	N 4	O 4	0	0
4	C	1	Total 23	C 15	N 4	O 4	0	0
4	D	1	Total 23	C 15	N 4	O 4	0	0
4	E	1	Total 23	C 15	N 4	O 4	0	0
4	F	1	Total 23	C 15	N 4	O 4	0	0
4	G	1	Total 23	C 15	N 4	O 4	0	0
4	H	1	Total 23	C 15	N 4	O 4	0	0
4	I	1	Total 23	C 15	N 4	O 4	0	0
4	J	1	Total 23	C 15	N 4	O 4	0	0
4	K	1	Total 23	C 15	N 4	O 4	0	0
4	L	1	Total 23	C 15	N 4	O 4	0	0
4	M	1	Total 23	C 15	N 4	O 4	0	0
4	N	1	Total 23	C 15	N 4	O 4	0	0
4	O	1	Total 23	C 15	N 4	O 4	0	0
4	P	1	Total 23	C 15	N 4	O 4	0	0

- Molecule 5 is YTTRIUM (III) ION (three-letter code: YT3) (formula: Y).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total 1	Y 1	0	0
5	E	1	Total 1	Y 1	0	0
5	I	1	Total 1	Y 1	0	0
5	M	1	Total 1	Y 1	0	0

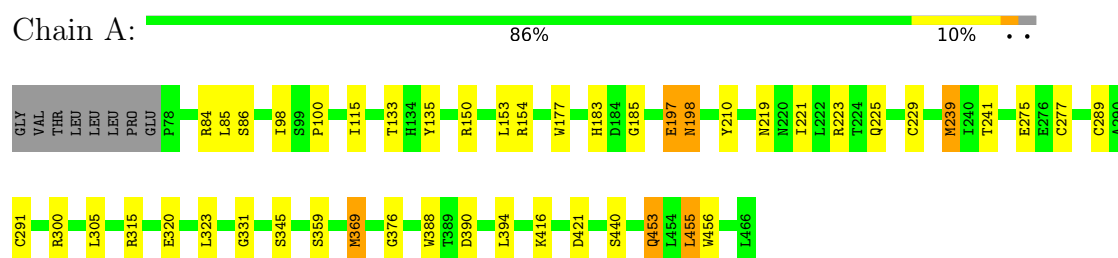
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	56	Total 56	O 56	0	0
6	B	56	Total 56	O 56	0	0
6	C	61	Total 61	O 61	0	0
6	D	56	Total 56	O 56	0	0
6	E	62	Total 62	O 62	0	0
6	F	58	Total 58	O 58	0	0
6	G	58	Total 58	O 58	0	0
6	H	57	Total 57	O 57	0	0
6	I	56	Total 56	O 56	0	0
6	J	57	Total 57	O 57	0	0
6	K	56	Total 56	O 56	0	0
6	L	59	Total 59	O 59	0	0
6	M	58	Total 58	O 58	0	0
6	N	58	Total 58	O 58	0	0
6	O	62	Total 62	O 62	0	0
6	P	58	Total 58	O 58	0	0

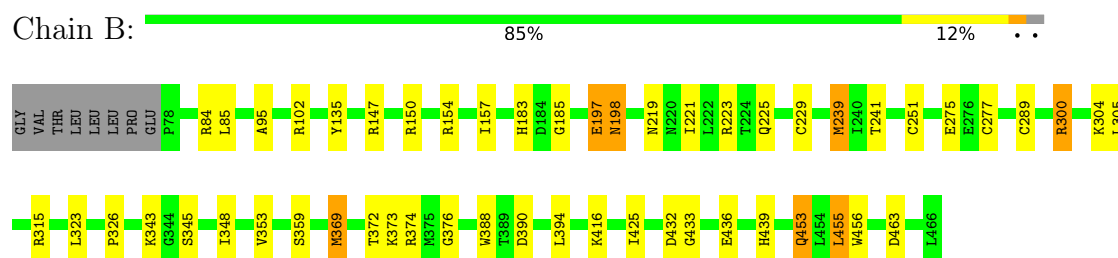
3 Residue-property plots [i](#)

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. 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. 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.

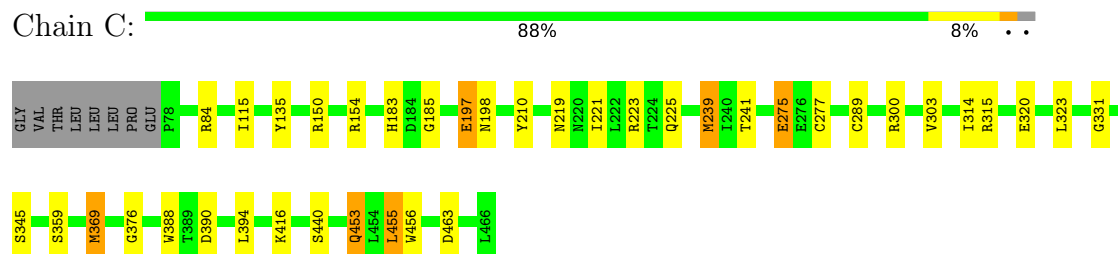
• Molecule 1: Neuraminidase



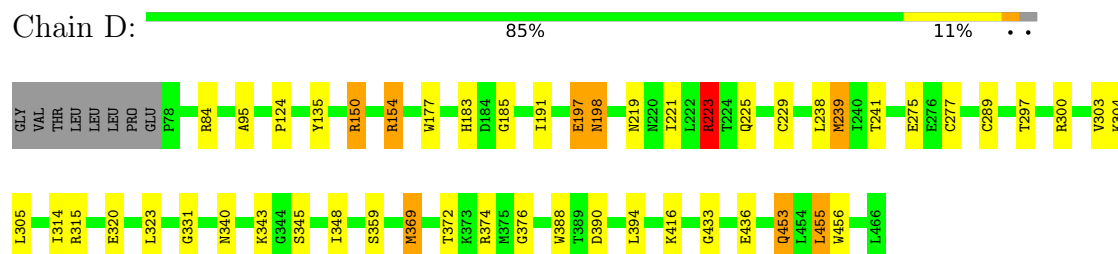
• Molecule 1: Neuraminidase




• Molecule 1: Neuraminidase

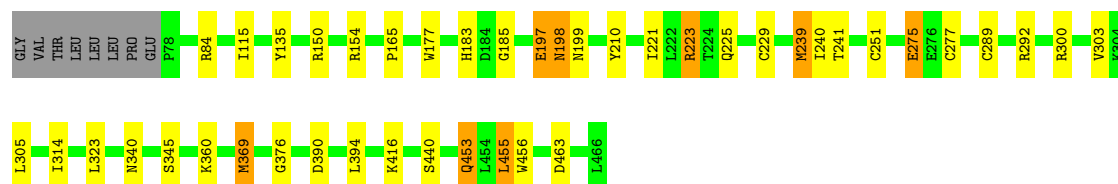


• Molecule 1: Neuraminidase




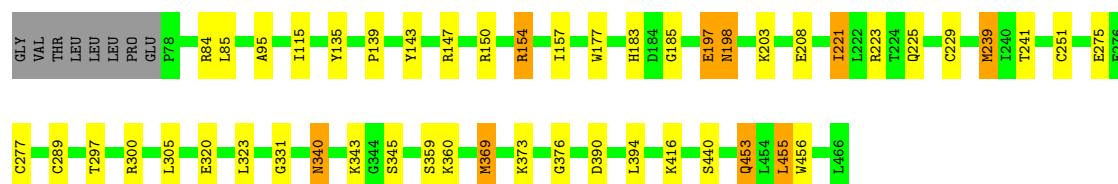
- Molecule 1: Neuraminidase

Chain E:  87% 9% ..



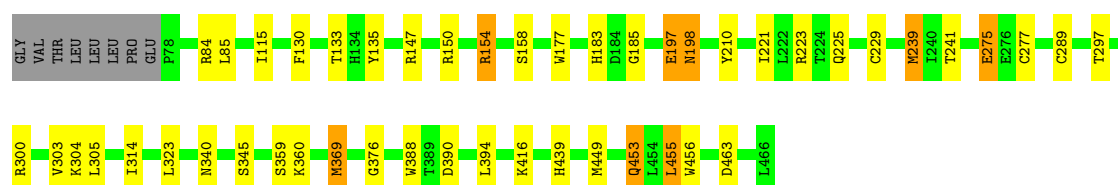
- Molecule 1: Neuraminidase

Chain F:  86% 10% ..



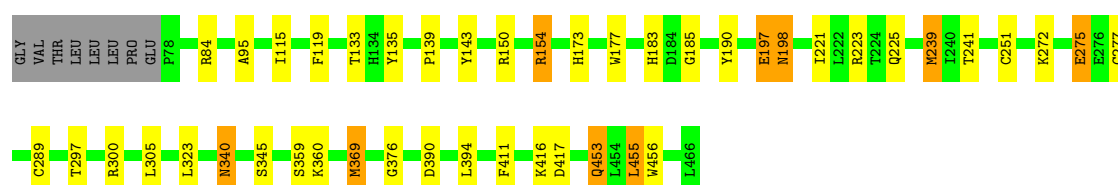
- Molecule 1: Neuraminidase

Chain G:  86% 10% ..




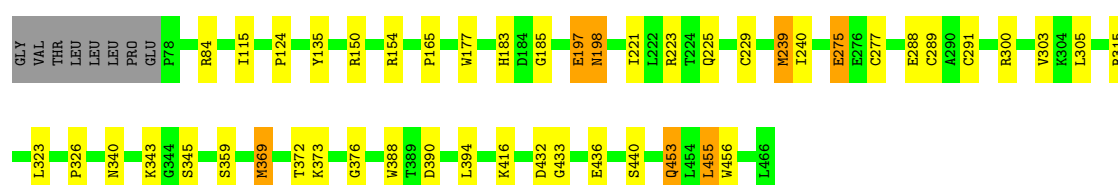
- Molecule 1: Neuraminidase

Chain H:  87% 9% ..

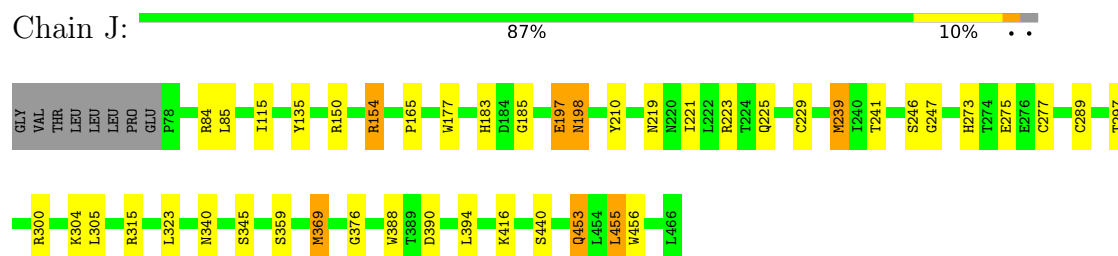


- Molecule 1: Neuraminidase

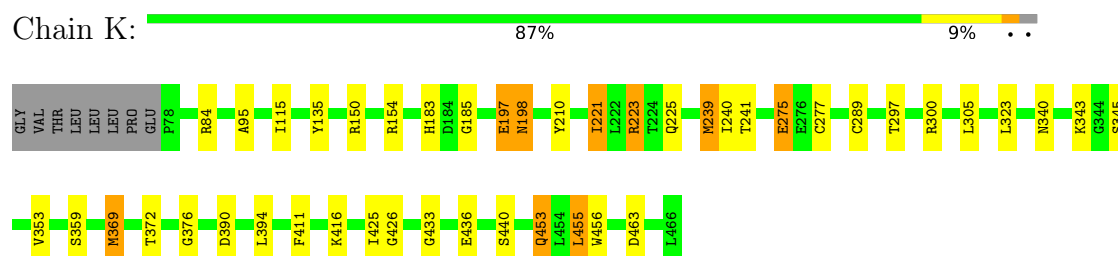
Chain I:  86% 10% ..



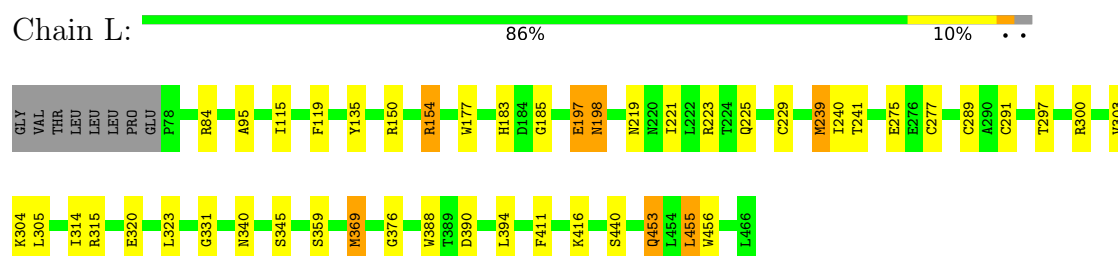
● Molecule 1: Neuraminidase



● Molecule 1: Neuraminidase



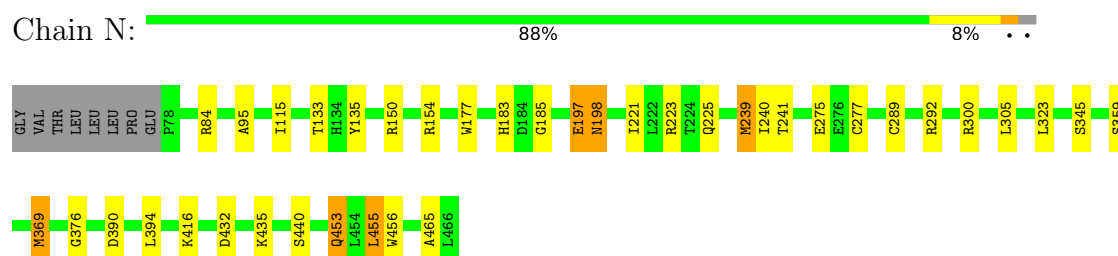
● Molecule 1: Neuraminidase



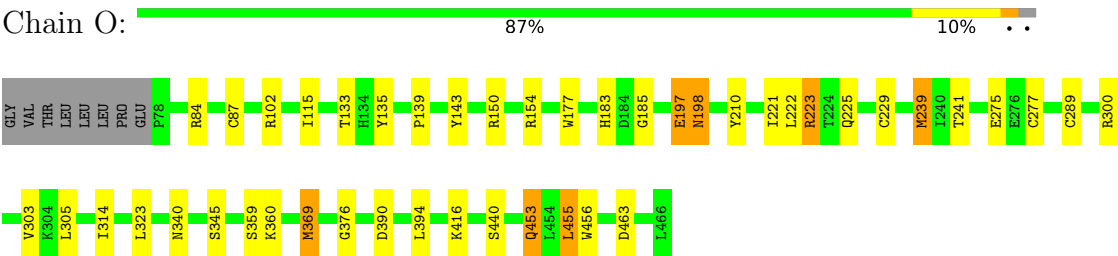
● Molecule 1: Neuraminidase



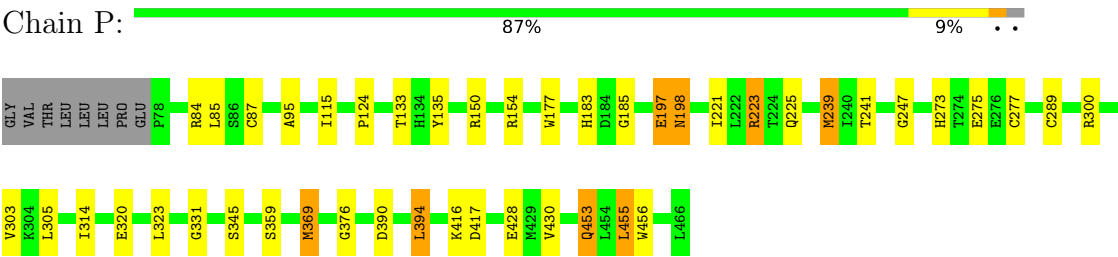
● Molecule 1: Neuraminidase



● Molecule 1: Neuraminidase



● Molecule 1: Neuraminidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	111.96Å 124.87Å 125.25Å 90.03° 92.11° 91.27°	Depositor
Resolution (Å)	55.90 – 2.54 55.83 – 2.30	Depositor EDS
% Data completeness (in resolution range)	90.6 (55.90-2.54) 95.2 (55.83-2.30)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.16 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.198 , 0.214 0.215 , 0.219	Depositor DCC
R_{free} test set	14501 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	12.4	Xtriage
Anisotropy	0.423	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 2.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.119 for h,l,-k 0.119 for h,-l,k 0.118 for h,-k,-l 0.179 for -h,k,-l 0.125 for -h,-k,l 0.099 for -h,l,k 0.189 for -h,-l,-k	Xtriage
Reported twinning fraction	0.758 for H, K, L 0.139 for -H, -L, -K 0.103 for -H, K, -L	Depositor
Outliers	0 of 286793 reflections	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	49796	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.20% of the height of the origin peak. No significant pseudotranslation is detected.*

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: BCZ, YT3, NAG, CA

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	0/3089	0.75	0/4171
1	B	0.76	0/3089	0.75	1/4171 (0.0%)
1	C	0.75	0/3089	0.75	0/4171
1	D	0.74	0/3089	0.74	1/4171 (0.0%)
1	E	0.79	0/3089	0.76	1/4171 (0.0%)
1	F	0.83	1/3089 (0.0%)	0.77	0/4171
1	G	0.79	0/3089	0.76	0/4171
1	H	0.78	0/3089	0.76	1/4171 (0.0%)
1	I	0.77	0/3089	0.76	0/4171
1	J	0.78	0/3089	0.74	0/4171
1	K	0.76	0/3089	0.74	0/4171
1	L	0.77	0/3089	0.76	0/4171
1	M	0.77	0/3089	0.74	1/4171 (0.0%)
1	N	0.80	0/3089	0.77	1/4171 (0.0%)
1	O	0.78	1/3089 (0.0%)	0.76	1/4171 (0.0%)
1	P	0.80	1/3089 (0.0%)	0.78	2/4171 (0.0%)
All	All	0.78	3/49424 (0.0%)	0.76	9/66736 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	1
1	F	0	1
1	H	0	1
1	I	0	1
1	O	0	2
All	All	0	6

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	87	CYS	CB-SG	5.64	1.91	1.82
1	F	208	GLU	CG-CD	5.15	1.59	1.51
1	O	87	CYS	CB-SG	5.06	1.90	1.82

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	292	ARG	NE-CZ-NH1	6.63	123.61	120.30
1	P	417	ASP	CB-CG-OD1	6.27	123.94	118.30
1	H	417	ASP	CB-CG-OD1	6.24	123.92	118.30
1	E	292	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	B	300	ARG	NE-CZ-NH2	-5.37	117.62	120.30

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	340	ASN	Peptide
1	F	340	ASN	Peptide
1	H	340	ASN	Peptide
1	I	340	ASN	Peptide
1	O	222	LEU	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3016	0	2912	25	1
1	B	3016	0	2912	47	0
1	C	3016	0	2912	22	1
1	D	3016	0	2912	23	5
1	E	3016	0	2912	23	1
1	F	3016	0	2912	47	0
1	G	3016	0	2912	28	1
1	H	3016	0	2912	23	1
1	I	3016	0	2912	47	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	J	3016	0	2912	22	1
1	K	3016	0	2912	24	4
1	L	3016	0	2912	28	1
1	M	3016	0	2912	25	1
1	N	3016	0	2912	43	0
1	O	3016	0	2912	22	1
1	P	3016	0	2912	25	0
2	A	14	0	13	0	0
2	B	14	0	13	0	0
2	C	14	0	13	0	0
2	D	14	0	13	0	0
2	E	14	0	13	0	0
2	F	14	0	13	0	0
2	G	14	0	13	0	0
2	H	14	0	13	0	0
2	I	14	0	13	0	0
2	J	14	0	13	0	0
2	K	14	0	13	0	0
2	L	14	0	13	0	0
2	M	14	0	13	0	0
2	N	14	0	13	0	0
2	O	14	0	13	0	0
2	P	14	0	13	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
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
4	A	23	0	27	1	0
4	B	23	0	27	1	0
4	C	23	0	27	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	23	0	27	1	0
4	E	23	0	27	1	0
4	F	23	0	27	1	0
4	G	23	0	27	2	0
4	H	23	0	27	1	0
4	I	23	0	27	2	0
4	J	23	0	27	1	0
4	K	23	0	27	1	0
4	L	23	0	27	1	0
4	M	23	0	27	2	0
4	N	23	0	27	1	0
4	O	23	0	27	1	0
4	P	23	0	27	2	0
5	A	1	0	0	0	0
5	E	1	0	0	0	0
5	I	1	0	0	0	0
5	M	1	0	0	0	0
6	A	56	0	0	1	0
6	B	56	0	0	1	0
6	C	61	0	0	1	0
6	D	56	0	0	1	0
6	E	62	0	0	2	0
6	F	58	0	0	1	0
6	G	58	0	0	2	0
6	H	57	0	0	2	0
6	I	56	0	0	2	0
6	J	57	0	0	2	0
6	K	56	0	0	1	0
6	L	59	0	0	1	0
6	M	58	0	0	2	0
6	N	58	0	0	1	0
6	O	62	0	0	1	0
6	P	58	0	0	1	0
All	All	49796	0	47232	417	9

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.

The worst 5 of 417 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:F:343:LYS:CE	1:N:465:ALA:HB1	1.36	1.49
1:B:372:THR:HG21	1:I:433:GLY:O	1.14	1.30
1:F:343:LYS:HZ1	1:N:465:ALA:CB	1.43	1.30
1:B:433:GLY:O	1:I:372:THR:CG2	1.80	1.30
1:F:343:LYS:NZ	1:N:465:ALA:CB	1.95	1.27

The worst 5 of 9 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:433:GLY:O	1:K:372:THR:CG2[1_545]	1.78	0.42
1:D:372:THR:CG2	1:K:433:GLY:O[1_545]	1.81	0.39
1:A:219:ASN:OD1	1:G:360:LYS:NZ[1_556]	1.90	0.30
1:J:219:ASN:OD1	1:M:360:LYS:NZ[1_665]	1.94	0.26
1:C:219:ASN:OD1	1:E:360:LYS:NZ[1_545]	1.96	0.24

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	388/397 (98%)	367 (95%)	21 (5%)	0	100	100
1	B	388/397 (98%)	370 (95%)	18 (5%)	0	100	100
1	C	388/397 (98%)	367 (95%)	21 (5%)	0	100	100
1	D	388/397 (98%)	365 (94%)	23 (6%)	0	100	100
1	E	388/397 (98%)	369 (95%)	18 (5%)	1 (0%)	41	51
1	F	388/397 (98%)	369 (95%)	18 (5%)	1 (0%)	41	51
1	G	388/397 (98%)	368 (95%)	20 (5%)	0	100	100
1	H	388/397 (98%)	368 (95%)	20 (5%)	0	100	100
1	I	388/397 (98%)	371 (96%)	17 (4%)	0	100	100
1	J	388/397 (98%)	368 (95%)	20 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	K	388/397 (98%)	370 (95%)	17 (4%)	1 (0%)	41	51
1	L	388/397 (98%)	372 (96%)	16 (4%)	0	100	100
1	M	388/397 (98%)	369 (95%)	18 (5%)	1 (0%)	41	51
1	N	388/397 (98%)	369 (95%)	19 (5%)	0	100	100
1	O	388/397 (98%)	367 (95%)	21 (5%)	0	100	100
1	P	388/397 (98%)	371 (96%)	17 (4%)	0	100	100
All	All	6208/6352 (98%)	5900 (95%)	304 (5%)	4 (0%)	51	65

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	199	ASN
1	M	199	ASN
1	K	221	ILE
1	F	221	ILE

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	323/329 (98%)	303 (94%)	20 (6%)	18	24
1	B	323/329 (98%)	302 (94%)	21 (6%)	17	23
1	C	323/329 (98%)	306 (95%)	17 (5%)	22	30
1	D	323/329 (98%)	302 (94%)	21 (6%)	17	23
1	E	323/329 (98%)	304 (94%)	19 (6%)	19	25
1	F	323/329 (98%)	302 (94%)	21 (6%)	17	23
1	G	323/329 (98%)	303 (94%)	20 (6%)	18	24
1	H	323/329 (98%)	304 (94%)	19 (6%)	19	25
1	I	323/329 (98%)	305 (94%)	18 (6%)	21	28
1	J	323/329 (98%)	302 (94%)	21 (6%)	17	23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	K	323/329 (98%)	304 (94%)	19 (6%)	19	25
1	L	323/329 (98%)	304 (94%)	19 (6%)	19	25
1	M	323/329 (98%)	302 (94%)	21 (6%)	17	23
1	N	323/329 (98%)	305 (94%)	18 (6%)	21	28
1	O	323/329 (98%)	303 (94%)	20 (6%)	18	24
1	P	323/329 (98%)	303 (94%)	20 (6%)	18	24
All	All	5168/5264 (98%)	4854 (94%)	314 (6%)	18	24

5 of 314 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	416	LYS
1	O	359	SER
1	M	154	ARG
1	N	198	ASN
1	P	223	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 77 such sidechains are listed below:

Mol	Chain	Res	Type
1	L	453	GLN
1	O	439	HIS
1	M	198	ASN
1	N	225	GLN
1	P	225	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 52 ligands modelled in this entry, 20 are monoatomic - leaving 32 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	BCZ	G	1001	-	19,23,23	0.89	1 (5%)	21,32,32	1.51	4 (19%)
4	BCZ	D	1001	-	19,23,23	1.03	1 (5%)	21,32,32	1.58	4 (19%)
4	BCZ	A	1001	-	19,23,23	1.13	1 (5%)	21,32,32	1.40	4 (19%)
2	NAG	E	900	1	14,14,15	0.76	0	17,19,21	1.87	4 (23%)
2	NAG	M	900	1	14,14,15	0.67	0	17,19,21	2.23	4 (23%)
4	BCZ	B	1001	-	19,23,23	0.86	1 (5%)	21,32,32	1.49	3 (14%)
2	NAG	G	900	1	14,14,15	0.54	0	17,19,21	2.14	3 (17%)
2	NAG	J	900	1	14,14,15	0.66	0	17,19,21	2.00	2 (11%)
4	BCZ	P	1001	-	19,23,23	0.89	1 (5%)	21,32,32	1.43	3 (14%)
2	NAG	H	900	1	14,14,15	0.85	0	17,19,21	1.94	3 (17%)
4	BCZ	E	1001	-	19,23,23	1.15	2 (10%)	21,32,32	1.49	4 (19%)
4	BCZ	M	1001	-	19,23,23	1.43	3 (15%)	21,32,32	1.17	3 (14%)
4	BCZ	L	1001	-	19,23,23	1.13	1 (5%)	21,32,32	1.42	3 (14%)
2	NAG	I	900	1	14,14,15	0.73	0	17,19,21	2.28	4 (23%)
4	BCZ	C	1001	-	19,23,23	1.33	2 (10%)	21,32,32	1.28	3 (14%)
4	BCZ	J	1001	-	19,23,23	0.97	1 (5%)	21,32,32	1.52	4 (19%)
4	BCZ	N	1001	-	19,23,23	1.28	1 (5%)	21,32,32	1.35	4 (19%)
4	BCZ	K	1001	-	19,23,23	1.23	1 (5%)	21,32,32	1.59	4 (19%)
2	NAG	F	900	1	14,14,15	0.87	0	17,19,21	1.93	2 (11%)
2	NAG	A	900	1	14,14,15	0.61	0	17,19,21	2.10	3 (17%)
4	BCZ	I	1001	-	19,23,23	1.14	1 (5%)	21,32,32	1.57	3 (14%)
2	NAG	O	900	1	14,14,15	0.62	0	17,19,21	2.27	3 (17%)
4	BCZ	H	1001	-	19,23,23	1.43	2 (10%)	21,32,32	1.38	5 (23%)
2	NAG	K	900	1	14,14,15	0.69	0	17,19,21	1.85	3 (17%)
4	BCZ	F	1001	-	19,23,23	1.22	1 (5%)	21,32,32	1.35	3 (14%)
2	NAG	B	900	1	14,14,15	0.66	0	17,19,21	2.13	4 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	L	900	1	14,14,15	0.57	0	17,19,21	2.05	4 (23%)
2	NAG	C	900	1	14,14,15	0.73	0	17,19,21	2.08	2 (11%)
4	BCZ	O	1001	-	19,23,23	1.05	1 (5%)	21,32,32	1.69	6 (28%)
2	NAG	P	900	1	14,14,15	0.72	0	17,19,21	1.83	3 (17%)
2	NAG	N	900	1	14,14,15	0.79	0	17,19,21	1.98	3 (17%)
2	NAG	D	900	1	14,14,15	0.92	0	17,19,21	2.03	5 (29%)

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	BCZ	G	1001	-	-	0/20/40/40	0/1/1/1
4	BCZ	D	1001	-	-	0/20/40/40	0/1/1/1
4	BCZ	A	1001	-	-	0/20/40/40	0/1/1/1
2	NAG	E	900	1	-	1/6/23/26	0/1/1/1
2	NAG	M	900	1	-	0/6/23/26	0/1/1/1
4	BCZ	B	1001	-	-	0/20/40/40	0/1/1/1
2	NAG	G	900	1	-	0/6/23/26	0/1/1/1
2	NAG	J	900	1	-	0/6/23/26	0/1/1/1
4	BCZ	P	1001	-	-	2/20/40/40	0/1/1/1
2	NAG	H	900	1	-	0/6/23/26	0/1/1/1
4	BCZ	E	1001	-	-	0/20/40/40	0/1/1/1
4	BCZ	M	1001	-	-	0/20/40/40	0/1/1/1
4	BCZ	L	1001	-	-	0/20/40/40	0/1/1/1
2	NAG	I	900	1	-	0/6/23/26	0/1/1/1
4	BCZ	C	1001	-	-	0/20/40/40	0/1/1/1
4	BCZ	J	1001	-	-	0/20/40/40	0/1/1/1
4	BCZ	N	1001	-	-	0/20/40/40	0/1/1/1
4	BCZ	K	1001	-	-	0/20/40/40	0/1/1/1
2	NAG	F	900	1	-	0/6/23/26	0/1/1/1
2	NAG	A	900	1	-	0/6/23/26	0/1/1/1
4	BCZ	I	1001	-	-	0/20/40/40	0/1/1/1
2	NAG	O	900	1	-	0/6/23/26	0/1/1/1
4	BCZ	H	1001	-	-	0/20/40/40	0/1/1/1
2	NAG	K	900	1	-	0/6/23/26	0/1/1/1
4	BCZ	F	1001	-	-	0/20/40/40	0/1/1/1
2	NAG	B	900	1	-	0/6/23/26	0/1/1/1
2	NAG	L	900	1	-	0/6/23/26	0/1/1/1
2	NAG	C	900	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BCZ	O	1001	-	-	2/20/40/40	0/1/1/1
2	NAG	P	900	1	-	0/6/23/26	0/1/1/1
2	NAG	N	900	1	-	0/6/23/26	0/1/1/1
2	NAG	D	900	1	-	0/6/23/26	0/1/1/1

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	1001	BCZ	C26-N25	4.54	1.41	1.33
4	M	1001	BCZ	C26-N25	4.45	1.40	1.33
4	F	1001	BCZ	C26-N25	4.03	1.40	1.33
4	N	1001	BCZ	C26-N25	3.92	1.40	1.33
4	C	1001	BCZ	C26-N25	3.91	1.40	1.33

The worst 5 of 112 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	900	NAG	C1-O5-C5	7.47	122.31	112.19
2	O	900	NAG	C1-O5-C5	7.35	122.15	112.19
2	M	900	NAG	C1-O5-C5	7.30	122.09	112.19
2	G	900	NAG	C1-O5-C5	7.01	121.69	112.19
2	C	900	NAG	C1-O5-C5	6.65	121.20	112.19

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	P	1001	BCZ	C10-C24-C36-C39
2	E	900	NAG	O5-C5-C6-O6
4	O	1001	BCZ	C10-C24-C36-C39
4	O	1001	BCZ	C37-C24-C36-C39
4	P	1001	BCZ	C37-C24-C36-C39

There are no ring outliers.

16 monomers are involved in 20 short contacts:

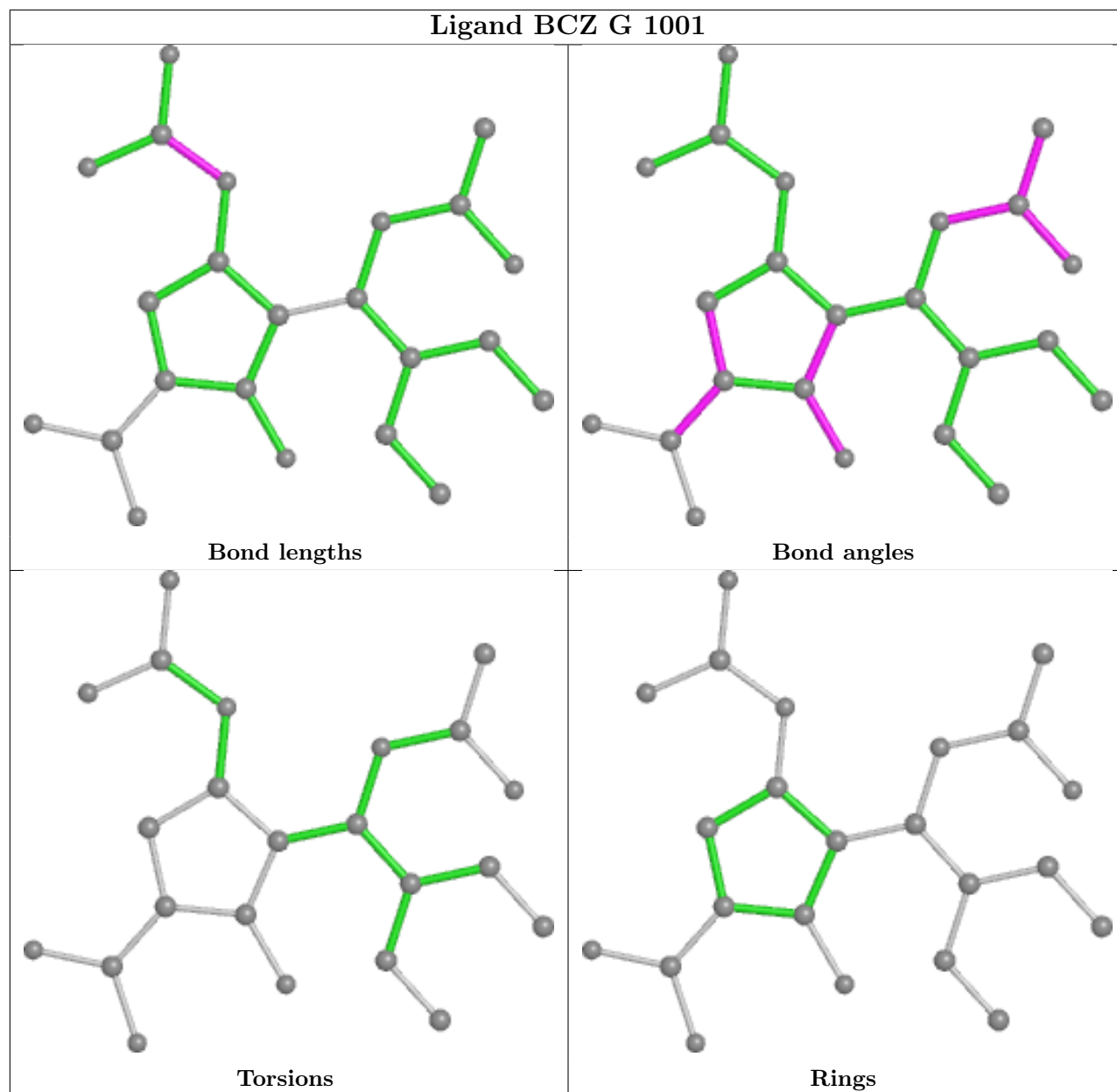
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	1001	BCZ	2	0
4	D	1001	BCZ	1	0
4	A	1001	BCZ	1	0

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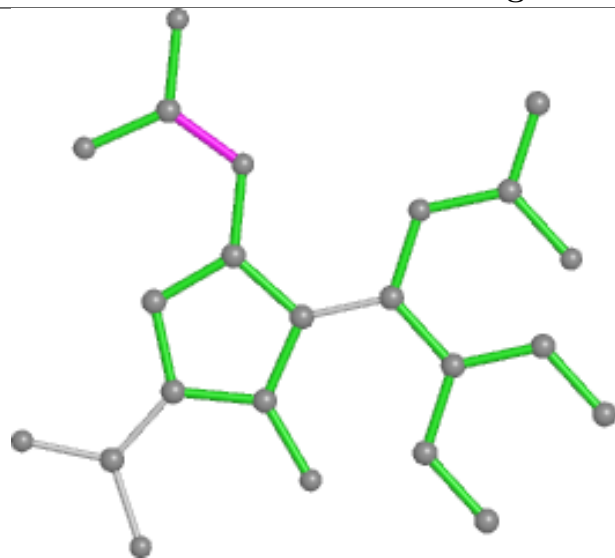
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1001	BCZ	1	0
4	P	1001	BCZ	2	0
4	E	1001	BCZ	1	0
4	M	1001	BCZ	2	0
4	L	1001	BCZ	1	0
4	C	1001	BCZ	1	0
4	J	1001	BCZ	1	0
4	N	1001	BCZ	1	0
4	K	1001	BCZ	1	0
4	I	1001	BCZ	2	0
4	H	1001	BCZ	1	0
4	F	1001	BCZ	1	0
4	O	1001	BCZ	1	0

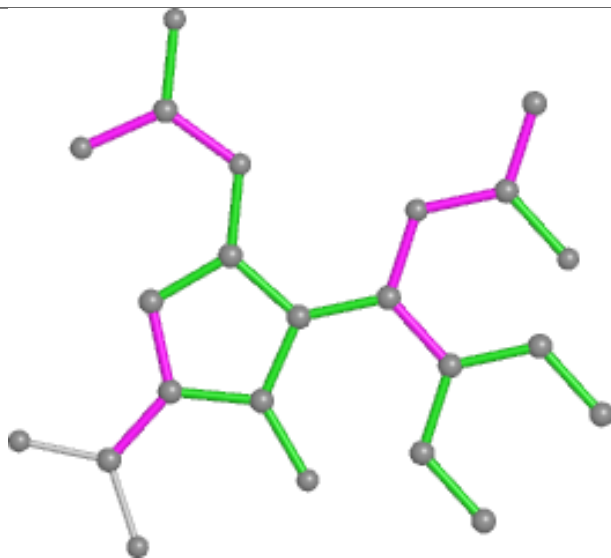
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



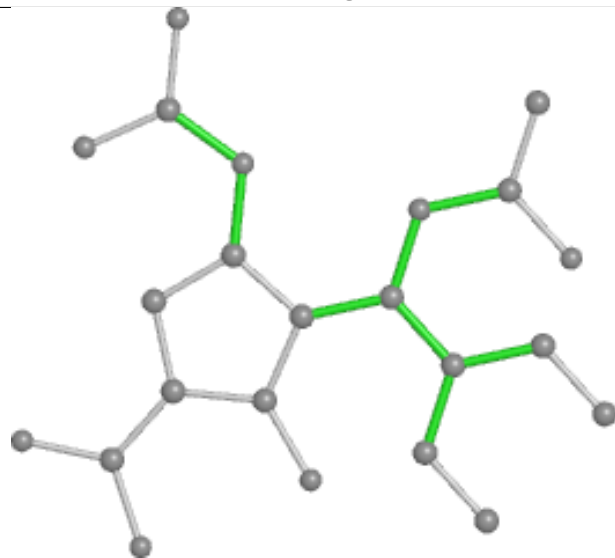
Ligand BCZ D 1001



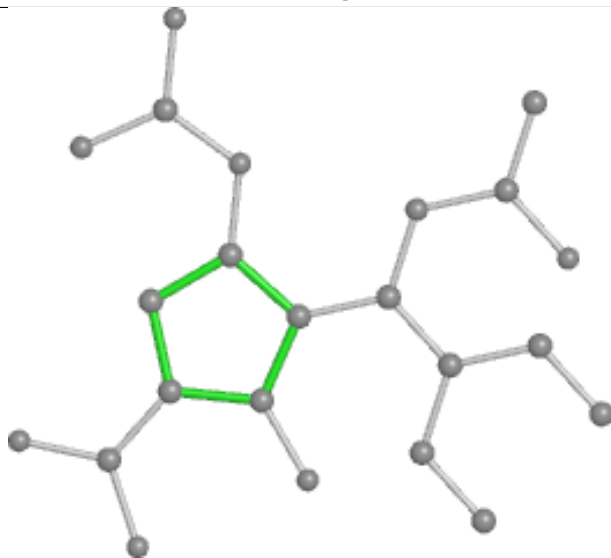
Bond lengths



Bond angles

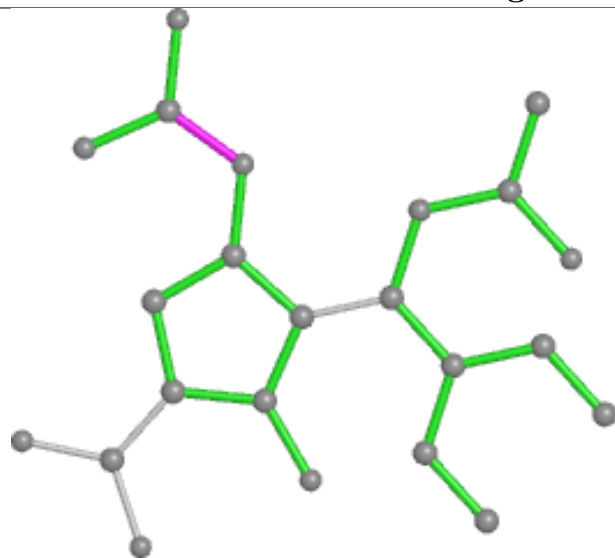


Torsions

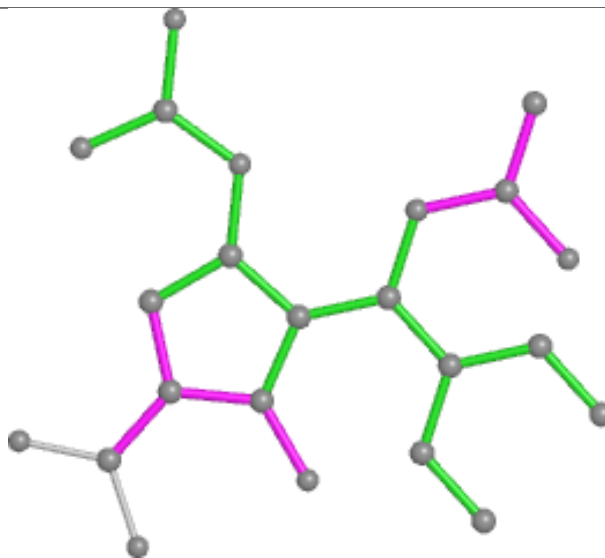


Rings

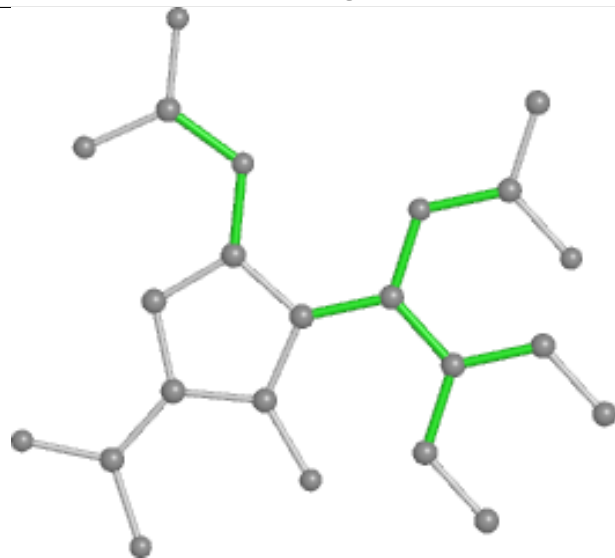
Ligand BCZ A 1001



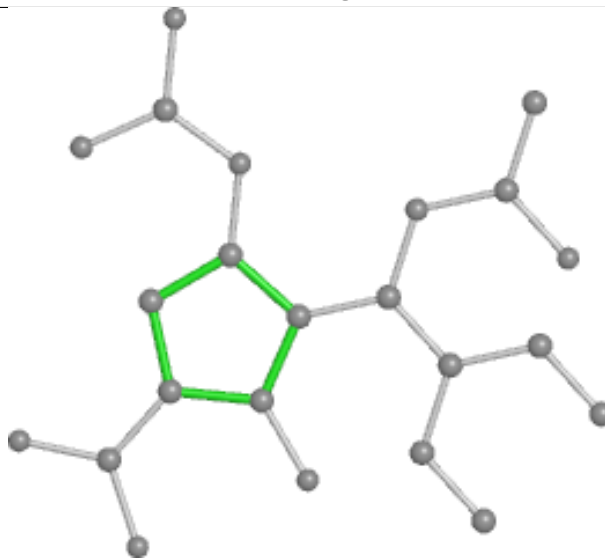
Bond lengths



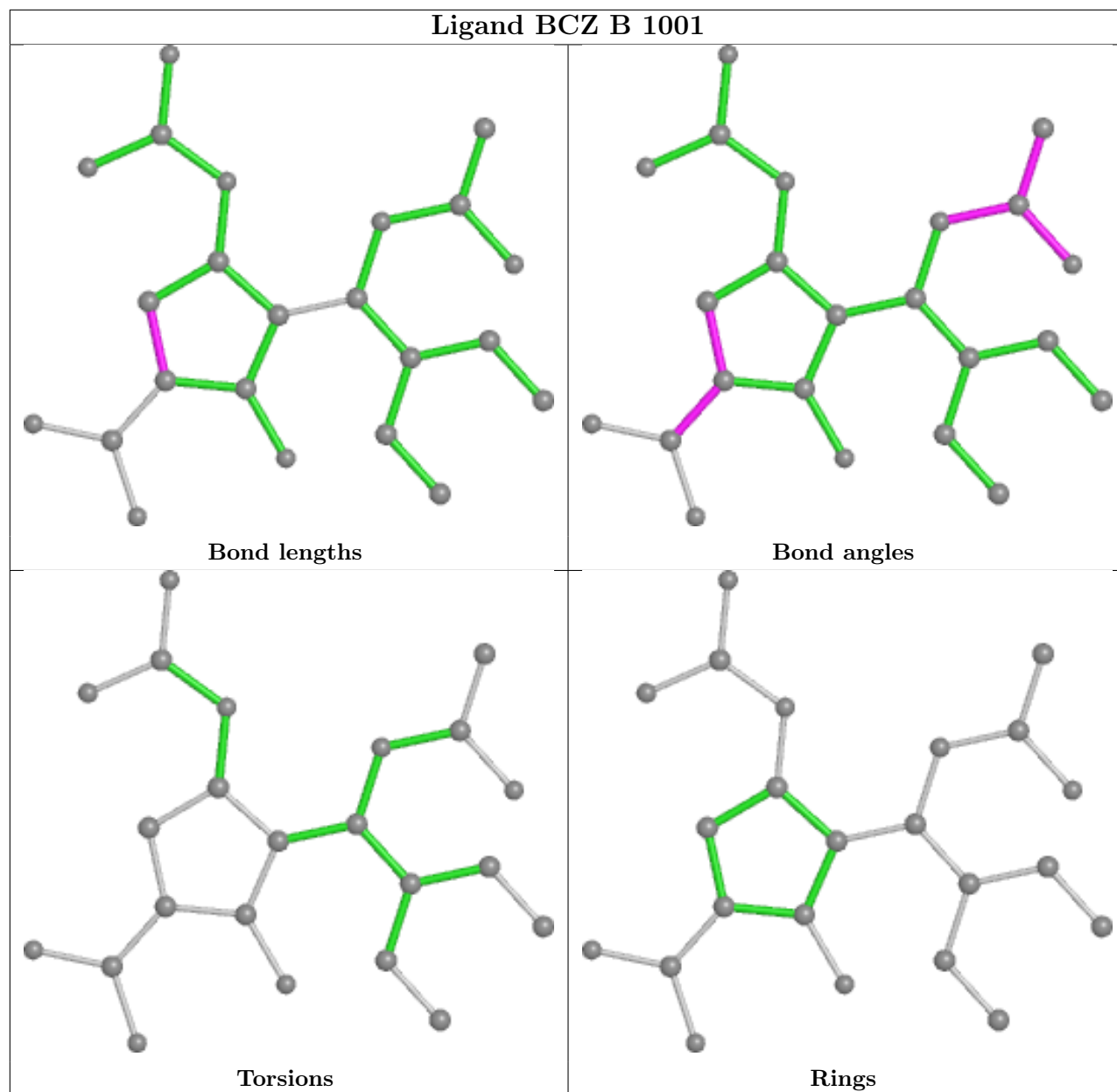
Bond angles

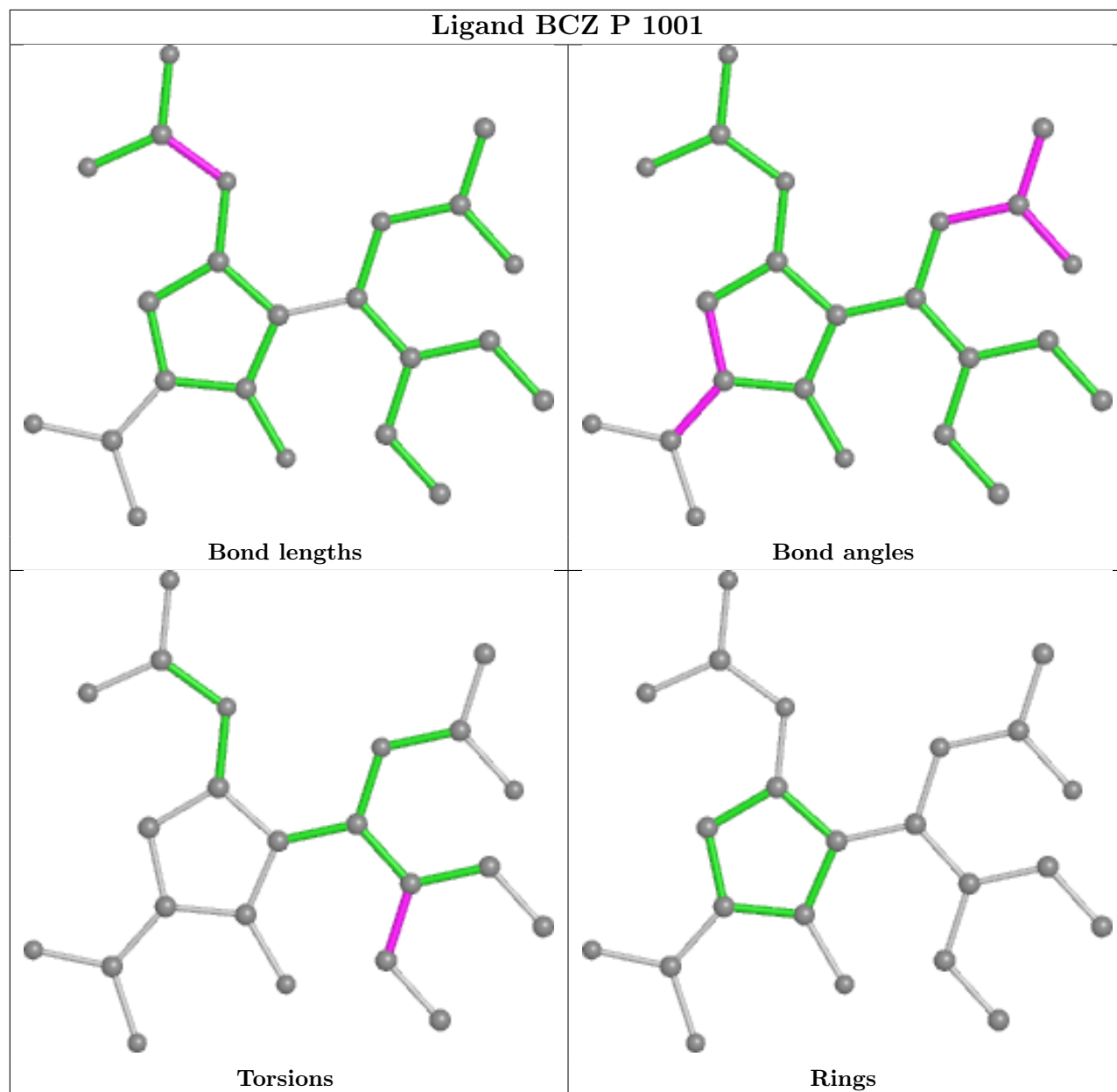


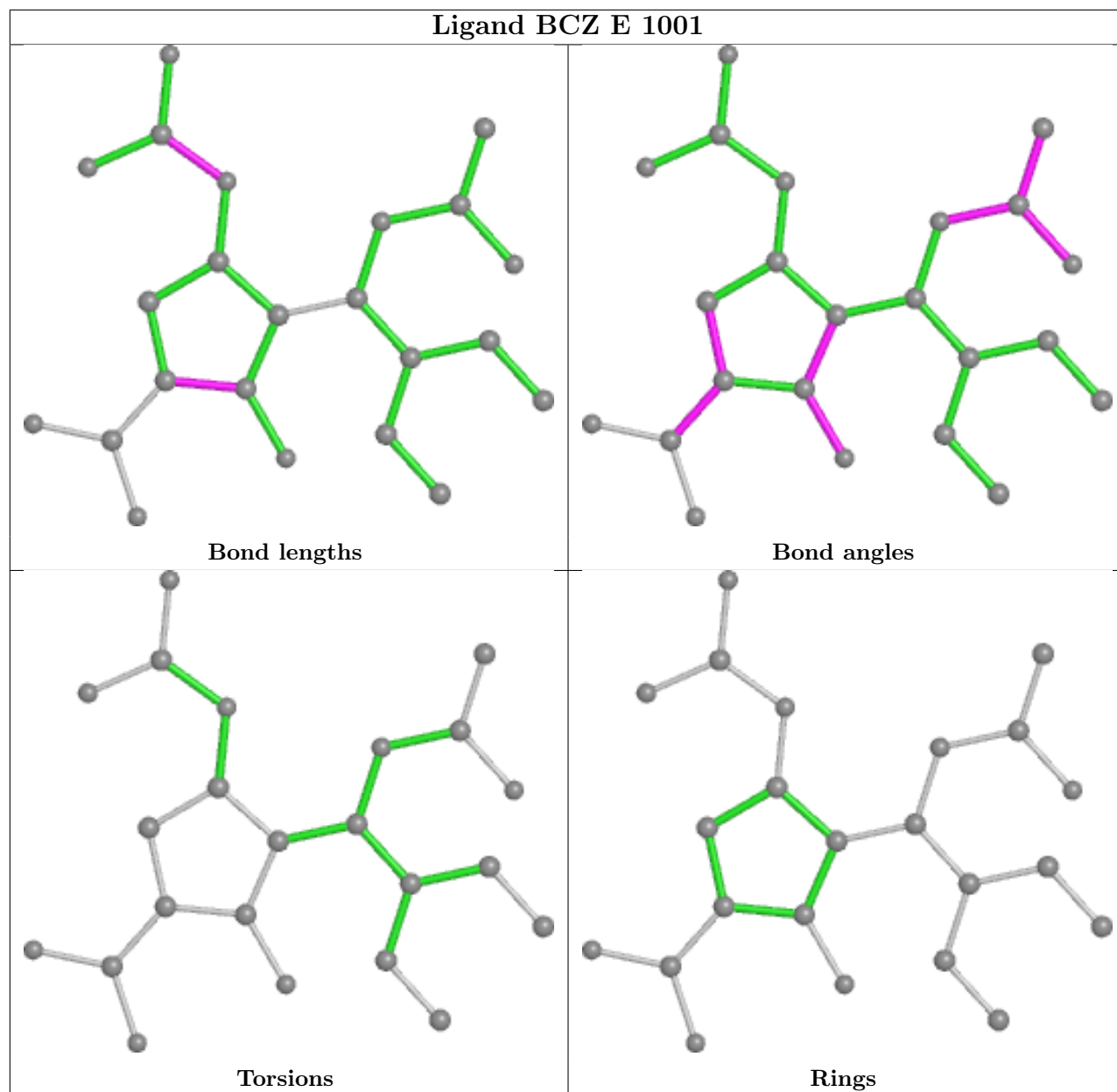
Torsions



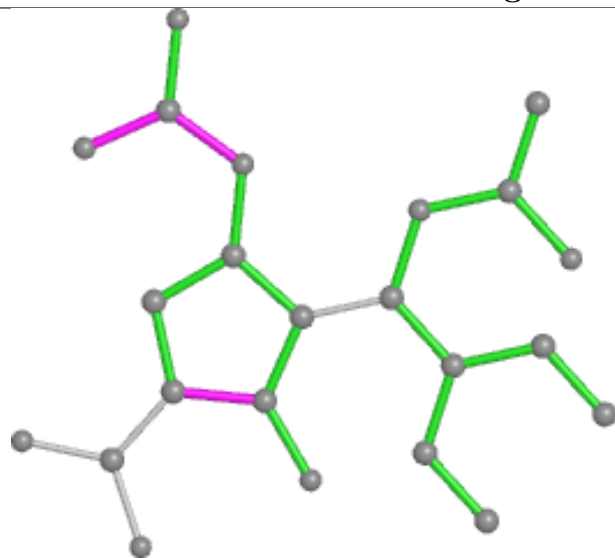
Rings



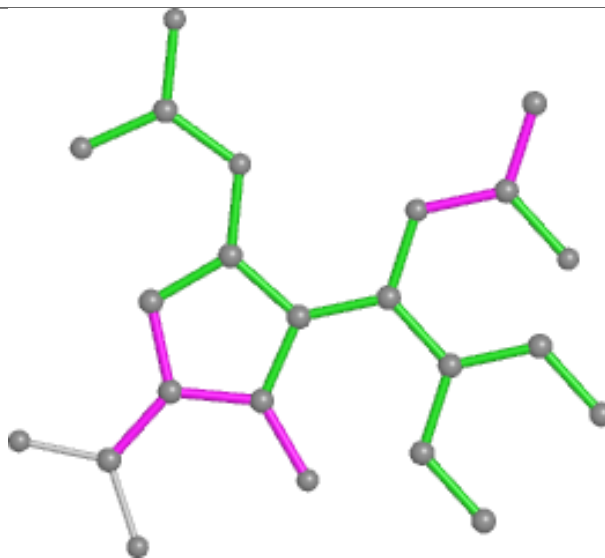




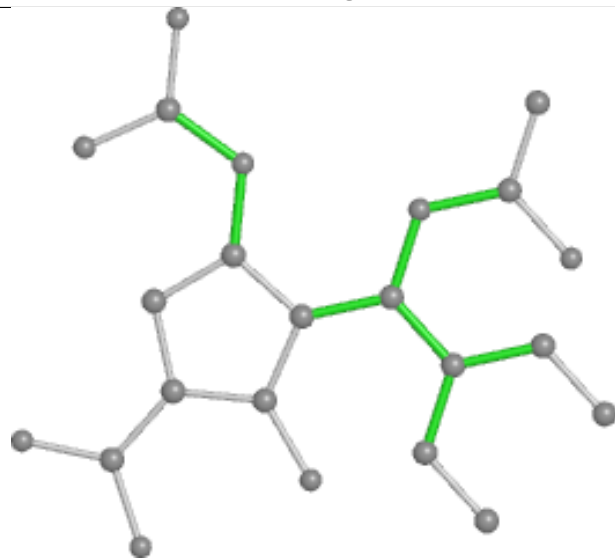
Ligand BCZ M 1001



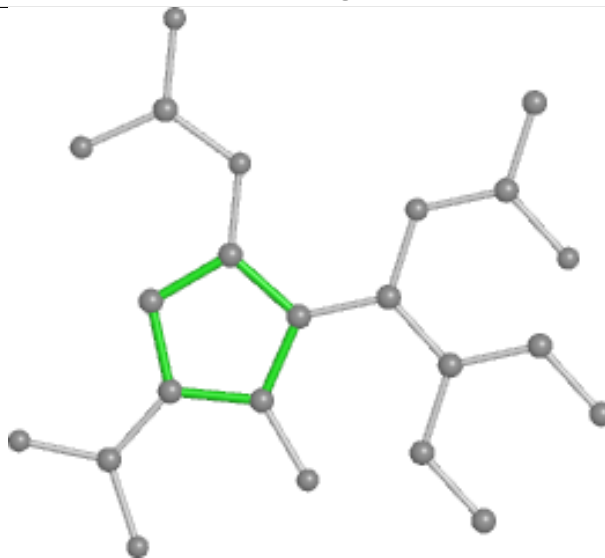
Bond lengths



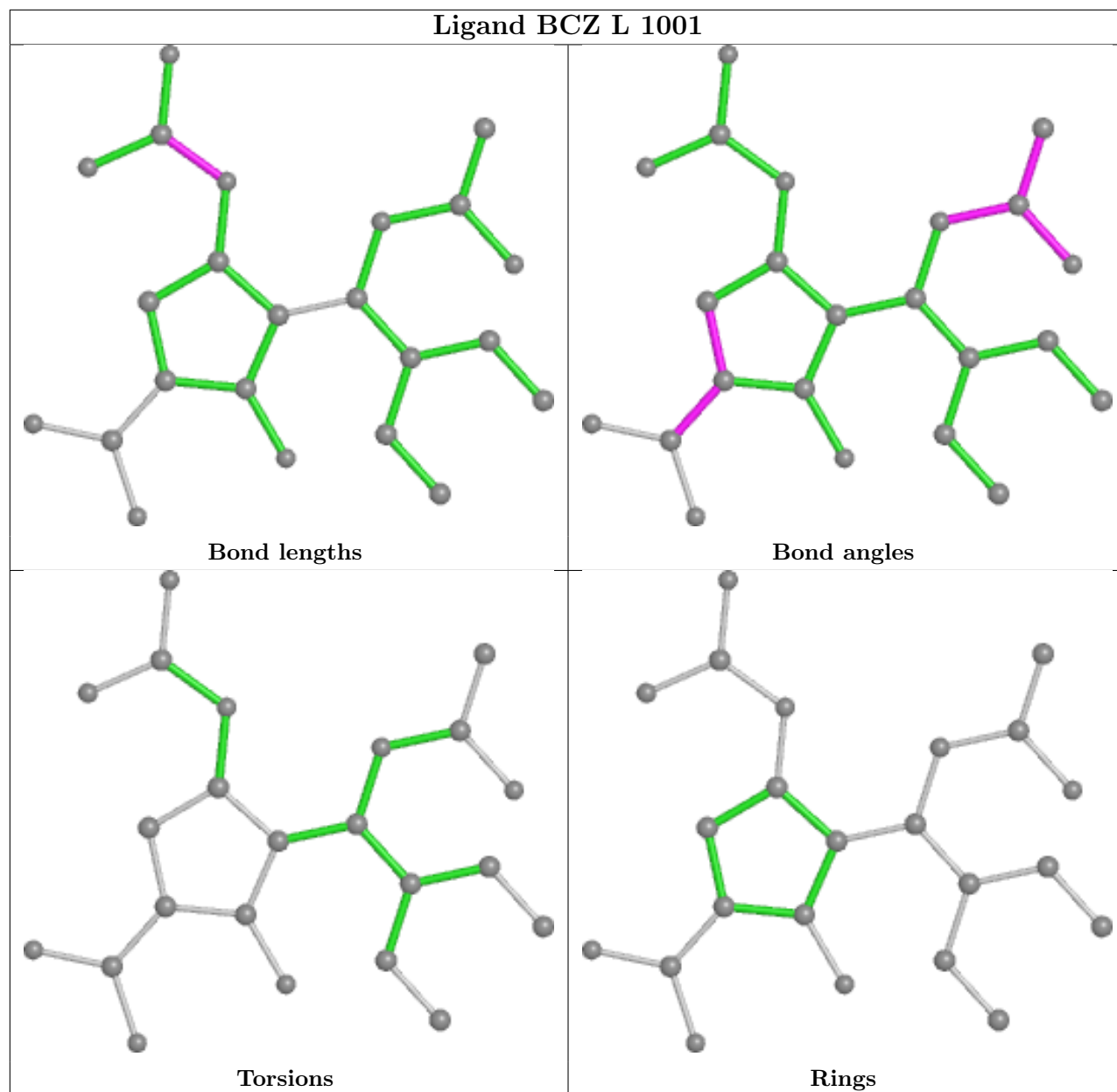
Bond angles

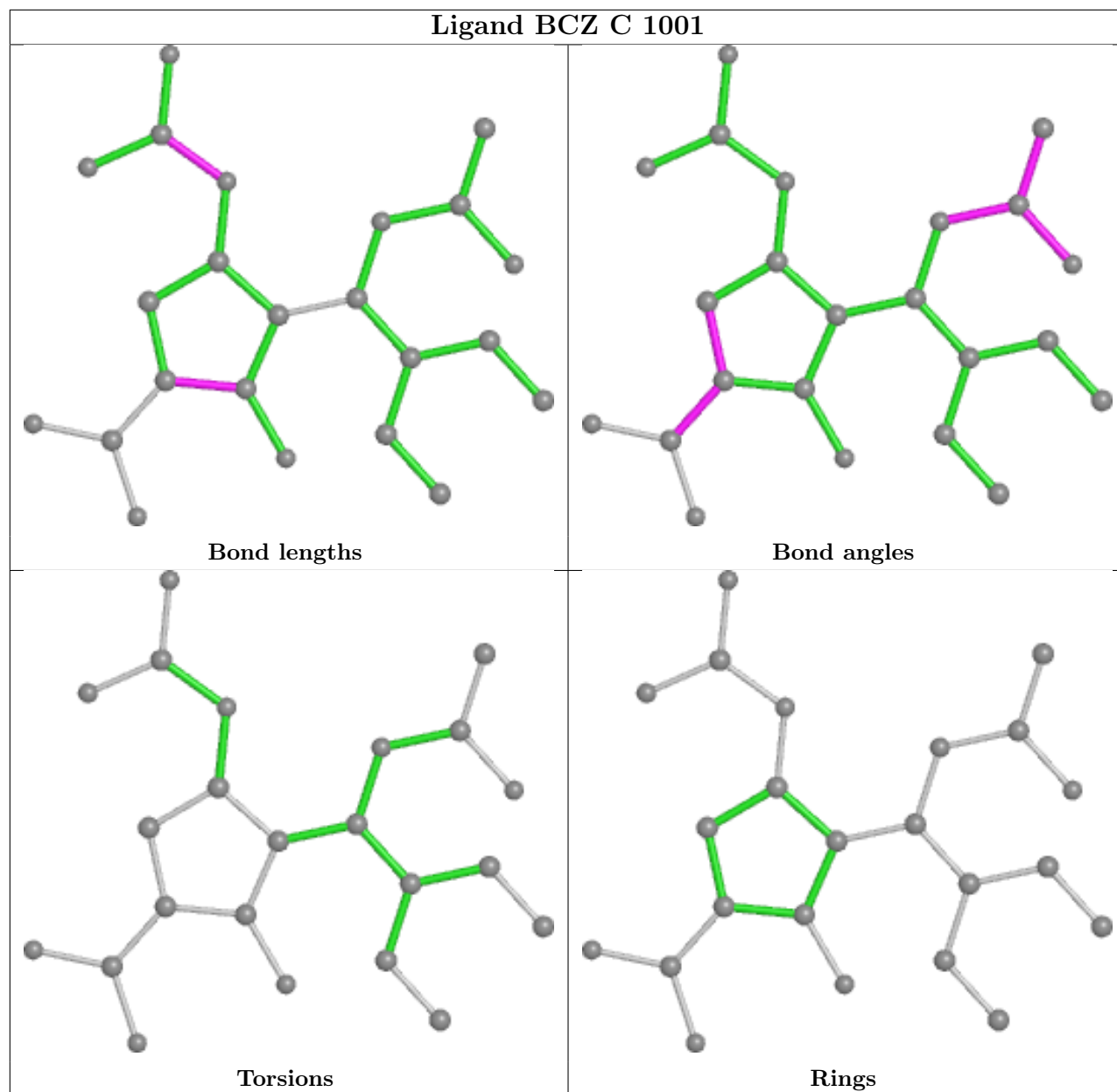


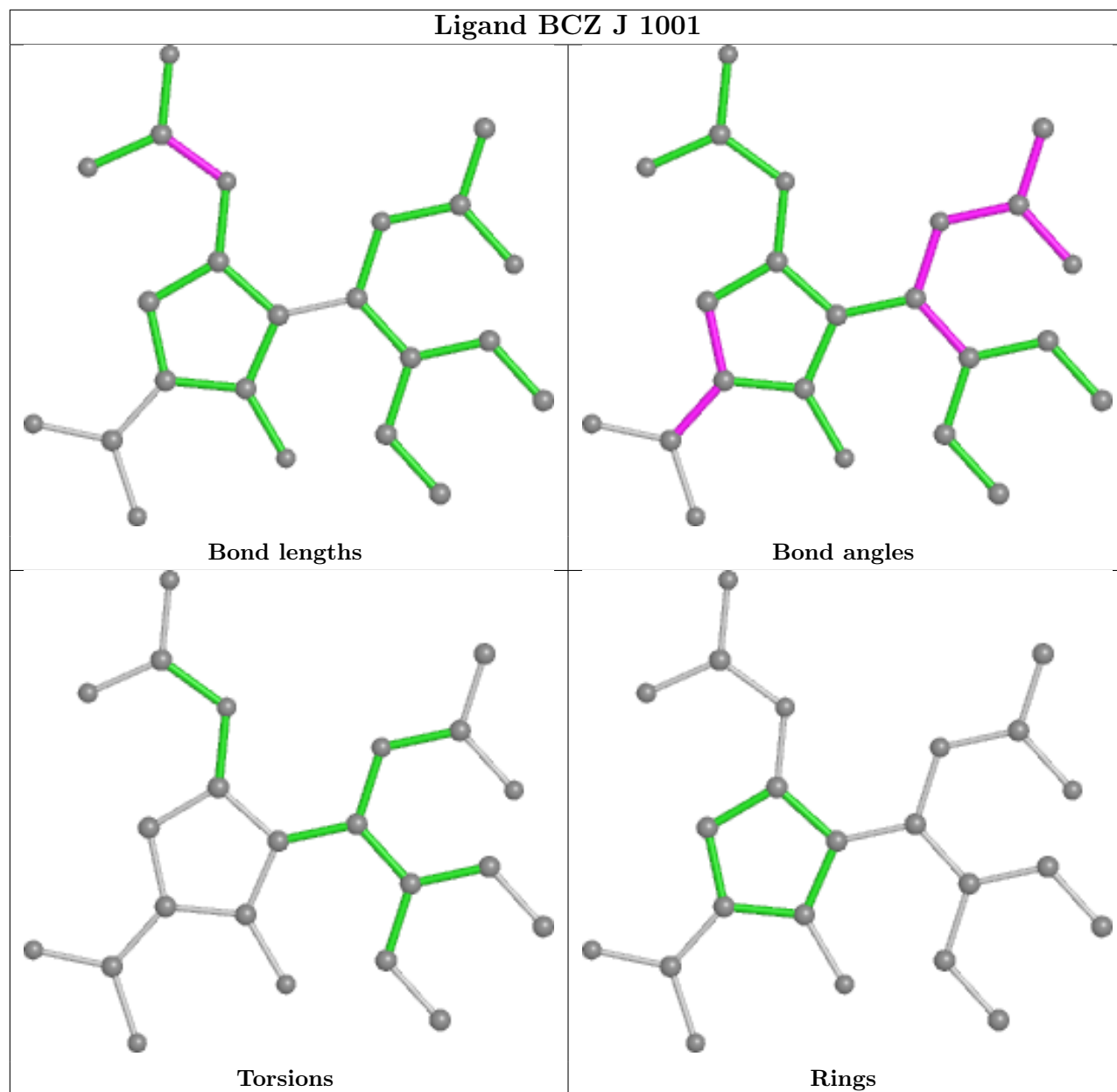
Torsions



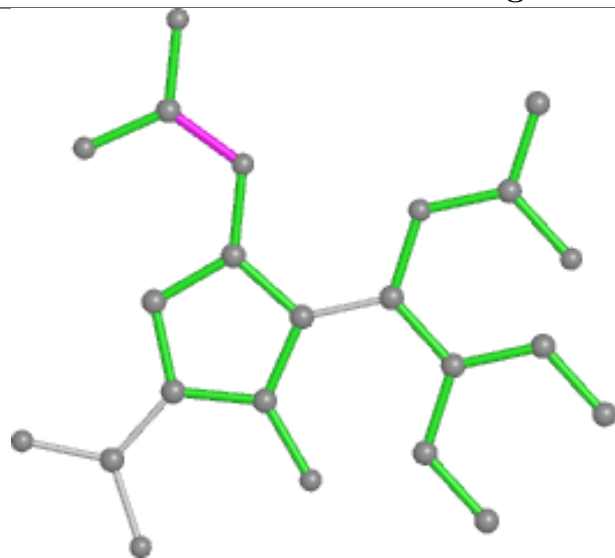
Rings



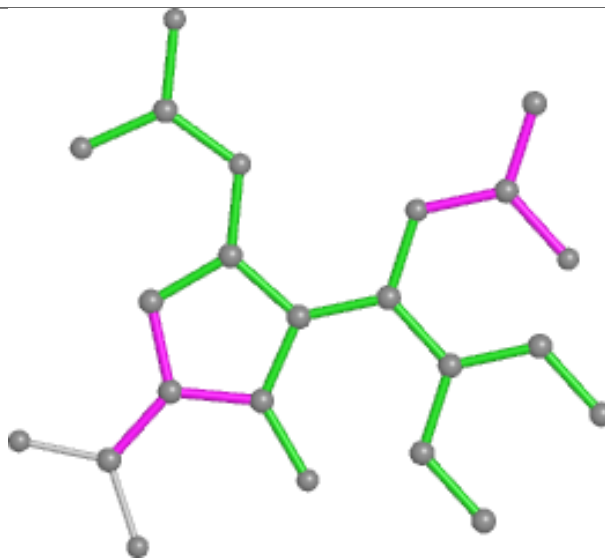




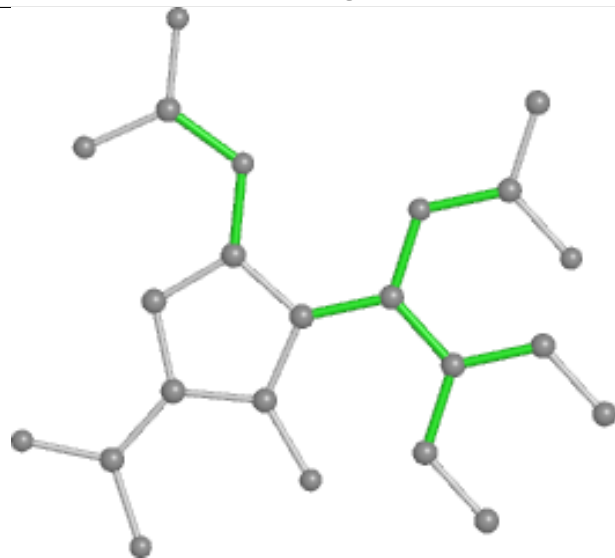
Ligand BCZ N 1001



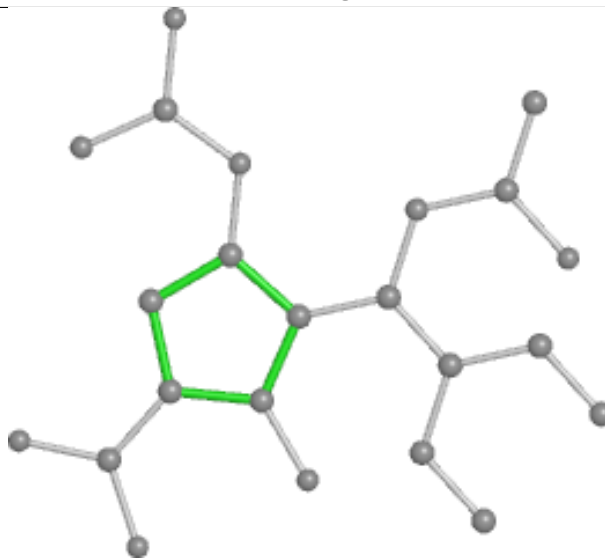
Bond lengths



Bond angles

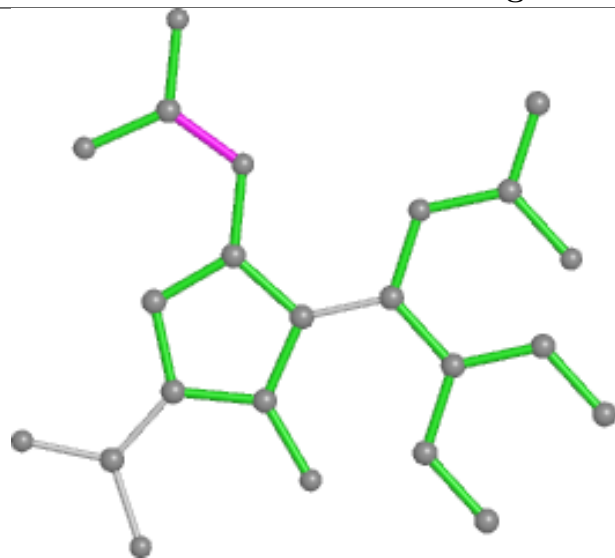


Torsions

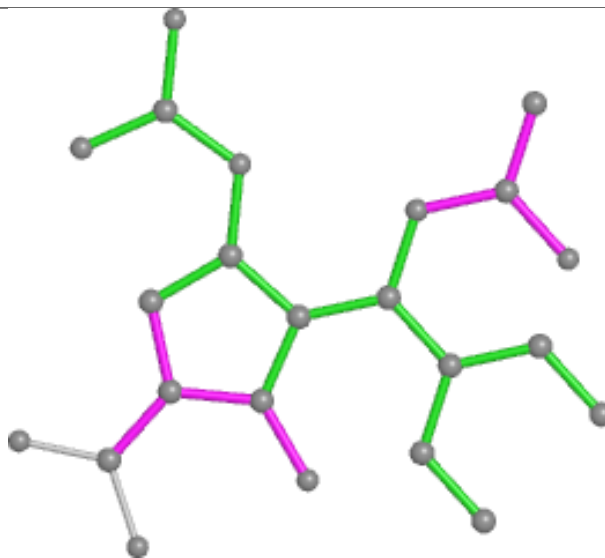


Rings

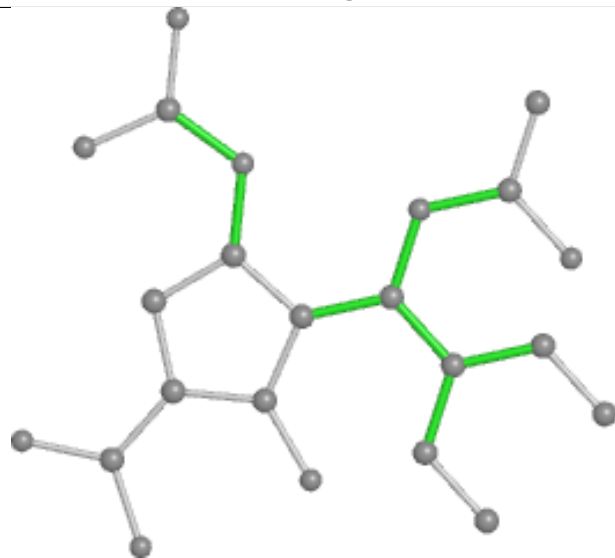
Ligand BCZ K 1001



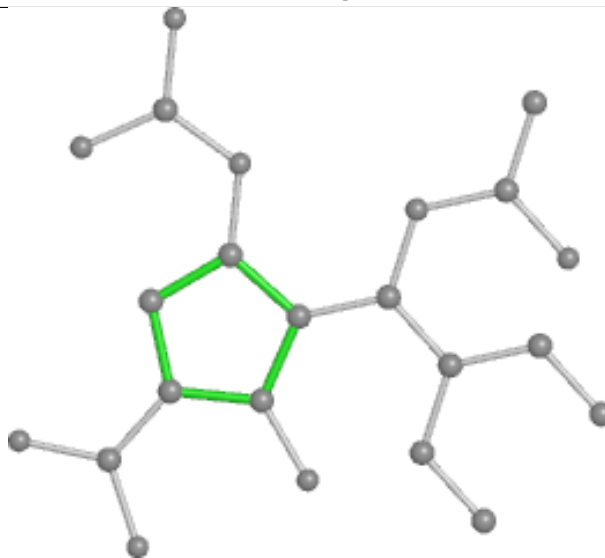
Bond lengths



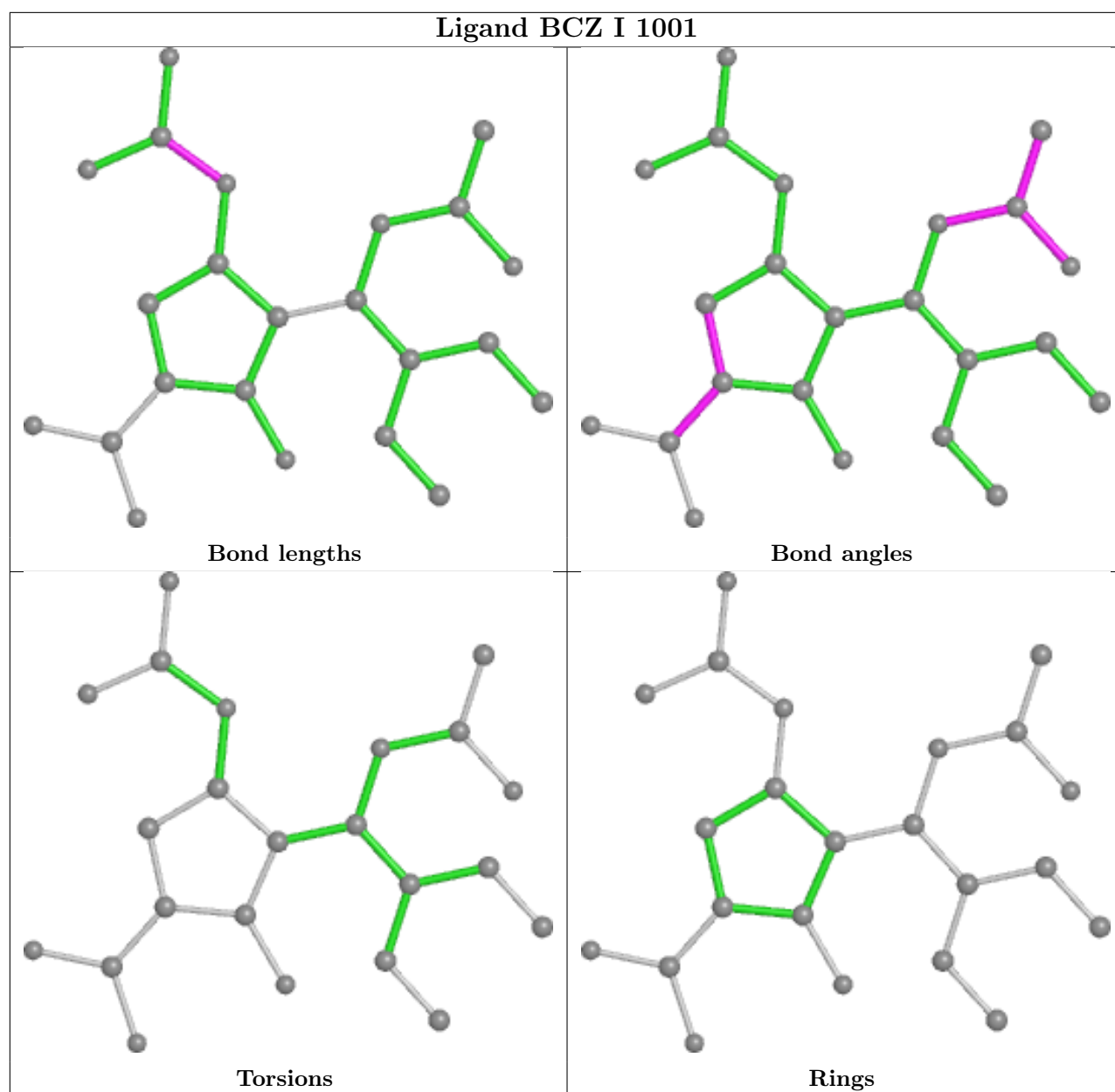
Bond angles



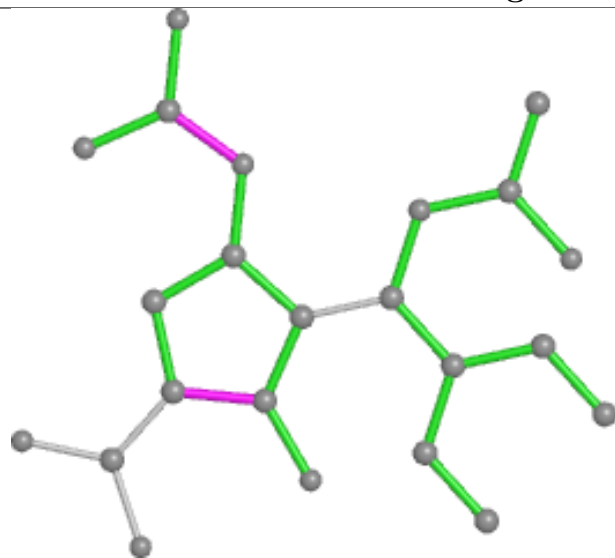
Torsions



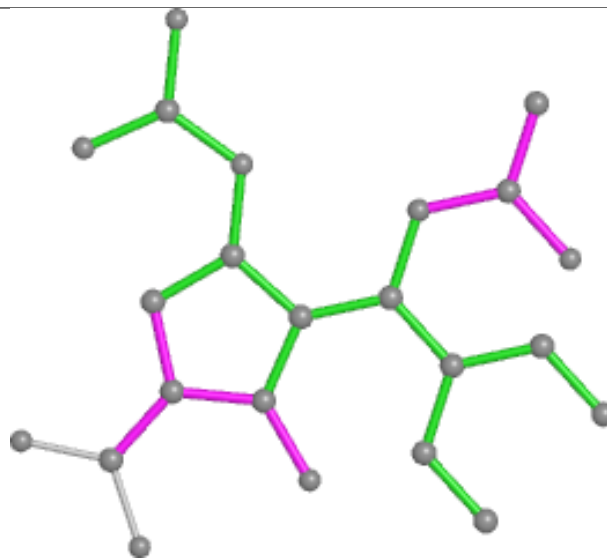
Rings



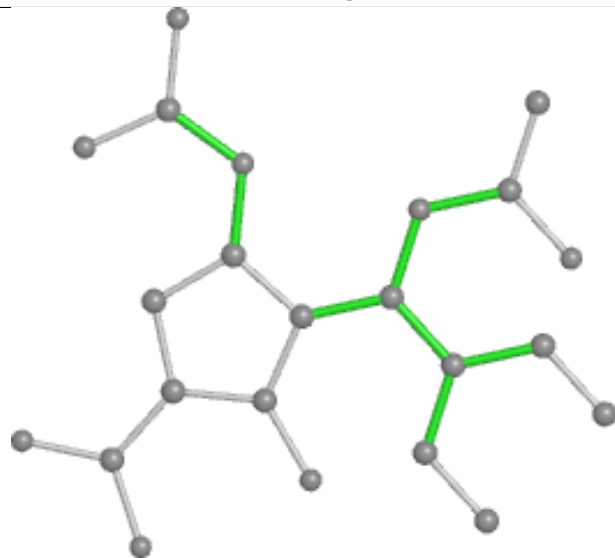
Ligand BCZ H 1001



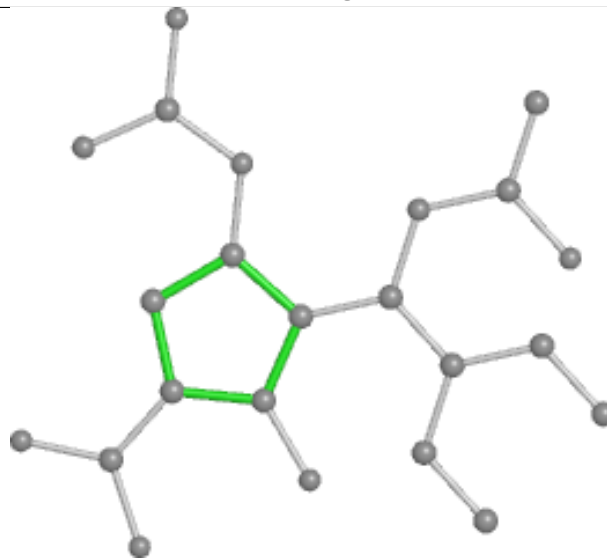
Bond lengths



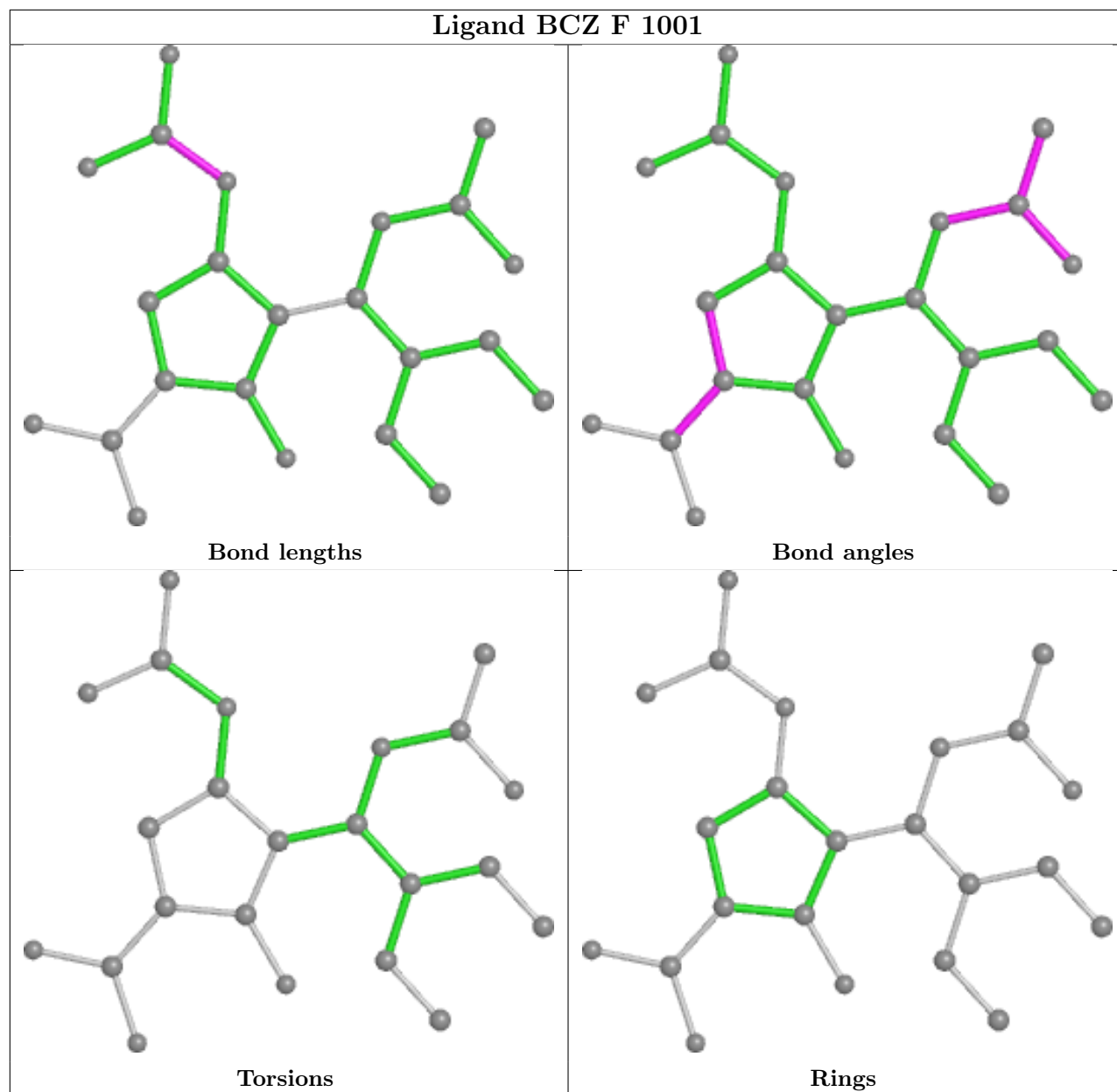
Bond angles

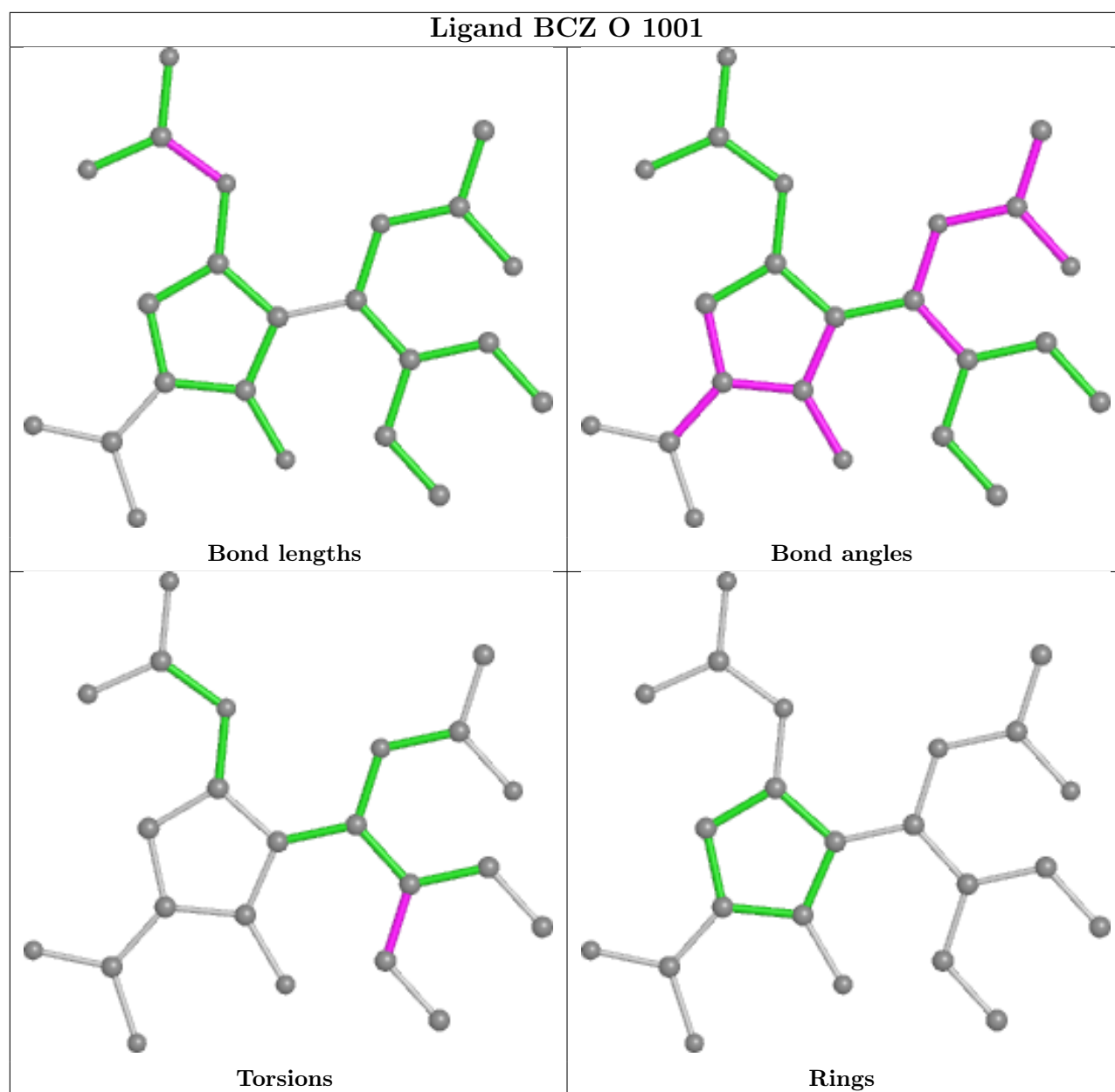


Torsions



Rings





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

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

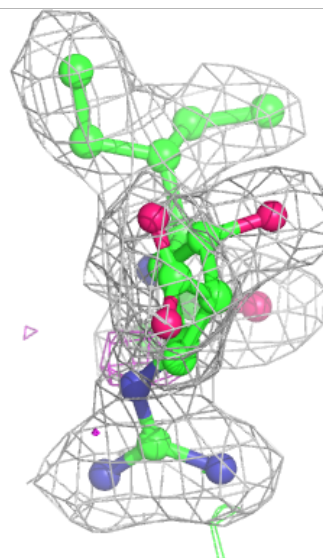
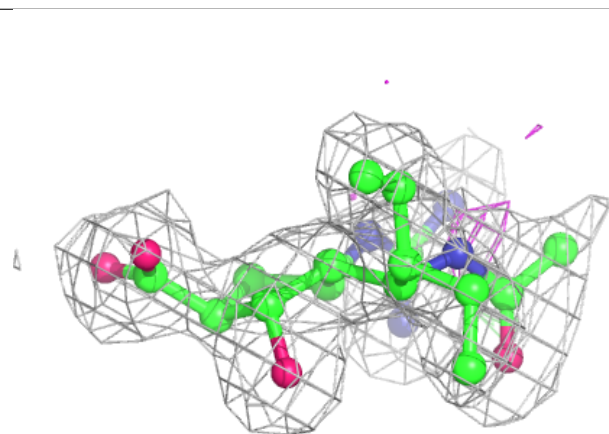
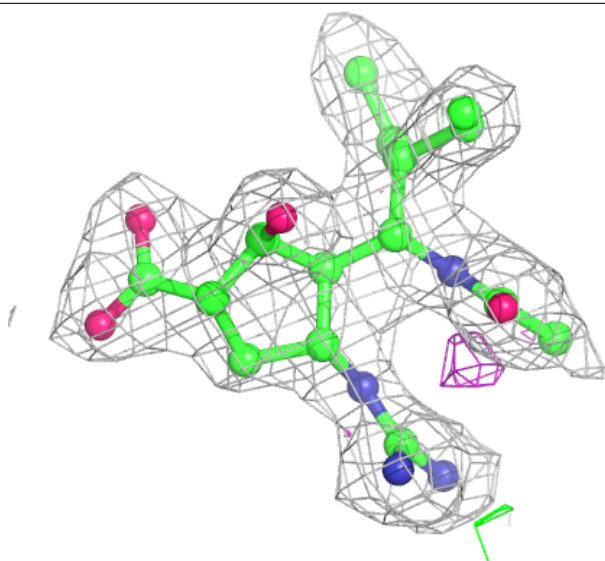
6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

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.

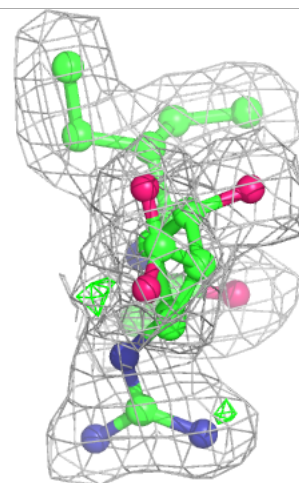
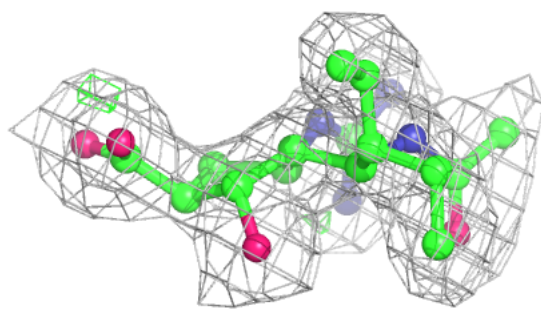
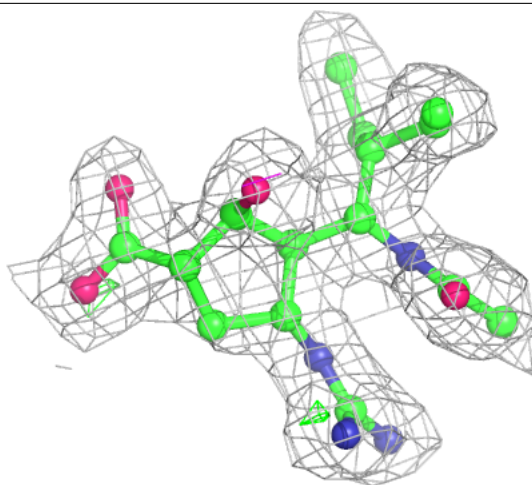
Electron density around BCZ A 1001:

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



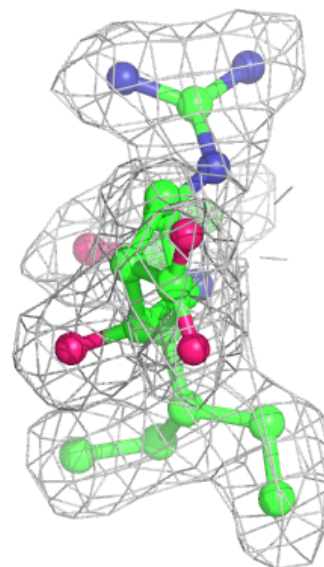
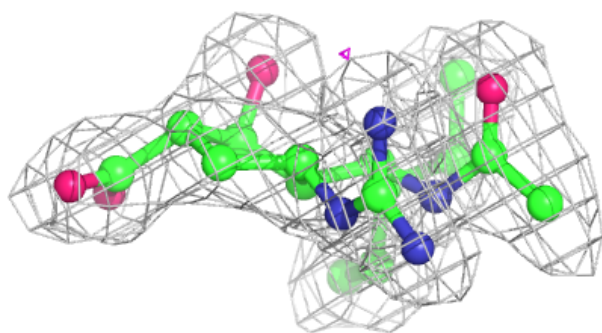
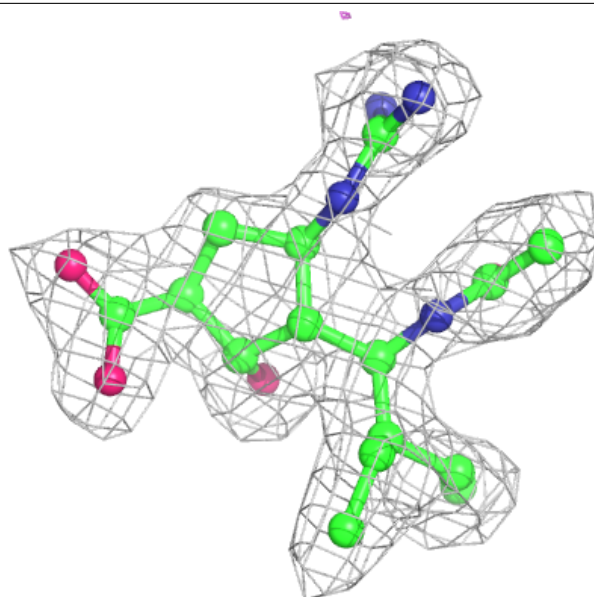
Electron density around BCZ B 1001:

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



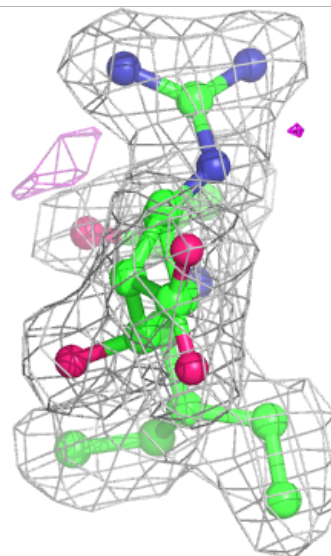
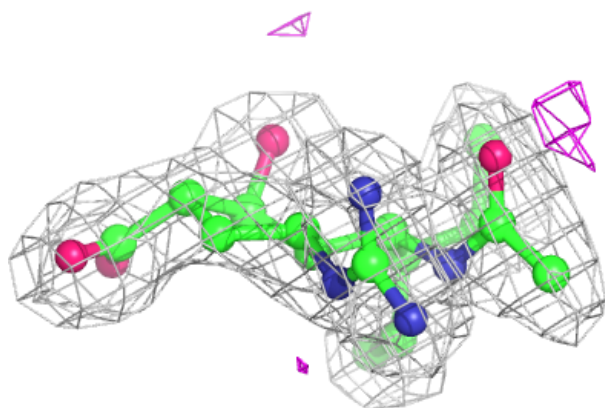
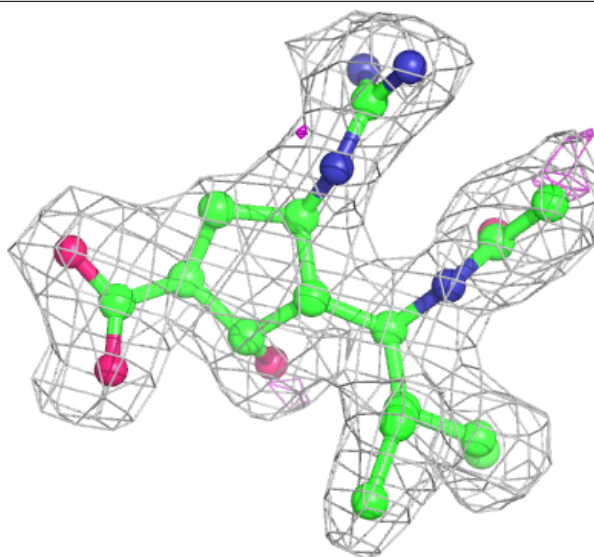
Electron density around BCZ C 1001:

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



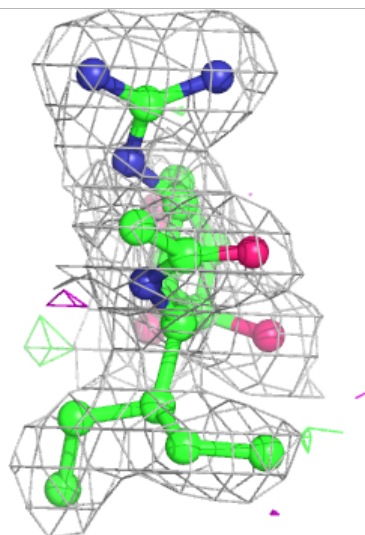
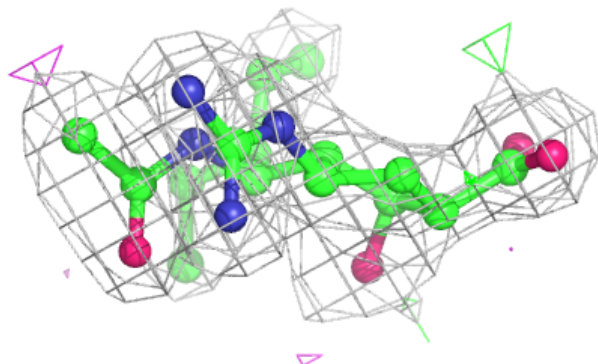
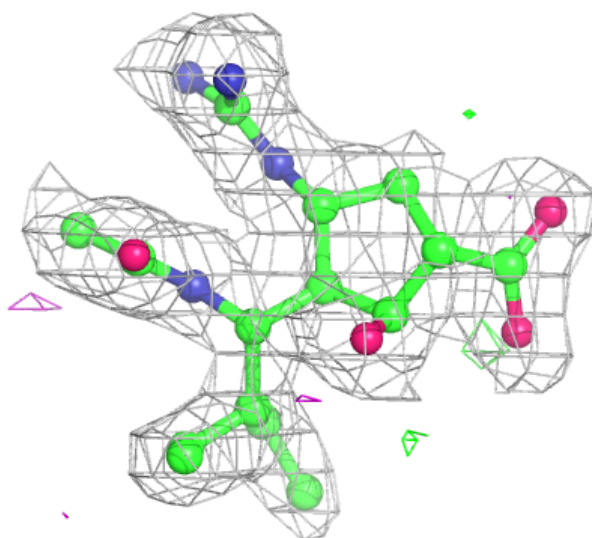
Electron density around BCZ D 1001:

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



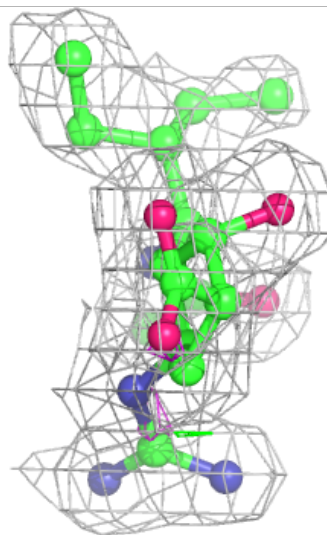
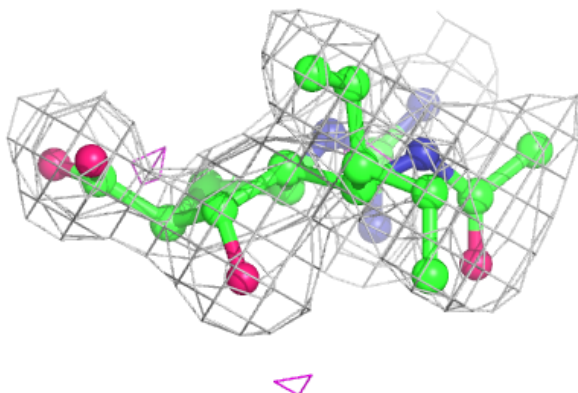
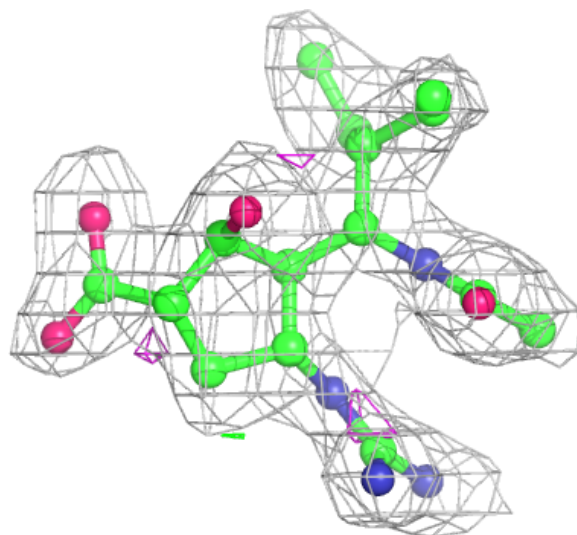
Electron density around BCZ E 1001:

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



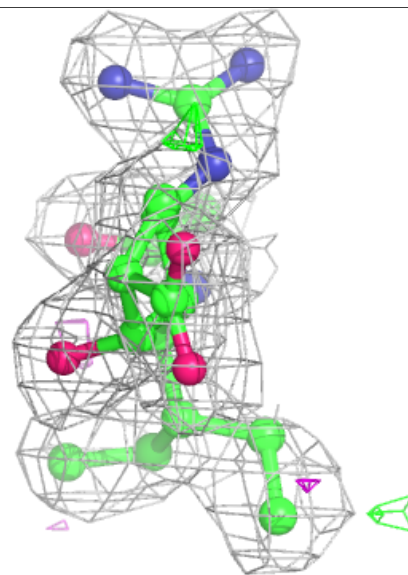
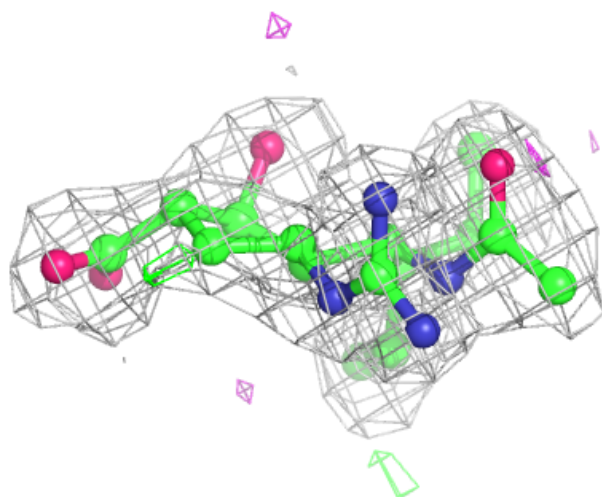
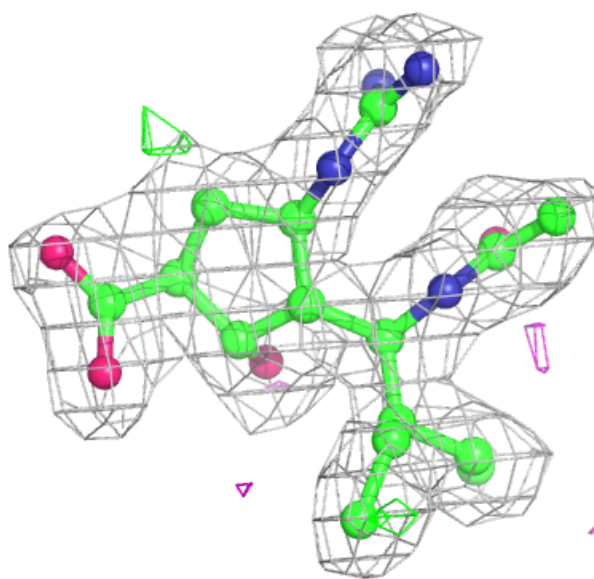
Electron density around BCZ F 1001:

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



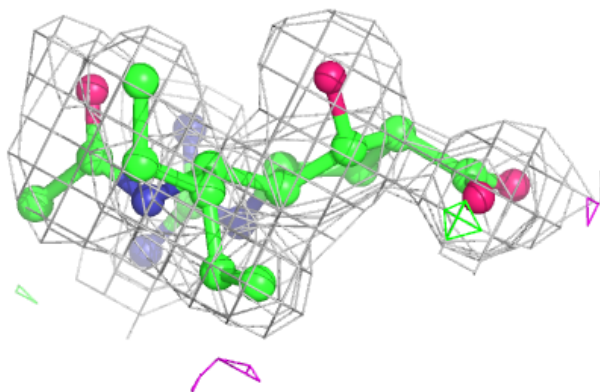
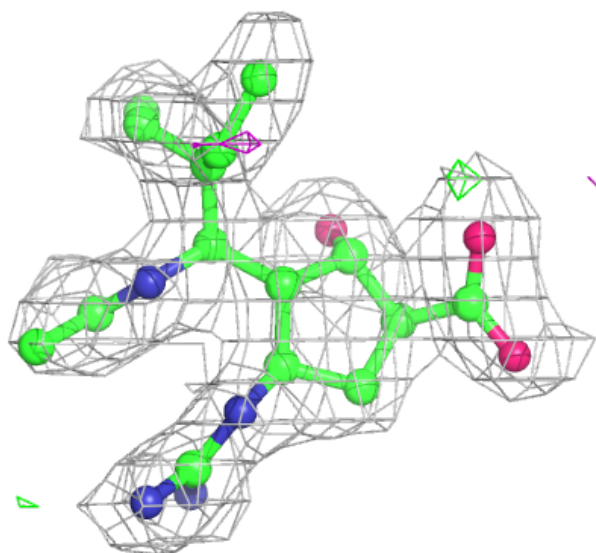
Electron density around BCZ G 1001:

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



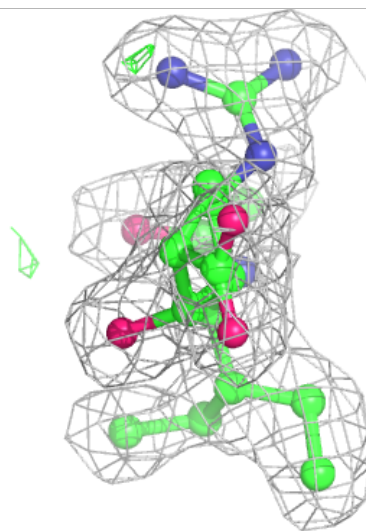
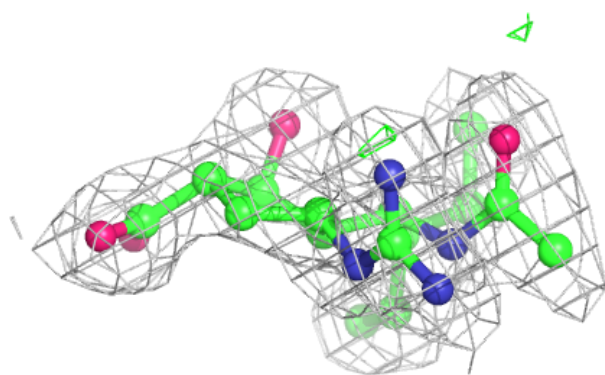
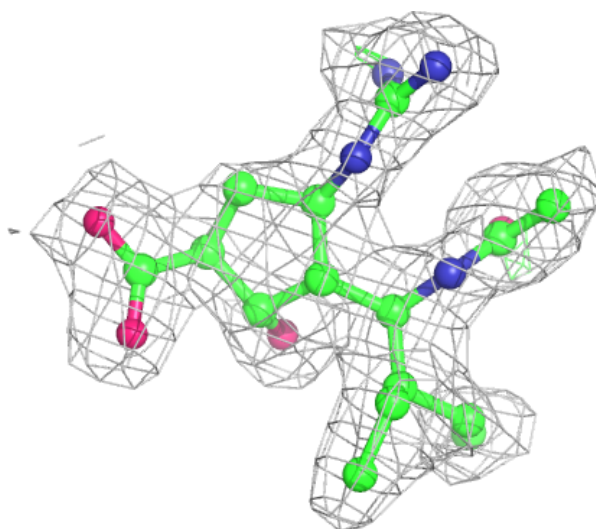
Electron density around BCZ H 1001:

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



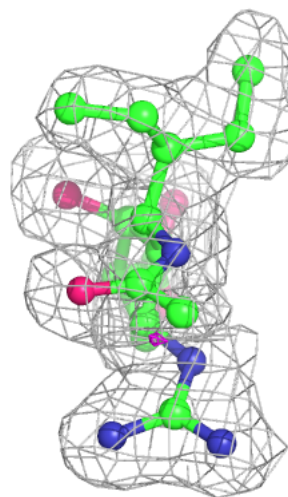
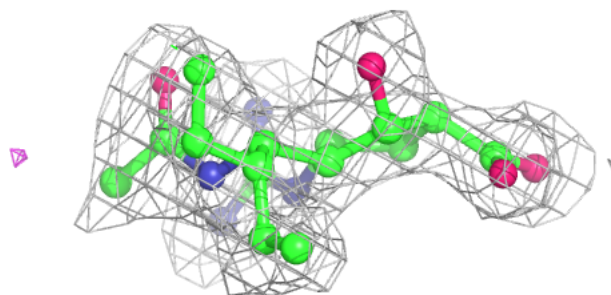
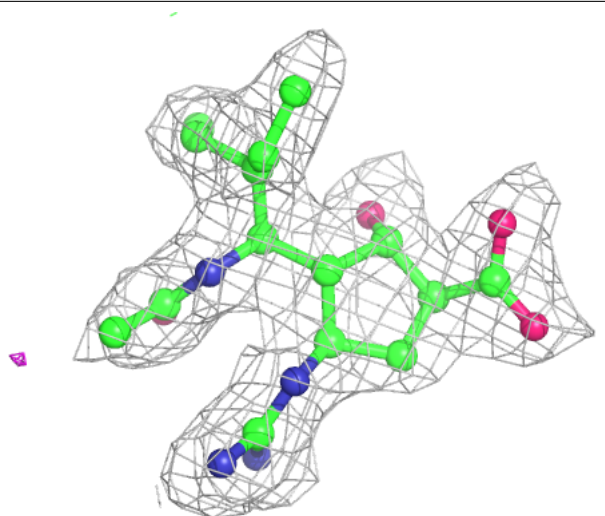
Electron density around BCZ I 1001:

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



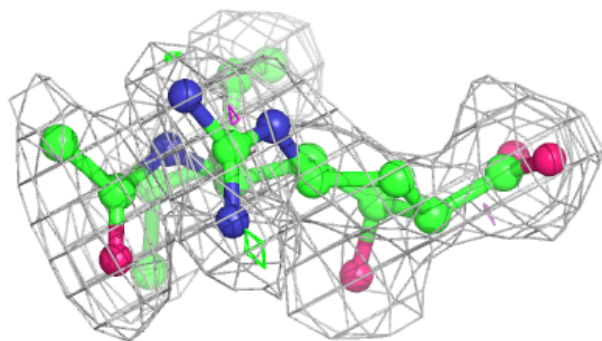
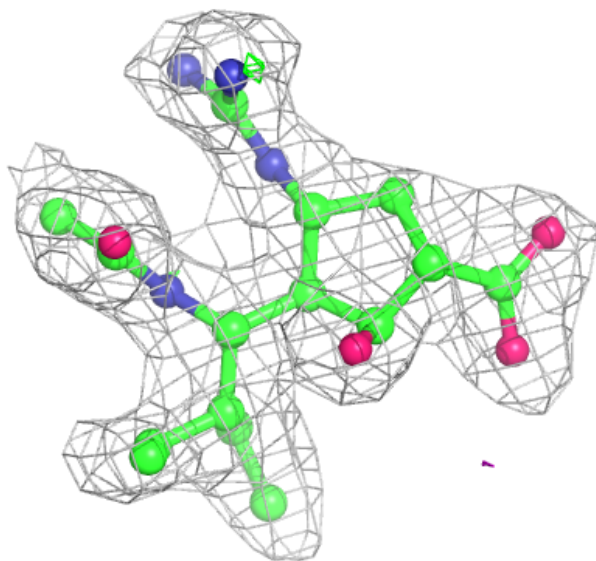
Electron density around BCZ J 1001:

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



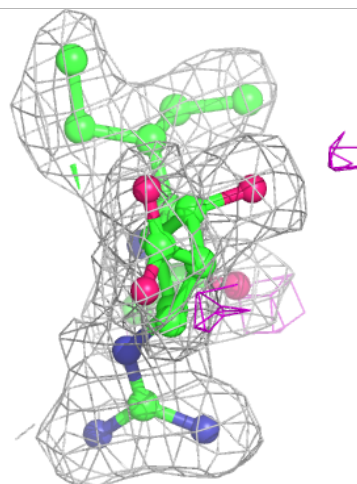
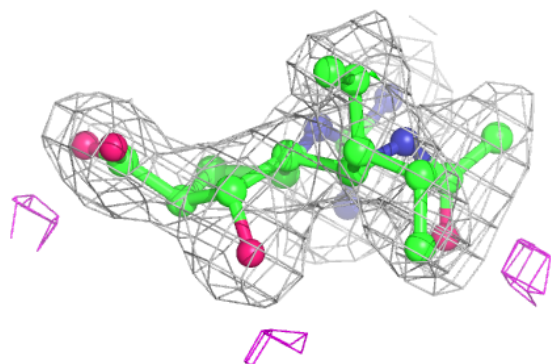
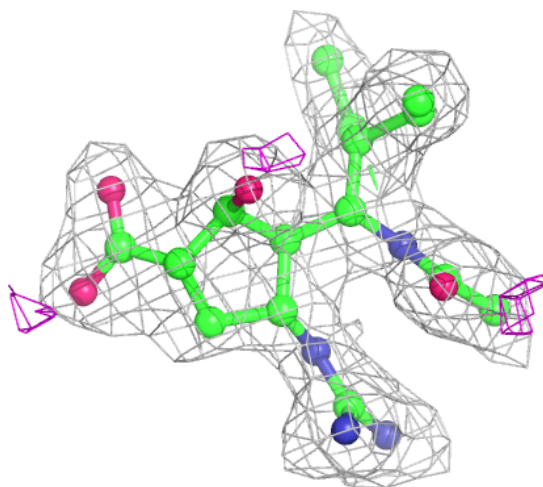
Electron density around BCZ K 1001:

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



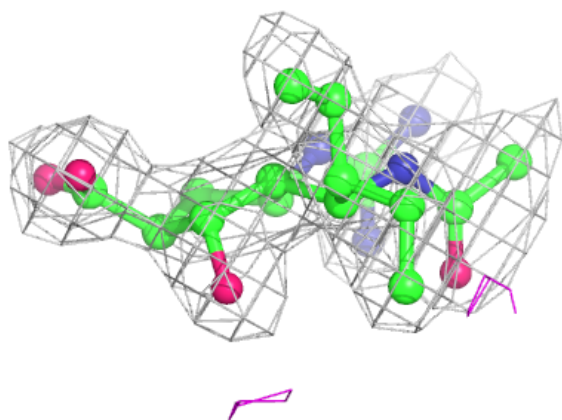
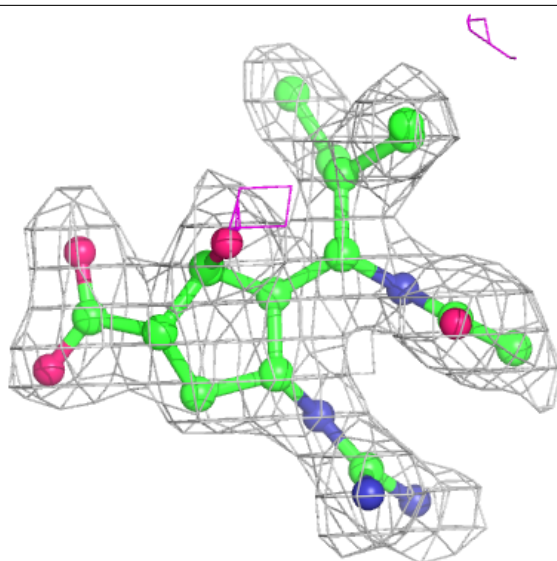
Electron density around BCZ L 1001:

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



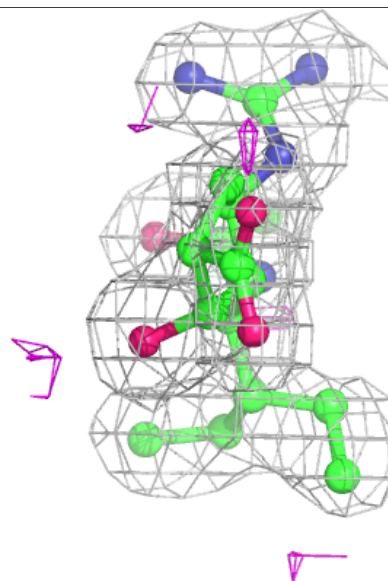
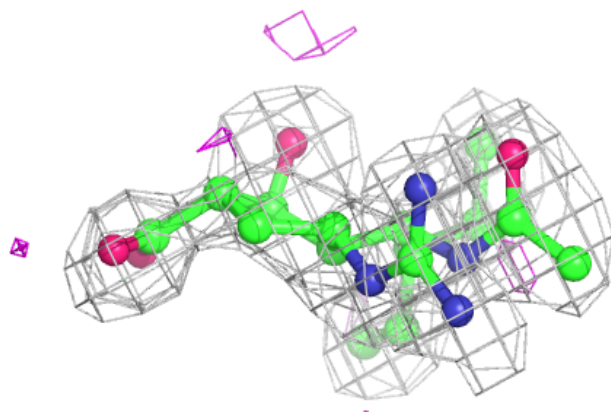
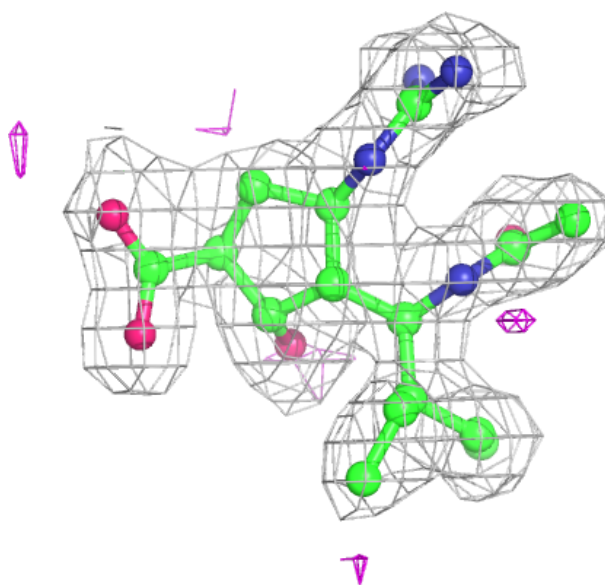
Electron density around BCZ M 1001:

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



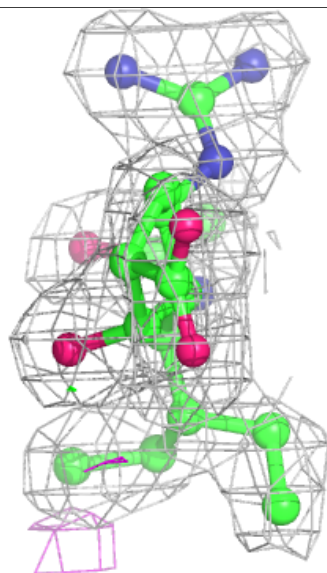
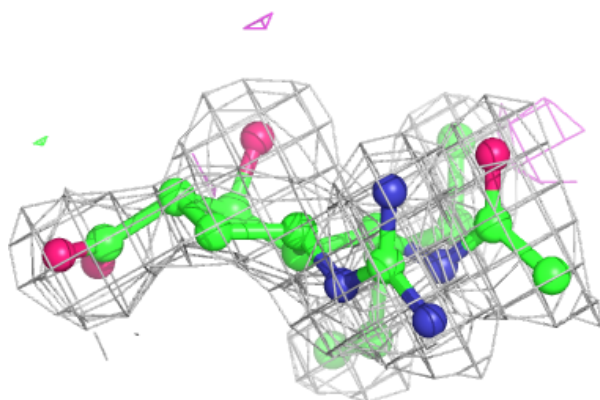
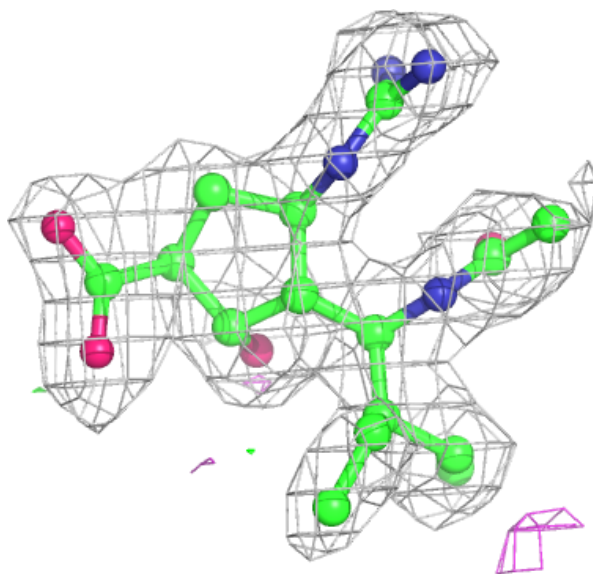
Electron density around BCZ N 1001:

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



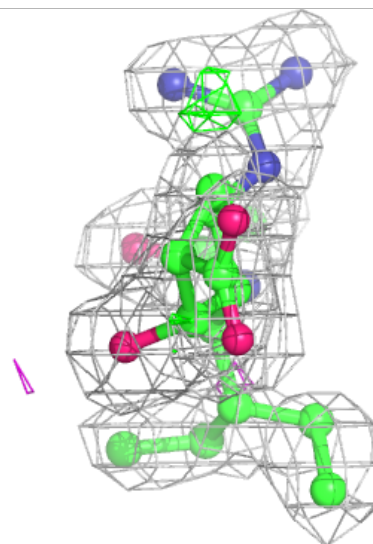
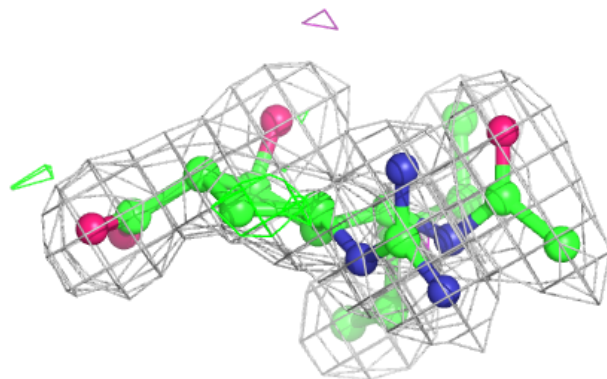
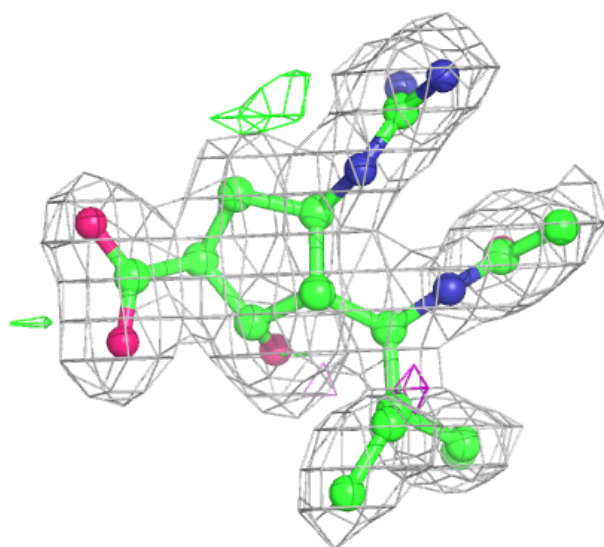
Electron density around BCZ O 1001:

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



Electron density around BCZ P 1001:

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



6.5 Other polymers [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.