



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:40 AM UTC

PDB ID : 3K39 / pdb_00003k39
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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

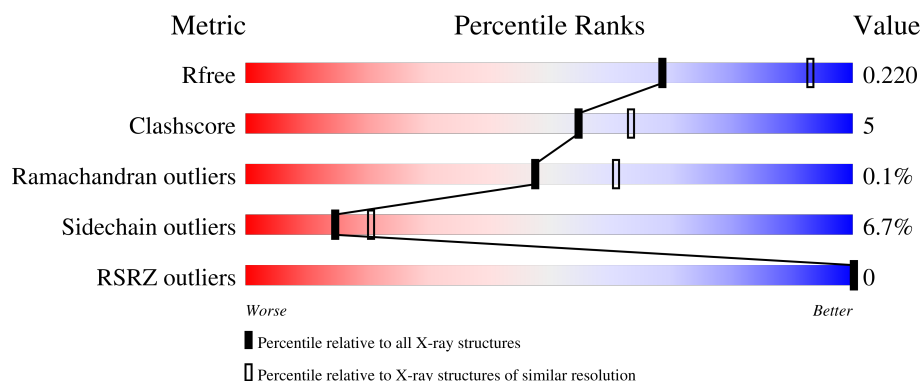
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.54 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}	180053	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

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	397	
1	B	397	
1	C	397	
1	D	397	
1	E	397	

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Mol	Chain	Length	Quality of chain
1	F	397	 85% 10% . . .
1	G	397	 85% 10% . . .
1	H	397	 86% 9% . . .
1	I	397	 83% 12% . . .
1	J	397	 85% 10% . . .
1	K	397	 85% 10% . .
1	L	397	 85% 10% . .
1	M	397	 85% 10% . .
1	N	397	 87% 9% . .
1	O	397	 86% 9% . .
1	P	397	 85% 10% . . .

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.

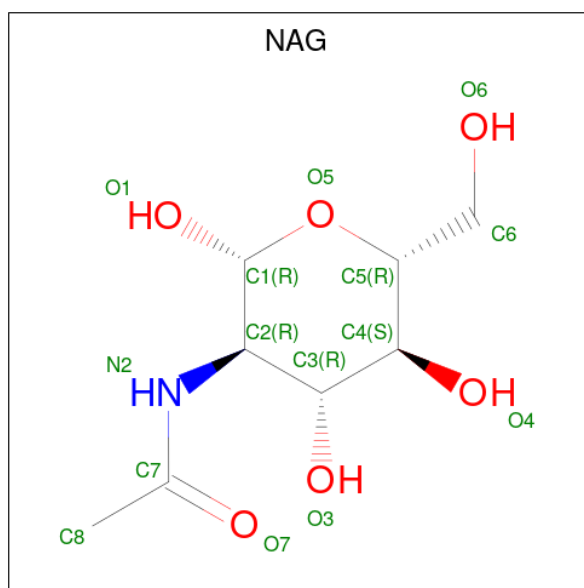
- Molecule 1 is a protein called Neuraminidase.

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 (CCD ID: 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 (CCD ID: CA) (formula: Ca).

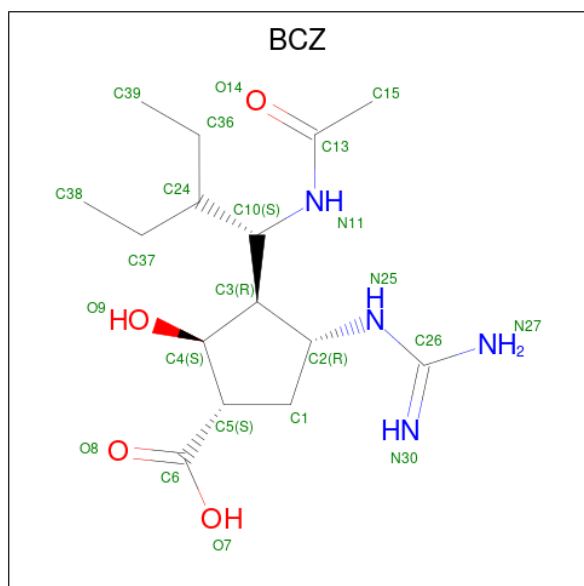
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ca	0	0
			1	1		
3	B	1	Total	Ca	0	0
			1	1		
3	C	1	Total	Ca	0	0
			1	1		
3	D	1	Total	Ca	0	0
			1	1		
3	E	1	Total	Ca	0	0
			1	1		

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

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



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

- Molecule 5 is YTTRIUM (III) ION (CCD ID: YT3) (formula: Y).

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

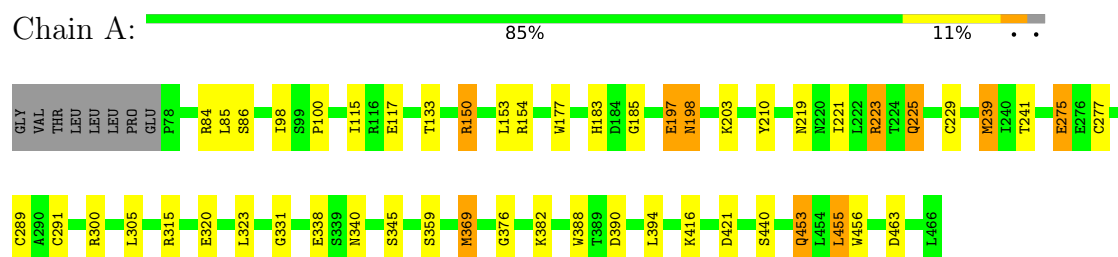
- Molecule 6 is water.

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

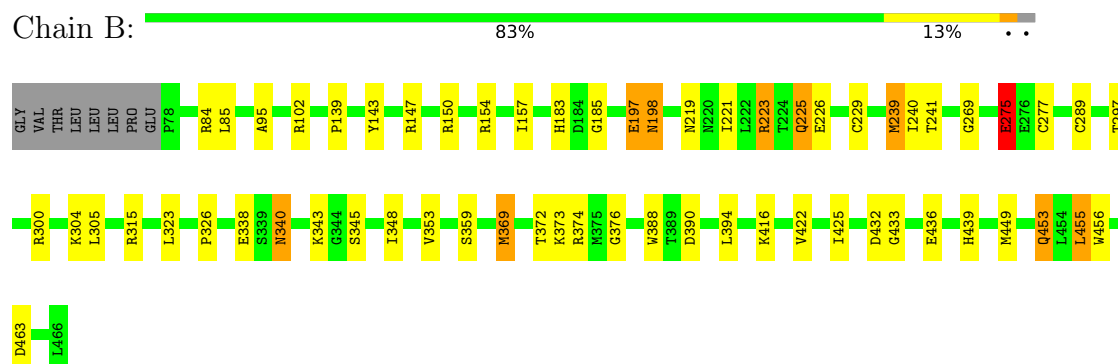
3 Residue-property plots

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.

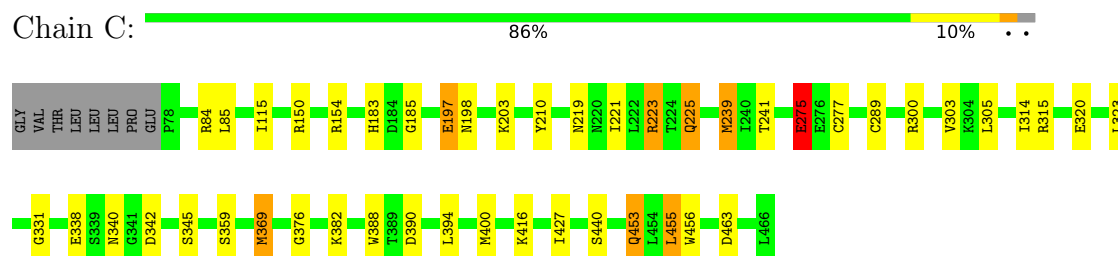
• Molecule 1: Neuraminidase



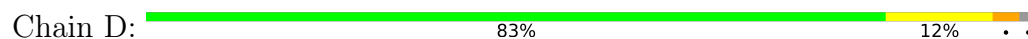
• Molecule 1: Neuraminidase

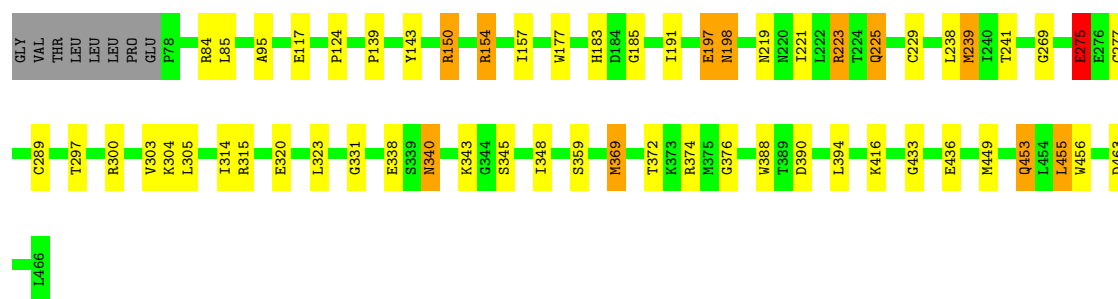


• Molecule 1: Neuraminidase



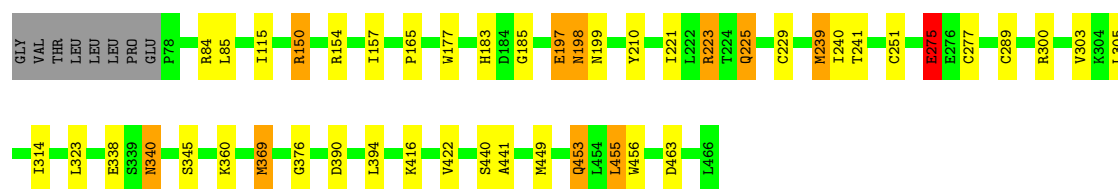
• Molecule 1: Neuraminidase





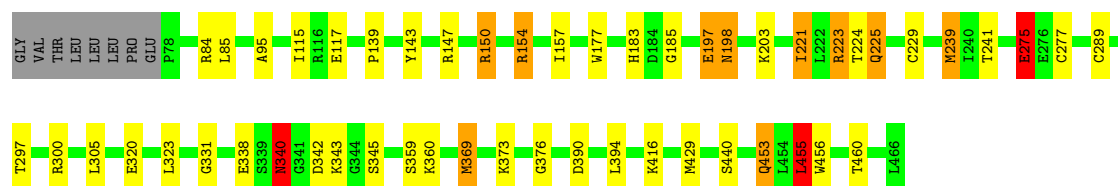
- Molecule 1: Neuraminidase

Chain E: 86% 9% . .



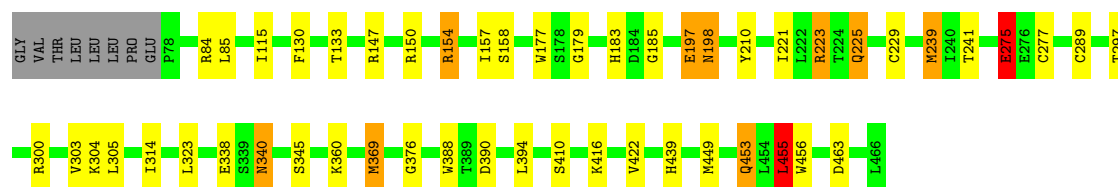
- Molecule 1: Neuraminidase

Chain F: 85% 10% . . .



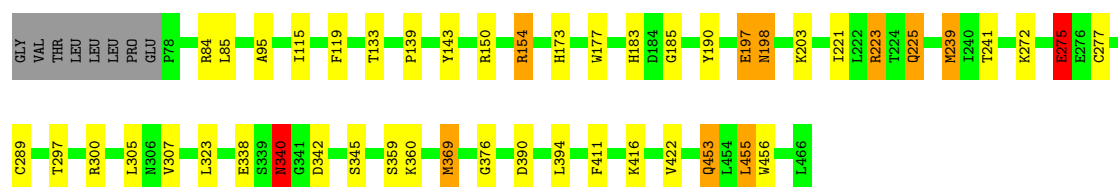
- Molecule 1: Neuraminidase

Chain G: 85% 10% . . .

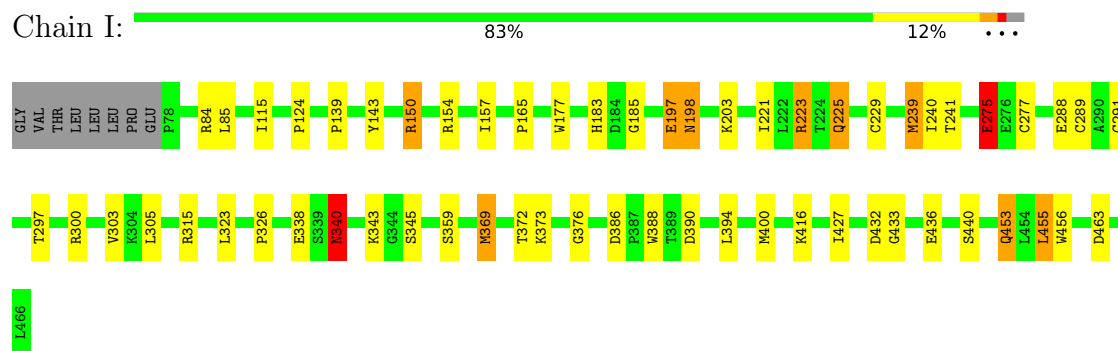


- Molecule 1: Neuraminidase

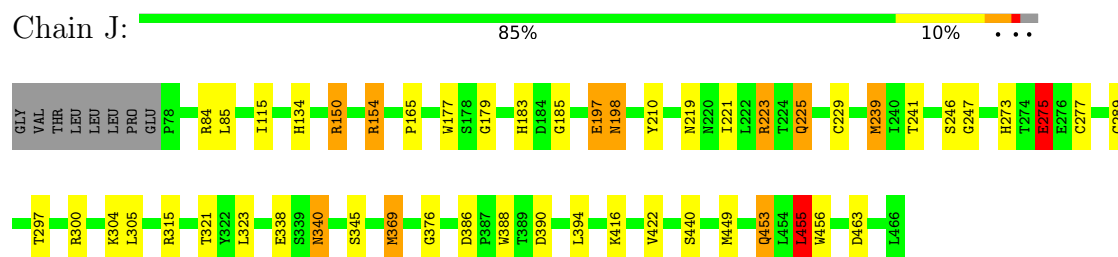
Chain H: 86% 9% . . .



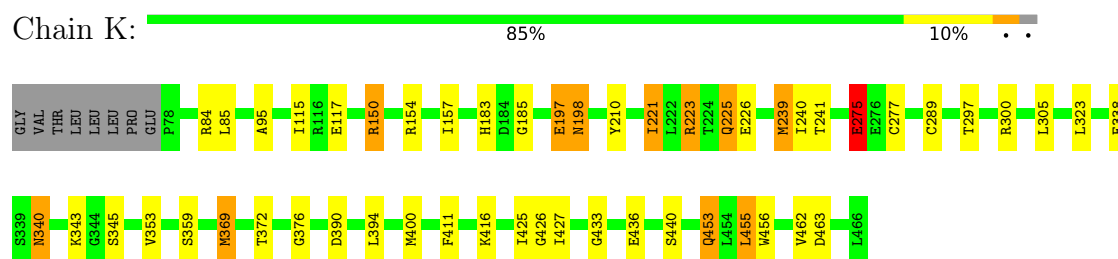
- Molecule 1: Neuraminidase



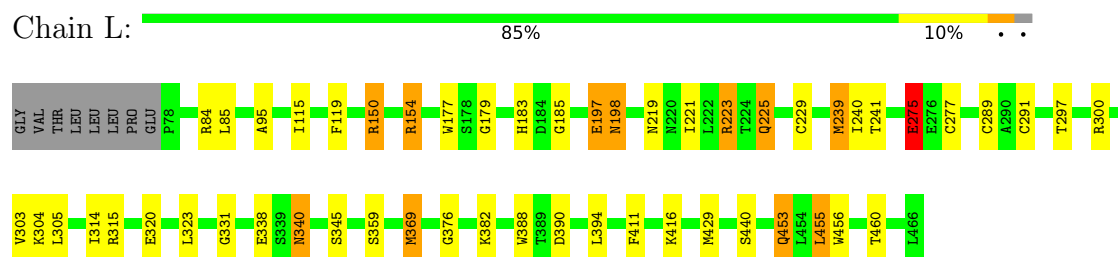
- Molecule 1: Neuraminidase



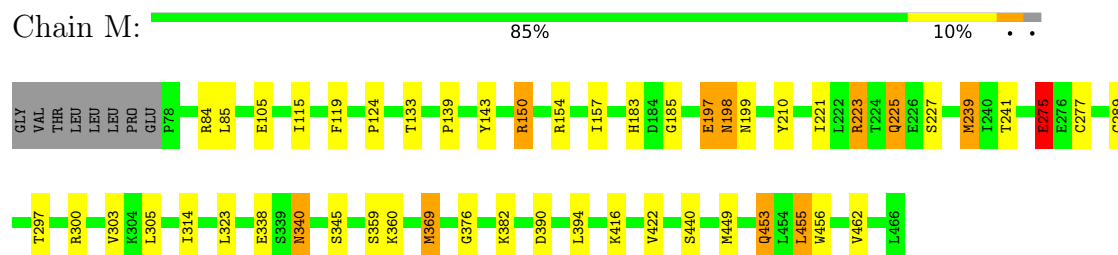
- Molecule 1: Neuraminidase



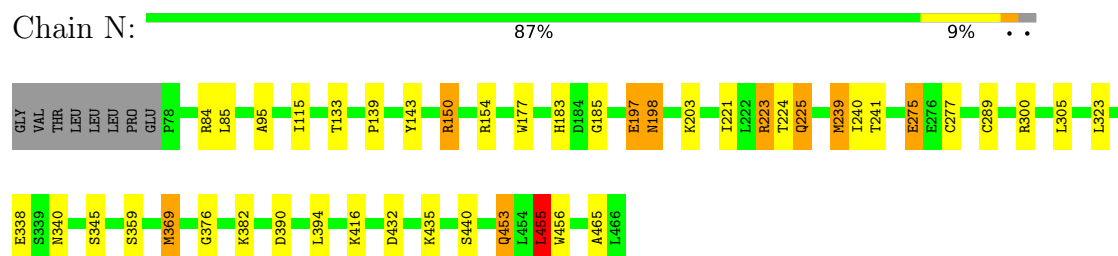
- Molecule 1: Neuraminidase



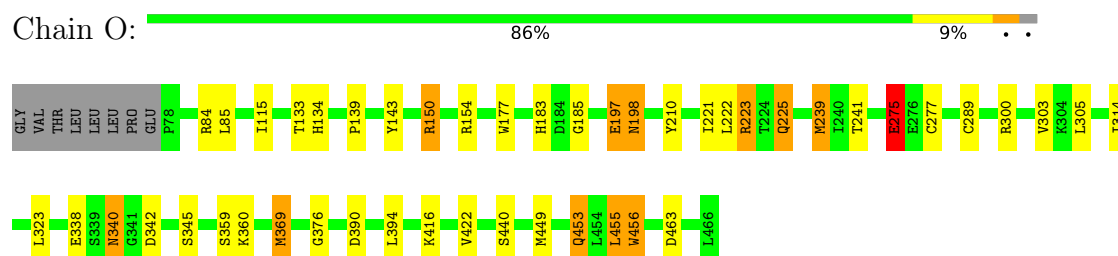
- Molecule 1: Neuraminidase



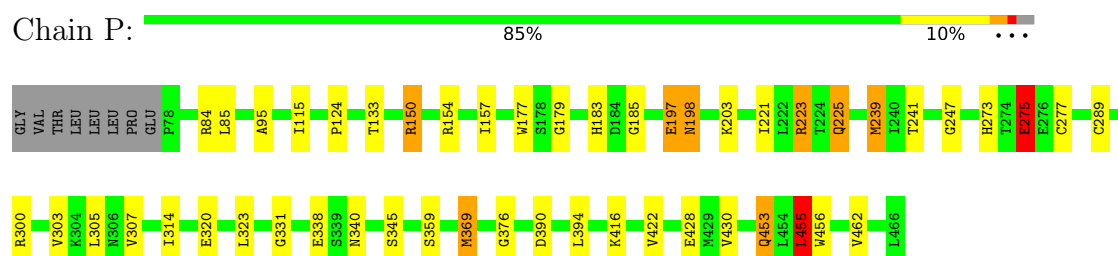
● Molecule 1: Neuraminidase



● 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 55.90 – 2.54	Depositor EDS
% Data completeness (in resolution range)	90.6 (55.90-2.54) 96.6 (55.90-2.54)	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 0.216 , 0.220	Depositor DCC
R_{free} test set	14501 reflections (4.82%)	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)	0.35 , 0.0	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	0.90	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: NAG, CA, YT3, BCZ

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	0.94	1/3089 (0.0%)	0.97	3/4171 (0.1%)
1	B	0.93	0/3089	0.97	5/4171 (0.1%)
1	C	0.90	0/3089	0.97	4/4171 (0.1%)
1	D	0.91	1/3089 (0.0%)	0.98	4/4171 (0.1%)
1	E	0.94	1/3089 (0.0%)	0.98	4/4171 (0.1%)
1	F	0.99	1/3089 (0.0%)	0.98	6/4171 (0.1%)
1	G	0.96	0/3089	0.99	6/4171 (0.1%)
1	H	0.94	2/3089 (0.1%)	0.99	5/4171 (0.1%)
1	I	0.94	0/3089	0.98	5/4171 (0.1%)
1	J	0.95	2/3089 (0.1%)	0.97	7/4171 (0.2%)
1	K	0.95	2/3089 (0.1%)	0.97	3/4171 (0.1%)
1	L	0.92	0/3089	0.96	4/4171 (0.1%)
1	M	0.94	0/3089	0.96	5/4171 (0.1%)
1	N	0.95	1/3089 (0.0%)	0.98	4/4171 (0.1%)
1	O	0.97	1/3089 (0.0%)	0.97	6/4171 (0.1%)
1	P	0.93	2/3089 (0.1%)	0.98	6/4171 (0.1%)
All	All	0.94	14/49424 (0.0%)	0.97	77/66736 (0.1%)

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 (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	117	GLU	C-O	-6.09	1.21	1.23
1	N	224	THR	CA-C	6.03	1.59	1.53
1	J	386	ASP	C-O	-5.79	1.20	1.25
1	H	307	VAL	CA-CB	5.70	1.61	1.54
1	F	224	THR	CA-C	5.67	1.58	1.53
1	K	117	GLU	CA-CB	5.49	1.56	1.52
1	P	462	VAL	CA-CB	5.47	1.61	1.54
1	O	134	HIS	N-CA	5.28	1.52	1.46
1	H	342	ASP	N-CA	5.27	1.52	1.45
1	E	441	ALA	CA-CB	-5.24	1.44	1.53
1	P	307	VAL	CA-CB	5.12	1.60	1.54
1	J	321	THR	CA-CB	5.04	1.59	1.52
1	D	117	GLU	C-O	5.03	1.26	1.23
1	K	462	VAL	CA-CB	5.03	1.60	1.54

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	225	GLN	N-CA-C	9.46	121.59	111.28
1	J	225	GLN	N-CA-C	8.96	121.05	111.28
1	H	340	ASN	N-CA-C	8.44	120.17	110.97
1	P	340	ASN	N-CA-C	8.43	120.16	110.97
1	D	225	GLN	N-CA-C	8.03	120.11	111.36
1	J	340	ASN	N-CA-C	7.89	119.79	111.03
1	C	340	ASN	N-CA-C	7.83	119.60	111.14
1	I	340	ASN	N-CA-C	7.81	119.48	110.97
1	D	340	ASN	N-CA-C	7.64	119.51	111.03
1	B	225	GLN	N-CA-C	7.52	120.36	111.71
1	L	225	GLN	N-CA-C	7.47	119.43	111.28
1	E	340	ASN	N-CA-C	7.42	119.06	110.97
1	M	340	ASN	N-CA-C	7.36	118.99	110.97
1	P	225	GLN	N-CA-C	7.32	120.31	111.82
1	B	340	ASN	N-CA-C	7.30	119.13	111.03
1	G	340	ASN	N-CA-C	7.22	119.04	111.03
1	I	275	GLU	N-CA-C	7.18	120.08	109.24
1	M	225	GLN	N-CA-C	7.16	120.12	111.82
1	A	340	ASN	N-CA-C	7.14	118.75	110.97
1	I	225	GLN	N-CA-C	7.12	120.07	111.82
1	L	340	ASN	N-CA-C	7.06	118.86	111.03
1	J	275	GLU	N-CA-C	7.05	119.89	109.24
1	E	275	GLU	N-CA-C	6.98	119.54	109.14
1	H	225	GLN	N-CA-C	6.91	119.84	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	225	GLN	N-CA-C	6.90	119.65	111.71
1	D	275	GLU	N-CA-C	6.88	119.40	109.14
1	G	225	GLN	N-CA-C	6.86	119.78	111.82
1	O	225	GLN	N-CA-C	6.80	119.71	111.82
1	P	455	LEU	N-CA-C	6.77	121.58	113.12
1	E	225	GLN	N-CA-C	6.68	119.58	111.82
1	H	275	GLU	N-CA-C	6.63	119.25	109.24
1	O	340	ASN	N-CA-C	6.62	118.29	111.14
1	F	340	ASN	N-CA-C	6.58	118.25	111.14
1	G	422	VAL	N-CA-C	6.57	114.63	107.60
1	O	275	GLU	N-CA-C	6.55	119.37	109.41
1	K	340	ASN	N-CA-C	6.54	118.29	111.03
1	B	275	GLU	N-CA-C	6.49	119.03	109.24
1	F	275	GLU	N-CA-C	6.46	118.99	109.24
1	N	225	GLN	N-CA-C	6.45	119.31	111.82
1	E	422	VAL	N-CA-C	6.40	114.44	107.60
1	K	275	GLU	N-CA-C	6.35	119.36	109.52
1	N	340	ASN	N-CA-C	6.30	118.02	111.03
1	M	422	VAL	N-CA-C	6.26	113.75	107.55
1	L	275	GLU	N-CA-C	6.26	118.69	109.24
1	G	275	GLU	N-CA-C	6.25	118.45	109.14
1	A	275	GLU	N-CA-C	6.17	118.56	109.24
1	C	275	GLU	N-CA-C	6.11	118.47	109.24
1	N	275	GLU	N-CA-C	6.03	118.34	109.24
1	M	275	GLU	N-CA-C	6.02	118.86	109.52
1	P	275	GLU	N-CA-C	5.98	118.27	109.24
1	C	225	GLN	N-CA-C	5.94	118.71	111.82
1	P	179	GLY	N-CA-C	5.90	119.71	111.10
1	F	455	LEU	N-CA-C	5.75	120.31	113.12
1	J	422	VAL	N-CA-C	5.61	113.60	107.60
1	O	422	VAL	N-CA-C	5.59	113.58	107.60
1	F	225	GLN	N-CA-C	5.57	118.28	111.82
1	M	462	VAL	N-CA-C	5.54	116.71	108.23
1	H	342	ASP	N-CA-C	5.51	118.68	110.14
1	J	455	LEU	N-CA-C	5.47	119.96	113.12
1	J	134	HIS	N-CA-C	-5.45	106.51	112.72
1	G	179	GLY	N-CA-C	5.43	119.03	111.10
1	D	269	GLY	N-CA-C	5.37	118.05	111.45
1	O	342	ASP	N-CA-C	5.37	118.46	110.14
1	F	342	ASP	N-CA-C	5.35	118.44	110.14
1	G	455	LEU	N-CA-C	5.31	119.76	113.12
1	H	422	VAL	N-CA-C	5.31	113.28	107.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	455	LEU	N-CA-C	5.26	119.70	113.12
1	O	456	TRP	N-CA-C	5.26	117.38	109.23
1	B	269	GLY	N-CA-C	5.14	118.90	111.24
1	F	117	GLU	CB-CA-C	-5.13	107.56	111.20
1	J	179	GLY	N-CA-C	5.09	118.53	111.10
1	I	386	ASP	CA-C-N	5.08	124.74	119.56
1	I	386	ASP	C-N-CA	5.08	124.74	119.56
1	L	179	GLY	N-CA-C	5.06	118.49	111.10
1	P	422	VAL	N-CA-C	5.06	113.02	107.60
1	B	422	VAL	N-CA-C	5.01	112.96	107.60
1	C	342	ASP	N-CA-C	5.00	117.49	110.14

There are no chirality outliers.

All (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
1	O	340	ASN	Peptide

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	3016	0	2912	27	1
1	B	3016	0	2912	52	0
1	C	3016	0	2912	23	1
1	D	3016	0	2912	28	5
1	E	3016	0	2912	26	1
1	F	3016	0	2912	52	0
1	G	3016	0	2912	30	1
1	H	3016	0	2912	25	1
1	I	3016	0	2912	53	0
1	J	3016	0	2912	25	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	K	3016	0	2912	26	4
1	L	3016	0	2912	31	1
1	M	3016	0	2912	28	1
1	N	3016	0	2912	47	0
1	O	3016	0	2912	25	1
1	P	3016	0	2912	28	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
4	D	23	0	27	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	461	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 5.

All (461) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:F:343:LYS:NZ	1:N:465:ALA:CA	1.98	1.27
1:B:433:GLY:O	1:I:372:THR:HG21	1.17	1.26
1:F:343:LYS:HE2	1:N:465:ALA:O	1.34	1.26
1:B:372:THR:CG2	1:I:433:GLY:O	1.84	1.25
1:F:343:LYS:CE	1:N:465:ALA:CB	2.18	1.21
1:F:343:LYS:NZ	1:N:465:ALA:HA	1.56	1.18
1:F:343:LYS:HZ3	1:N:465:ALA:CA	1.55	1.18
1:B:433:GLY:HA2	1:I:373:LYS:HE3	1.32	1.10
1:F:373:LYS:HE3	1:N:432:ASP:O	1.50	1.09
1:B:373:LYS:HE3	1:I:433:GLY:HA2	1.29	1.07
1:F:343:LYS:NZ	1:N:465:ALA:HB1	1.63	1.06
1:F:343:LYS:HE3	1:N:465:ALA:CB	1.82	1.04
1:B:436:GLU:O	1:I:343:LYS:NZ	1.92	1.01
1:F:343:LYS:HZ3	1:N:465:ALA:HA	0.87	1.01
1:B:343:LYS:NZ	1:I:436:GLU:O	2.02	0.93
1:F:343:LYS:HE2	1:N:465:ALA:C	1.94	0.93
1:F:343:LYS:HZ1	1:N:465:ALA:HB2	1.35	0.92
1:F:147:ARG:NH2	1:N:435:LYS:HD3	1.87	0.90
1:H:225:GLN:HE21	1:H:239:MET:H	1.16	0.89
1:F:343:LYS:HE3	1:N:465:ALA:HB1	0.91	0.88
1:F:343:LYS:CE	1:N:465:ALA:O	2.22	0.88
1:D:225:GLN:HE21	1:D:239:MET:H	1.22	0.87
1:F:373:LYS:CE	1:N:432:ASP:O	2.22	0.87
1:J:225:GLN:HE21	1:J:239:MET:H	1.24	0.85
1:L:225:GLN:HE21	1:L:239:MET:H	1.26	0.84
1:C:225:GLN:HE21	1:C:239:MET:H	1.21	0.83
1:P:225:GLN:HE21	1:P:239:MET:H	1.23	0.83
1:N:225:GLN:HE21	1:N:239:MET:H	1.23	0.82
1:B:433:GLY:O	1:I:372:THR:HG22	1.78	0.82
1:F:225:GLN:HE21	1:F:239:MET:H	1.28	0.81
1:F:343:LYS:CE	1:N:465:ALA:CA	2.57	0.81
1:B:225:GLN:HE21	1:B:239:MET:H	1.27	0.80
1:I:225:GLN:HE21	1:I:239:MET:H	1.29	0.80
1:A:225:GLN:HE21	1:A:239:MET:H	1.30	0.79
1:K:225:GLN:HE21	1:K:239:MET:H	1.31	0.78
1:F:343:LYS:CE	1:N:465:ALA:C	2.58	0.77
1:O:225:GLN:HE21	1:O:239:MET:H	1.32	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:225:GLN:NE2	1:P:239:MET:H	1.85	0.75
1:A:150:ARG:NH1	1:A:197:GLU:OE1	2.19	0.74
1:E:225:GLN:HE21	1:E:239:MET:H	1.33	0.74
1:C:225:GLN:NE2	1:C:239:MET:H	1.86	0.73
1:J:225:GLN:NE2	1:J:239:MET:H	1.87	0.73
1:H:225:GLN:NE2	1:H:239:MET:H	1.87	0.72
1:I:150:ARG:NH1	1:I:197:GLU:OE1	2.23	0.72
1:A:225:GLN:NE2	1:A:239:MET:H	1.88	0.71
1:H:221:ILE:O	1:H:223:ARG:HD3	1.91	0.70
1:B:433:GLY:HA2	1:I:373:LYS:CE	2.18	0.70
1:O:198:ASN:HD22	1:O:198:ASN:H	1.39	0.70
1:K:225:GLN:NE2	1:K:239:MET:H	1.90	0.70
1:G:225:GLN:NE2	1:G:239:MET:H	1.90	0.70
1:M:198:ASN:HD22	1:M:198:ASN:H	1.38	0.69
1:G:198:ASN:H	1:G:198:ASN:HD22	1.40	0.69
1:B:373:LYS:CE	1:I:433:GLY:HA2	2.17	0.69
1:E:221:ILE:O	1:E:223:ARG:HD3	1.93	0.69
1:E:198:ASN:HD22	1:E:198:ASN:H	1.40	0.69
1:B:225:GLN:NE2	1:B:239:MET:H	1.92	0.68
1:M:225:GLN:HE21	1:M:239:MET:H	1.42	0.67
1:G:225:GLN:HE21	1:G:239:MET:H	1.42	0.67
1:I:225:GLN:NE2	1:I:239:MET:H	1.92	0.67
1:K:223:ARG:HG2	6:K:2018:HOH:O	1.94	0.66
1:N:225:GLN:NE2	1:N:239:MET:H	1.92	0.66
1:D:225:GLN:NE2	1:D:239:MET:H	1.92	0.66
1:P:150:ARG:NH1	1:P:197:GLU:OE1	2.29	0.66
1:L:223:ARG:HG2	6:L:2018:HOH:O	1.95	0.66
1:D:223:ARG:HG2	6:D:2018:HOH:O	1.96	0.66
1:E:223:ARG:HG2	6:E:2018:HOH:O	1.96	0.66
1:B:150:ARG:NH1	1:B:197:GLU:OE1	2.30	0.65
1:B:372:THR:HG22	1:I:433:GLY:O	1.89	0.65
1:H:150:ARG:NH1	1:H:197:GLU:OE1	2.28	0.65
1:I:300:ARG:HG3	1:I:323:LEU:HB2	1.78	0.65
1:L:225:GLN:NE2	1:L:239:MET:H	1.94	0.65
1:C:150:ARG:NH1	1:C:197:GLU:OE1	2.28	0.65
1:O:225:GLN:NE2	1:O:239:MET:H	1.95	0.65
1:E:150:ARG:NH1	1:E:197:GLU:OE1	2.29	0.65
1:I:223:ARG:HG2	6:I:2018:HOH:O	1.98	0.64
1:C:223:ARG:HG2	6:C:2018:HOH:O	1.95	0.64
1:P:223:ARG:HG2	6:P:2018:HOH:O	1.96	0.64
1:F:225:GLN:NE2	1:F:239:MET:H	1.95	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:223:ARG:HG2	6:O:2018:HOH:O	1.98	0.63
1:F:221:ILE:O	1:F:223:ARG:HD3	1.98	0.63
1:J:223:ARG:HG2	6:J:2018:HOH:O	1.99	0.63
1:M:225:GLN:NE2	1:M:239:MET:H	1.97	0.63
1:E:225:GLN:NE2	1:E:239:MET:H	1.97	0.63
1:D:297:THR:OG1	1:D:340:ASN:O	2.11	0.62
1:N:150:ARG:NH1	1:N:197:GLU:OE1	2.31	0.62
1:K:150:ARG:NH1	1:K:197:GLU:OE1	2.31	0.62
1:C:221:ILE:O	1:C:223:ARG:HD3	2.00	0.61
1:H:198:ASN:HD22	1:H:198:ASN:H	1.46	0.61
1:L:150:ARG:NH1	1:L:197:GLU:OE1	2.34	0.61
1:L:300:ARG:HG3	1:L:323:LEU:HB2	1.83	0.61
1:L:183:HIS:CD2	1:L:185:GLY:H	2.18	0.61
1:F:150:ARG:NH1	1:F:197:GLU:OE1	2.34	0.61
1:A:300:ARG:HG3	1:A:323:LEU:HB2	1.83	0.60
1:K:183:HIS:CD2	1:K:185:GLY:H	2.19	0.60
1:N:223:ARG:HG3	4:N:1001:BCZ:H152	1.83	0.60
1:A:277:CYS:HB3	1:A:289:CYS:HB3	1.82	0.60
1:B:223:ARG:HG3	4:B:1001:BCZ:H152	1.84	0.60
1:P:183:HIS:CD2	1:P:185:GLY:H	2.19	0.60
1:B:432:ASP:O	1:I:373:LYS:CE	2.49	0.60
1:B:223:ARG:HG2	6:B:2018:HOH:O	2.01	0.60
1:M:198:ASN:HD22	1:M:198:ASN:N	2.01	0.59
1:O:221:ILE:O	1:O:223:ARG:HD3	2.03	0.59
1:O:198:ASN:HD22	1:O:198:ASN:N	2.01	0.59
1:N:198:ASN:H	1:N:198:ASN:HD22	1.48	0.59
1:P:223:ARG:HG3	4:P:1001:BCZ:H152	1.85	0.59
1:M:221:ILE:O	1:M:223:ARG:HD3	2.03	0.59
1:M:223:ARG:HG3	4:M:1001:BCZ:H152	1.83	0.59
1:L:369:MET:HB2	1:L:376:GLY:HA3	1.85	0.58
1:C:300:ARG:HG3	1:C:323:LEU:HB2	1.84	0.58
1:A:183:HIS:CD2	1:A:185:GLY:H	2.22	0.58
1:J:221:ILE:O	1:J:223:ARG:HD3	2.04	0.58
1:G:303:VAL:HG22	1:G:314:ILE:HG12	1.86	0.58
1:I:198:ASN:H	1:I:198:ASN:HD22	1.51	0.58
1:O:223:ARG:HG3	4:O:1001:BCZ:H152	1.85	0.58
1:G:150:ARG:NH1	1:G:197:GLU:OE1	2.37	0.58
1:K:277:CYS:HB3	1:K:289:CYS:HB3	1.85	0.58
1:N:223:ARG:HG2	6:N:2018:HOH:O	2.03	0.58
1:B:373:LYS:CE	1:I:432:ASP:O	2.52	0.58
1:I:277:CYS:HB3	1:I:289:CYS:HB3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:198:ASN:H	1:K:198:ASN:HD22	1.52	0.57
1:A:223:ARG:HG2	6:A:2018:HOH:O	2.03	0.57
1:A:369:MET:HB2	1:A:376:GLY:HA3	1.85	0.57
1:P:453:GLN:O	1:P:455:LEU:HD22	2.04	0.57
1:G:183:HIS:CD2	1:G:185:GLY:H	2.21	0.57
1:J:223:ARG:HG3	4:J:1001:BCZ:H152	1.85	0.57
1:B:277:CYS:HB3	1:B:289:CYS:HB3	1.86	0.57
1:D:300:ARG:HG3	1:D:323:LEU:HB2	1.87	0.57
1:H:223:ARG:HG3	4:H:1001:BCZ:H152	1.86	0.57
1:K:300:ARG:HG3	1:K:323:LEU:HB2	1.84	0.57
1:L:223:ARG:HG3	4:L:1001:BCZ:H152	1.87	0.57
1:M:150:ARG:NH1	1:M:197:GLU:OE1	2.38	0.56
1:I:369:MET:HB2	1:I:376:GLY:HA3	1.86	0.56
1:L:198:ASN:H	1:L:198:ASN:HD22	1.53	0.56
1:A:221:ILE:O	1:A:223:ARG:HD3	2.05	0.56
1:B:453:GLN:O	1:B:455:LEU:HD22	2.05	0.56
1:D:150:ARG:NH1	1:D:197:GLU:OE1	2.37	0.56
1:E:198:ASN:HD22	1:E:198:ASN:N	2.00	0.56
1:F:223:ARG:HG3	4:F:1001:BCZ:H152	1.87	0.56
1:G:453:GLN:O	1:G:455:LEU:HD22	2.05	0.56
1:I:223:ARG:HG3	4:I:1001:BCZ:H152	1.87	0.56
1:O:150:ARG:NH1	1:O:197:GLU:OE1	2.38	0.56
1:D:223:ARG:HG3	4:D:1001:BCZ:H152	1.87	0.56
1:G:223:ARG:HG2	6:G:2018:HOH:O	2.06	0.56
1:K:400:MET:HE3	1:K:427:ILE:HD11	1.88	0.56
1:C:277:CYS:HB3	1:C:289:CYS:HB3	1.88	0.56
1:E:303:VAL:HG22	1:E:314:ILE:HG12	1.88	0.56
1:E:453:GLN:O	1:E:455:LEU:HD22	2.06	0.56
1:F:203:LYS:HB3	1:G:449:MET:HE1	1.88	0.56
1:G:198:ASN:HD22	1:G:198:ASN:N	2.02	0.56
1:B:221:ILE:O	1:B:223:ARG:HD3	2.06	0.55
1:M:297:THR:OG1	1:M:340:ASN:O	2.12	0.55
1:G:223:ARG:HG3	4:G:1001:BCZ:H152	1.87	0.55
1:C:183:HIS:CD2	1:C:185:GLY:H	2.24	0.55
1:F:223:ARG:HG2	6:F:2018:HOH:O	2.06	0.55
1:N:277:CYS:HB3	1:N:289:CYS:HB3	1.88	0.55
1:E:183:HIS:CD2	1:E:185:GLY:H	2.24	0.55
1:M:449:MET:HE1	1:P:203:LYS:HB3	1.89	0.55
1:F:183:HIS:CD2	1:F:185:GLY:H	2.25	0.55
1:J:277:CYS:HB3	1:J:289:CYS:HB3	1.89	0.55
1:N:183:HIS:CD2	1:N:185:GLY:H	2.25	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:223:ARG:HG3	4:E:1001:BCZ:H152	1.89	0.55
1:J:183:HIS:CD2	1:J:185:GLY:H	2.25	0.55
1:B:198:ASN:H	1:B:198:ASN:HD22	1.55	0.54
1:O:183:HIS:CD2	1:O:185:GLY:H	2.24	0.54
1:M:223:ARG:HG2	6:M:2018:HOH:O	2.06	0.54
1:P:198:ASN:H	1:P:198:ASN:HD22	1.55	0.54
1:P:225:GLN:HE21	1:P:239:MET:N	1.99	0.54
1:L:277:CYS:HB3	1:L:289:CYS:HB3	1.89	0.54
1:B:183:HIS:CD2	1:B:185:GLY:H	2.26	0.54
1:L:183:HIS:HD2	1:L:185:GLY:H	1.55	0.54
1:A:223:ARG:HG3	4:A:1001:BCZ:H152	1.89	0.54
1:L:221:ILE:O	1:L:223:ARG:HD3	2.08	0.54
1:M:183:HIS:CD2	1:M:185:GLY:H	2.26	0.54
1:B:369:MET:HB2	1:B:376:GLY:HA3	1.90	0.53
1:F:369:MET:HB2	1:F:376:GLY:HA3	1.91	0.53
1:F:300:ARG:HG3	1:F:323:LEU:HB2	1.90	0.53
1:K:223:ARG:HG3	4:K:1001:BCZ:H152	1.89	0.53
1:B:300:ARG:HG3	1:B:323:LEU:HB2	1.89	0.53
1:B:219:ASN:OD1	1:F:360:LYS:NZ	2.37	0.52
1:J:150:ARG:NH1	1:J:197:GLU:OE1	2.42	0.52
1:H:198:ASN:HD22	1:H:198:ASN:N	2.07	0.52
1:J:198:ASN:HD22	1:J:198:ASN:H	1.57	0.52
1:L:453:GLN:O	1:L:455:LEU:HD22	2.09	0.52
1:L:239:MET:HE3	1:L:240:ILE:HA	1.92	0.52
1:H:277:CYS:HB3	1:H:289:CYS:HB3	1.92	0.52
1:B:326:PRO:CB	1:I:436:GLU:HG3	2.39	0.52
1:O:453:GLN:O	1:O:455:LEU:HD22	2.09	0.52
1:C:369:MET:HB2	1:C:376:GLY:HA3	1.92	0.52
1:J:369:MET:HB2	1:J:376:GLY:HA3	1.91	0.52
1:E:210:TYR:CZ	1:F:95:ALA:HB1	2.45	0.52
1:G:297:THR:OG1	1:G:340:ASN:O	2.13	0.52
1:G:300:ARG:HG3	1:G:323:LEU:HB2	1.92	0.52
1:D:277:CYS:HB3	1:D:289:CYS:HB3	1.91	0.52
1:G:221:ILE:O	1:G:223:ARG:HD3	2.10	0.52
1:H:183:HIS:CD2	1:H:185:GLY:H	2.28	0.52
1:H:300:ARG:HG3	1:H:323:LEU:HB2	1.92	0.52
1:J:453:GLN:O	1:J:455:LEU:HD22	2.10	0.52
1:E:463:ASP:OD2	1:E:463:ASP:C	2.53	0.51
1:D:183:HIS:CD2	1:D:185:GLY:H	2.29	0.51
1:D:304:LYS:HD2	1:D:388:TRP:CH2	2.44	0.51
1:H:223:ARG:HH21	1:H:275:GLU:CD	2.19	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:369:MET:HB2	1:D:376:GLY:HA3	1.91	0.51
1:K:198:ASN:HD22	1:K:198:ASN:N	2.09	0.51
1:N:198:ASN:HD22	1:N:198:ASN:N	2.07	0.51
1:I:453:GLN:O	1:I:455:LEU:HD22	2.11	0.51
1:I:198:ASN:HD22	1:I:198:ASN:N	2.06	0.51
1:C:223:ARG:HG3	4:C:1001:BCZ:H152	1.91	0.50
1:A:183:HIS:HD2	1:A:185:GLY:H	1.58	0.50
1:P:221:ILE:O	1:P:223:ARG:HD3	2.10	0.50
1:I:221:ILE:O	1:I:223:ARG:HD3	2.12	0.50
1:C:183:HIS:HD2	1:C:185:GLY:H	1.60	0.50
1:G:277:CYS:HB3	1:G:289:CYS:HB3	1.93	0.50
1:I:203:LYS:HB3	1:J:449:MET:HE1	1.93	0.50
1:E:277:CYS:HB3	1:E:289:CYS:HB3	1.92	0.49
1:H:223:ARG:HG2	6:H:2018:HOH:O	2.12	0.49
1:J:297:THR:OG1	1:J:340:ASN:O	2.25	0.49
1:P:277:CYS:HB3	1:P:289:CYS:HB3	1.94	0.49
1:M:369:MET:HB2	1:M:376:GLY:HA3	1.94	0.49
1:M:453:GLN:O	1:M:455:LEU:HD22	2.12	0.49
1:I:400:MET:HE3	1:I:427:ILE:HD11	1.94	0.49
1:D:198:ASN:H	1:D:198:ASN:HD22	1.59	0.49
1:F:343:LYS:HZ1	1:N:465:ALA:CA	1.90	0.49
1:E:198:ASN:H	1:E:198:ASN:ND2	2.10	0.49
1:J:300:ARG:HG3	1:J:323:LEU:HB2	1.94	0.49
1:I:183:HIS:CD2	1:I:185:GLY:H	2.30	0.49
1:F:297:THR:OG1	1:F:340:ASN:O	2.25	0.49
1:M:157:ILE:HD12	1:M:157:ILE:C	2.38	0.49
1:K:239:MET:HE3	1:K:240:ILE:HA	1.95	0.49
1:B:326:PRO:CG	1:I:436:GLU:HG3	2.42	0.48
1:K:453:GLN:O	1:K:455:LEU:HD22	2.13	0.48
1:A:453:GLN:O	1:A:455:LEU:HD22	2.13	0.48
1:E:223:ARG:HH21	1:E:275:GLU:CD	2.21	0.48
1:N:221:ILE:O	1:N:223:ARG:HD3	2.12	0.48
1:B:463:ASP:C	1:B:463:ASP:OD2	2.57	0.48
1:I:225:GLN:HE21	1:I:239:MET:N	2.06	0.48
1:A:225:GLN:HE21	1:A:239:MET:N	2.04	0.48
1:C:223:ARG:HH21	1:C:275:GLU:CD	2.22	0.48
1:D:453:GLN:O	1:D:455:LEU:HD22	2.13	0.48
1:J:210:TYR:CZ	1:K:95:ALA:HB1	2.47	0.48
1:L:198:ASN:HD22	1:L:198:ASN:N	2.09	0.48
1:F:139:PRO:HA	1:F:143:TYR:HH	1.78	0.48
1:N:369:MET:HB2	1:N:376:GLY:HA3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:198:ASN:HD22	1:D:198:ASN:N	2.12	0.47
1:B:198:ASN:HD22	1:B:198:ASN:N	2.11	0.47
1:E:300:ARG:HG3	1:E:323:LEU:HB2	1.95	0.47
1:F:147:ARG:HH22	1:N:435:LYS:HD3	1.74	0.47
1:D:221:ILE:O	1:D:223:ARG:HD3	2.14	0.47
1:H:225:GLN:HE21	1:H:239:MET:N	1.98	0.47
1:H:453:GLN:O	1:H:455:LEU:HD22	2.13	0.47
1:O:303:VAL:HG22	1:O:314:ILE:HG12	1.95	0.47
1:P:115:ILE:HG22	1:P:133:THR:HA	1.96	0.47
1:N:203:LYS:HB3	1:O:449:MET:HE1	1.97	0.47
1:F:157:ILE:C	1:F:157:ILE:HD12	2.40	0.47
1:J:198:ASN:HD22	1:J:198:ASN:N	2.12	0.47
1:K:463:ASP:OD2	1:K:463:ASP:C	2.56	0.47
1:A:115:ILE:O	1:A:440:SER:HA	2.14	0.47
1:D:191:ILE:HD13	1:D:238:LEU:HD13	1.97	0.47
1:I:139:PRO:HA	1:I:143:TYR:HH	1.80	0.47
1:L:304:LYS:HD2	1:L:388:TRP:CH2	2.49	0.47
1:B:436:GLU:HG3	1:I:326:PRO:CG	2.44	0.47
1:B:157:ILE:C	1:B:157:ILE:HD12	2.39	0.47
1:E:239:MET:HE3	1:E:240:ILE:HA	1.97	0.47
1:K:225:GLN:HE21	1:K:239:MET:N	2.07	0.47
1:B:436:GLU:HG3	1:I:326:PRO:CB	2.45	0.46
1:K:369:MET:HB2	1:K:376:GLY:HA3	1.97	0.46
1:B:139:PRO:HA	1:B:143:TYR:HH	1.81	0.46
1:C:225:GLN:HE21	1:C:239:MET:N	2.02	0.46
1:I:115:ILE:O	1:I:440:SER:HA	2.16	0.46
1:M:303:VAL:HG22	1:M:314:ILE:HG12	1.96	0.46
1:O:115:ILE:HG22	1:O:133:THR:HA	1.97	0.46
1:K:223:ARG:HH21	1:K:275:GLU:CD	2.24	0.46
1:E:150:ARG:HG2	1:E:177:TRP:CD2	2.51	0.46
1:O:300:ARG:HG3	1:O:323:LEU:HB2	1.97	0.46
1:F:277:CYS:HB3	1:F:289:CYS:HB3	1.97	0.46
1:K:183:HIS:HD2	1:K:185:GLY:H	1.60	0.46
1:O:463:ASP:OD2	1:O:463:ASP:C	2.59	0.46
1:I:223:ARG:HH21	1:I:275:GLU:CD	2.24	0.46
1:J:304:LYS:HD2	1:J:388:TRP:CH2	2.51	0.46
1:M:198:ASN:H	1:M:198:ASN:ND2	2.09	0.46
1:B:297:THR:OG1	1:B:340:ASN:O	2.28	0.46
1:M:115:ILE:O	1:M:440:SER:HA	2.16	0.46
1:N:139:PRO:HA	1:N:143:TYR:HH	1.80	0.46
1:O:277:CYS:HB3	1:O:289:CYS:HB3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:315:ARG:HB2	1:B:388:TRP:CD1	2.52	0.45
1:P:300:ARG:HG3	1:P:323:LEU:HB2	1.98	0.45
1:D:303:VAL:HG22	1:D:314:ILE:HG12	1.98	0.45
1:M:277:CYS:HB3	1:M:289:CYS:HB3	1.97	0.45
1:N:239:MET:HE3	1:N:240:ILE:HA	1.97	0.45
1:O:115:ILE:O	1:O:440:SER:HA	2.15	0.45
1:A:150:ARG:HG2	1:A:177:TRP:CD2	2.50	0.45
1:H:139:PRO:HA	1:H:143:TYR:HH	1.81	0.45
1:I:315:ARG:HB2	1:I:388:TRP:CD1	2.51	0.45
1:N:300:ARG:HG3	1:N:323:LEU:HB2	1.97	0.45
1:O:198:ASN:H	1:O:198:ASN:ND2	2.12	0.45
1:O:369:MET:HB2	1:O:376:GLY:HA3	1.98	0.45
1:A:315:ARG:HB2	1:A:388:TRP:CD1	2.52	0.45
1:K:221:ILE:O	1:K:223:ARG:HD3	2.16	0.45
1:C:115:ILE:O	1:C:440:SER:HA	2.17	0.45
1:C:400:MET:HE3	1:C:427:ILE:HD11	1.99	0.45
1:G:150:ARG:HH11	1:G:150:ARG:HB2	1.81	0.45
1:P:369:MET:HB2	1:P:376:GLY:HA3	1.98	0.45
1:H:369:MET:HB2	1:H:376:GLY:HA3	1.99	0.45
1:C:210:TYR:CZ	1:D:95:ALA:HB1	2.52	0.44
1:G:154:ARG:HG2	1:G:177:TRP:HA	1.99	0.44
1:G:463:ASP:C	1:G:463:ASP:OD2	2.58	0.44
1:D:124:PRO:HD3	1:D:183:HIS:CD2	2.52	0.44
1:G:369:MET:HB2	1:G:376:GLY:HA3	1.99	0.44
1:I:297:THR:OG1	1:I:340:ASN:O	2.32	0.44
1:C:453:GLN:O	1:C:455:LEU:HD22	2.18	0.44
1:F:343:LYS:NZ	1:N:465:ALA:C	2.71	0.44
1:N:453:GLN:O	1:N:455:LEU:HD22	2.17	0.44
1:J:154:ARG:HG2	1:J:177:TRP:HA	2.00	0.44
1:N:115:ILE:O	1:N:440:SER:HA	2.17	0.44
1:O:139:PRO:HA	1:O:143:TYR:HH	1.83	0.44
1:I:165:PRO:HG2	6:I:2046:HOH:O	2.18	0.44
1:A:463:ASP:OD2	1:A:463:ASP:C	2.61	0.44
1:C:463:ASP:OD2	1:C:463:ASP:C	2.60	0.44
1:N:115:ILE:HG22	1:N:133:THR:HA	2.00	0.44
1:K:115:ILE:O	1:K:440:SER:HA	2.18	0.44
1:L:197:GLU:CA	1:L:197:GLU:OE2	2.66	0.44
1:K:353:VAL:HG12	1:K:425:ILE:HD11	2.00	0.43
1:L:303:VAL:HG22	1:L:314:ILE:HG12	1.99	0.43
1:L:315:ARG:HB2	1:L:388:TRP:CD1	2.53	0.43
1:P:157:ILE:C	1:P:157:ILE:HD12	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:223:ARG:HH21	1:P:275:GLU:CD	2.26	0.43
1:E:369:MET:HB2	1:E:376:GLY:HA3	1.98	0.43
1:F:198:ASN:HD22	1:F:198:ASN:H	1.66	0.43
1:I:157:ILE:C	1:I:157:ILE:HD12	2.43	0.43
1:B:225:GLN:HE21	1:B:239:MET:N	2.04	0.43
1:B:239:MET:HE3	1:B:240:ILE:HA	2.00	0.43
1:C:303:VAL:HG22	1:C:314:ILE:HG12	2.01	0.43
1:B:304:LYS:HD2	1:B:388:TRP:CH2	2.54	0.43
1:L:223:ARG:HH21	1:L:275:GLU:CD	2.26	0.43
1:G:304:LYS:HD2	1:G:388:TRP:CH2	2.53	0.43
1:C:315:ARG:HB2	1:C:388:TRP:CD1	2.54	0.43
1:E:239:MET:HE3	1:E:240:ILE:CA	2.49	0.43
1:I:239:MET:HE3	1:I:240:ILE:HA	2.01	0.43
1:P:428:GLU:HG2	1:P:430:VAL:HG23	2.00	0.43
1:D:223:ARG:HH21	1:D:275:GLU:CD	2.27	0.43
1:D:463:ASP:OD2	1:D:463:ASP:C	2.62	0.43
1:F:154:ARG:HG2	1:F:177:TRP:HA	2.00	0.43
1:L:429:MET:HE2	1:L:460:THR:HG23	2.01	0.43
1:F:198:ASN:HD22	1:F:198:ASN:N	2.16	0.43
1:G:130:PHE:CD1	1:G:158:SER:HB3	2.53	0.43
1:J:463:ASP:OD2	1:J:463:ASP:C	2.62	0.43
1:P:247:GLY:O	1:P:273:HIS:ND1	2.52	0.43
1:E:157:ILE:HD12	1:E:157:ILE:C	2.44	0.43
1:P:197:GLU:OE2	1:P:197:GLU:CA	2.66	0.43
1:D:139:PRO:HA	1:D:143:TYR:HH	1.84	0.42
1:F:320:GLU:HB2	1:F:331:GLY:HA2	2.00	0.42
1:G:223:ARG:CG	4:G:1001:BCZ:H152	2.48	0.42
1:L:291:CYS:O	1:L:300:ARG:HD3	2.19	0.42
1:O:150:ARG:HG2	1:O:177:TRP:CD2	2.54	0.42
1:L:239:MET:HE3	1:L:240:ILE:CA	2.49	0.42
1:L:297:THR:OG1	1:L:340:ASN:O	2.22	0.42
1:P:150:ARG:HG2	1:P:177:TRP:CD2	2.54	0.42
1:D:154:ARG:HG2	1:D:177:TRP:HA	2.02	0.42
1:E:165:PRO:HG2	6:E:2046:HOH:O	2.19	0.42
1:G:225:GLN:HE21	1:G:239:MET:N	2.10	0.42
1:M:223:ARG:CG	4:M:1001:BCZ:H152	2.48	0.42
1:P:183:HIS:HD2	1:P:185:GLY:H	1.63	0.42
1:B:432:ASP:O	1:I:373:LYS:HE3	2.18	0.42
1:I:288:GLU:HA	1:I:303:VAL:O	2.19	0.42
1:M:124:PRO:HD3	1:M:183:HIS:CD2	2.54	0.42
1:P:198:ASN:HD22	1:P:198:ASN:N	2.14	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:291:CYS:O	1:A:300:ARG:HD3	2.19	0.42
1:A:320:GLU:HB2	1:A:331:GLY:HA2	2.01	0.42
1:F:150:ARG:HG2	1:F:177:TRP:CD2	2.55	0.42
1:J:247:GLY:O	1:J:273:HIS:ND1	2.53	0.42
1:A:153:LEU:HD13	1:B:102:ARG:CZ	2.49	0.42
1:G:223:ARG:HH21	1:G:275:GLU:CD	2.27	0.42
1:K:411:PHE:CZ	1:K:426:GLY:HA3	2.54	0.42
1:E:449:MET:HE1	1:H:203:LYS:HB3	2.01	0.42
1:G:150:ARG:HG2	1:G:177:TRP:CD2	2.54	0.42
1:J:223:ARG:HH21	1:J:275:GLU:CD	2.27	0.42
1:M:300:ARG:HG3	1:M:323:LEU:HB2	2.02	0.42
1:P:223:ARG:CG	4:P:1001:BCZ:H152	2.50	0.42
1:D:348:ILE:HD12	1:D:374:ARG:HG2	2.02	0.42
1:G:210:TYR:CZ	1:H:95:ALA:HB1	2.55	0.42
1:I:124:PRO:HD3	1:I:183:HIS:CD2	2.55	0.42
1:J:315:ARG:HB2	1:J:388:TRP:CD1	2.53	0.42
1:K:157:ILE:C	1:K:157:ILE:HD12	2.45	0.42
1:B:147:ARG:HG2	1:B:439:HIS:CD2	2.55	0.42
1:D:315:ARG:HB2	1:D:388:TRP:CD1	2.55	0.42
1:G:115:ILE:HG22	1:G:133:THR:HA	2.02	0.42
1:J:115:ILE:O	1:J:440:SER:HA	2.20	0.42
1:A:86:SER:HA	1:A:421:ASP:O	2.19	0.41
1:B:348:ILE:HD12	1:B:374:ARG:HG2	2.01	0.41
1:B:436:GLU:HG3	1:I:326:PRO:HG2	2.02	0.41
1:J:225:GLN:HE21	1:J:239:MET:N	2.05	0.41
1:L:119:PHE:HA	1:L:411:PHE:CZ	2.55	0.41
1:P:320:GLU:HB2	1:P:331:GLY:HA2	2.01	0.41
1:D:320:GLU:HB2	1:D:331:GLY:HA2	2.01	0.41
1:M:119:PHE:CG	1:M:227:SER:HA	2.55	0.41
1:N:198:ASN:H	1:N:198:ASN:ND2	2.17	0.41
1:F:147:ARG:NH2	1:N:435:LYS:CD	2.70	0.41
1:F:453:GLN:O	1:F:455:LEU:HD22	2.20	0.41
1:I:463:ASP:OD2	1:I:463:ASP:C	2.63	0.41
1:K:210:TYR:CZ	1:L:95:ALA:HB1	2.55	0.41
1:L:150:ARG:HG2	1:L:177:TRP:CD2	2.55	0.41
1:A:98:ILE:O	1:A:100:PRO:HD3	2.21	0.41
1:A:203:LYS:HB3	1:B:449:MET:HE1	2.03	0.41
1:B:436:GLU:OE1	1:I:343:LYS:HG2	2.20	0.41
1:D:157:ILE:C	1:D:157:ILE:HD12	2.45	0.41
1:F:429:MET:HE2	1:F:460:THR:HG23	2.03	0.41
1:G:157:ILE:C	1:G:157:ILE:HD12	2.44	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:150:ARG:HG2	1:I:177:TRP:CD2	2.55	0.41
1:N:150:ARG:HG2	1:N:177:TRP:CD2	2.55	0.41
1:A:198:ASN:N	1:A:198:ASN:HD22	2.19	0.41
1:E:240:ILE:O	1:E:251:CYS:HB2	2.20	0.41
1:G:147:ARG:HG2	1:G:439:HIS:CG	2.55	0.41
1:H:115:ILE:HG22	1:H:133:THR:HA	2.02	0.41
1:H:119:PHE:HA	1:H:411:PHE:CZ	2.56	0.41
1:I:223:ARG:CG	4:I:1001:BCZ:H152	2.50	0.41
1:L:225:GLN:HE21	1:L:239:MET:N	2.07	0.41
1:M:210:TYR:CZ	1:N:95:ALA:HB1	2.55	0.41
1:O:223:ARG:HH21	1:O:275:GLU:CD	2.29	0.41
1:P:303:VAL:HG22	1:P:314:ILE:HG12	2.03	0.41
1:A:197:GLU:OE2	1:A:197:GLU:CA	2.69	0.41
1:A:210:TYR:CZ	1:B:95:ALA:HB1	2.56	0.41
1:C:203:LYS:HB3	1:D:449:MET:HE1	2.03	0.41
1:F:139:PRO:HA	1:F:143:TYR:OH	2.21	0.41
1:F:320:GLU:HB2	1:F:331:GLY:CA	2.50	0.41
1:I:291:CYS:O	1:I:300:ARG:HD3	2.20	0.41
1:M:150:ARG:HH11	1:M:150:ARG:HB2	1.85	0.41
1:N:225:GLN:HE21	1:N:239:MET:N	2.02	0.41
1:B:432:ASP:O	1:I:373:LYS:HE2	2.20	0.41
1:J:165:PRO:HG2	6:J:2046:HOH:O	2.21	0.41
1:L:115:ILE:O	1:L:440:SER:HA	2.20	0.41
1:P:124:PRO:HD3	1:P:183:HIS:CD2	2.56	0.41
1:B:223:ARG:HH21	1:B:275:GLU:CD	2.28	0.41
1:E:115:ILE:O	1:E:440:SER:HA	2.20	0.41
1:H:154:ARG:HG2	1:H:177:TRP:HA	2.03	0.41
1:O:139:PRO:HA	1:O:143:TYR:OH	2.21	0.41
1:A:115:ILE:HG22	1:A:133:THR:HA	2.03	0.41
1:H:297:THR:OG1	1:H:340:ASN:O	2.30	0.41
1:M:105:GLU:HB3	6:M:2031:HOH:O	2.21	0.41
1:B:373:LYS:HE2	1:I:432:ASP:O	2.20	0.40
1:H:139:PRO:HA	1:H:143:TYR:OH	2.21	0.40
1:H:173:HIS:CE1	1:H:190:TYR:CE1	3.09	0.40
1:O:210:TYR:CZ	1:P:95:ALA:HB1	2.56	0.40
1:F:223:ARG:HH21	1:F:275:GLU:CD	2.29	0.40
1:H:272:LYS:HB2	6:H:2062:HOH:O	2.22	0.40
1:L:154:ARG:HG2	1:L:177:TRP:HA	2.02	0.40
1:L:320:GLU:HB2	1:L:331:GLY:HA2	2.03	0.40
1:O:453:GLN:HE21	1:O:453:GLN:HB3	1.74	0.40
1:B:353:VAL:HG12	1:B:425:ILE:HD11	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:453:GLN:HE21	1:C:453:GLN:HB3	1.77	0.40
1:F:115:ILE:O	1:F:440:SER:HA	2.21	0.40
1:F:343:LYS:HZ3	1:N:465:ALA:C	2.22	0.40
1:K:297:THR:OG1	1:K:340:ASN:O	2.31	0.40
1:M:115:ILE:HG22	1:M:133:THR:HA	2.02	0.40
1:C:320:GLU:HB2	1:C:331:GLY:HA2	2.04	0.40
1:G:275:GLU:HB3	6:G:2009:HOH:O	2.22	0.40
1:M:139:PRO:HA	1:M:143:TYR:HH	1.86	0.40
1:M:223:ARG:HH21	1:M:275:GLU:CD	2.30	0.40

All (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
1:D:436:GLU:O	1:K:343:LYS:NZ[1_545]	1.96	0.24
1:L:219:ASN:OD1	1:O:360:LYS:NZ[1_656]	1.97	0.23
1:D:343:LYS:NZ	1:K:436:GLU:O[1_545]	2.06	0.14
1:D:219:ASN:OD1	1:H:360:LYS:NZ[1_546]	2.13	0.07

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	388/397 (98%)	365 (94%)	23 (6%)	0	100	100
1	E	388/397 (98%)	369 (95%)	18 (5%)	1 (0%)	36	45
1	F	388/397 (98%)	369 (95%)	18 (5%)	1 (0%)	36	45
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
1	K	388/397 (98%)	370 (95%)	17 (4%)	1 (0%)	36	45
1	L	388/397 (98%)	372 (96%)	16 (4%)	0	100	100
1	M	388/397 (98%)	369 (95%)	18 (5%)	1 (0%)	36	45
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%)	48	61

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%)	300 (93%)	23 (7%)	13	19
1	B	323/329 (98%)	300 (93%)	23 (7%)	13	19
1	C	323/329 (98%)	302 (94%)	21 (6%)	15	22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	323/329 (98%)	301 (93%)	22 (7%)	14	20
1	E	323/329 (98%)	302 (94%)	21 (6%)	15	22
1	F	323/329 (98%)	301 (93%)	22 (7%)	14	20
1	G	323/329 (98%)	302 (94%)	21 (6%)	15	22
1	H	323/329 (98%)	303 (94%)	20 (6%)	16	24
1	I	323/329 (98%)	301 (93%)	22 (7%)	14	20
1	J	323/329 (98%)	301 (93%)	22 (7%)	14	20
1	K	323/329 (98%)	300 (93%)	23 (7%)	13	19
1	L	323/329 (98%)	300 (93%)	23 (7%)	13	19
1	M	323/329 (98%)	301 (93%)	22 (7%)	14	20
1	N	323/329 (98%)	301 (93%)	22 (7%)	14	20
1	O	323/329 (98%)	302 (94%)	21 (6%)	15	22
1	P	323/329 (98%)	302 (94%)	21 (6%)	15	22
All	All	5168/5264 (98%)	4819 (93%)	349 (7%)	15	20

All (349) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	84	ARG
1	A	85	LEU
1	A	150	ARG
1	A	154	ARG
1	A	197	GLU
1	A	198	ASN
1	A	223	ARG
1	A	229	CYS
1	A	239	MET
1	A	241	THR
1	A	275	GLU
1	A	305	LEU
1	A	338	GLU
1	A	345	SER
1	A	359	SER
1	A	369	MET
1	A	382	LYS
1	A	390	ASP
1	A	394	LEU

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Mol	Chain	Res	Type
1	A	416	LYS
1	A	453	GLN
1	A	455	LEU
1	A	456	TRP
1	B	84	ARG
1	B	85	LEU
1	B	154	ARG
1	B	197	GLU
1	B	198	ASN
1	B	223	ARG
1	B	226[A]	GLU
1	B	226[B]	GLU
1	B	229	CYS
1	B	239	MET
1	B	241	THR
1	B	275	GLU
1	B	305	LEU
1	B	338	GLU
1	B	345	SER
1	B	359	SER
1	B	369	MET
1	B	390	ASP
1	B	394	LEU
1	B	416	LYS
1	B	453	GLN
1	B	455	LEU
1	B	456	TRP
1	C	84	ARG
1	C	85	LEU
1	C	154	ARG
1	C	197	GLU
1	C	198	ASN
1	C	223	ARG
1	C	239	MET
1	C	241	THR
1	C	275	GLU
1	C	305	LEU
1	C	338	GLU
1	C	345	SER
1	C	359	SER
1	C	369	MET
1	C	382	LYS

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Mol	Chain	Res	Type
1	C	390	ASP
1	C	394	LEU
1	C	416	LYS
1	C	453	GLN
1	C	455	LEU
1	C	456	TRP
1	D	84	ARG
1	D	85	LEU
1	D	150	ARG
1	D	154	ARG
1	D	197	GLU
1	D	198	ASN
1	D	223	ARG
1	D	229	CYS
1	D	239	MET
1	D	241	THR
1	D	275	GLU
1	D	305	LEU
1	D	338	GLU
1	D	345	SER
1	D	359	SER
1	D	369	MET
1	D	390	ASP
1	D	394	LEU
1	D	416	LYS
1	D	453	GLN
1	D	455	LEU
1	D	456	TRP
1	E	84	ARG
1	E	85	LEU
1	E	150	ARG
1	E	154	ARG
1	E	197	GLU
1	E	198	ASN
1	E	223	ARG
1	E	229	CYS
1	E	239	MET
1	E	241	THR
1	E	275	GLU
1	E	305	LEU
1	E	338	GLU
1	E	345	SER

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Mol	Chain	Res	Type
1	E	369	MET
1	E	390	ASP
1	E	394	LEU
1	E	416	LYS
1	E	453	GLN
1	E	455	LEU
1	E	456	TRP
1	F	84	ARG
1	F	85	LEU
1	F	150	ARG
1	F	154	ARG
1	F	197	GLU
1	F	198	ASN
1	F	223	ARG
1	F	229	CYS
1	F	239	MET
1	F	241	THR
1	F	275	GLU
1	F	305	LEU
1	F	338	GLU
1	F	345	SER
1	F	359	SER
1	F	369	MET
1	F	390	ASP
1	F	394	LEU
1	F	416	LYS
1	F	453	GLN
1	F	455	LEU
1	F	456	TRP
1	G	84	ARG
1	G	85	LEU
1	G	154	ARG
1	G	197	GLU
1	G	198	ASN
1	G	223	ARG
1	G	229	CYS
1	G	239	MET
1	G	241	THR
1	G	275	GLU
1	G	305	LEU
1	G	338	GLU
1	G	345	SER

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Mol	Chain	Res	Type
1	G	369	MET
1	G	390	ASP
1	G	394	LEU
1	G	410	SER
1	G	416	LYS
1	G	453	GLN
1	G	455	LEU
1	G	456	TRP
1	H	84	ARG
1	H	85	LEU
1	H	154	ARG
1	H	197	GLU
1	H	198	ASN
1	H	223	ARG
1	H	239	MET
1	H	241	THR
1	H	275	GLU
1	H	305	LEU
1	H	338	GLU
1	H	345	SER
1	H	359	SER
1	H	369	MET
1	H	390	ASP
1	H	394	LEU
1	H	416	LYS
1	H	453	GLN
1	H	455	LEU
1	H	456	TRP
1	I	84	ARG
1	I	85	LEU
1	I	150	ARG
1	I	154	ARG
1	I	197	GLU
1	I	198	ASN
1	I	223	ARG
1	I	229	CYS
1	I	239	MET
1	I	241	THR
1	I	275	GLU
1	I	305	LEU
1	I	338	GLU
1	I	345	SER

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Mol	Chain	Res	Type
1	I	359	SER
1	I	369	MET
1	I	390	ASP
1	I	394	LEU
1	I	416	LYS
1	I	453	GLN
1	I	455	LEU
1	I	456	TRP
1	J	84	ARG
1	J	85	LEU
1	J	150	ARG
1	J	154	ARG
1	J	197	GLU
1	J	198	ASN
1	J	223	ARG
1	J	229	CYS
1	J	239	MET
1	J	241	THR
1	J	246	SER
1	J	275	GLU
1	J	305	LEU
1	J	338	GLU
1	J	345	SER
1	J	369	MET
1	J	390	ASP
1	J	394	LEU
1	J	416	LYS
1	J	453	GLN
1	J	455	LEU
1	J	456	TRP
1	K	84	ARG
1	K	85	LEU
1	K	150	ARG
1	K	154	ARG
1	K	197	GLU
1	K	198	ASN
1	K	223	ARG
1	K	226[A]	GLU
1	K	226[B]	GLU
1	K	239	MET
1	K	241	THR
1	K	275	GLU

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Mol	Chain	Res	Type
1	K	305	LEU
1	K	338	GLU
1	K	345	SER
1	K	359	SER
1	K	369	MET
1	K	390	ASP
1	K	394	LEU
1	K	416	LYS
1	K	453	GLN
1	K	455	LEU
1	K	456	TRP
1	L	84	ARG
1	L	85	LEU
1	L	150	ARG
1	L	154	ARG
1	L	197	GLU
1	L	198	ASN
1	L	223	ARG
1	L	229	CYS
1	L	239	MET
1	L	241	THR
1	L	275	GLU
1	L	305	LEU
1	L	338	GLU
1	L	345	SER
1	L	359	SER
1	L	369	MET
1	L	382	LYS
1	L	390	ASP
1	L	394	LEU
1	L	416	LYS
1	L	453	GLN
1	L	455	LEU
1	L	456	TRP
1	M	84	ARG
1	M	85	LEU
1	M	150	ARG
1	M	154	ARG
1	M	197	GLU
1	M	198	ASN
1	M	223	ARG
1	M	239	MET

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Mol	Chain	Res	Type
1	M	241	THR
1	M	275	GLU
1	M	305	LEU
1	M	338	GLU
1	M	345	SER
1	M	359	SER
1	M	369	MET
1	M	382	LYS
1	M	390	ASP
1	M	394	LEU
1	M	416	LYS
1	M	453	GLN
1	M	455	LEU
1	M	456	TRP
1	N	84	ARG
1	N	85	LEU
1	N	150	ARG
1	N	154	ARG
1	N	197	GLU
1	N	198	ASN
1	N	223	ARG
1	N	239	MET
1	N	241	THR
1	N	275	GLU
1	N	305	LEU
1	N	338	GLU
1	N	345	SER
1	N	359	SER
1	N	369	MET
1	N	382	LYS
1	N	390	ASP
1	N	394	LEU
1	N	416	LYS
1	N	453	GLN
1	N	455	LEU
1	N	456	TRP
1	O	84	ARG
1	O	85	LEU
1	O	150	ARG
1	O	154	ARG
1	O	197	GLU
1	O	198	ASN

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Mol	Chain	Res	Type
1	O	223	ARG
1	O	239	MET
1	O	241	THR
1	O	275	GLU
1	O	305	LEU
1	O	338	GLU
1	O	345	SER
1	O	359	SER
1	O	369	MET
1	O	390	ASP
1	O	394	LEU
1	O	416	LYS
1	O	453	GLN
1	O	455	LEU
1	O	456	TRP
1	P	84	ARG
1	P	85	LEU
1	P	150	ARG
1	P	154	ARG
1	P	197	GLU
1	P	198	ASN
1	P	223	ARG
1	P	239	MET
1	P	241	THR
1	P	275	GLU
1	P	305	LEU
1	P	338	GLU
1	P	345	SER
1	P	359	SER
1	P	369	MET
1	P	390	ASP
1	P	394	LEU
1	P	416	LYS
1	P	453	GLN
1	P	455	LEU
1	P	456	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (83) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	129	HIS
1	A	183	HIS

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Mol	Chain	Res	Type
1	A	198	ASN
1	A	225	GLN
1	A	439	HIS
1	A	453	GLN
1	B	129	HIS
1	B	183	HIS
1	B	198	ASN
1	B	225	GLN
1	B	439	HIS
1	B	453	GLN
1	C	183	HIS
1	C	198	ASN
1	C	225	GLN
1	C	235	ASN
1	C	439	HIS
1	C	453	GLN
1	D	183	HIS
1	D	198	ASN
1	D	225	GLN
1	D	439	HIS
1	D	453	GLN
1	E	183	HIS
1	E	198	ASN
1	E	225	GLN
1	E	439	HIS
1	E	453	GLN
1	F	183	HIS
1	F	198	ASN
1	F	225	GLN
1	F	453	GLN
1	G	129	HIS
1	G	183	HIS
1	G	198	ASN
1	G	225	GLN
1	G	235	ASN
1	G	439	HIS
1	G	453	GLN
1	H	183	HIS
1	H	198	ASN
1	H	225	GLN
1	H	453	GLN
1	I	183	HIS

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Mol	Chain	Res	Type
1	I	198	ASN
1	I	225	GLN
1	I	439	HIS
1	I	453	GLN
1	J	183	HIS
1	J	198	ASN
1	J	225	GLN
1	J	235	ASN
1	J	439	HIS
1	J	453	GLN
1	K	183	HIS
1	K	198	ASN
1	K	225	GLN
1	K	439	HIS
1	K	453	GLN
1	L	109	ASN
1	L	183	HIS
1	L	198	ASN
1	L	225	GLN
1	L	439	HIS
1	L	453	GLN
1	M	183	HIS
1	M	198	ASN
1	M	225	GLN
1	M	439	HIS
1	M	453	GLN
1	N	183	HIS
1	N	198	ASN
1	N	225	GLN
1	N	439	HIS
1	N	453	GLN
1	O	183	HIS
1	O	198	ASN
1	O	225	GLN
1	O	453	GLN
1	P	183	HIS
1	P	198	ASN
1	P	225	GLN
1	P	453	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 oligosaccharides 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$
2	NAG	E	900	1	14,14,15	0.80	1 (7%)	17,19,21	1.90	4 (23%)
2	NAG	K	900	1	14,14,15	0.69	0	17,19,21	1.86	3 (17%)
4	BCZ	E	1001	-	22,23,23	1.15	2 (9%)	24,32,32	1.54	5 (20%)
4	BCZ	A	1001	-	22,23,23	1.24	3 (13%)	24,32,32	1.40	4 (16%)
2	NAG	P	900	1	14,14,15	0.72	0	17,19,21	1.86	2 (11%)
4	BCZ	O	1001	-	22,23,23	1.13	1 (4%)	24,32,32	1.73	7 (29%)
4	BCZ	B	1001	-	22,23,23	0.96	1 (4%)	24,32,32	1.44	3 (12%)
4	BCZ	L	1001	-	22,23,23	1.21	1 (4%)	24,32,32	1.40	3 (12%)
2	NAG	F	900	1	14,14,15	0.90	1 (7%)	17,19,21	1.94	2 (11%)
4	BCZ	J	1001	-	22,23,23	1.09	1 (4%)	24,32,32	1.47	4 (16%)
4	BCZ	M	1001	-	22,23,23	1.44	2 (9%)	24,32,32	1.20	4 (16%)
4	BCZ	F	1001	-	22,23,23	1.33	2 (9%)	24,32,32	1.32	4 (16%)
4	BCZ	K	1001	-	22,23,23	1.24	1 (4%)	24,32,32	1.57	5 (20%)
4	BCZ	D	1001	-	22,23,23	1.07	1 (4%)	24,32,32	1.63	5 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	N	900	1	14,14,15	0.81	0	17,19,21	2.00	3 (17%)
2	NAG	L	900	1	14,14,15	0.59	0	17,19,21	2.07	4 (23%)
4	BCZ	H	1001	-	22,23,23	1.52	3 (13%)	24,32,32	1.37	5 (20%)
2	NAG	G	900	1	14,14,15	0.56	0	17,19,21	2.16	3 (17%)
4	BCZ	C	1001	-	22,23,23	1.38	2 (9%)	24,32,32	1.27	3 (12%)
2	NAG	A	900	1	14,14,15	0.62	0	17,19,21	2.12	4 (23%)
2	NAG	D	900	1	14,14,15	0.94	0	17,19,21	2.04	4 (23%)
2	NAG	M	900	1	14,14,15	0.68	0	17,19,21	2.25	3 (17%)
2	NAG	C	900	1	14,14,15	0.76	0	17,19,21	2.09	2 (11%)
4	BCZ	I	1001	-	22,23,23	1.23	2 (9%)	24,32,32	1.56	4 (16%)
4	BCZ	N	1001	-	22,23,23	1.40	3 (13%)	24,32,32	1.38	4 (16%)
4	BCZ	P	1001	-	22,23,23	0.98	1 (4%)	24,32,32	1.51	5 (20%)
2	NAG	J	900	1	14,14,15	0.67	0	17,19,21	2.00	3 (17%)
4	BCZ	G	1001	-	22,23,23	0.99	2 (9%)	24,32,32	1.50	4 (16%)
2	NAG	I	900	1	14,14,15	0.74	0	17,19,21	2.29	4 (23%)
2	NAG	H	900	1	14,14,15	0.87	0	17,19,21	1.98	3 (17%)
2	NAG	O	900	1	14,14,15	0.63	0	17,19,21	2.30	4 (23%)
2	NAG	B	900	1	14,14,15	0.66	0	17,19,21	2.15	4 (23%)

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
2	NAG	E	900	1	-	1/6/23/26	0/1/1/1
2	NAG	K	900	1	-	0/6/23/26	0/1/1/1
4	BCZ	E	1001	-	-	0/24/40/40	0/1/1/1
4	BCZ	A	1001	-	-	0/24/40/40	0/1/1/1
2	NAG	P	900	1	-	0/6/23/26	0/1/1/1
4	BCZ	O	1001	-	-	1/24/40/40	0/1/1/1
4	BCZ	B	1001	-	-	1/24/40/40	0/1/1/1
4	BCZ	L	1001	-	-	2/24/40/40	0/1/1/1
2	NAG	F	900	1	-	0/6/23/26	0/1/1/1
4	BCZ	J	1001	-	-	0/24/40/40	0/1/1/1
4	BCZ	M	1001	-	-	0/24/40/40	0/1/1/1
4	BCZ	F	1001	-	-	0/24/40/40	0/1/1/1
4	BCZ	K	1001	-	-	1/24/40/40	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BCZ	D	1001	-	-	2/24/40/40	0/1/1/1
2	NAG	N	900	1	-	0/6/23/26	0/1/1/1
2	NAG	L	900	1	-	0/6/23/26	0/1/1/1
4	BCZ	H	1001	-	-	0/24/40/40	0/1/1/1
2	NAG	G	900	1	-	0/6/23/26	0/1/1/1
4	BCZ	C	1001	-	-	0/24/40/40	0/1/1/1
2	NAG	A	900	1	-	0/6/23/26	0/1/1/1
2	NAG	D	900	1	-	0/6/23/26	0/1/1/1
2	NAG	M	900	1	-	0/6/23/26	0/1/1/1
2	NAG	C	900	1	-	0/6/23/26	0/1/1/1
4	BCZ	I	1001	-	-	2/24/40/40	0/1/1/1
4	BCZ	N	1001	-	-	2/24/40/40	0/1/1/1
4	BCZ	P	1001	-	-	2/24/40/40	0/1/1/1
2	NAG	J	900	1	-	0/6/23/26	0/1/1/1
4	BCZ	G	1001	-	-	0/24/40/40	0/1/1/1
2	NAG	I	900	1	-	0/6/23/26	0/1/1/1
2	NAG	H	900	1	-	0/6/23/26	0/1/1/1
2	NAG	O	900	1	-	0/6/23/26	0/1/1/1
2	NAG	B	900	1	-	0/6/23/26	0/1/1/1

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	1001	BCZ	C26-N25	4.61	1.41	1.33
4	M	1001	BCZ	C26-N25	4.52	1.40	1.33
4	F	1001	BCZ	C26-N25	4.09	1.40	1.33
4	N	1001	BCZ	C26-N25	3.98	1.40	1.33
4	C	1001	BCZ	C26-N25	3.97	1.40	1.33
4	K	1001	BCZ	C26-N25	3.36	1.38	1.33
4	A	1001	BCZ	C26-N25	3.27	1.38	1.33
4	O	1001	BCZ	C26-N25	3.14	1.38	1.33
4	L	1001	BCZ	C26-N25	3.12	1.38	1.33
4	H	1001	BCZ	C5-C6	3.05	1.56	1.51
4	N	1001	BCZ	C5-C6	2.81	1.56	1.51
4	M	1001	BCZ	C26-N30	2.68	1.41	1.32
4	E	1001	BCZ	C26-N25	2.56	1.37	1.33
4	I	1001	BCZ	C26-N25	2.46	1.37	1.33
4	J	1001	BCZ	C26-N25	2.40	1.37	1.33
4	I	1001	BCZ	C5-C6	2.33	1.55	1.51
4	P	1001	BCZ	C26-N25	2.33	1.37	1.33
4	D	1001	BCZ	C26-N25	2.21	1.36	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	1001	BCZ	C5-C4	-2.20	1.50	1.54
4	G	1001	BCZ	C26-N25	2.15	1.36	1.33
2	F	900	NAG	C1-C2	2.15	1.55	1.52
4	B	1001	BCZ	C5-C6	2.14	1.55	1.51
4	H	1001	BCZ	C26-N30	2.13	1.39	1.32
4	F	1001	BCZ	C5-C6	2.13	1.55	1.51
4	C	1001	BCZ	C5-C6	2.12	1.55	1.51
4	G	1001	BCZ	C26-N30	2.10	1.39	1.32
2	E	900	NAG	C1-C2	2.09	1.55	1.52
4	A	1001	BCZ	O7-C6	-2.05	1.24	1.30
4	N	1001	BCZ	C26-N30	2.05	1.39	1.32
4	A	1001	BCZ	C26-N30	2.03	1.39	1.32

All (121) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	900	NAG	C1-O5-C5	7.55	122.31	112.19
2	O	900	NAG	C1-O5-C5	7.44	122.15	112.19
2	M	900	NAG	C1-O5-C5	7.39	122.09	112.19
2	G	900	NAG	C1-O5-C5	7.09	121.69	112.19
2	C	900	NAG	C1-O5-C5	6.73	121.20	112.19
2	J	900	NAG	C1-O5-C5	6.71	121.17	112.19
2	L	900	NAG	C1-O5-C5	6.68	121.14	112.19
2	A	900	NAG	C1-O5-C5	6.68	121.14	112.19
2	B	900	NAG	C1-O5-C5	6.57	120.99	112.19
2	F	900	NAG	C1-O5-C5	6.45	120.83	112.19
2	N	900	NAG	C1-O5-C5	6.37	120.73	112.19
2	D	900	NAG	C1-O5-C5	6.18	120.46	112.19
2	H	900	NAG	C1-O5-C5	5.87	120.05	112.19
2	P	900	NAG	C1-O5-C5	5.66	119.77	112.19
2	K	900	NAG	C1-O5-C5	5.61	119.70	112.19
2	E	900	NAG	C1-O5-C5	5.22	119.18	112.19
4	O	1001	BCZ	C15-C13-N11	-4.22	109.12	116.12
4	I	1001	BCZ	O14-C13-N11	3.87	128.82	121.98
4	K	1001	BCZ	O14-C13-N11	3.81	128.72	121.98
4	I	1001	BCZ	C15-C13-N11	-3.74	109.91	116.12
4	J	1001	BCZ	C15-C13-N11	-3.68	110.02	116.12
4	D	1001	BCZ	C1-C5-C6	-3.57	106.50	114.55
4	P	1001	BCZ	C15-C13-N11	-3.57	110.20	116.12
4	E	1001	BCZ	C15-C13-N11	-3.55	110.23	116.12
4	K	1001	BCZ	C15-C13-N11	-3.47	110.36	116.12
4	B	1001	BCZ	C15-C13-N11	-3.45	110.39	116.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	900	NAG	C1-C2-N2	-3.42	105.04	110.43
4	D	1001	BCZ	C15-C13-N11	-3.34	110.59	116.12
4	B	1001	BCZ	C1-C5-C6	-3.30	107.12	114.55
4	J	1001	BCZ	O14-C13-N11	3.29	127.79	121.98
4	G	1001	BCZ	C15-C13-N11	-3.28	110.67	116.12
2	H	900	NAG	C1-C2-N2	-3.26	105.29	110.43
4	B	1001	BCZ	O14-C13-N11	3.25	127.72	121.98
4	L	1001	BCZ	C1-C5-C6	-3.24	107.24	114.55
4	P	1001	BCZ	C1-C5-C6	-3.20	107.34	114.55
4	A	1001	BCZ	C15-C13-N11	-3.19	110.82	116.12
4	G	1001	BCZ	C1-C5-C6	-3.19	107.36	114.55
4	E	1001	BCZ	C1-C5-C6	-3.17	107.42	114.55
4	L	1001	BCZ	C15-C13-N11	-3.15	110.89	116.12
4	N	1001	BCZ	O8-C6-C5	-3.15	115.57	123.01
4	N	1001	BCZ	C1-C5-C6	-3.15	107.45	114.55
4	P	1001	BCZ	O8-C6-C5	-3.12	115.65	123.01
4	F	1001	BCZ	C15-C13-N11	-3.10	110.97	116.12
4	O	1001	BCZ	O8-C6-C5	-3.05	115.81	123.01
4	I	1001	BCZ	C1-C5-C6	-3.00	107.78	114.55
4	C	1001	BCZ	C1-C5-C6	-2.99	107.81	114.55
2	O	900	NAG	C1-C2-N2	-2.98	105.73	110.43
4	C	1001	BCZ	C15-C13-N11	-2.94	111.24	116.12
2	B	900	NAG	C1-C2-N2	-2.89	105.87	110.43
4	A	1001	BCZ	O14-C13-N11	2.88	127.08	121.98
4	D	1001	BCZ	O8-C6-C5	-2.88	116.21	123.01
4	F	1001	BCZ	O14-C13-N11	2.88	127.07	121.98
4	A	1001	BCZ	C1-C5-C6	-2.87	108.08	114.55
2	J	900	NAG	C6-C5-C4	-2.84	106.06	113.02
4	H	1001	BCZ	O9-C4-C5	-2.80	104.16	111.37
4	H	1001	BCZ	O14-C13-N11	2.79	126.92	121.98
4	K	1001	BCZ	O9-C4-C5	-2.78	104.21	111.37
4	E	1001	BCZ	O8-C6-C5	-2.78	116.45	123.01
4	H	1001	BCZ	C15-C13-N11	-2.77	111.52	116.12
4	E	1001	BCZ	O14-C13-N11	2.69	126.74	121.98
2	D	900	NAG	O5-C1-C2	2.69	115.45	111.29
4	F	1001	BCZ	C1-C5-C6	-2.67	108.53	114.55
2	M	900	NAG	C1-C2-N2	-2.67	106.22	110.43
4	H	1001	BCZ	O8-C6-C5	-2.67	116.71	123.01
4	O	1001	BCZ	C1-C5-C6	-2.66	108.56	114.55
4	P	1001	BCZ	O14-C13-N11	2.66	126.68	121.98
2	C	900	NAG	C6-C5-C4	-2.63	106.56	113.02
4	L	1001	BCZ	O14-C13-N11	2.61	126.59	121.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1001	BCZ	N25-C26-N30	-2.59	116.14	120.58
2	B	900	NAG	C6-C5-C4	-2.59	106.67	113.02
4	K	1001	BCZ	C1-C5-C6	-2.58	108.74	114.55
4	A	1001	BCZ	O9-C4-C5	-2.57	104.75	111.37
2	D	900	NAG	C1-C2-N2	-2.57	106.38	110.43
2	E	900	NAG	C1-C2-N2	-2.57	106.38	110.43
4	G	1001	BCZ	O14-C13-N11	2.56	126.51	121.98
4	J	1001	BCZ	C24-C10-N11	-2.54	106.71	110.69
4	M	1001	BCZ	C1-C5-C6	-2.53	108.84	114.55
2	A	900	NAG	C6-C5-C4	-2.53	106.81	113.02
2	A	900	NAG	O5-C1-C2	2.52	115.19	111.29
4	J	1001	BCZ	C1-C5-C6	-2.50	108.93	114.55
4	O	1001	BCZ	O14-C13-N11	2.46	126.33	121.98
4	N	1001	BCZ	C15-C13-N11	-2.46	112.05	116.12
2	I	900	NAG	O7-C7-C8	-2.46	117.68	122.05
4	G	1001	BCZ	O8-C6-C5	-2.45	117.23	123.01
2	O	900	NAG	C6-C5-C4	-2.44	107.03	113.02
4	D	1001	BCZ	C24-C10-N11	-2.44	106.87	110.69
4	M	1001	BCZ	O8-C6-C5	-2.42	117.29	123.01
2	B	900	NAG	C2-N2-C7	2.40	126.12	122.90
2	M	900	NAG	O5-C1-C2	2.38	114.97	111.29
4	O	1001	BCZ	C24-C10-N11	-2.37	106.97	110.69
2	K	900	NAG	C1-C2-N2	-2.36	106.71	110.43
2	K	900	NAG	C6-C5-C4	-2.36	107.23	113.02
2	D	900	NAG	O5-C5-C4	2.34	116.53	110.83
2	N	900	NAG	C1-C2-N2	-2.33	106.76	110.43
2	H	900	NAG	O5-C1-C2	2.32	114.88	111.29
4	O	1001	BCZ	O9-C4-C5	-2.31	105.42	111.37
2	G	900	NAG	C6-C5-C4	-2.31	107.36	113.02
2	E	900	NAG	C6-C5-C4	-2.30	107.37	113.02
2	N	900	NAG	O5-C1-C2	2.30	114.84	111.29
2	G	900	NAG	C1-C2-N2	-2.29	106.82	110.43
2	I	900	NAG	C6-C5-C4	-2.29	107.39	113.02
2	F	900	NAG	C1-C2-N2	-2.28	106.84	110.43
2	E	900	NAG	O5-C1-C2	2.27	114.80	111.29
4	C	1001	BCZ	O14-C13-N11	2.24	125.95	121.98
4	F	1001	BCZ	O8-C6-C5	-2.23	117.75	123.01
4	O	1001	BCZ	O7-C6-O8	2.23	129.14	124.08
2	L	900	NAG	O7-C7-C8	-2.21	118.13	122.05
4	M	1001	BCZ	C15-C13-N11	-2.19	112.49	116.12
2	L	900	NAG	O5-C1-C2	2.19	114.67	111.29
4	K	1001	BCZ	O8-C6-C5	-2.18	117.87	123.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	900	NAG	C1-C2-N2	-2.15	107.05	110.43
4	H	1001	BCZ	C1-C5-C6	-2.13	109.75	114.55
4	M	1001	BCZ	O9-C4-C5	-2.13	105.90	111.37
2	O	900	NAG	C2-N2-C7	2.12	125.75	122.90
4	N	1001	BCZ	O14-C13-N11	2.10	125.69	121.98
2	J	900	NAG	C1-C2-N2	-2.10	107.13	110.43
2	L	900	NAG	C6-C5-C4	-2.06	107.97	113.02
4	I	1001	BCZ	O8-C6-C5	-2.04	118.19	123.01
2	A	900	NAG	C1-C2-N2	-2.03	107.23	110.43
4	P	1001	BCZ	O7-C6-O8	2.03	128.68	124.08
4	E	1001	BCZ	O9-C4-C3	-2.01	106.14	112.42

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	900	NAG	O5-C5-C6-O6
4	P	1001	BCZ	C10-C24-C36-C39
4	B	1001	BCZ	C4-C5-C6-O7
4	D	1001	BCZ	C4-C5-C6-O8
4	D	1001	BCZ	C4-C5-C6-O7
4	I	1001	BCZ	C4-C5-C6-O8
4	I	1001	BCZ	C4-C5-C6-O7
4	K	1001	BCZ	C4-C5-C6-O7
4	L	1001	BCZ	C4-C5-C6-O8
4	L	1001	BCZ	C4-C5-C6-O7
4	N	1001	BCZ	C4-C5-C6-O8
4	N	1001	BCZ	C4-C5-C6-O7
4	O	1001	BCZ	C10-C24-C36-C39
4	P	1001	BCZ	C37-C24-C36-C39

There are no ring outliers.

16 monomers are involved in 20 short contacts:

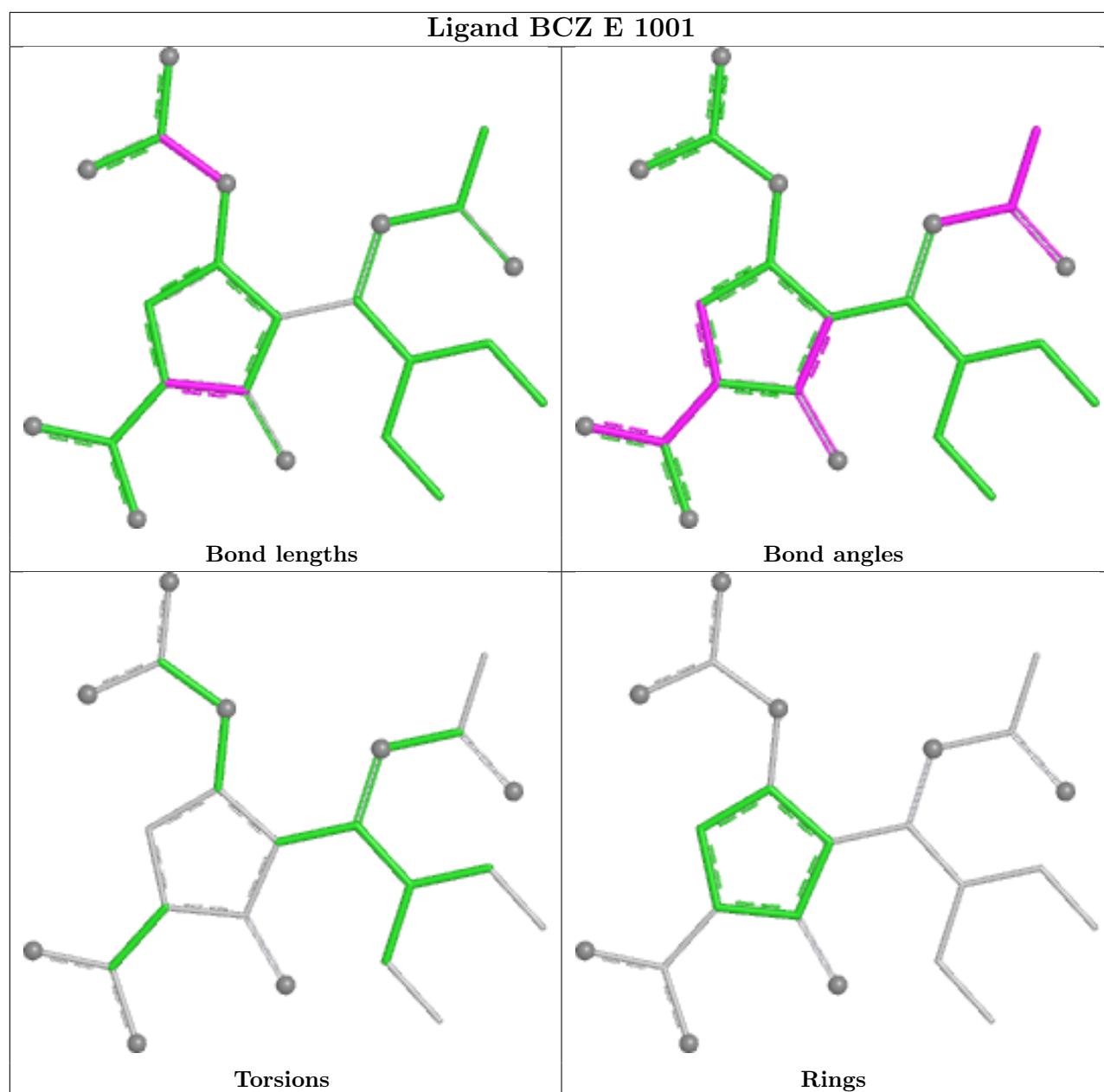
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	1001	BCZ	1	0
4	A	1001	BCZ	1	0
4	O	1001	BCZ	1	0
4	B	1001	BCZ	1	0
4	L	1001	BCZ	1	0
4	J	1001	BCZ	1	0

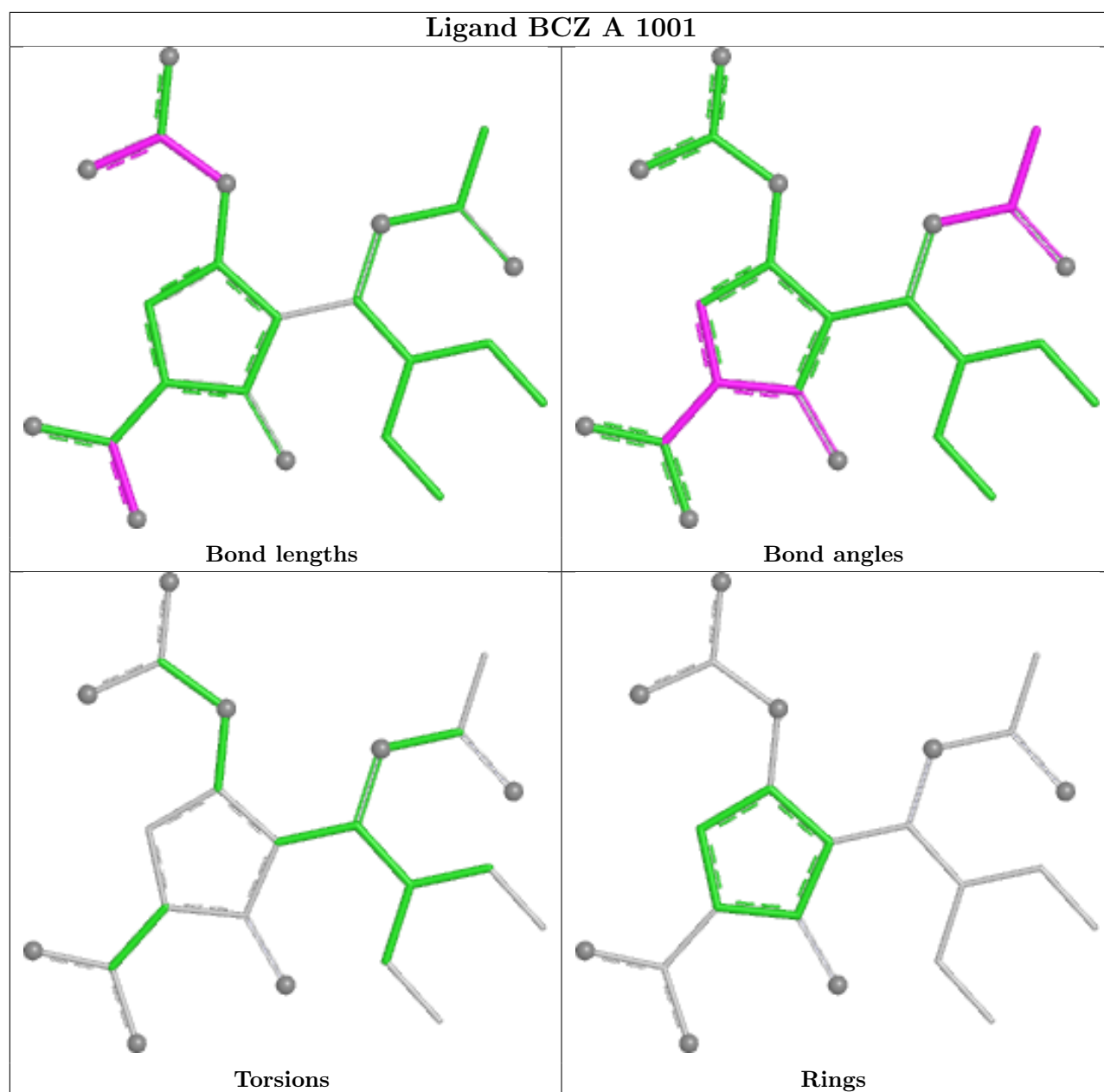
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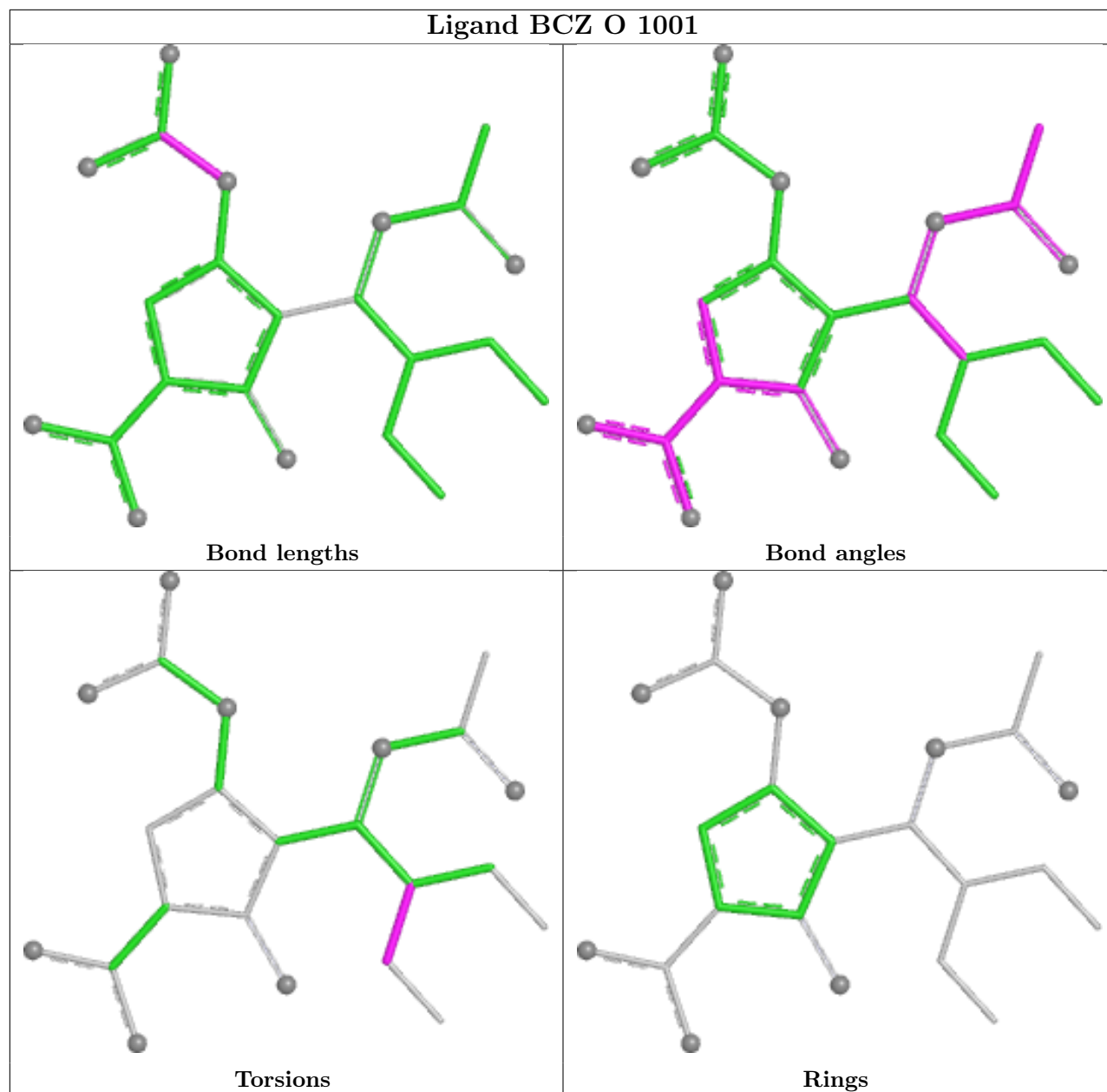
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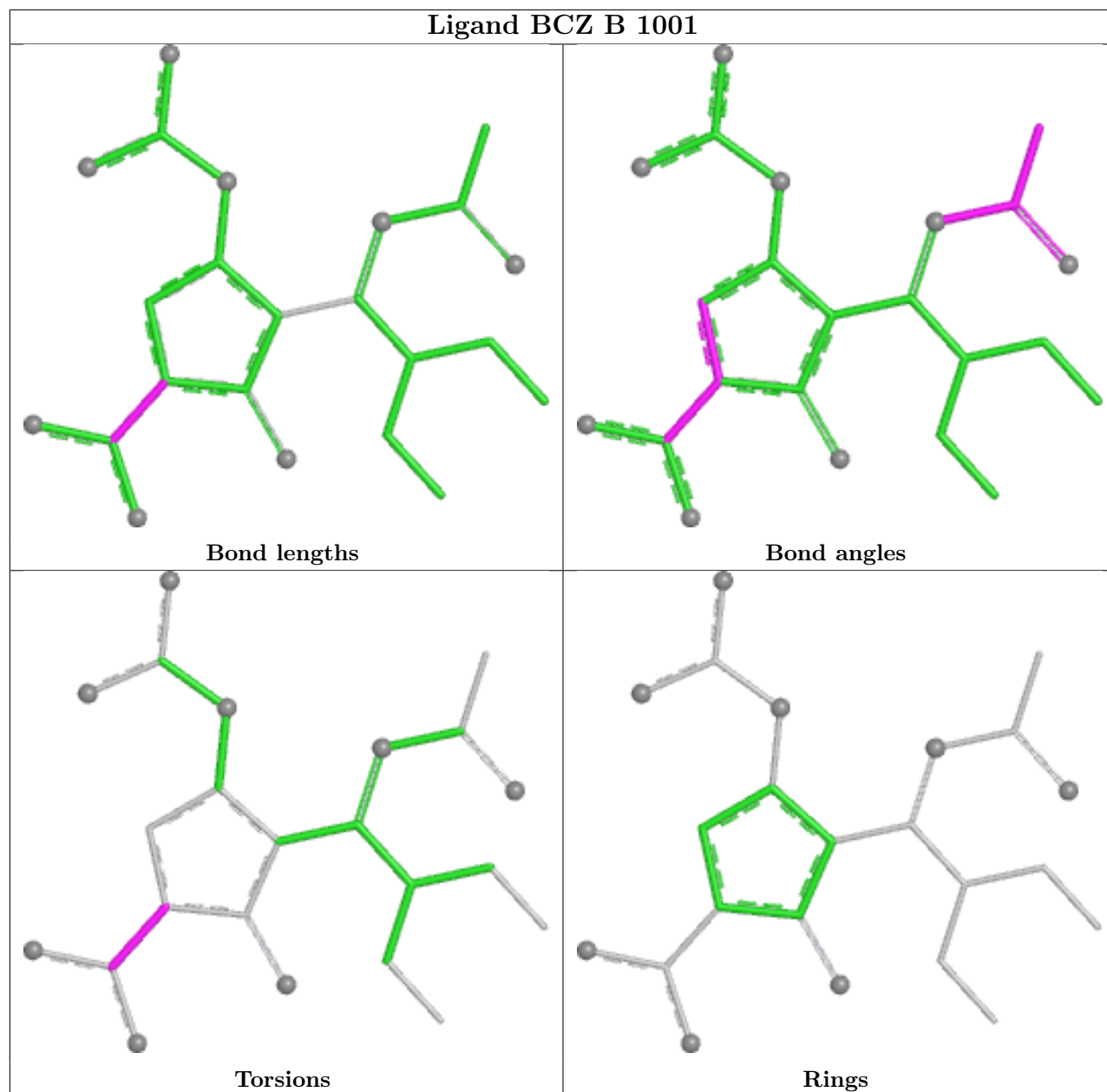
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	M	1001	BCZ	2	0
4	F	1001	BCZ	1	0
4	K	1001	BCZ	1	0
4	D	1001	BCZ	1	0
4	H	1001	BCZ	1	0
4	C	1001	BCZ	1	0
4	I	1001	BCZ	2	0
4	N	1001	BCZ	1	0
4	P	1001	BCZ	2	0
4	G	1001	BCZ	2	0

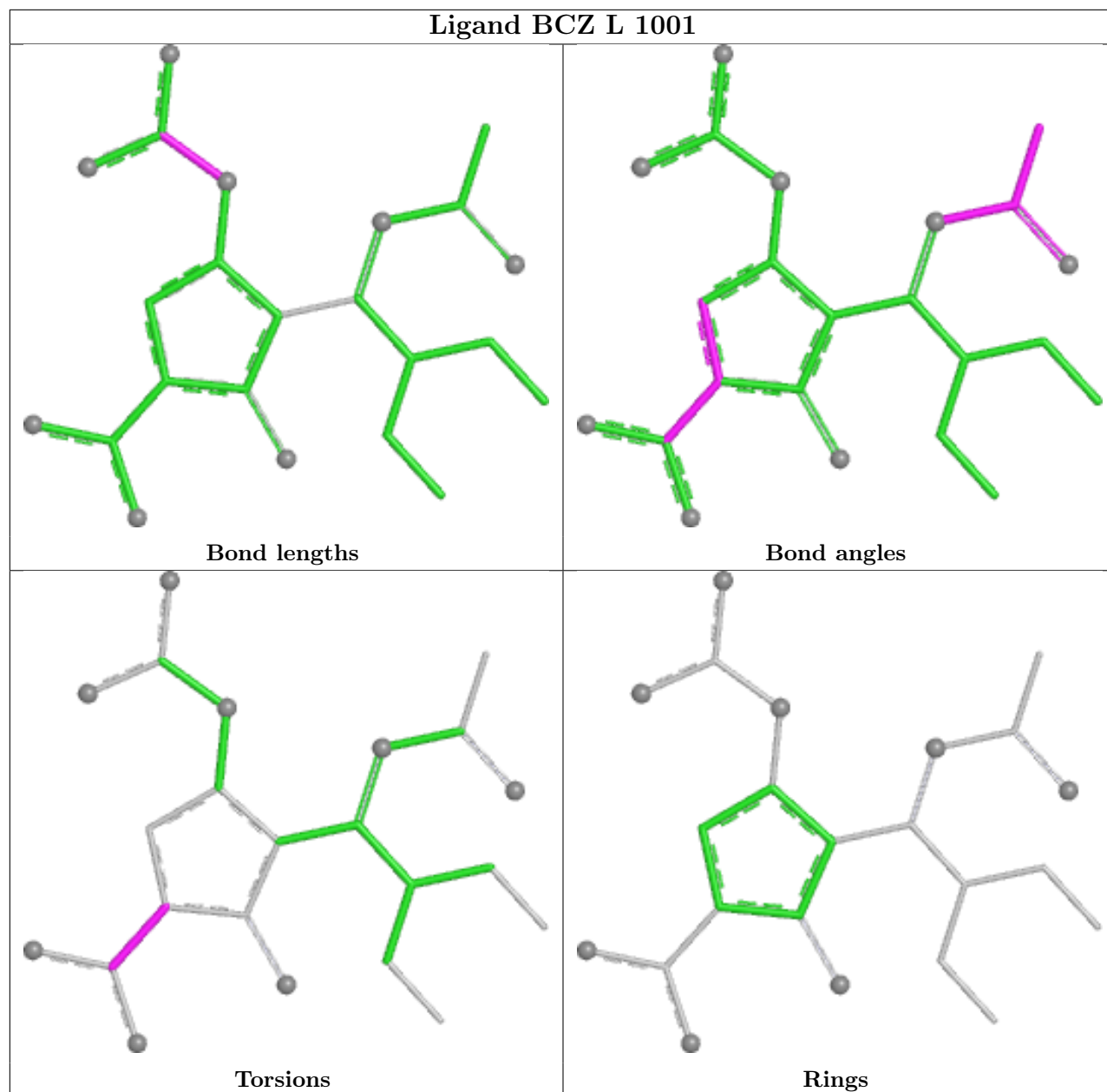
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

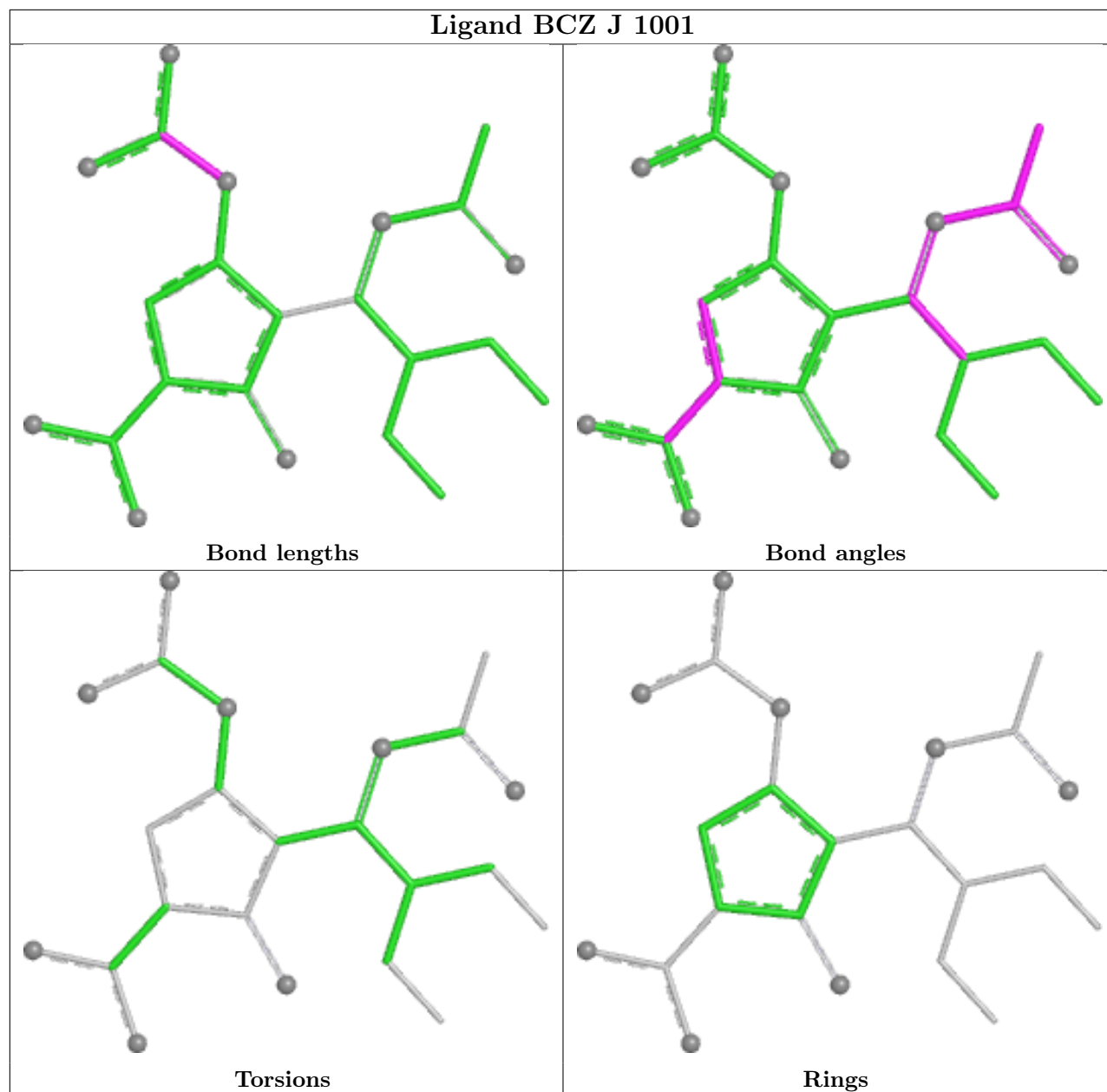


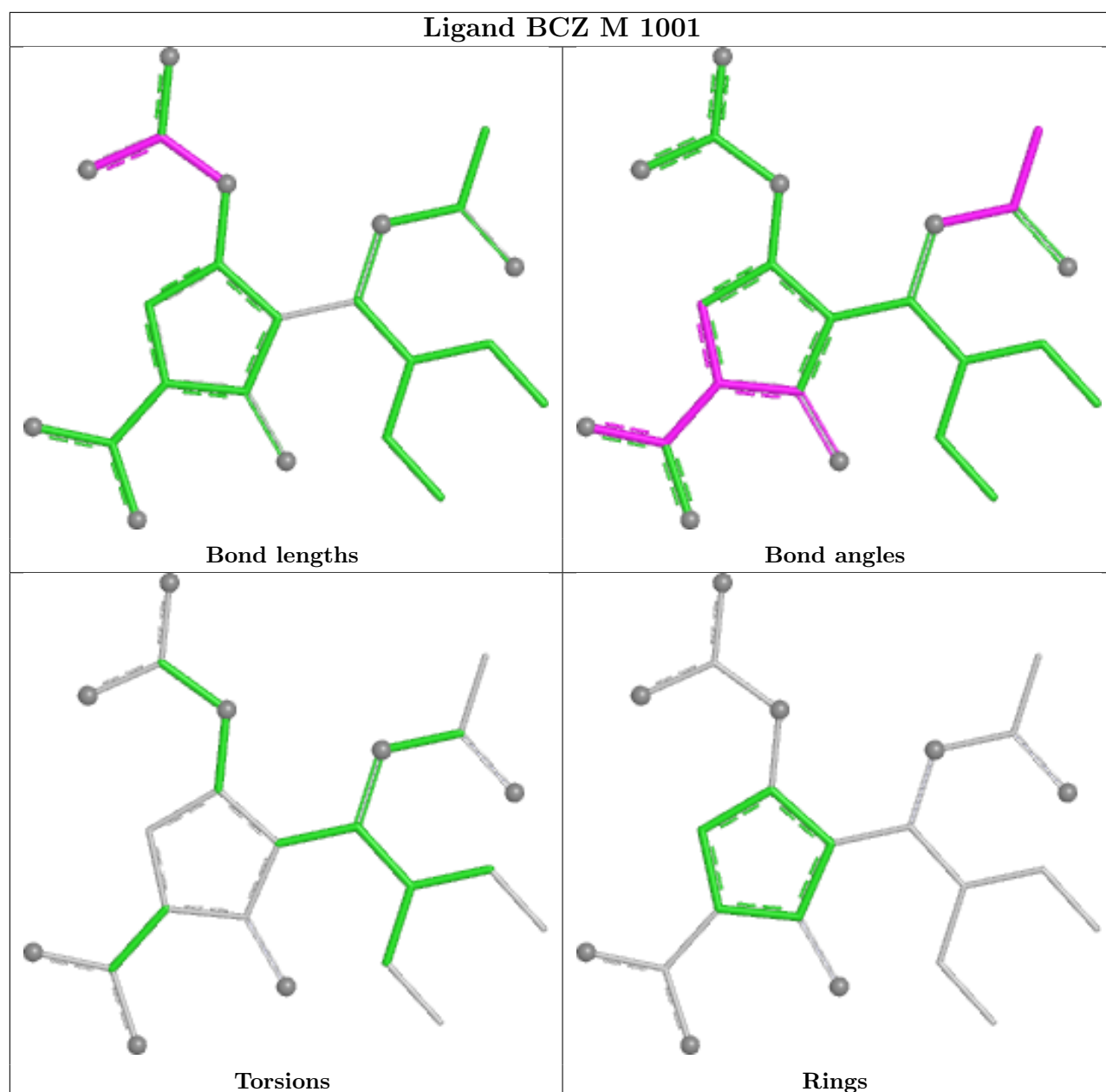


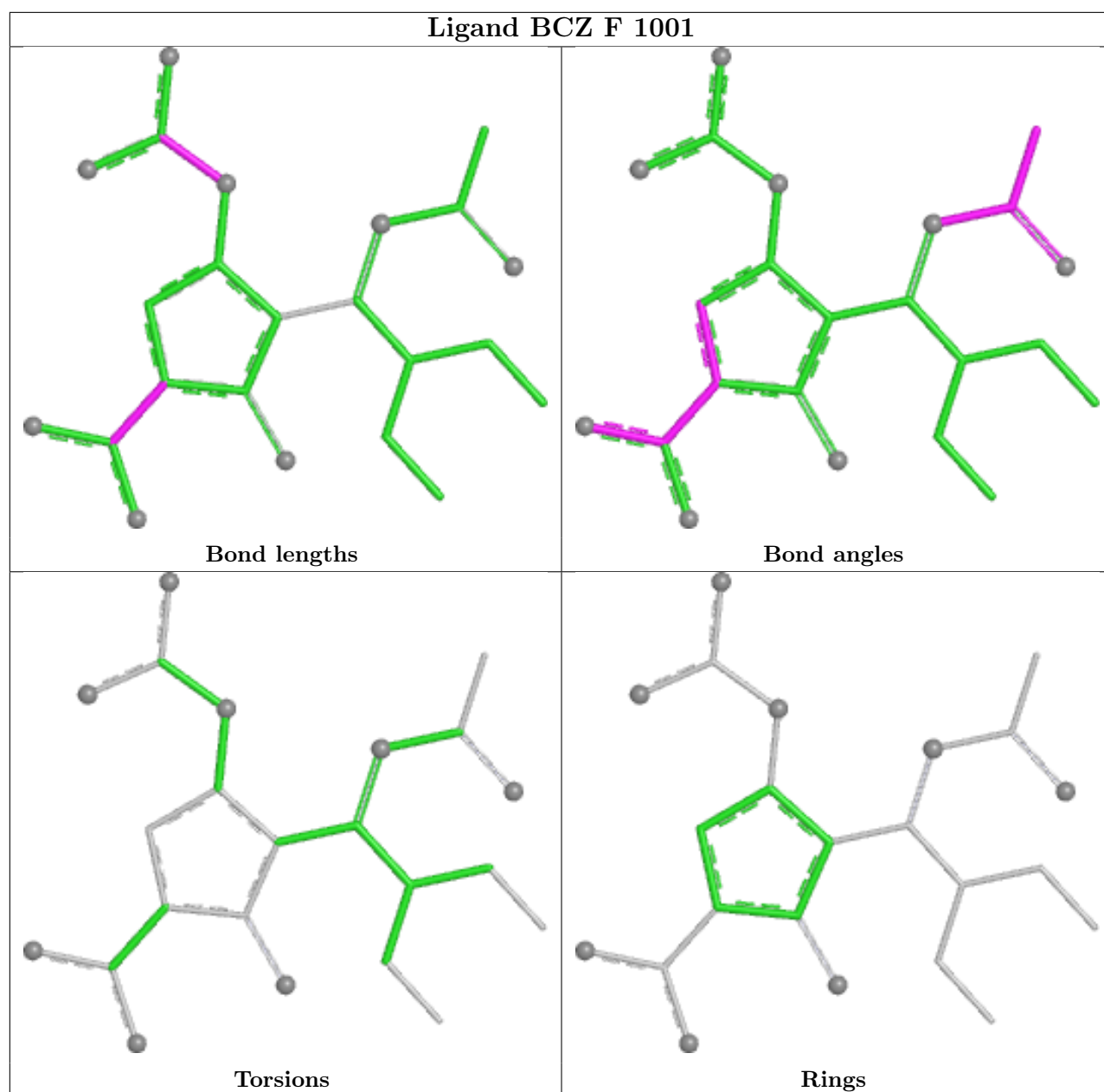


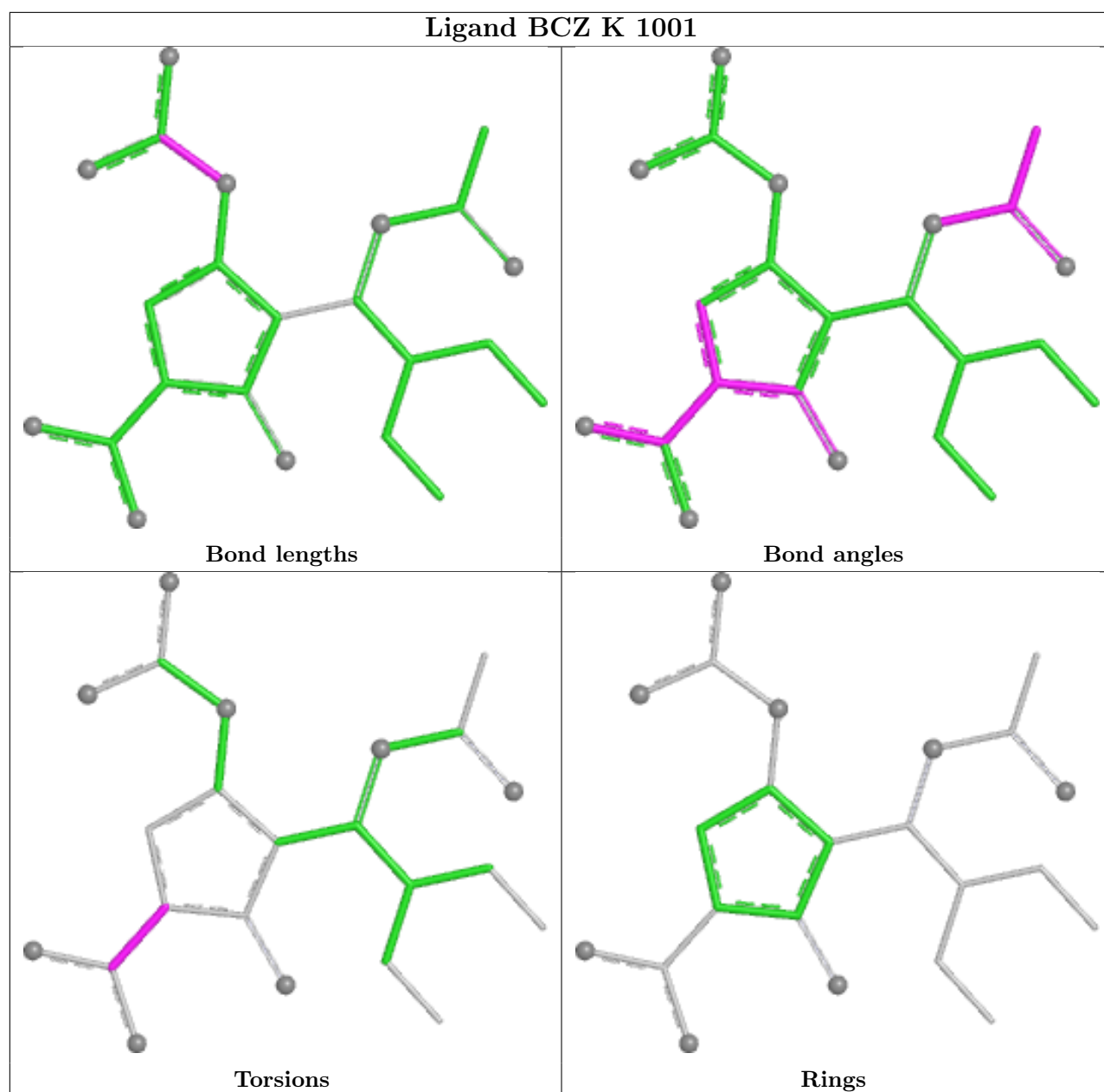


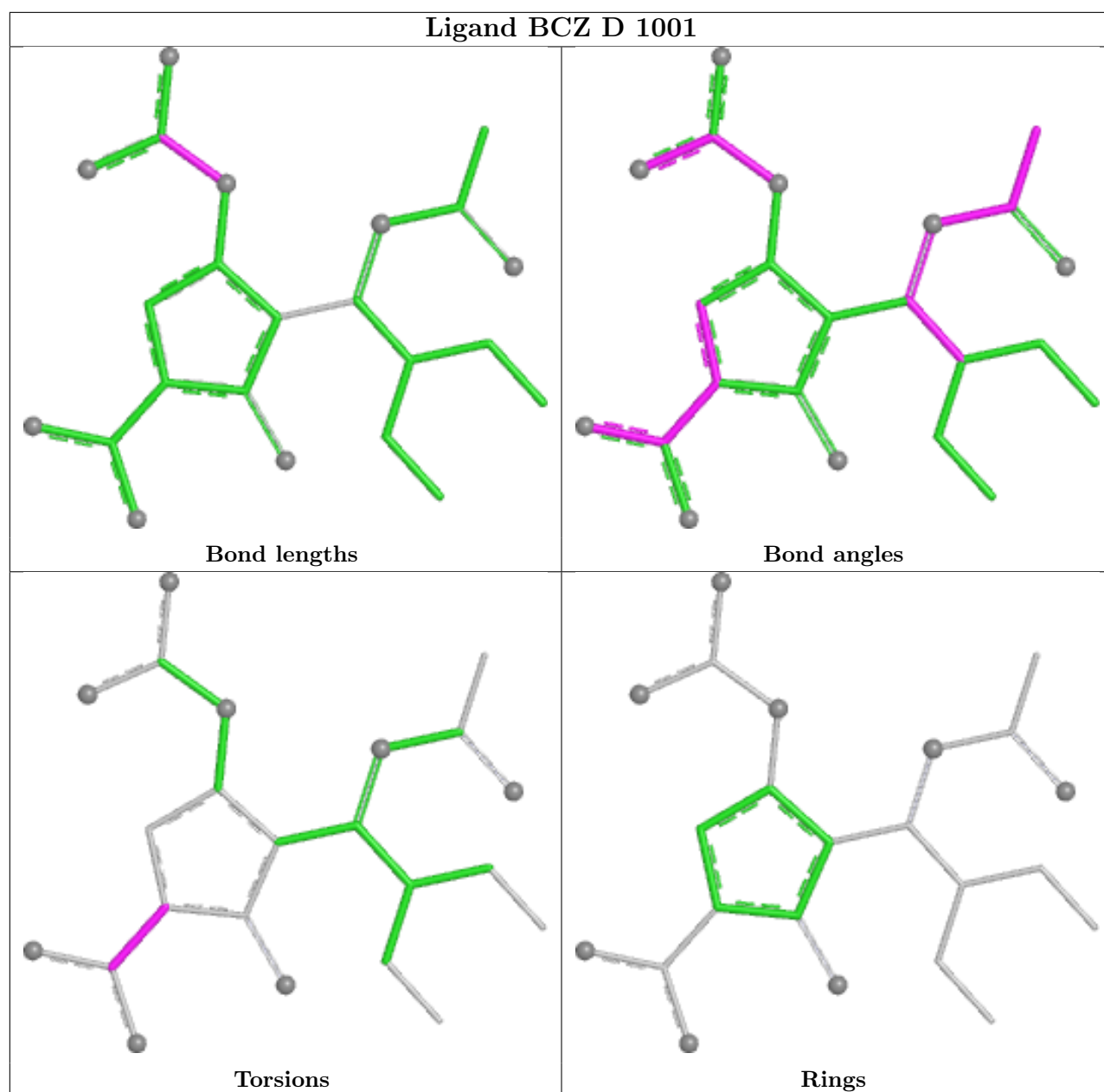


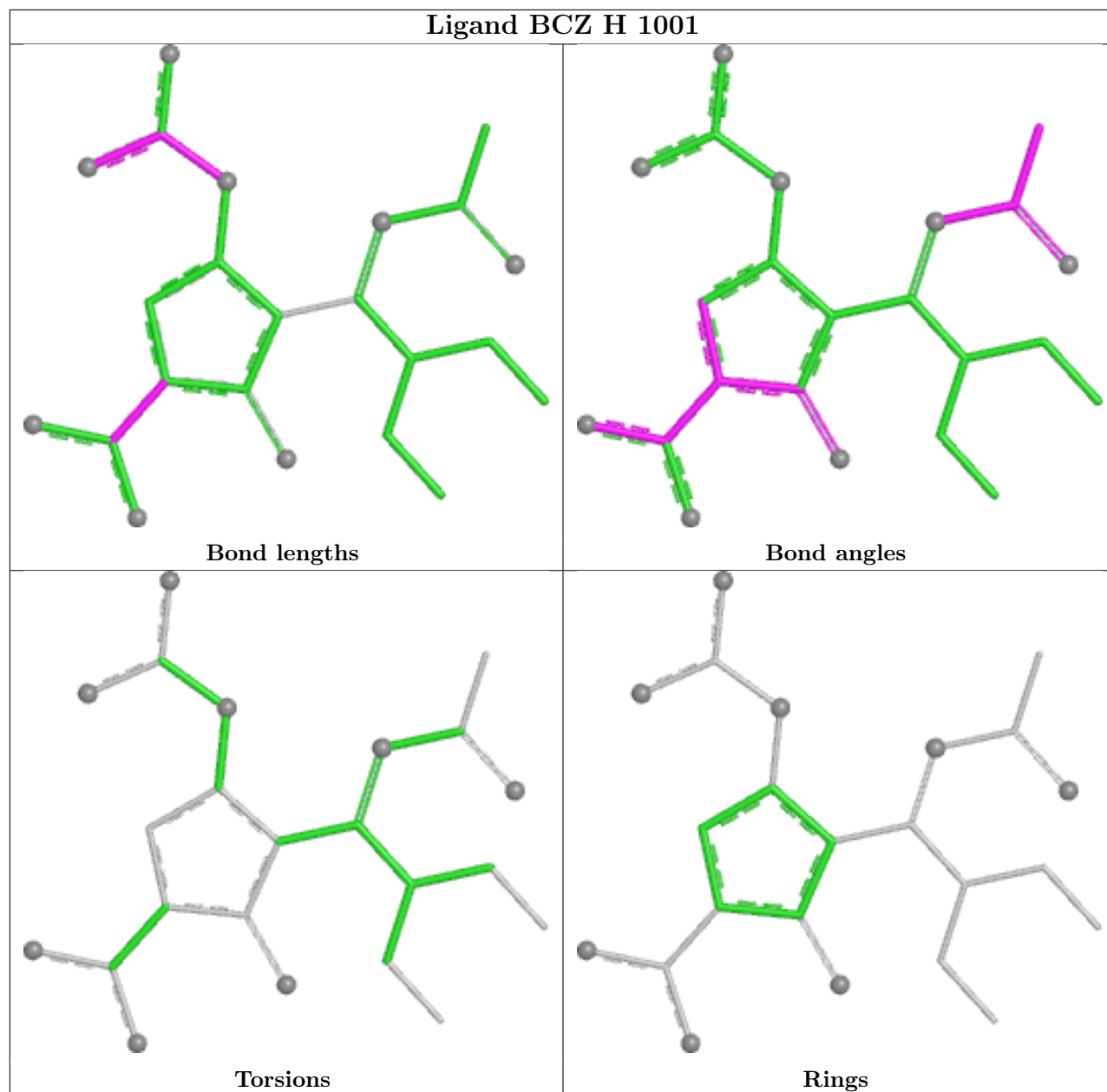


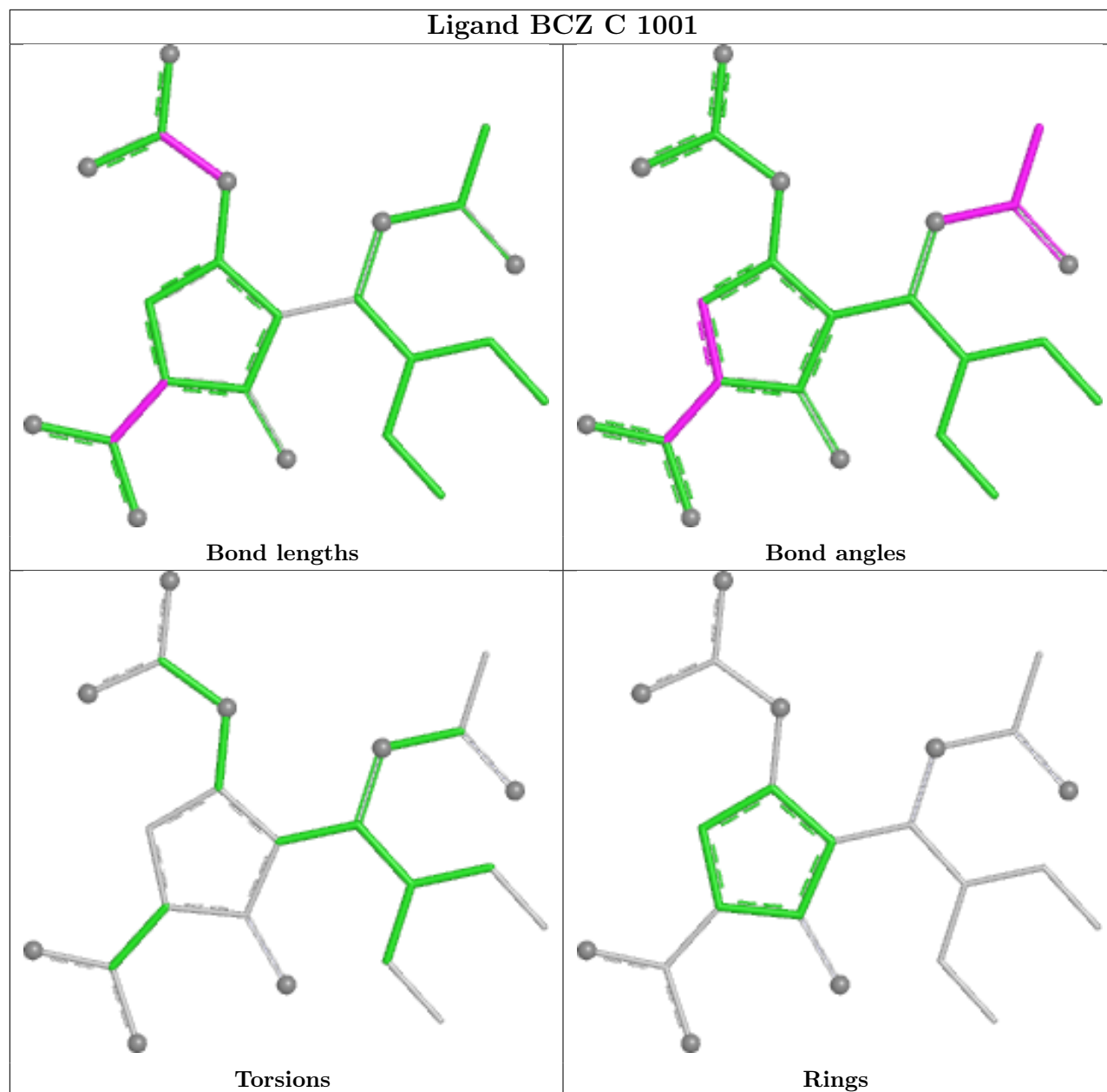


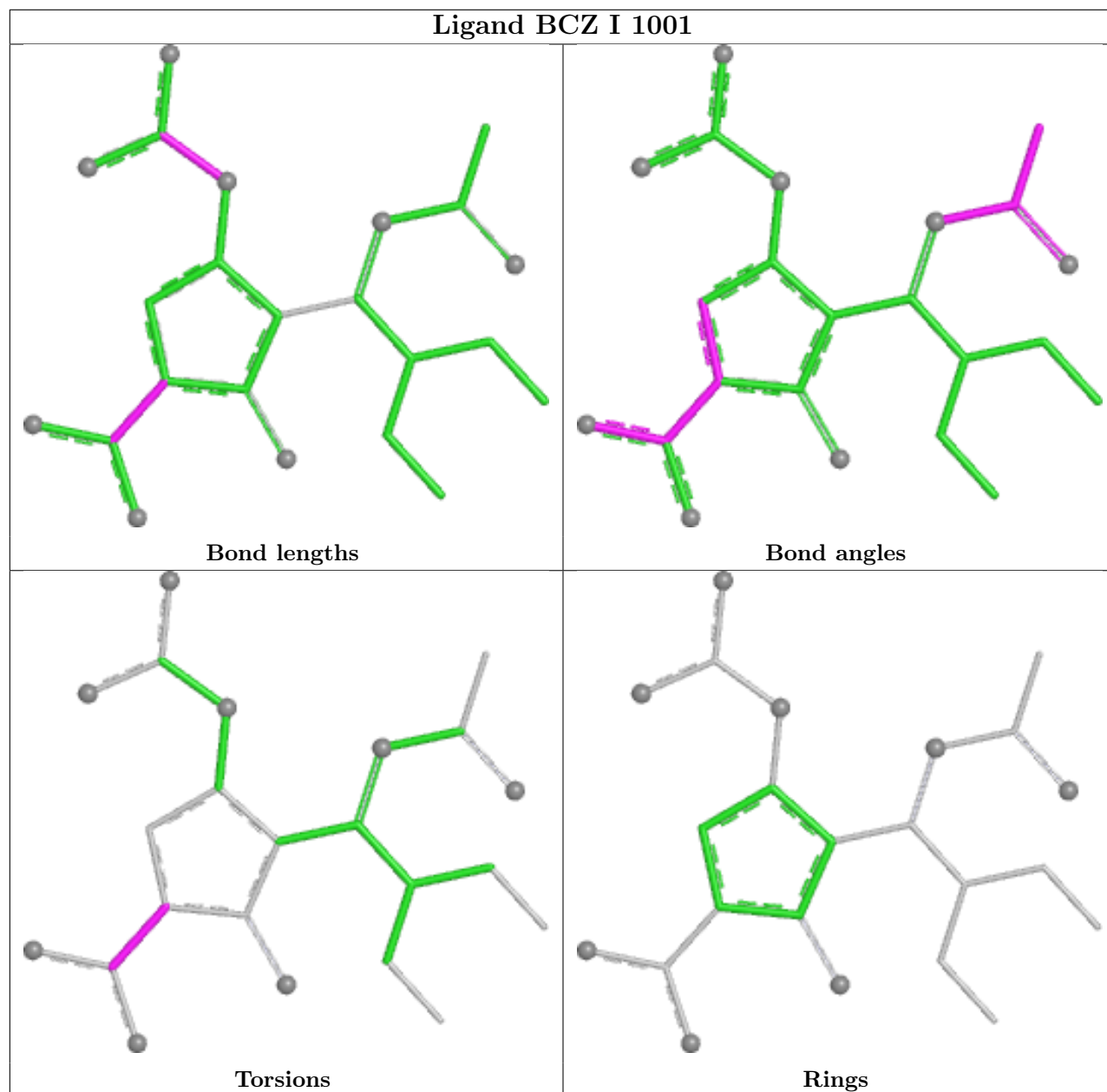


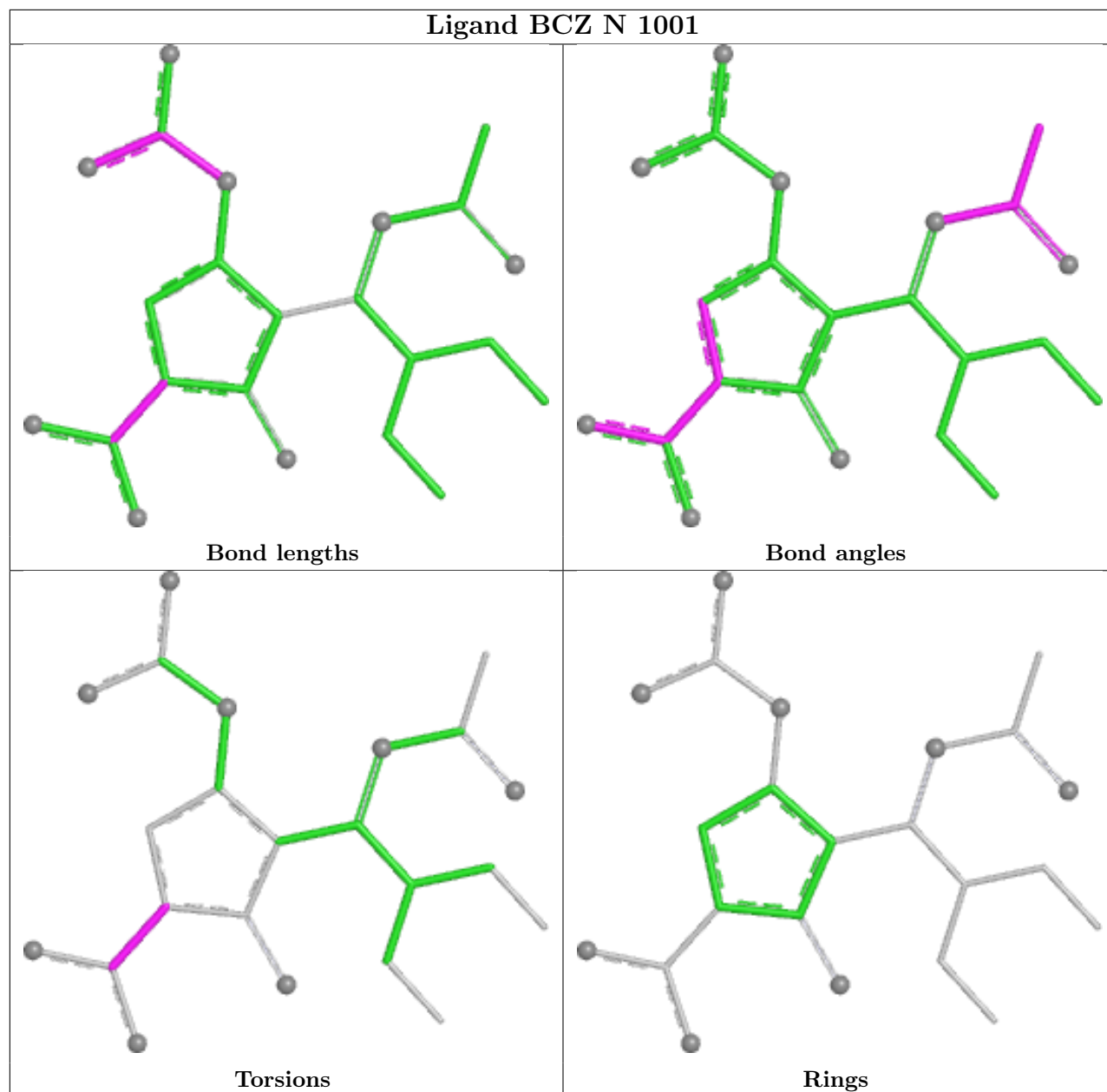


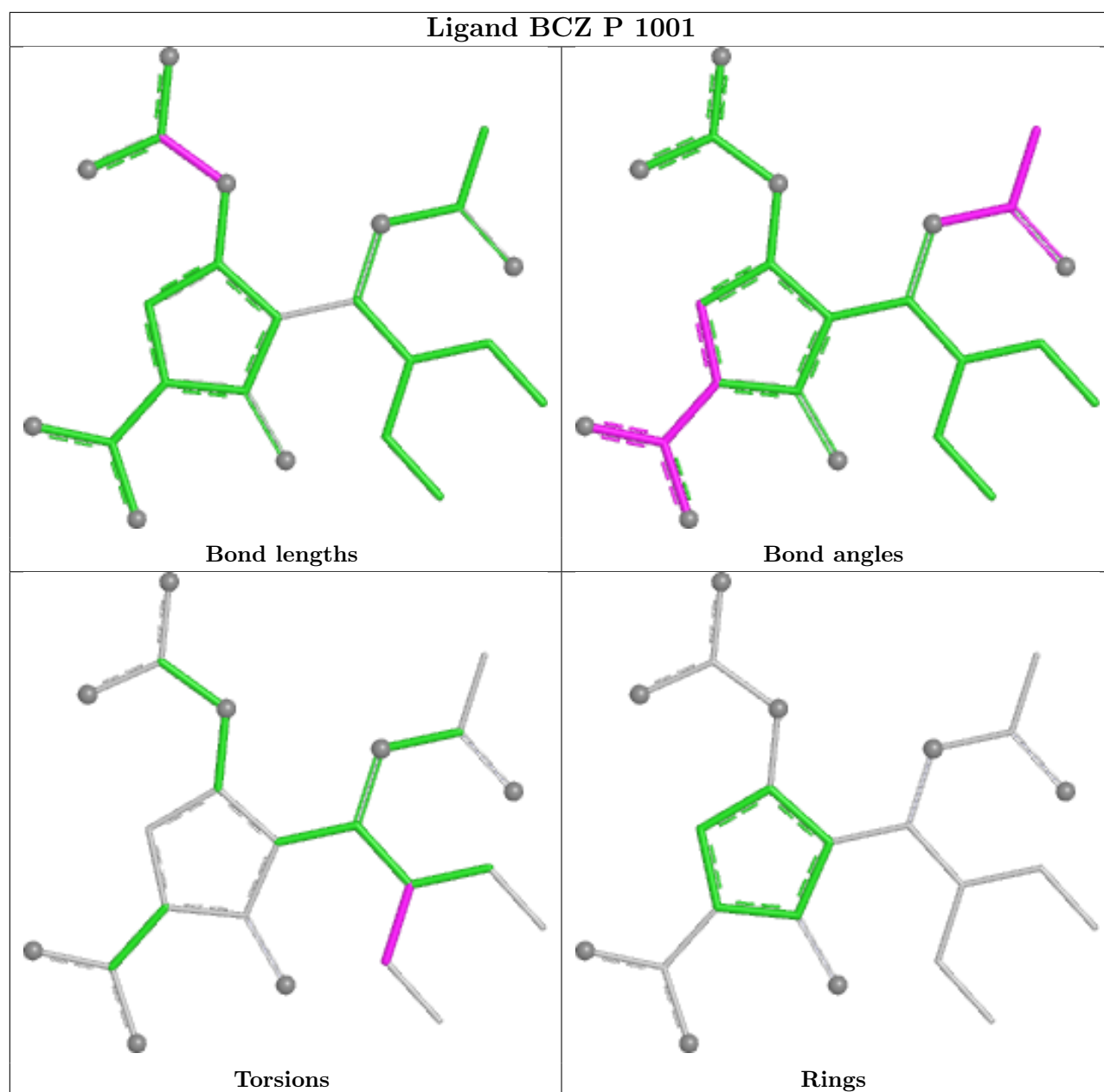


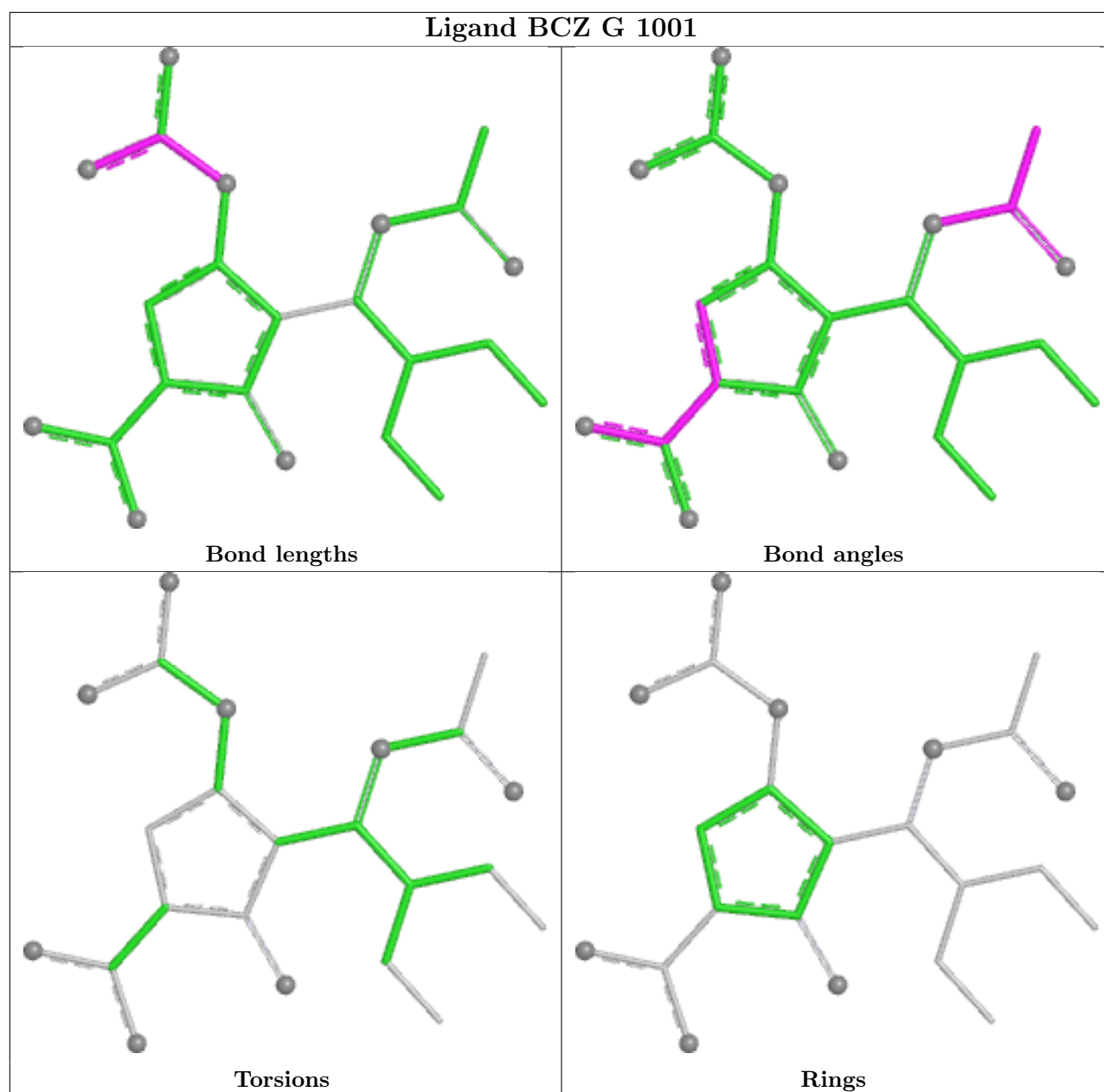












5.7 Other polymers [i](#)

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	389/397 (97%)	-1.62	0 100 100	9, 22, 30, 36	4 (1%)
1	B	389/397 (97%)	-1.62	0 100 100	9, 22, 30, 36	4 (1%)
1	C	389/397 (97%)	-1.62	0 100 100	9, 22, 30, 36	4 (1%)
1	D	389/397 (97%)	-1.63	0 100 100	9, 22, 30, 36	4 (1%)
1	E	389/397 (97%)	-1.60	0 100 100	9, 22, 30, 36	4 (1%)
1	F	389/397 (97%)	-1.57	0 100 100	9, 22, 30, 36	4 (1%)
1	G	389/397 (97%)	-1.60	0 100 100	9, 22, 30, 36	4 (1%)
1	H	389/397 (97%)	-1.61	0 100 100	9, 22, 30, 36	4 (1%)
1	I	389/397 (97%)	-1.63	0 100 100	9, 22, 30, 36	4 (1%)
1	J	389/397 (97%)	-1.62	0 100 100	9, 22, 30, 36	4 (1%)
1	K	389/397 (97%)	-1.63	0 100 100	9, 22, 30, 36	4 (1%)
1	L	389/397 (97%)	-1.62	0 100 100	9, 22, 30, 36	4 (1%)
1	M	389/397 (97%)	-1.60	0 100 100	9, 22, 30, 36	4 (1%)
1	N	389/397 (97%)	-1.59	0 100 100	9, 22, 30, 36	4 (1%)
1	O	389/397 (97%)	-1.60	0 100 100	9, 22, 30, 36	4 (1%)
1	P	389/397 (97%)	-1.60	0 100 100	9, 22, 30, 36	4 (1%)
All	All	6224/6352 (97%)	-1.61	0 100 100	9, 22, 30, 36	64 (1%)

There are no RSRZ outliers to report.

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
2	NAG	H	900	14/15	0.97	0.05	33,38,41,41	0
2	NAG	C	900	14/15	0.98	0.04	33,38,40,41	0
2	NAG	D	900	14/15	0.98	0.04	33,38,41,41	0
2	NAG	E	900	14/15	0.98	0.04	33,38,40,41	0
2	NAG	F	900	14/15	0.98	0.05	33,38,41,41	0
2	NAG	B	900	14/15	0.98	0.04	33,38,40,41	0
2	NAG	I	900	14/15	0.98	0.04	34,39,41,41	0
2	NAG	J	900	14/15	0.98	0.04	33,38,41,41	0
2	NAG	K	900	14/15	0.98	0.04	33,38,41,42	0
2	NAG	M	900	14/15	0.98	0.04	33,39,40,41	0
2	NAG	N	900	14/15	0.98	0.04	33,39,40,41	0
2	NAG	O	900	14/15	0.98	0.04	34,39,41,41	0
2	NAG	P	900	14/15	0.98	0.04	33,38,40,41	0
2	NAG	G	900	14/15	0.99	0.04	33,39,40,41	0
2	NAG	L	900	14/15	0.99	0.03	33,38,40,41	0
2	NAG	A	900	14/15	0.99	0.04	33,38,41,42	0
3	CA	A	1000	1/1	0.99	0.04	53,53,53,53	0
3	CA	C	1000	1/1	0.99	0.04	53,53,53,53	0
3	CA	D	1000	1/1	0.99	0.04	53,53,53,53	0
3	CA	E	1000	1/1	0.99	0.03	53,53,53,53	0
3	CA	F	1000	1/1	0.99	0.04	53,53,53,53	0
3	CA	G	1000	1/1	0.99	0.03	53,53,53,53	0
3	CA	H	1000	1/1	0.99	0.03	53,53,53,53	0
3	CA	I	1000	1/1	0.99	0.04	53,53,53,53	0
3	CA	J	1000	1/1	0.99	0.05	53,53,53,53	0
3	CA	K	1000	1/1	0.99	0.04	52,52,52,52	0
3	CA	L	1000	1/1	0.99	0.03	53,53,53,53	0
3	CA	M	1000	1/1	0.99	0.04	53,53,53,53	0
3	CA	N	1000	1/1	0.99	0.02	53,53,53,53	0
3	CA	O	1000	1/1	0.99	0.03	53,53,53,53	0
4	BCZ	A	1001	23/23	0.99	0.03	15,25,27,29	0
4	BCZ	B	1001	23/23	0.99	0.03	15,25,27,28	0

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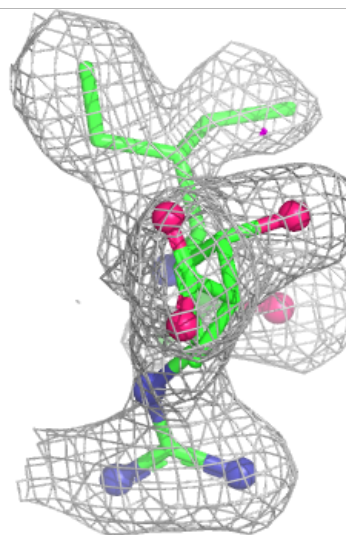
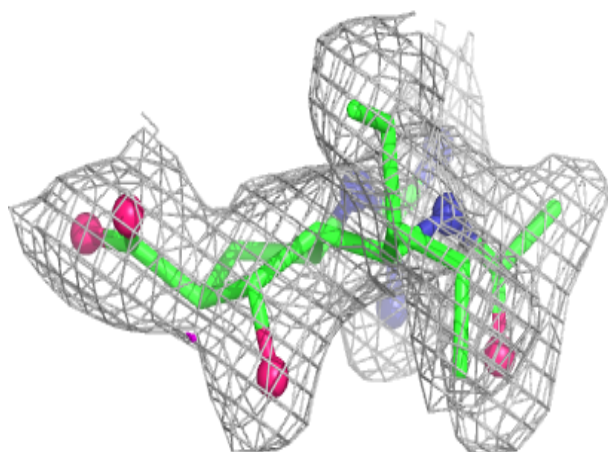
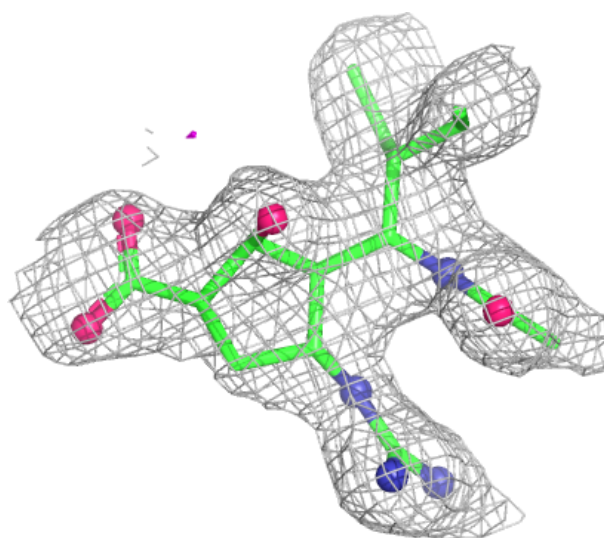
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	BCZ	C	1001	23/23	0.99	0.03	15,25,27,29	0
4	BCZ	D	1001	23/23	0.99	0.03	15,25,27,29	0
4	BCZ	E	1001	23/23	0.99	0.03	15,25,27,29	0
4	BCZ	G	1001	23/23	0.99	0.03	15,25,27,29	0
4	BCZ	H	1001	23/23	0.99	0.03	15,25,27,29	0
4	BCZ	I	1001	23/23	0.99	0.03	15,25,27,29	0
4	BCZ	J	1001	23/23	0.99	0.03	15,25,27,29	0
4	BCZ	L	1001	23/23	0.99	0.03	15,25,27,28	0
4	BCZ	M	1001	23/23	0.99	0.03	15,25,27,29	0
4	BCZ	N	1001	23/23	0.99	0.03	15,25,27,29	0
4	BCZ	O	1001	23/23	0.99	0.03	15,25,27,29	0
4	BCZ	P	1001	23/23	0.99	0.03	15,25,27,29	0
4	BCZ	F	1001	23/23	1.00	0.02	15,25,27,29	0
3	CA	P	1000	1/1	1.00	0.02	53,53,53,53	0
4	BCZ	K	1001	23/23	1.00	0.03	15,25,27,28	0
3	CA	B	1000	1/1	1.00	0.03	53,53,53,53	0
5	YT3	A	1	1/1	1.00	0.01	28,28,28,28	0
5	YT3	E	2	1/1	1.00	0.01	28,28,28,28	0
5	YT3	I	3	1/1	1.00	0.01	29,29,29,29	0
5	YT3	M	4	1/1	1.00	0.01	30,30,30,30	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.

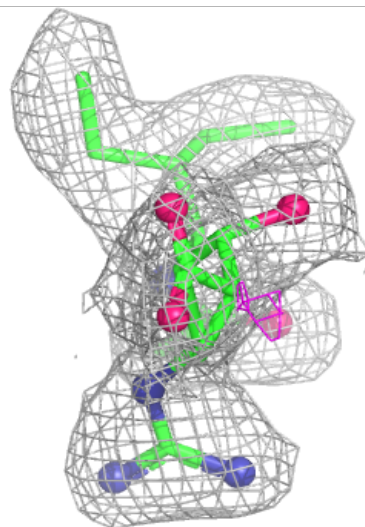
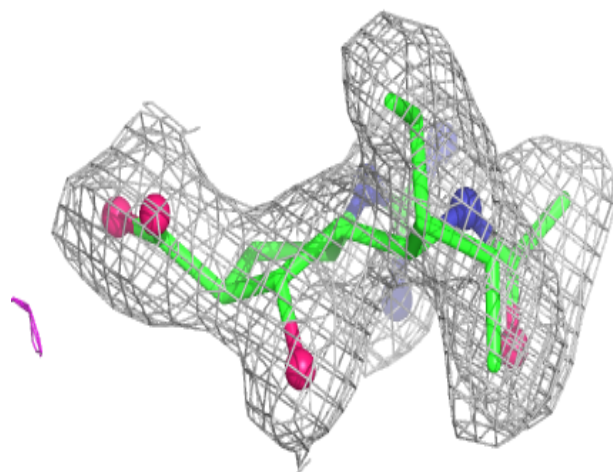
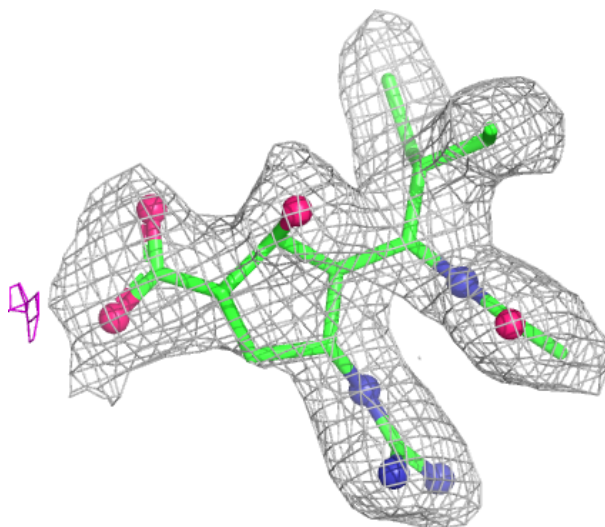
Electron density around BCZ A 1001:

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



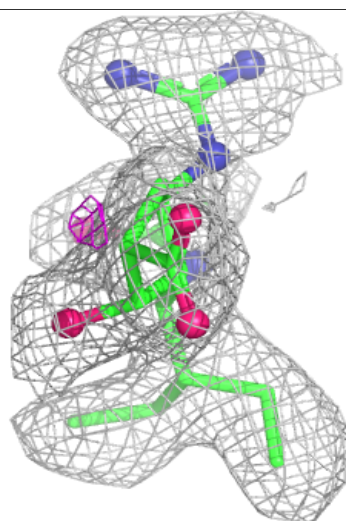
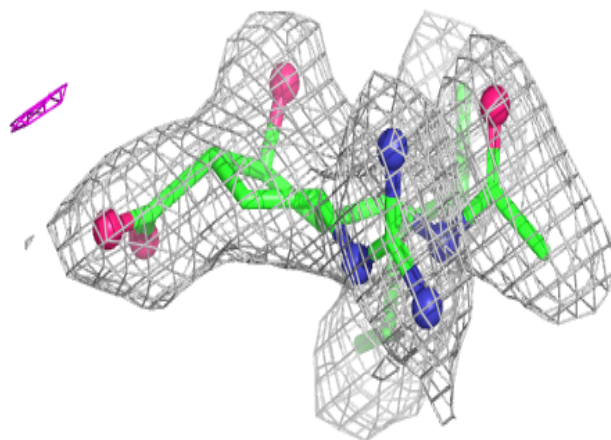
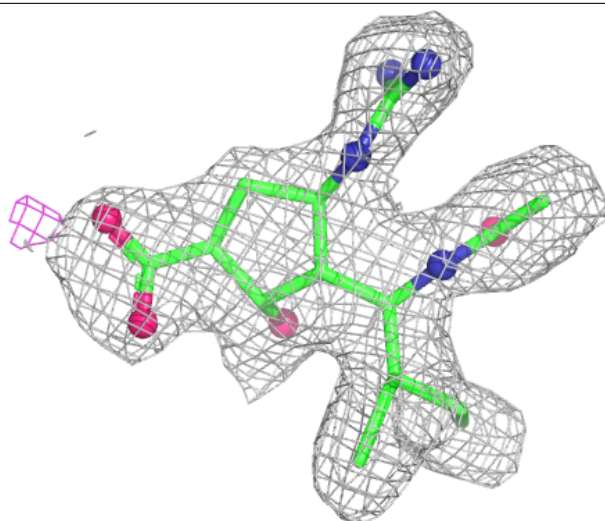
Electron density around BCZ B 1001:

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and green (positive)



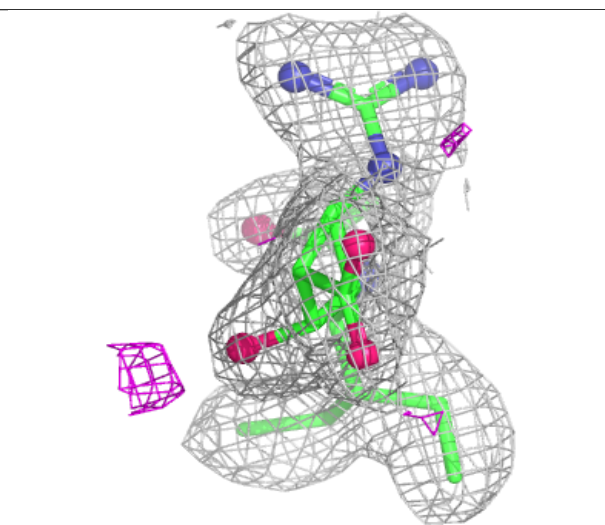
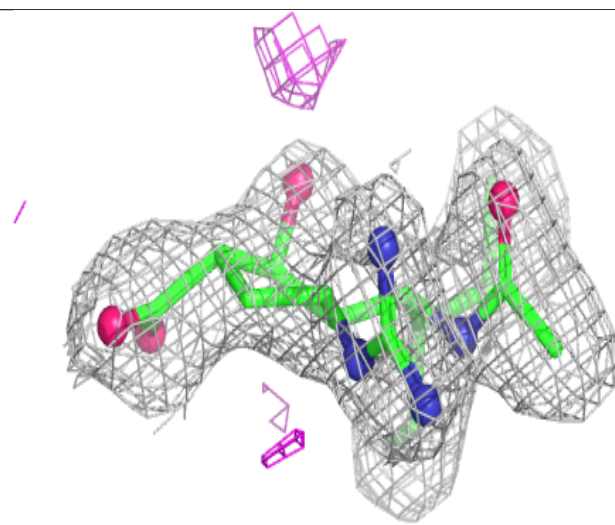
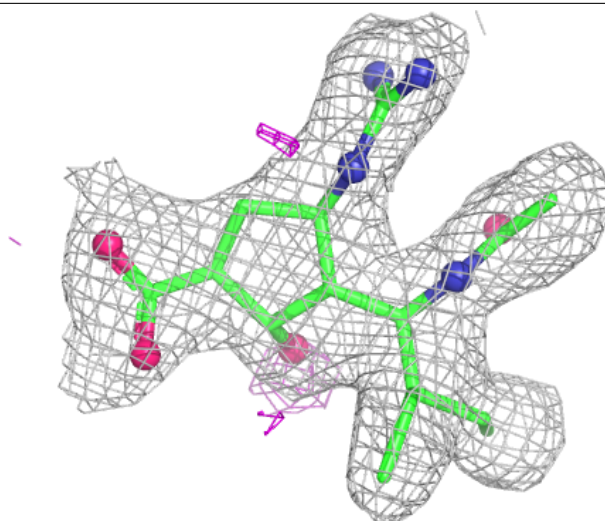
Electron density around BCZ C 1001:

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



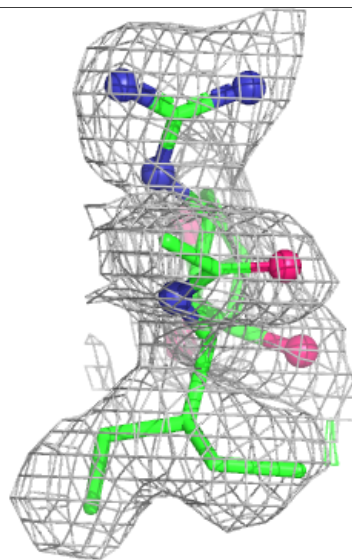
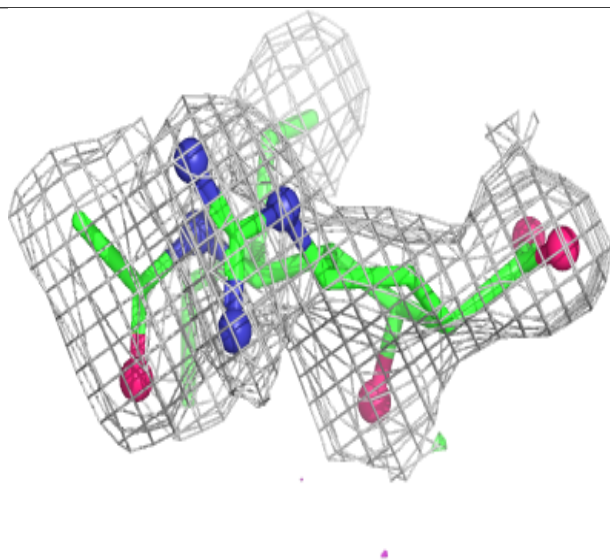
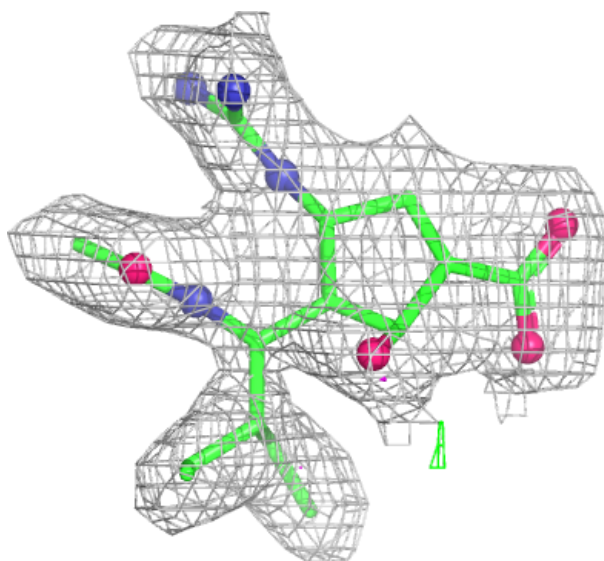
Electron density around BCZ D 1001:

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



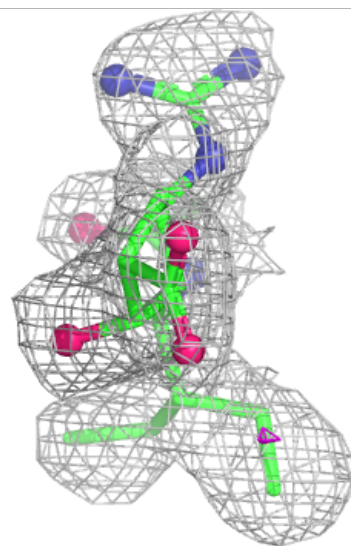
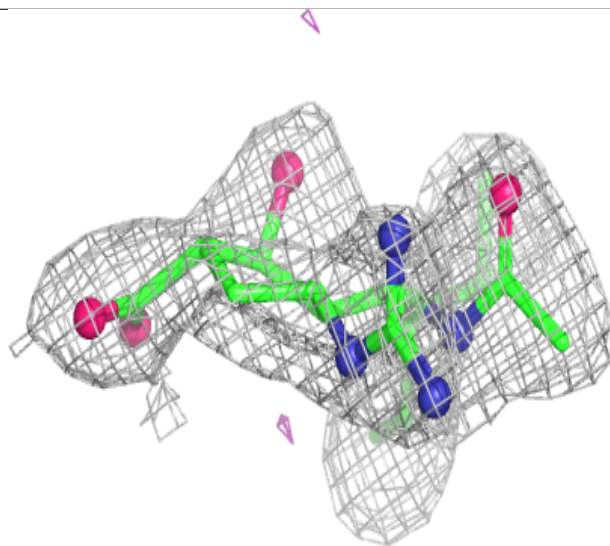
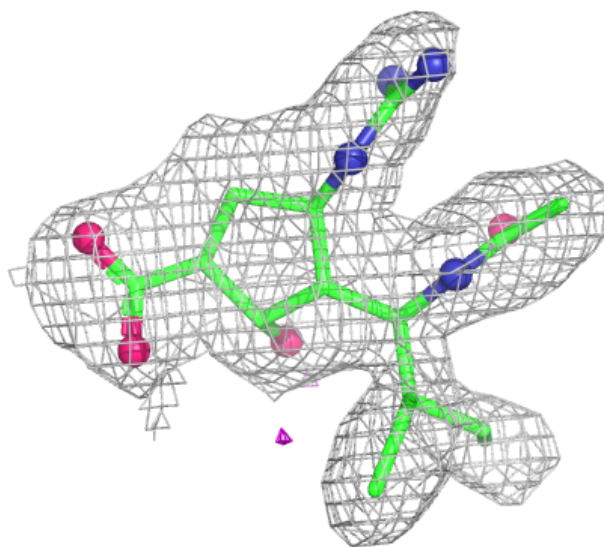
Electron density around BCZ E 1001:

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



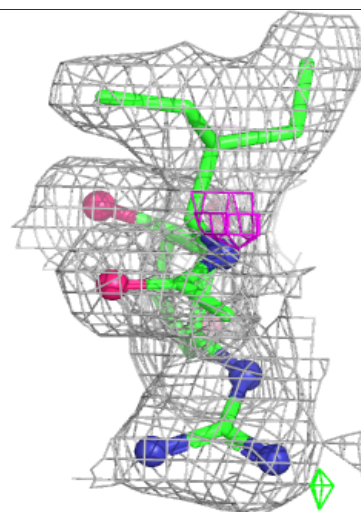
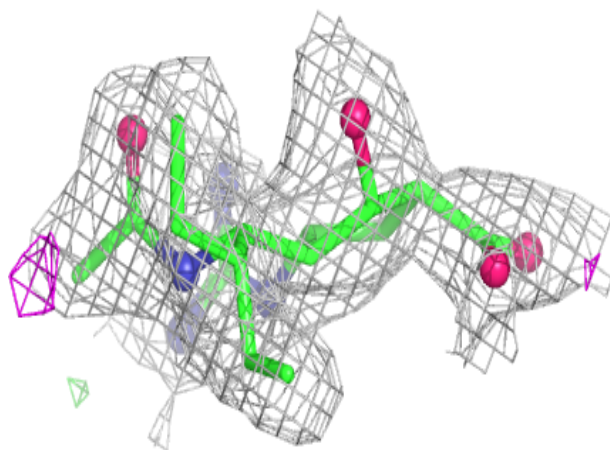
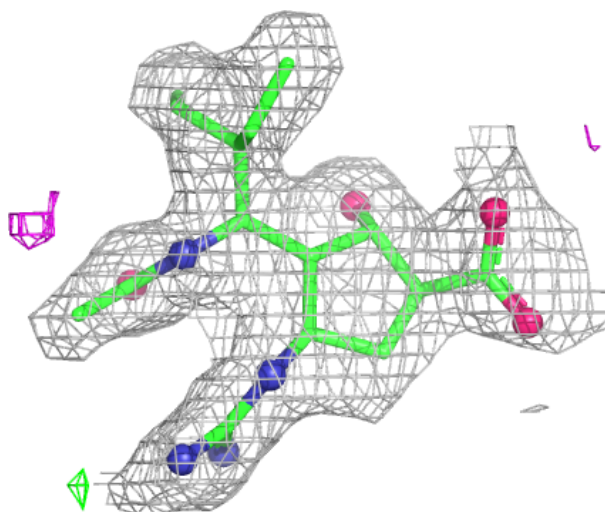
Electron density around BCZ G 1001:

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



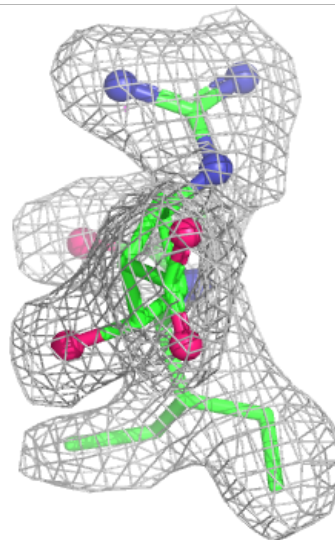
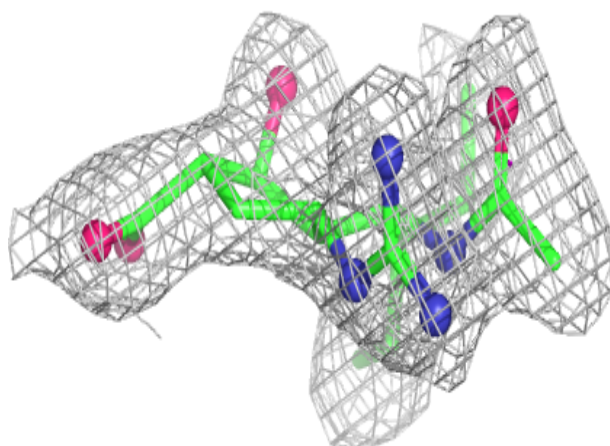
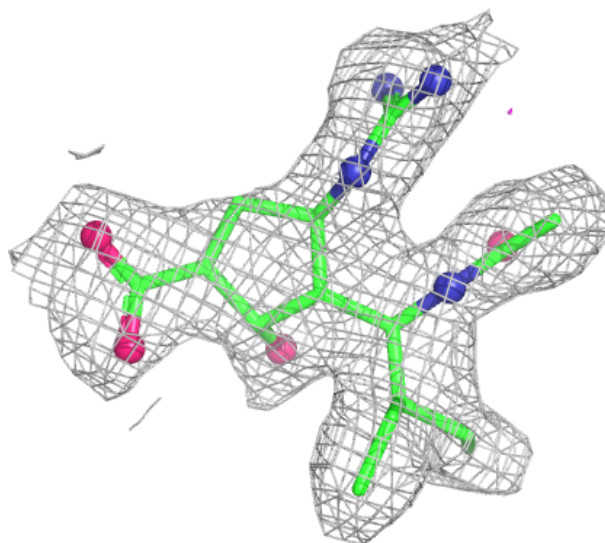
Electron density around BCZ H 1001:

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



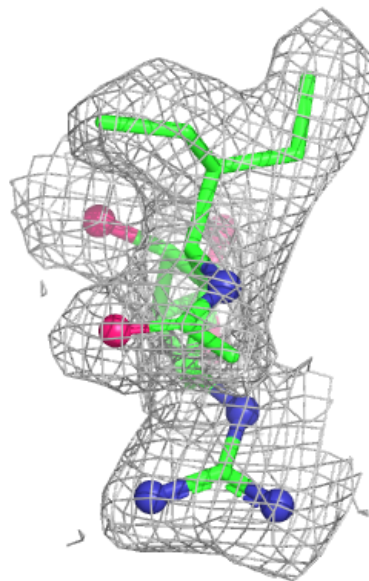
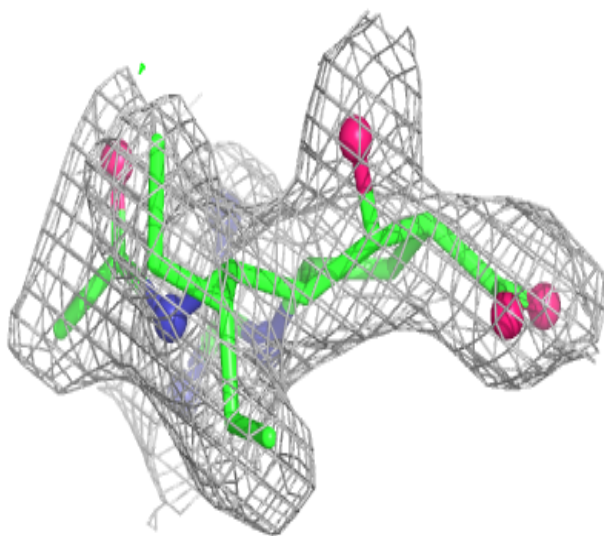
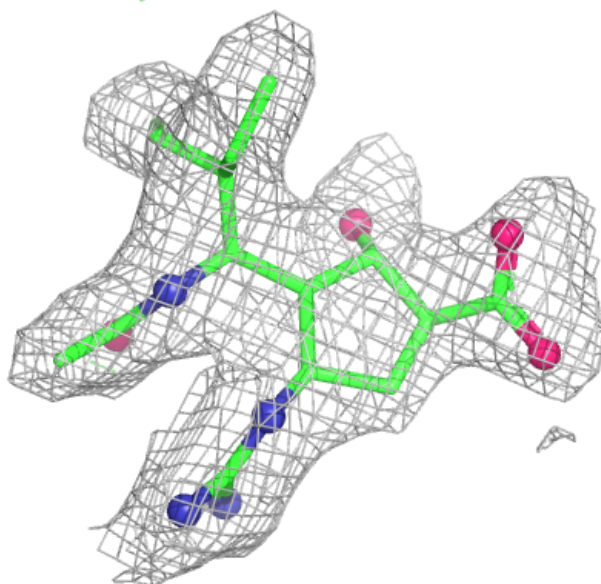
Electron density around BCZ I 1001:

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



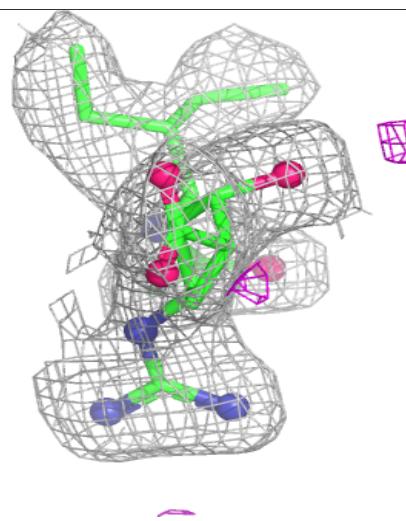
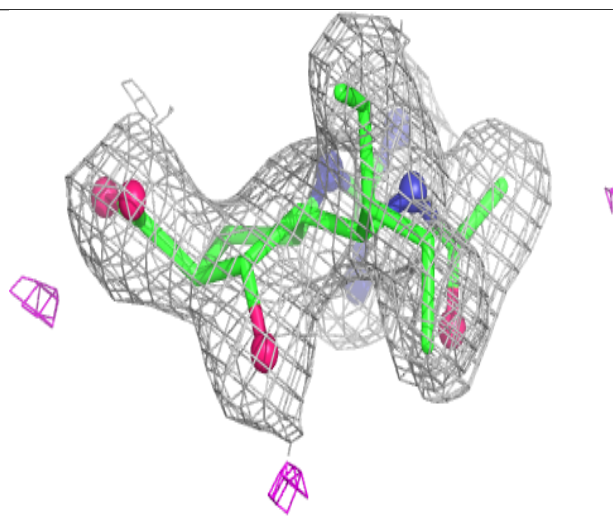
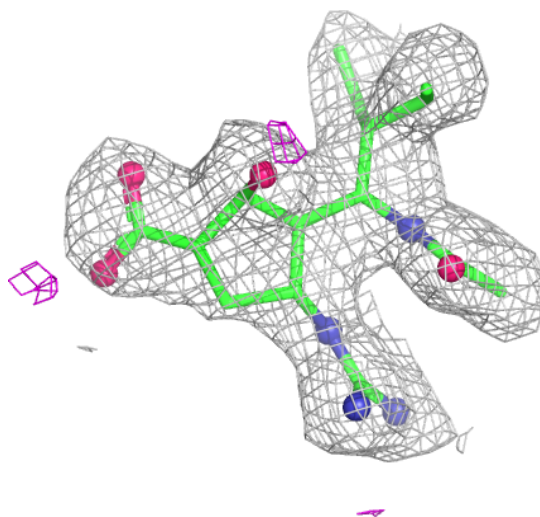
Electron density around BCZ J 1001:

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



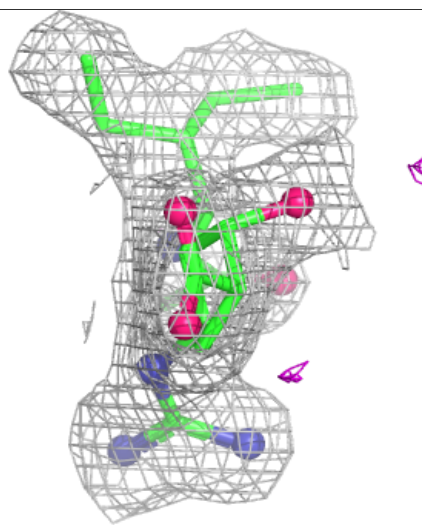
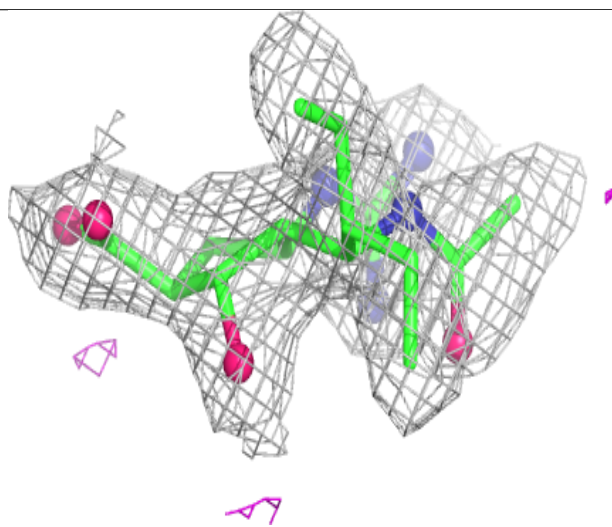
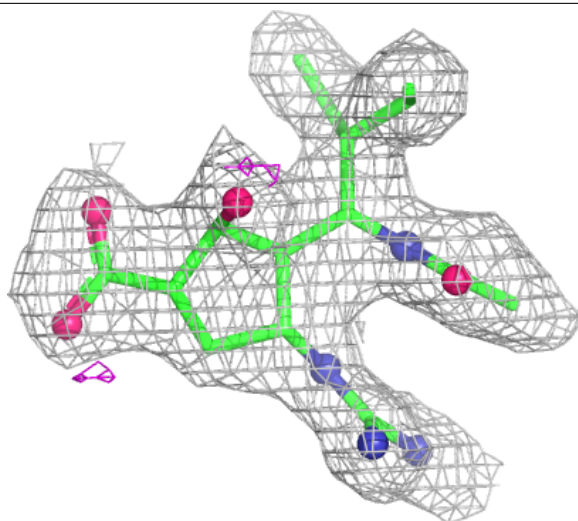
Electron density around BCZ L 1001:

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



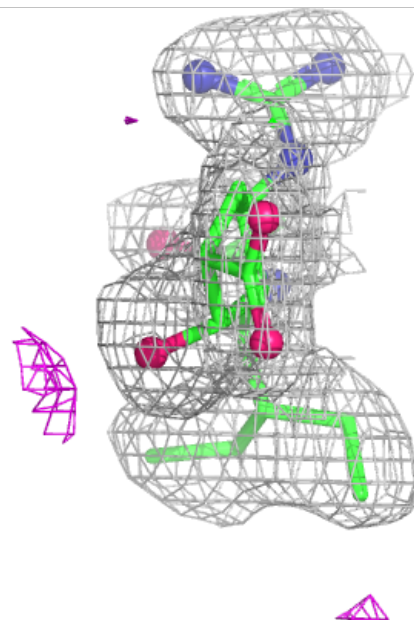
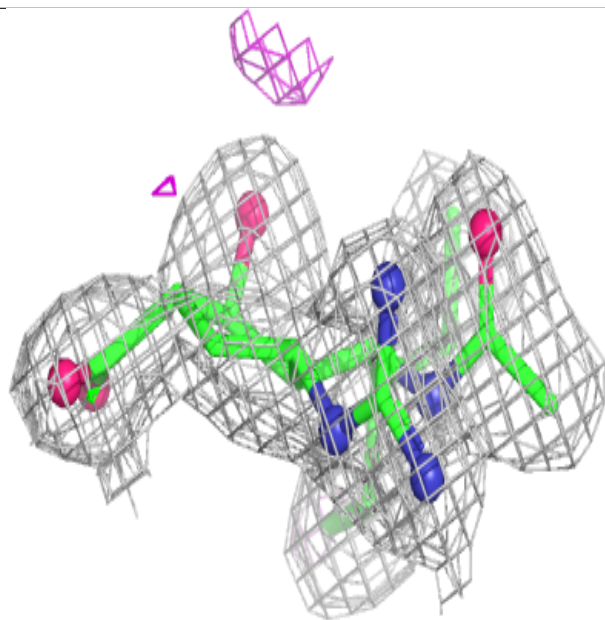
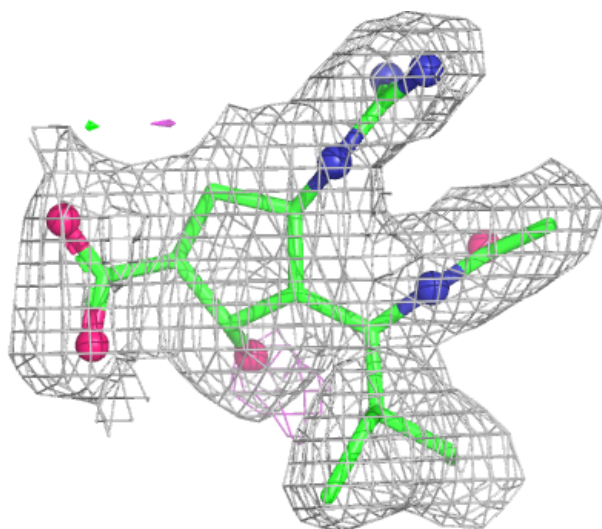
Electron density around BCZ M 1001:

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



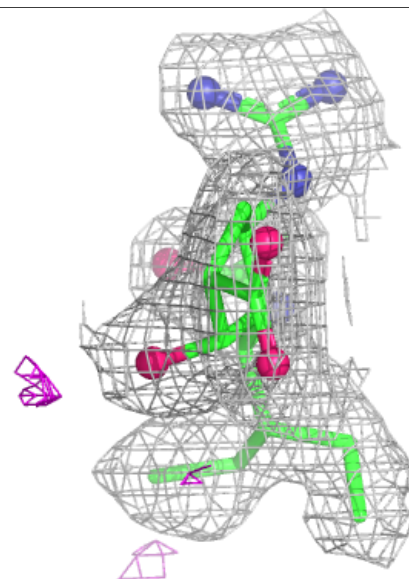
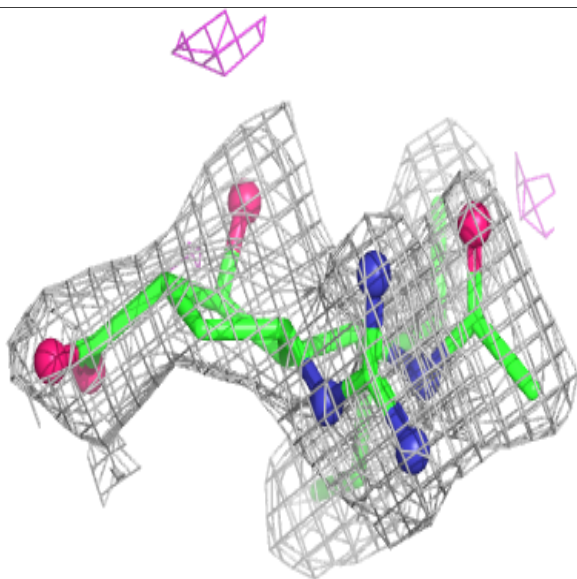
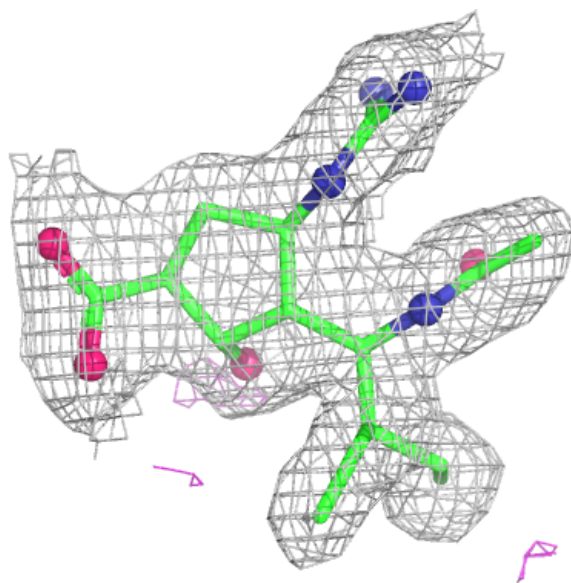
Electron density around BCZ N 1001:

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



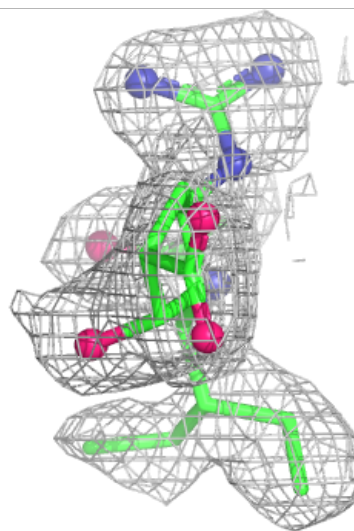
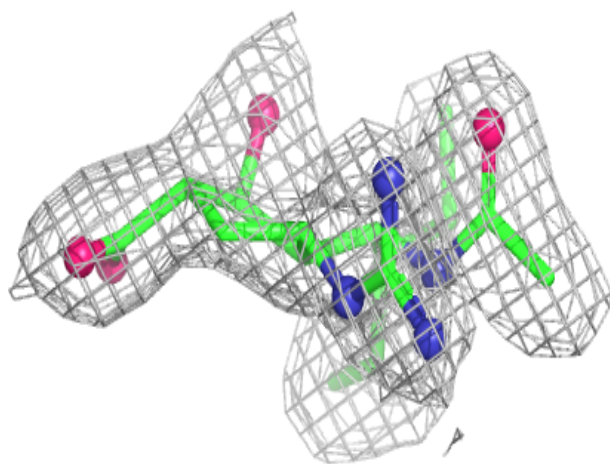
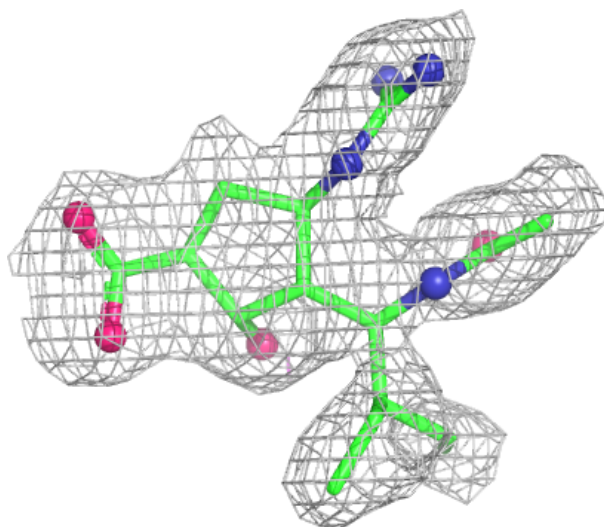
Electron density around BCZ O 1001:

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



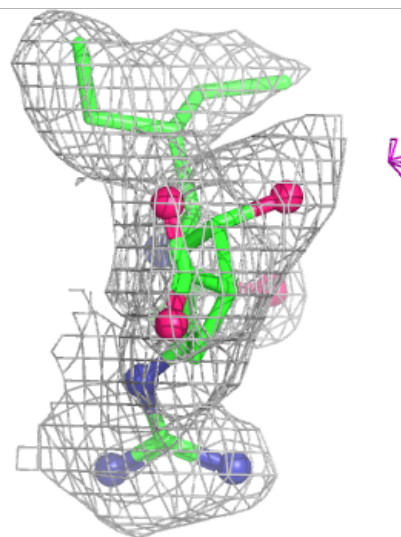
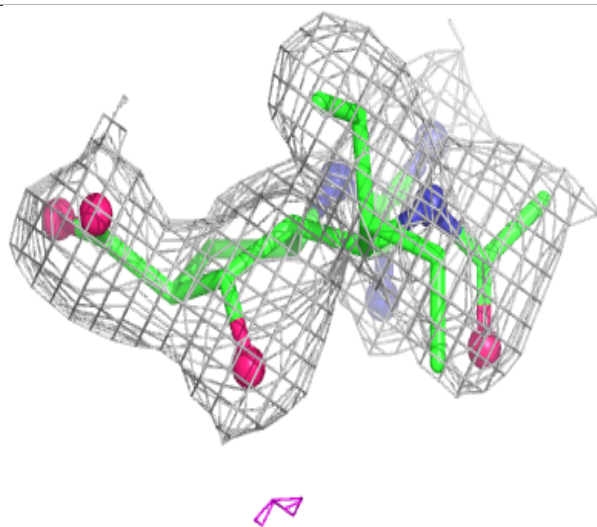
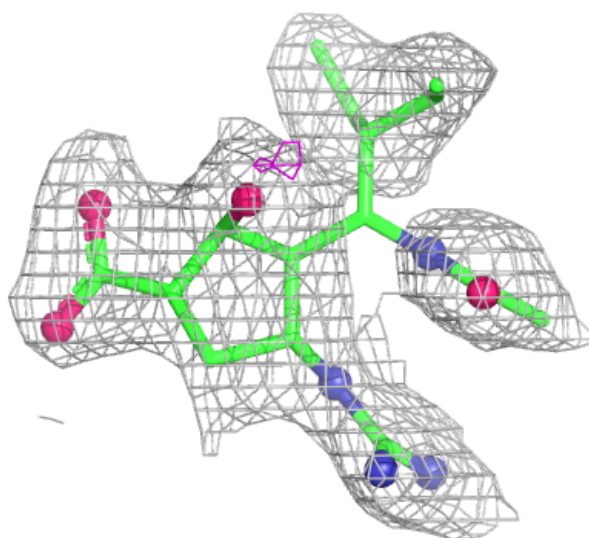
Electron density around BCZ P 1001:

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



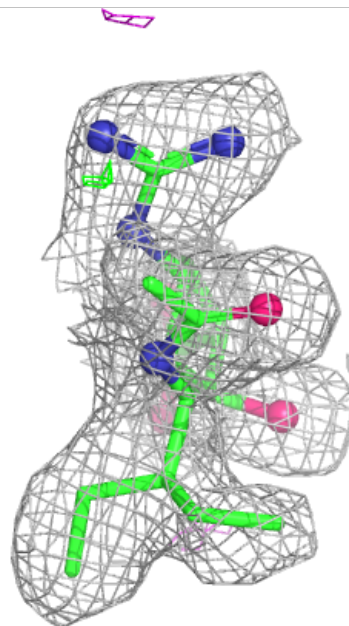
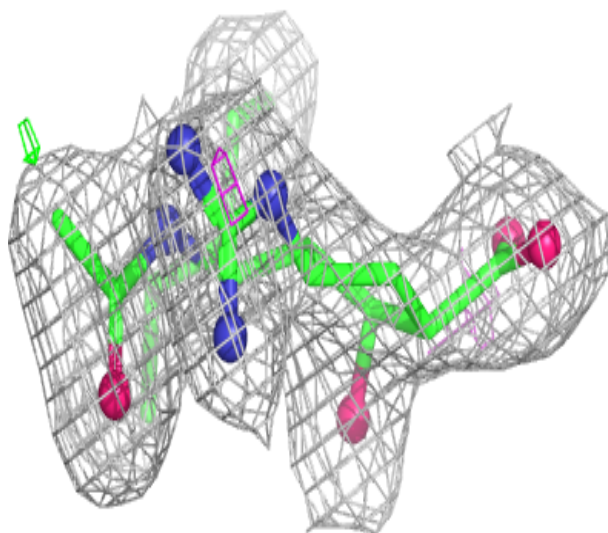
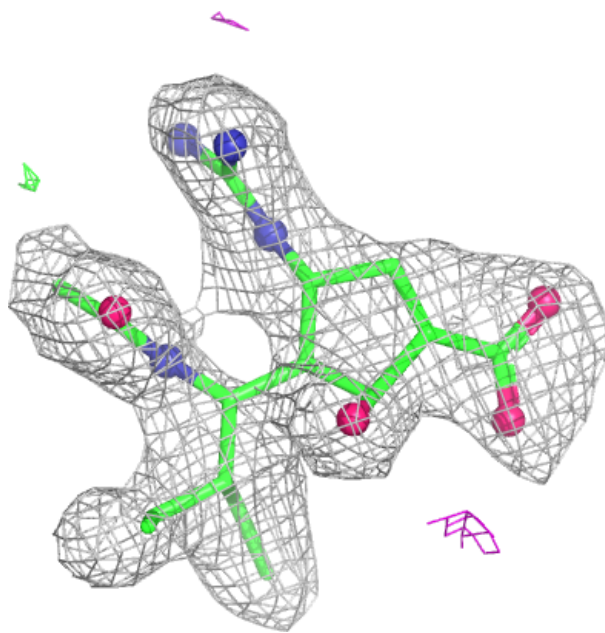
Electron density around BCZ F 1001:

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



Electron density around BCZ 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)



6.5 Other polymers ⓘ

There are no such residues in this entry.