



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 03:27 AM UTC

PDB ID : 3K3A / pdb_00003k3a
Title : Crystal Structure of B/Perth Neuraminidase D197E mutant in complex with Oseltamivir
Authors : Oakley, A.J.; McKimm-Breschkin, J.L.
Deposited on : 2009-10-02
Resolution : 2.59 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

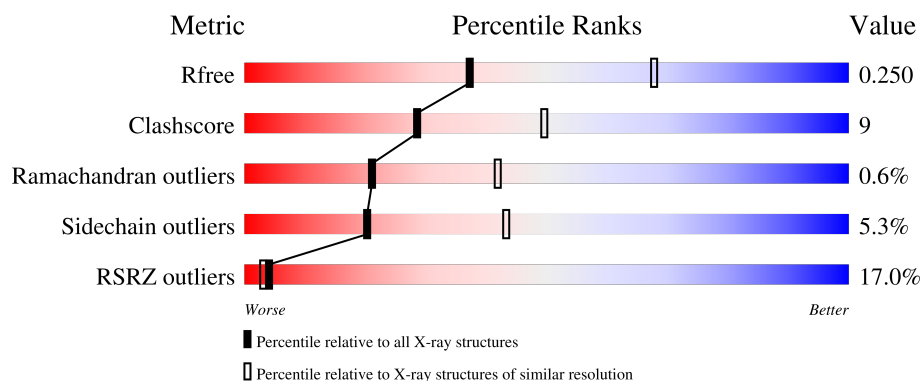
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.59 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	16% 79% 18% ..
1	B	397	17% 78% 18% ..
1	C	397	15% 79% 18% ..
1	D	397	18% 74% 23% ..
1	E	397	17% 74% 22% ..

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Mol	Chain	Length	Quality of chain
1	F	397	
1	G	397	
1	H	397	
1	I	397	
1	J	397	
1	K	397	
1	L	397	
1	M	397	
1	N	397	
1	O	397	
1	P	397	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 49183 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.

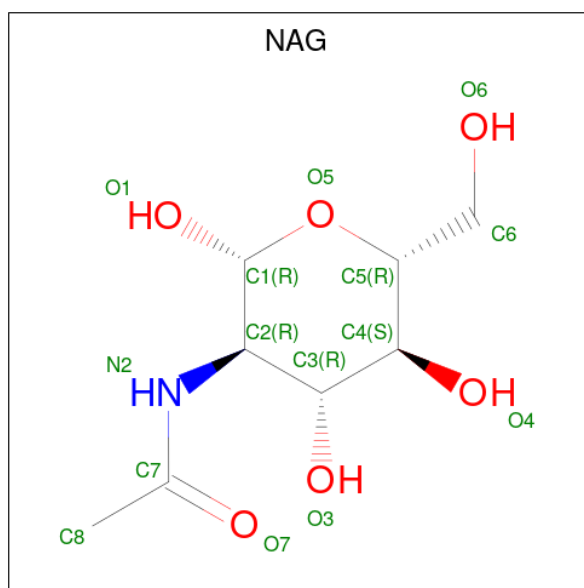
- Molecule 1 is a protein called Neuraminidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	389	Total	C	N	O	S	0	0	0
			2999	1882	519	569	29			
1	B	389	Total	C	N	O	S	0	0	0
			2999	1882	519	569	29			
1	C	389	Total	C	N	O	S	0	0	0
			2999	1882	519	569	29			
1	D	389	Total	C	N	O	S	0	0	0
			2999	1882	519	569	29			
1	E	389	Total	C	N	O	S	0	0	0
			2999	1882	519	569	29			
1	F	389	Total	C	N	O	S	0	0	0
			2999	1882	519	569	29			
1	G	389	Total	C	N	O	S	0	0	0
			2999	1882	519	569	29			
1	H	389	Total	C	N	O	S	0	0	0
			2999	1882	519	569	29			
1	I	389	Total	C	N	O	S	0	0	0
			2999	1882	519	569	29			
1	J	389	Total	C	N	O	S	0	0	0
			2999	1882	519	569	29			
1	K	389	Total	C	N	O	S	0	0	0
			2999	1882	519	569	29			
1	L	389	Total	C	N	O	S	0	0	0
			2999	1882	519	569	29			
1	M	389	Total	C	N	O	S	0	0	0
			2999	1882	519	569	29			
1	N	389	Total	C	N	O	S	0	0	0
			2999	1882	519	569	29			
1	O	389	Total	C	N	O	S	0	0	0
			2999	1882	519	569	29			
1	P	389	Total	C	N	O	S	0	0	0
			2999	1882	519	569	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).

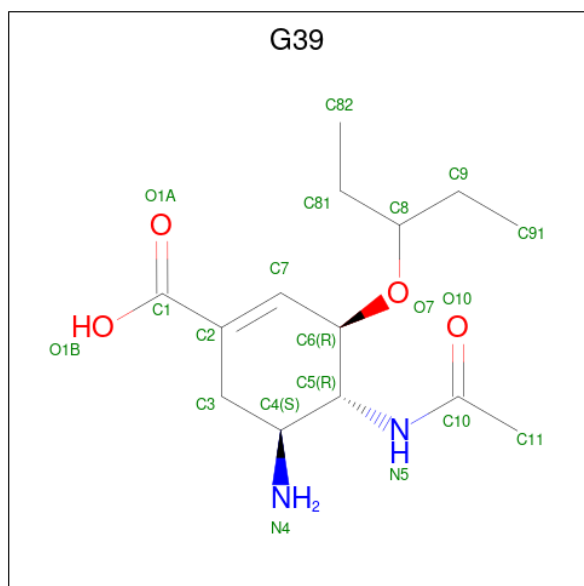
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ca	0	0
			1	1		
3	B	1	Total	Ca	0	0
			1	1		
3	C	1	Total	Ca	0	0
			1	1		
3	D	1	Total	Ca	0	0
			1	1		
3	E	1	Total	Ca	0	0
			1	1		

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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 (3R,4R,5S)-4-(acetylamino)-5-amino-3-(pentan-3-yloxy)cyclohex-1-ene-1-carboxylic acid (CCD ID: G39) (formula: C₁₄H₂₄N₂O₄).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 20 14 2 4	0	0
4	B	1	Total C N O 20 14 2 4	0	0
4	C	1	Total C N O 20 14 2 4	0	0
4	D	1	Total C N O 20 14 2 4	0	0
4	E	1	Total C N O 20 14 2 4	0	0
4	F	1	Total C N O 20 14 2 4	0	0
4	G	1	Total C N O 20 14 2 4	0	0
4	H	1	Total C N O 20 14 2 4	0	0
4	I	1	Total C N O 20 14 2 4	0	0
4	J	1	Total C N O 20 14 2 4	0	0
4	K	1	Total C N O 20 14 2 4	0	0
4	L	1	Total C N O 20 14 2 4	0	0
4	M	1	Total C N O 20 14 2 4	0	0
4	N	1	Total C N O 20 14 2 4	0	0
4	O	1	Total C N O 20 14 2 4	0	0
4	P	1	Total C N O 20 14 2 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	J	1	Total Y 1 1	0	0
5	P	1	Total Y 1 1	0	0

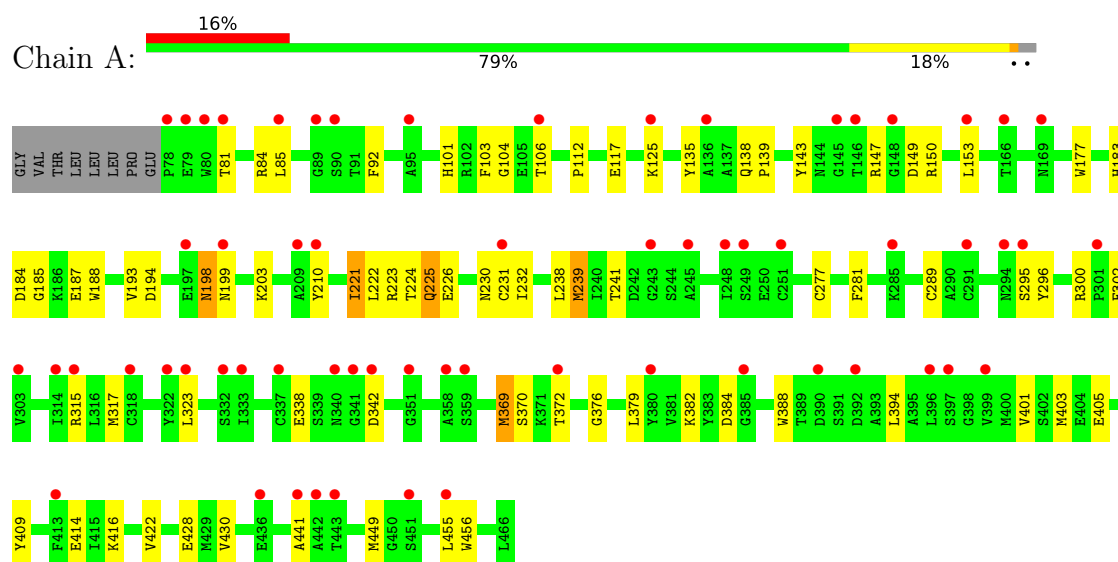
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	43	Total O 43 43	0	0
6	B	40	Total O 40 40	0	0
6	C	40	Total O 40 40	0	0
6	D	37	Total O 37 37	0	0
6	E	42	Total O 42 42	0	0
6	F	36	Total O 36 36	0	0
6	G	42	Total O 42 42	0	0
6	H	37	Total O 37 37	0	0
6	I	43	Total O 43 43	0	0
6	J	37	Total O 37 37	0	0
6	K	42	Total O 42 42	0	0
6	L	38	Total O 38 38	0	0
6	M	40	Total O 40 40	0	0
6	N	42	Total O 42 42	0	0
6	O	39	Total O 39 39	0	0
6	P	37	Total O 37 37	0	0

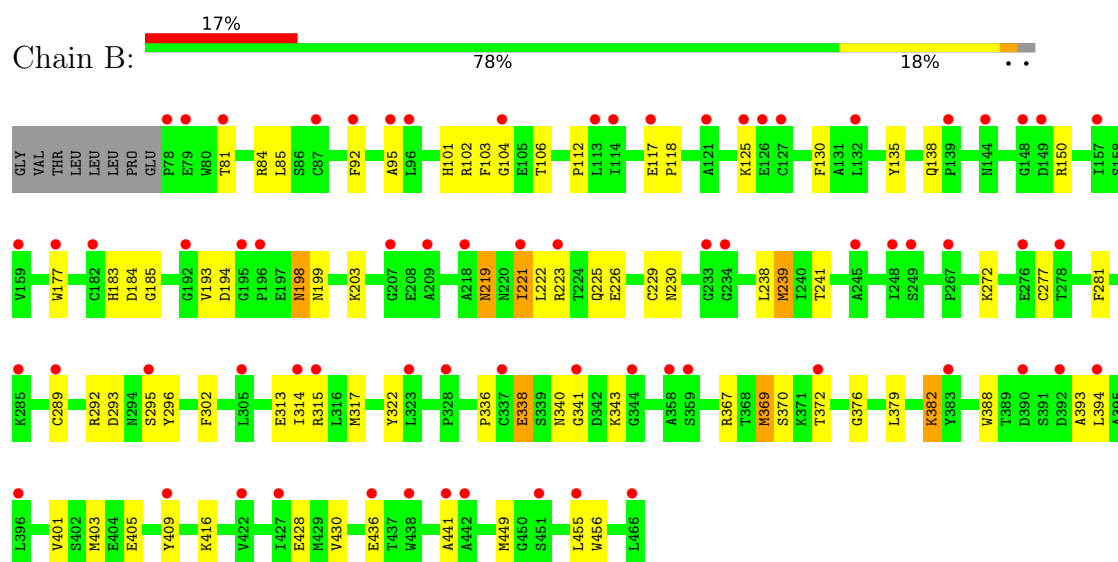
3 Residue-property plots [i](#)

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

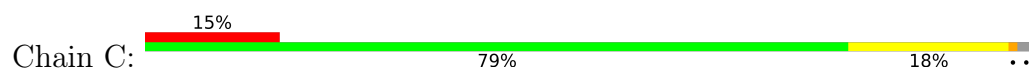
• Molecule 1: Neuraminidase

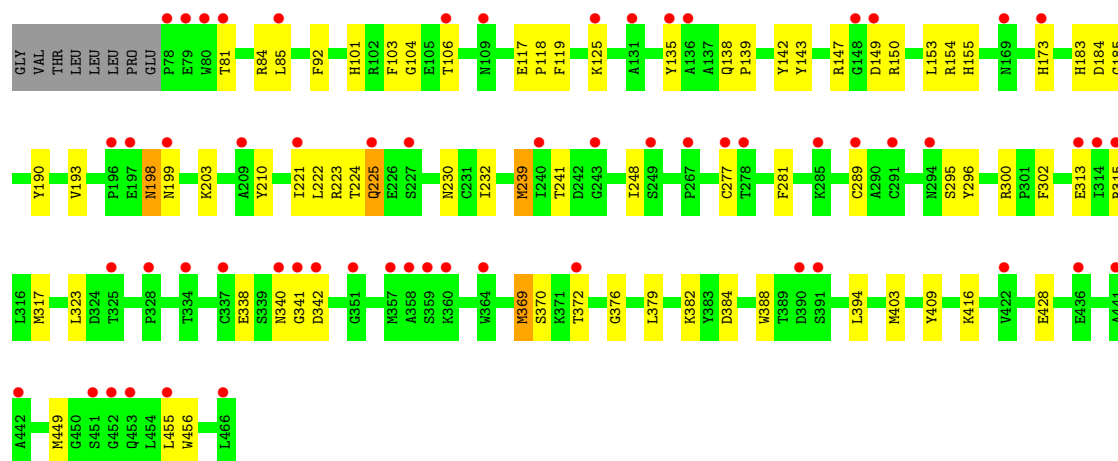


• Molecule 1: Neuraminidase

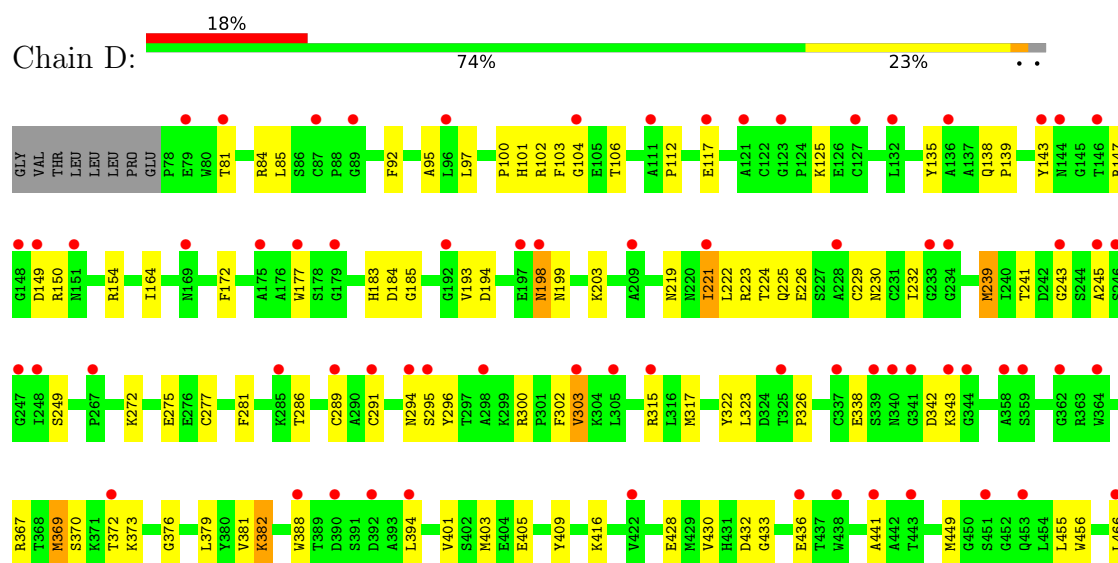


• Molecule 1: Neuraminidase

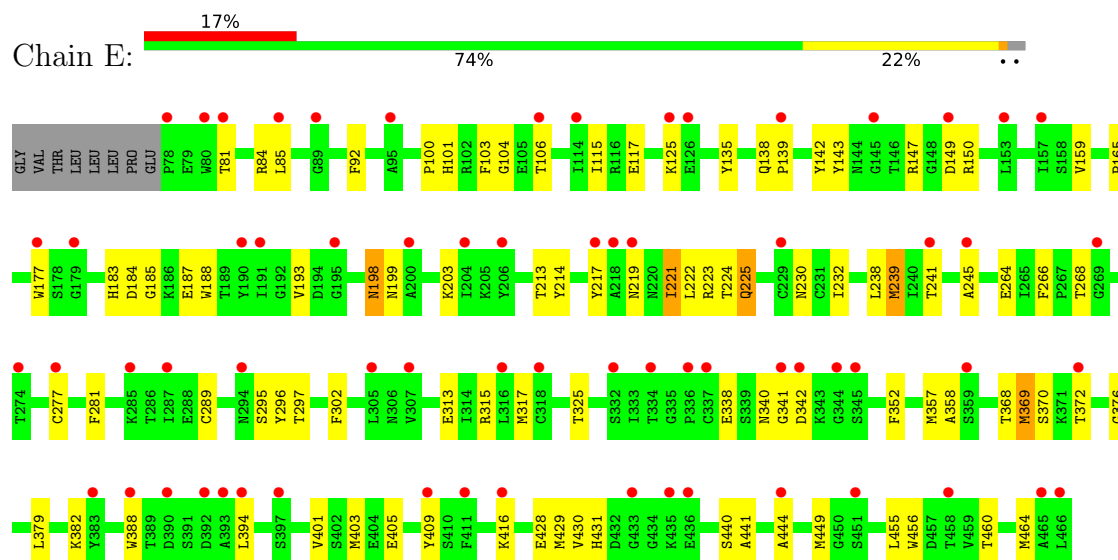




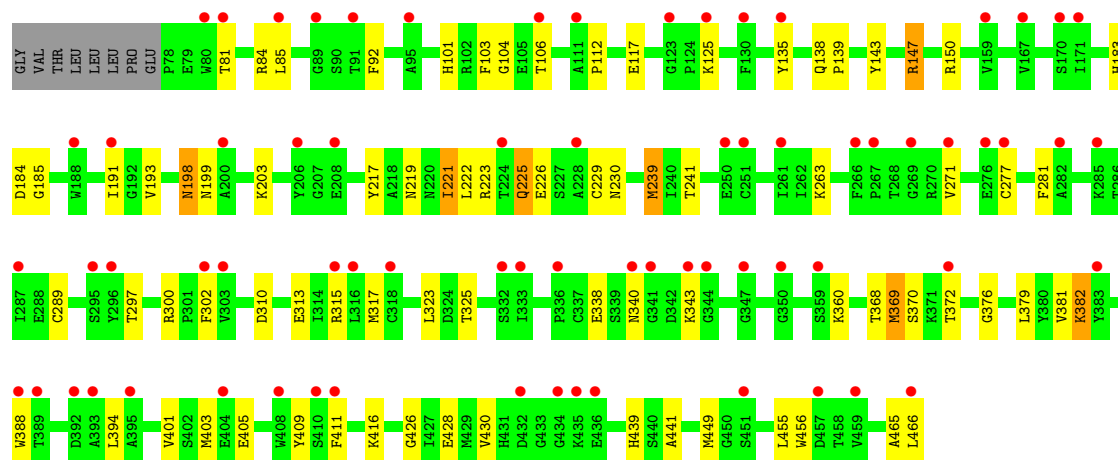
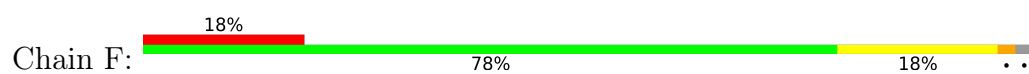
• Molecule 1: Neuraminidase



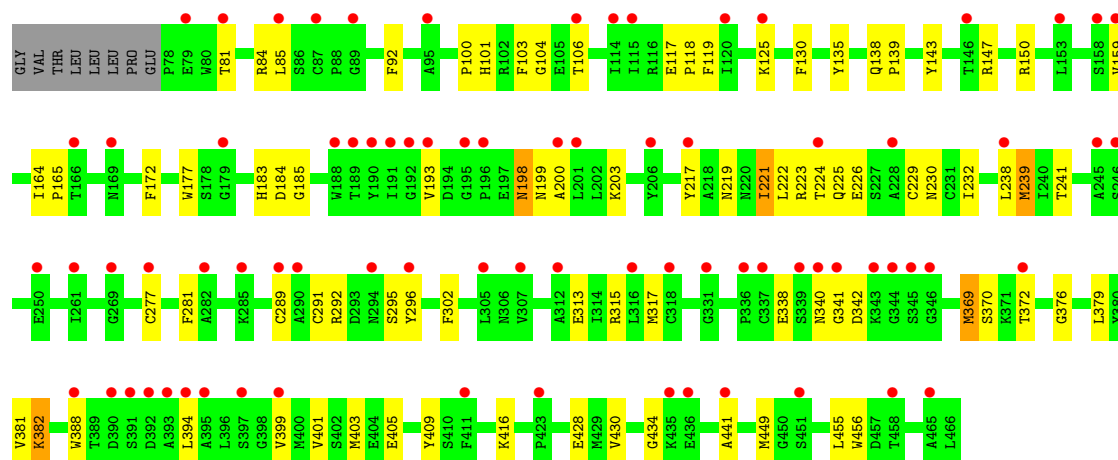
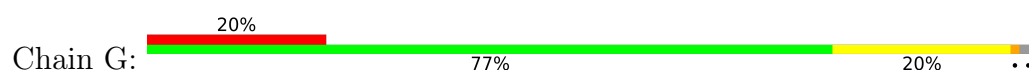
• Molecule 1: Neuraminidase



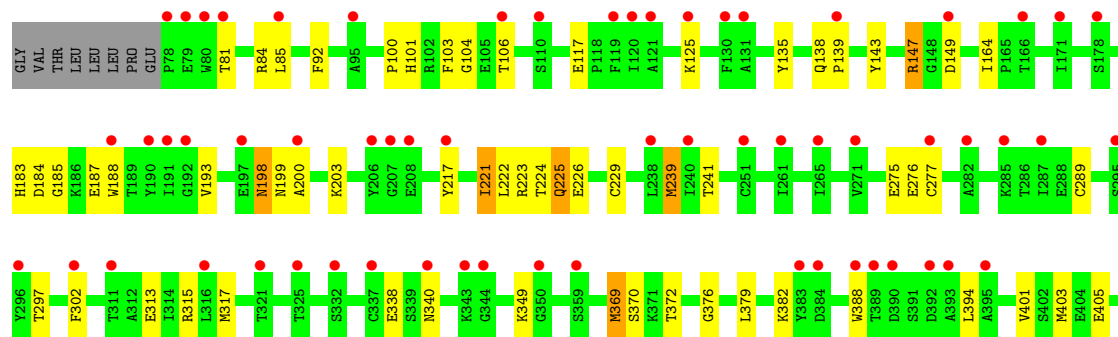
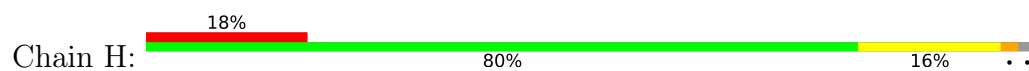
• Molecule 1: Neuraminidase

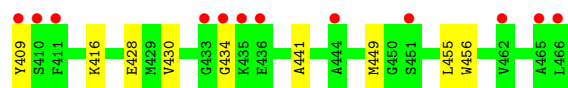


• Molecule 1: Neuraminidase

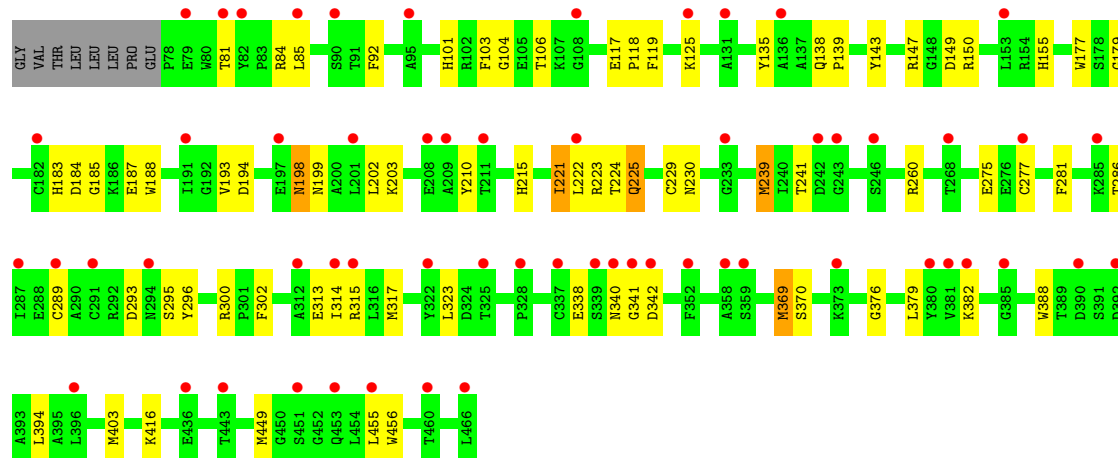
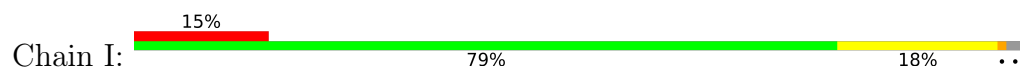


• Molecule 1: Neuraminidase

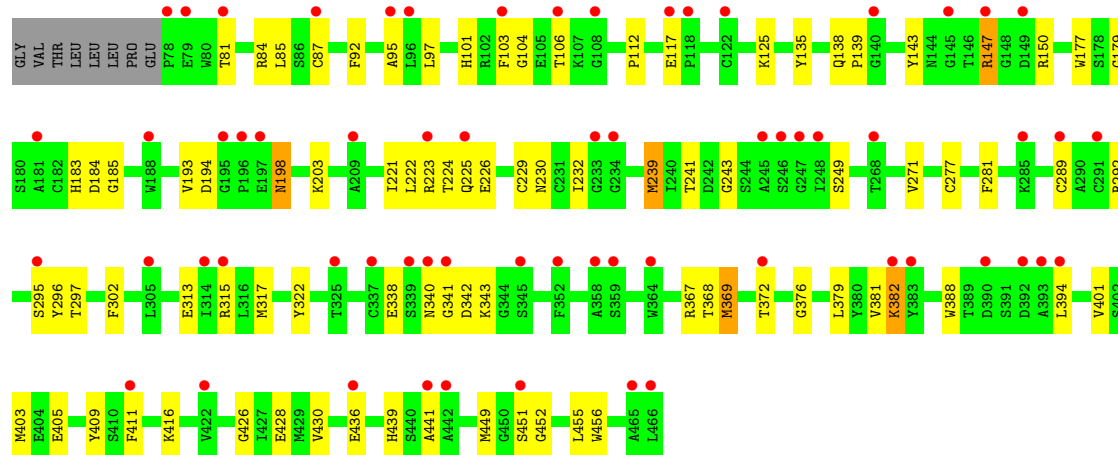
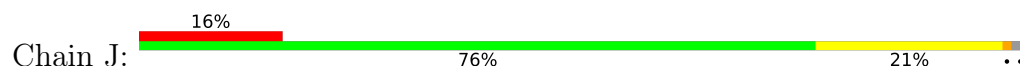




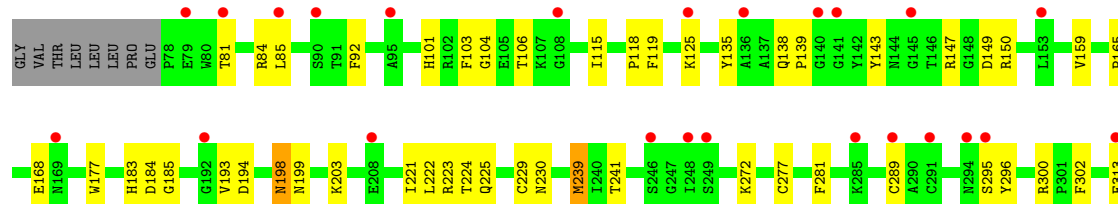
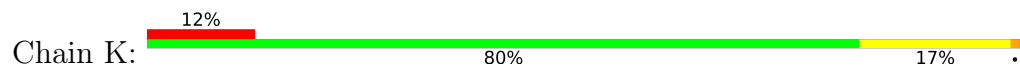
● Molecule 1: Neuraminidase

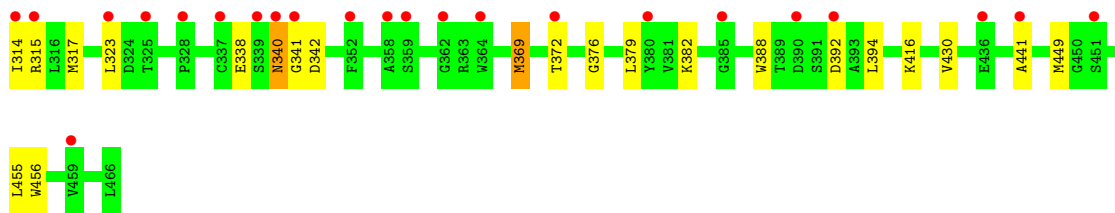


● Molecule 1: Neuraminidase

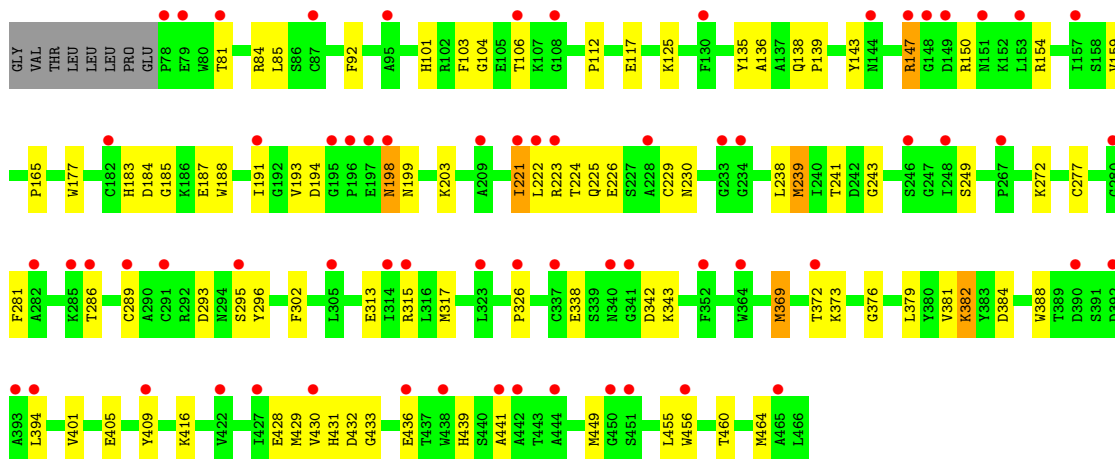
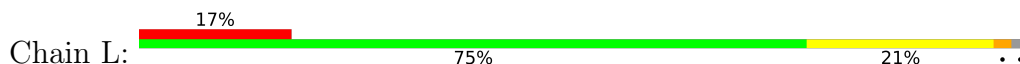


● Molecule 1: Neuraminidase

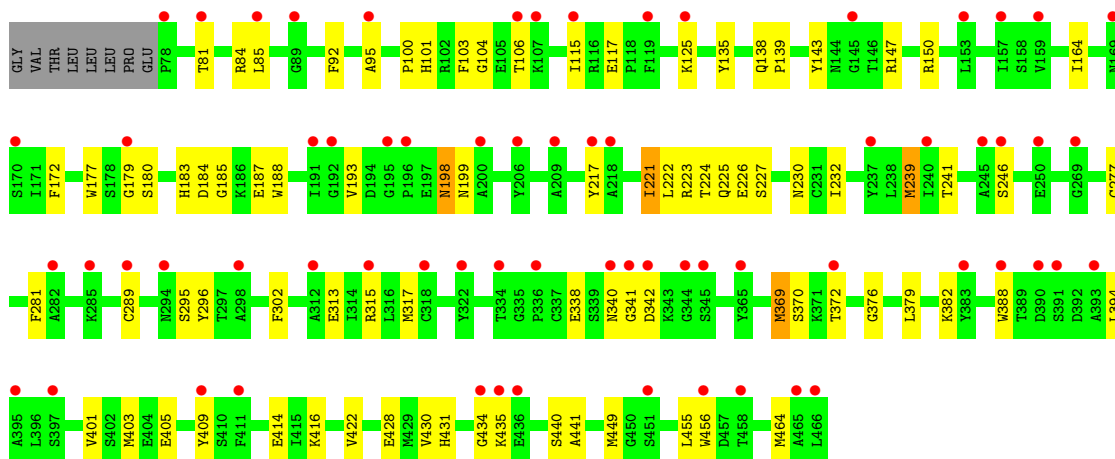
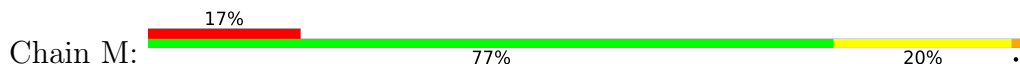




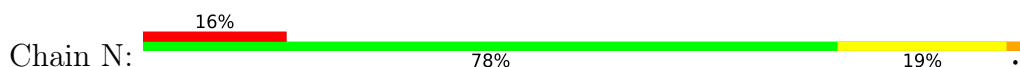
- Molecule 1: Neuraminidase

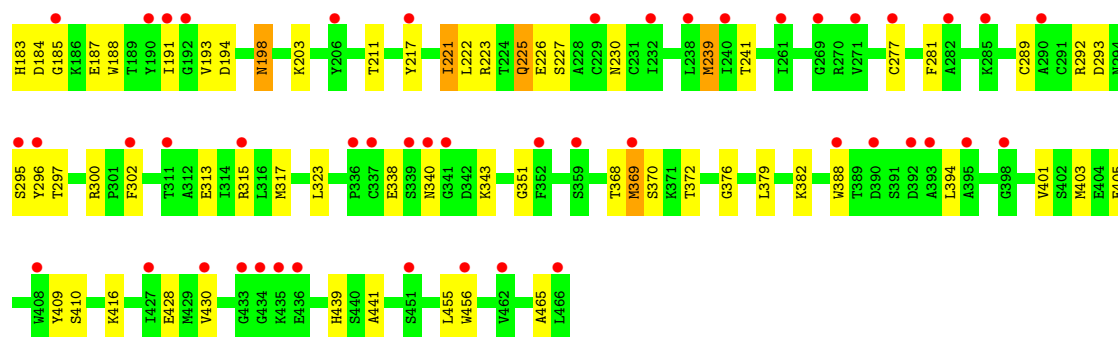


- Molecule 1: Neuraminidase

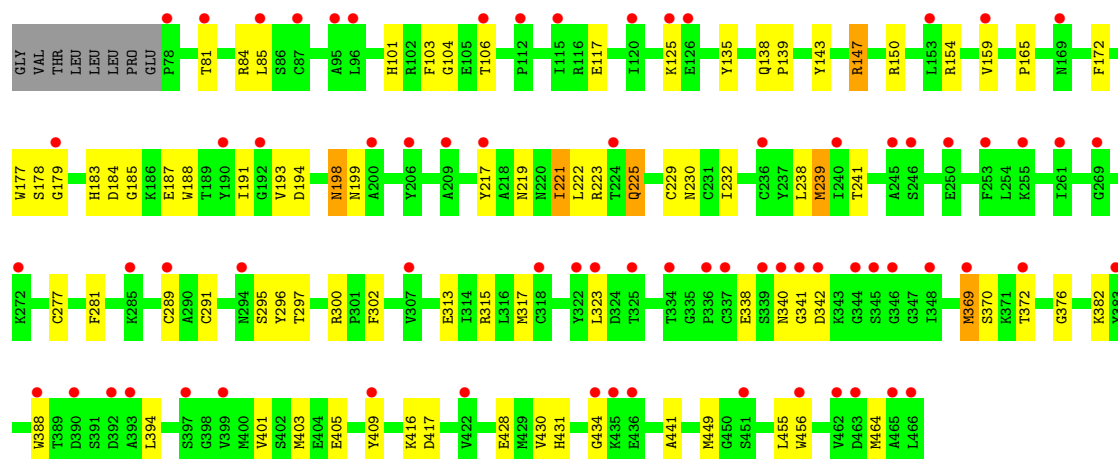
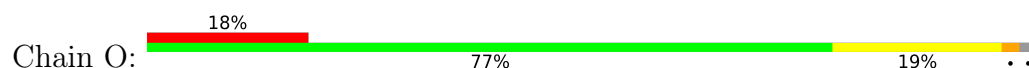


- Molecule 1: Neuraminidase

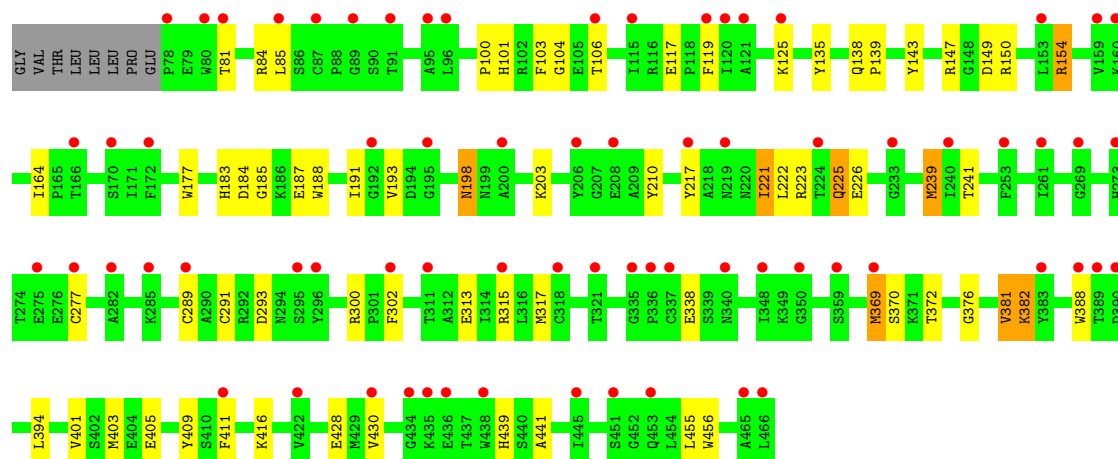
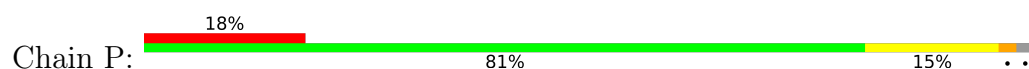




● Molecule 1: Neuraminidase



● Molecule 1: Neuraminidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	111.80Å 123.84Å 123.97Å 90.04° 90.17° 90.10°	Depositor
Resolution (Å)	49.69 – 2.59 49.69 – 2.59	Depositor EDS
% Data completeness (in resolution range)	96.3 (49.69-2.59) 97.4 (49.69-2.59)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.60 (at 2.25Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.207 , 0.229 (Not available) , 0.250	Depositor DCC
R_{free} test set	14641 reflections (4.64%)	wwPDB-VP
Wilson B-factor (Å ²)	22.4	Xtriage
Anisotropy	0.803	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 42.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.377 for h,l,-k 0.377 for h,-l,k 0.419 for h,-k,-l 0.417 for -h,k,-l 0.428 for -h,-k,l 0.367 for -h,l,k 0.370 for -h,-l,-k	Xtriage
Reported twinning fraction	0.323 for H, K, L 0.224 for -H, K, -L 0.097 for H, -L, K 0.100 for -h,-k,l 0.256 for -H, L, K	Depositor
Outliers	0 of 289439 reflections	Xtriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	49183	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.92% 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: G39, NAG, CA, YT3

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	0.91	0/3072	0.96	2/4150 (0.0%)
1	B	0.95	0/3072	0.98	0/4150
1	C	0.94	1/3072 (0.0%)	0.95	2/4150 (0.0%)
1	D	0.93	1/3072 (0.0%)	0.97	2/4150 (0.0%)
1	E	0.96	1/3072 (0.0%)	0.97	2/4150 (0.0%)
1	F	0.97	1/3072 (0.0%)	0.97	1/4150 (0.0%)
1	G	0.97	1/3072 (0.0%)	0.96	2/4150 (0.0%)
1	H	0.97	0/3072	0.96	1/4150 (0.0%)
1	I	0.93	0/3072	0.95	4/4150 (0.1%)
1	J	0.93	0/3072	0.95	5/4150 (0.1%)
1	K	0.92	0/3072	0.96	2/4150 (0.0%)
1	L	0.92	0/3072	0.94	2/4150 (0.0%)
1	M	0.96	1/3072 (0.0%)	0.96	2/4150 (0.0%)
1	N	0.95	0/3072	0.96	3/4150 (0.1%)
1	O	0.97	0/3072	0.96	4/4150 (0.1%)
1	P	0.97	1/3072 (0.0%)	0.97	2/4150 (0.0%)
All	All	0.95	7/49152 (0.0%)	0.96	36/66400 (0.1%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	399	VAL	CA-CB	5.81	1.60	1.53
1	C	248	ILE	CA-CB	5.80	1.60	1.54
1	F	271	VAL	N-CA	5.43	1.51	1.46
1	D	303	VAL	CA-CB	5.37	1.60	1.54
1	P	381	VAL	CA-CB	-5.27	1.50	1.55
1	E	444	ALA	CA-CB	-5.02	1.46	1.53
1	M	435	LYS	CA-C	5.02	1.59	1.52

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	452	GLY	N-CA-C	6.62	118.09	111.21
1	A	225	GLN	N-CA-C	6.31	119.83	111.75
1	O	179	GLY	N-CA-C	6.27	120.25	111.10
1	A	342	ASP	N-CA-C	6.08	119.84	110.42
1	O	225	GLN	N-CA-C	6.03	118.64	111.71
1	L	342	ASP	N-CA-C	6.00	119.73	110.42
1	G	342	ASP	N-CA-C	5.96	119.77	110.17
1	M	342	ASP	N-CA-C	5.92	119.70	110.17
1	P	225	GLN	N-CA-C	5.87	118.46	111.71
1	J	271	VAL	CA-C-N	5.80	128.37	120.54
1	J	271	VAL	C-N-CA	5.80	128.37	120.54
1	O	342	ASP	N-CA-C	5.78	119.48	110.17
1	E	225	GLN	N-CA-C	5.72	118.29	111.71
1	D	342	ASP	N-CA-C	5.64	119.16	110.42
1	P	291	CYS	N-CA-C	5.59	117.74	109.69
1	K	342	ASP	N-CA-C	5.57	119.14	110.17
1	N	225	GLN	N-CA-C	5.49	118.02	111.71
1	E	342	ASP	N-CA-C	5.44	118.93	110.17
1	J	342	ASP	N-CA-C	5.42	118.90	110.17
1	H	225	GLN	N-CA-C	5.39	117.91	111.71
1	I	179	GLY	N-CA-C	5.38	121.11	110.83
1	F	225	GLN	N-CA-C	5.32	117.82	111.71
1	J	179	GLY	N-CA-C	5.30	118.84	111.10
1	K	168	GLU	N-CA-C	5.30	118.21	111.69
1	N	179	GLY	N-CA-C	5.28	118.81	111.10
1	G	291	CYS	N-CA-C	5.28	117.30	109.69
1	M	179	GLY	N-CA-C	5.28	118.99	111.12
1	C	225	GLN	N-CA-C	5.28	117.78	111.71
1	I	342	ASP	N-CA-C	5.20	118.55	110.17
1	C	342	ASP	N-CA-C	5.16	118.47	110.17
1	L	286	THR	N-CA-C	5.14	116.77	108.34
1	O	291	CYS	N-CA-C	5.10	118.02	109.96
1	I	286	THR	N-CA-C	5.09	116.69	108.34
1	I	225	GLN	N-CA-C	5.07	117.54	111.71
1	N	227	SER	N-CA-C	5.03	115.17	108.38
1	D	286	THR	N-CA-C	5.01	116.55	108.34

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2999	0	2890	55	1
1	B	2999	0	2890	56	2
1	C	2999	0	2890	46	1
1	D	2999	0	2890	85	1
1	E	2999	0	2890	62	0
1	F	2999	0	2890	58	1
1	G	2999	0	2890	51	1
1	H	2999	0	2890	48	1
1	I	2999	0	2890	49	1
1	J	2999	0	2890	59	3
1	K	2999	0	2890	45	1
1	L	2999	0	2890	81	1
1	M	2999	0	2890	50	1
1	N	2999	0	2890	56	1
1	O	2999	0	2890	51	1
1	P	2999	0	2890	45	1
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
3	K	1	0	0	0	0
3	L	1	0	0	0	0
3	M	1	0	0	0	0
3	N	1	0	0	0	0
3	O	1	0	0	0	0
3	P	1	0	0	0	0
4	A	20	0	22	4	0
4	B	20	0	23	3	0
4	C	20	0	23	3	0
4	D	20	0	23	6	0
4	E	20	0	23	6	0
4	F	20	0	23	7	0
4	G	20	0	23	6	0
4	H	20	0	23	7	0
4	I	20	0	23	6	0
4	J	20	0	23	5	0
4	K	20	0	21	3	0
4	L	20	0	23	4	0
4	M	20	0	23	2	0
4	N	20	0	23	3	0
4	O	20	0	23	3	0
4	P	20	0	23	5	0
5	A	1	0	0	0	0
5	E	1	0	0	0	0
5	J	1	0	0	0	0
5	P	1	0	0	0	0
6	A	43	0	0	4	0
6	B	40	0	0	6	0
6	C	40	0	0	2	0
6	D	37	0	0	3	0
6	E	42	0	0	2	0
6	F	36	0	0	2	0
6	G	42	0	0	2	0
6	H	37	0	0	2	0
6	I	43	0	0	2	0
6	J	37	0	0	2	0
6	K	42	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	L	38	0	0	4	0
6	M	40	0	0	3	0
6	N	42	0	0	2	0
6	O	39	0	0	2	0
6	P	37	0	0	3	0
All	All	49183	0	46813	834	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 9.

All (834) 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:N:81:THR:HG23	6:N:2047:HOH:O	1.31	1.30
1:F:81:THR:HG23	6:F:2047:HOH:O	1.30	1.28
1:P:81:THR:HG23	6:P:2047:HOH:O	1.39	1.22
1:O:81:THR:HG23	6:O:2047:HOH:O	1.39	1.20
1:H:81:THR:HG23	6:H:2047:HOH:O	1.38	1.18
1:I:81:THR:HG23	6:I:2047:HOH:O	1.40	1.17
1:K:81:THR:HG23	6:K:2047:HOH:O	1.42	1.16
1:C:81:THR:HG23	6:C:2047:HOH:O	1.48	1.14
1:D:81:THR:HG23	6:D:2047:HOH:O	1.48	1.14
1:L:81:THR:HG23	6:L:2047:HOH:O	1.48	1.14
1:E:81:THR:HG23	6:E:2047:HOH:O	1.45	1.13
1:A:81:THR:HG23	6:A:2047:HOH:O	1.47	1.12
1:D:436:GLU:O	1:L:343:LYS:NZ	1.81	1.12
1:D:343:LYS:NZ	1:L:436:GLU:O	1.83	1.11
1:B:81:THR:HG23	6:B:2047:HOH:O	1.50	1.10
1:D:433:GLY:HA2	1:L:373:LYS:HE3	1.37	1.07
1:J:81:THR:HG23	6:J:2047:HOH:O	1.55	1.05
1:D:373:LYS:HE3	1:L:433:GLY:HA2	1.34	1.04
1:G:81:THR:HG23	6:G:2047:HOH:O	1.56	1.04
1:M:81:THR:HG23	6:M:2047:HOH:O	1.56	1.03
1:A:239:MET:HE1	6:A:2009:HOH:O	1.62	0.99
4:P:1:G39:H811	4:P:1:G39:H7	1.43	0.97
4:N:1:G39:H7	4:N:1:G39:H811	1.44	0.95
1:B:393:ALA:O	6:B:2013:HOH:O	1.85	0.95
1:D:326:PRO:HG2	1:L:436:GLU:HG3	1.48	0.94
1:D:225:GLN:HE21	1:D:239:MET:H	1.13	0.94
4:G:1:G39:H7	4:G:1:G39:H811	1.48	0.94
1:P:225:GLN:HE21	1:P:239:MET:H	1.11	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:198:ASN:HD22	1:H:198:ASN:H	1.19	0.91
1:K:225:GLN:HE21	1:K:239:MET:H	1.20	0.90
1:L:117:GLU:OE2	4:L:1:G39:N4	2.04	0.89
1:P:198:ASN:H	1:P:198:ASN:HD22	1.21	0.88
1:N:225:GLN:HE21	1:N:239:MET:H	1.22	0.87
1:D:436:GLU:HG3	1:L:326:PRO:HG2	1.56	0.87
1:H:183:HIS:HD2	1:H:185:GLY:H	1.20	0.87
1:F:198:ASN:HD22	1:F:198:ASN:H	1.22	0.86
1:C:225:GLN:HE21	1:C:239:MET:H	1.22	0.86
1:J:117:GLU:OE2	4:J:1:G39:N4	2.09	0.85
1:L:198:ASN:H	1:L:198:ASN:HD22	1.24	0.85
1:P:183:HIS:HD2	1:P:185:GLY:H	1.23	0.84
1:H:225:GLN:HE21	1:H:239:MET:H	1.20	0.84
1:D:373:LYS:CE	1:L:433:GLY:HA2	2.05	0.84
1:D:433:GLY:HA2	1:L:373:LYS:CE	2.08	0.84
1:G:225:GLN:HE21	1:G:239:MET:H	1.25	0.83
1:O:198:ASN:HD22	1:O:198:ASN:H	1.23	0.83
4:G:1:G39:H811	4:G:1:G39:C7	2.08	0.82
1:N:117:GLU:OE2	4:N:1:G39:N4	2.13	0.82
1:N:183:HIS:HD2	1:N:185:GLY:H	1.28	0.82
1:F:225:GLN:HE21	1:F:239:MET:H	1.27	0.81
1:G:198:ASN:H	1:G:198:ASN:HD22	1.25	0.81
1:J:225:GLN:HE21	1:J:239:MET:H	1.28	0.81
1:I:225:GLN:HE21	1:I:239:MET:H	1.25	0.81
1:N:198:ASN:H	1:N:198:ASN:HD22	1.29	0.81
1:M:225:GLN:HE21	1:M:239:MET:H	1.27	0.81
1:B:225:GLN:HE21	1:B:239:MET:H	1.27	0.80
1:J:198:ASN:HD22	1:J:198:ASN:H	1.29	0.80
1:K:221:ILE:O	1:K:223:ARG:HD3	1.82	0.80
1:B:313:GLU:OE2	1:B:315:ARG:NH2	2.14	0.80
1:M:198:ASN:HD22	1:M:198:ASN:H	1.27	0.79
1:H:223:ARG:HD2	4:H:1:G39:H912	1.63	0.79
1:B:183:HIS:HD2	1:B:185:GLY:H	1.31	0.79
1:O:225:GLN:HE21	1:O:239:MET:H	1.31	0.79
1:H:117:GLU:OE2	4:H:1:G39:N4	2.17	0.78
1:J:221:ILE:O	1:J:223:ARG:HD3	1.83	0.77
4:N:1:G39:H811	4:N:1:G39:C7	2.14	0.77
1:A:198:ASN:HD22	1:A:198:ASN:H	1.31	0.77
1:C:221:ILE:O	1:C:223:ARG:HD3	1.84	0.77
1:F:183:HIS:HD2	1:F:185:GLY:H	1.29	0.77
1:E:183:HIS:HD2	1:E:185:GLY:H	1.31	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:198:ASN:H	1:D:198:ASN:HD22	1.32	0.77
1:B:336:PRO:HD3	1:E:268:THR:HG22	1.66	0.76
1:J:223:ARG:HD2	4:J:1:G39:H912	1.68	0.76
1:F:150:ARG:NH1	4:F:1:G39:O10	2.19	0.75
1:D:225:GLN:NE2	1:D:239:MET:H	1.84	0.75
1:G:183:HIS:HD2	1:G:185:GLY:H	1.35	0.75
1:H:183:HIS:CD2	1:H:185:GLY:H	2.05	0.75
1:L:183:HIS:HD2	1:L:185:GLY:H	1.33	0.74
1:D:326:PRO:CG	1:L:436:GLU:HG3	2.16	0.74
1:A:225:GLN:HE21	1:A:239:MET:H	1.36	0.74
1:K:198:ASN:H	1:K:198:ASN:HD22	1.34	0.74
1:C:198:ASN:HD22	1:C:198:ASN:H	1.34	0.74
1:I:183:HIS:HD2	1:I:185:GLY:H	1.36	0.74
1:B:198:ASN:H	1:B:198:ASN:HD22	1.35	0.74
1:E:198:ASN:HD22	1:E:198:ASN:H	1.36	0.73
1:I:198:ASN:H	1:I:198:ASN:HD22	1.36	0.73
1:K:313:GLU:OE2	1:K:315:ARG:NH2	2.20	0.73
1:P:225:GLN:NE2	1:P:239:MET:H	1.86	0.73
1:C:239:MET:HE1	6:C:2009:HOH:O	1.88	0.72
1:N:225:GLN:NE2	1:N:239:MET:H	1.86	0.72
1:J:239:MET:HE1	6:J:2009:HOH:O	1.87	0.72
1:L:150:ARG:NH1	4:L:1:G39:O10	2.23	0.72
1:P:117:GLU:OE2	4:P:1:G39:N4	2.22	0.72
1:P:277:CYS:HB3	1:P:289:CYS:HB3	1.71	0.72
1:M:183:HIS:HD2	1:M:185:GLY:H	1.37	0.72
1:I:221:ILE:O	1:I:223:ARG:HD3	1.90	0.71
1:J:183:HIS:HD2	1:J:185:GLY:H	1.36	0.71
1:A:183:HIS:HD2	1:A:185:GLY:H	1.38	0.71
1:K:183:HIS:HD2	1:K:185:GLY:H	1.38	0.71
1:B:239:MET:HE1	6:B:2009:HOH:O	1.90	0.71
1:C:150:ARG:NH1	4:C:1:G39:O10	2.24	0.71
1:D:183:HIS:HD2	1:D:185:GLY:H	1.38	0.71
1:L:221:ILE:O	1:L:223:ARG:HD3	1.91	0.71
1:F:183:HIS:CD2	1:F:185:GLY:H	2.08	0.71
1:A:221:ILE:O	1:A:223:ARG:HD3	1.92	0.70
1:E:225:GLN:HE21	1:E:239:MET:H	1.39	0.70
1:C:183:HIS:HD2	1:C:185:GLY:H	1.39	0.70
1:A:449:MET:HE1	1:D:203:LYS:HB3	1.74	0.70
1:B:382:LYS:HE3	6:B:2013:HOH:O	1.90	0.70
1:H:225:GLN:NE2	1:H:239:MET:H	1.90	0.70
1:K:392:ASP:O	6:K:9:HOH:O	2.09	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:183:HIS:CD2	1:P:185:GLY:H	2.09	0.70
1:D:436:GLU:HG3	1:L:326:PRO:CG	2.21	0.69
1:I:117:GLU:OE2	4:I:1:G39:N4	2.25	0.69
1:B:221:ILE:O	1:B:223:ARG:HD3	1.91	0.69
1:D:225:GLN:HE21	1:D:239:MET:N	1.88	0.69
1:N:183:HIS:CD2	1:N:185:GLY:H	2.10	0.69
1:O:221:ILE:O	1:O:223:ARG:HD3	1.93	0.69
1:A:449:MET:CE	1:D:203:LYS:HB3	2.23	0.69
1:J:81:THR:HG22	1:J:184:ASP:C	2.18	0.69
1:D:432:ASP:O	1:L:373:LYS:CE	2.41	0.68
1:C:225:GLN:NE2	1:C:239:MET:H	1.90	0.68
1:L:239:MET:HE1	6:L:2009:HOH:O	1.92	0.68
1:O:183:HIS:HD2	1:O:185:GLY:H	1.40	0.68
1:I:225:GLN:NE2	1:I:239:MET:H	1.92	0.68
1:F:117:GLU:OE2	4:F:1:G39:N4	2.25	0.68
1:N:277:CYS:HB3	1:N:289:CYS:HB3	1.77	0.67
1:D:221:ILE:O	1:D:223:ARG:HD3	1.93	0.67
1:G:277:CYS:HB3	1:G:289:CYS:HB3	1.77	0.67
1:G:225:GLN:NE2	1:G:239:MET:H	1.92	0.67
1:M:225:GLN:NE2	1:M:239:MET:H	1.92	0.67
1:G:221:ILE:O	1:G:223:ARG:HD3	1.94	0.67
1:O:225:GLN:NE2	1:O:239:MET:H	1.92	0.66
1:G:183:HIS:CD2	1:G:185:GLY:H	2.13	0.66
1:D:373:LYS:CE	1:L:432:ASP:O	2.43	0.66
1:F:223:ARG:HD2	4:F:1:G39:H912	1.76	0.66
1:P:221:ILE:O	1:P:223:ARG:HD3	1.96	0.66
1:O:117:GLU:OE2	4:O:1:G39:N4	2.28	0.66
1:J:225:GLN:NE2	1:J:239:MET:H	1.93	0.66
1:K:225:GLN:NE2	1:K:239:MET:H	1.90	0.65
1:B:225:GLN:NE2	1:B:239:MET:H	1.94	0.65
1:N:203:LYS:HB3	1:O:449:MET:HE1	1.78	0.65
1:F:104:GLY:O	1:F:138:GLN:NE2	2.30	0.65
1:E:81:THR:HG22	1:E:184:ASP:C	2.22	0.65
1:F:225:GLN:NE2	1:F:239:MET:H	1.94	0.65
1:C:183:HIS:CD2	1:C:185:GLY:H	2.15	0.65
1:N:193:VAL:HG11	1:N:222:LEU:O	1.97	0.65
1:C:277:CYS:HB3	1:C:289:CYS:HB3	1.78	0.65
4:P:1:G39:H811	4:P:1:G39:C7	2.23	0.65
1:F:198:ASN:HD22	1:F:198:ASN:N	1.95	0.64
1:I:239:MET:HE1	6:I:2009:HOH:O	1.96	0.64
1:D:117:GLU:OE2	4:D:1:G39:N4	2.29	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:198:ASN:HD22	1:L:198:ASN:N	1.96	0.64
1:N:225:GLN:HE21	1:N:239:MET:N	1.94	0.64
1:H:225:GLN:HE21	1:H:239:MET:N	1.93	0.64
1:E:183:HIS:CD2	1:E:185:GLY:H	2.14	0.64
1:E:149:ASP:HB3	4:E:1:G39:O10	1.97	0.64
1:P:193:VAL:HG11	1:P:222:LEU:O	1.98	0.64
1:B:183:HIS:CD2	1:B:185:GLY:H	2.14	0.64
1:A:277:CYS:HB3	1:A:289:CYS:HB3	1.79	0.63
1:A:225:GLN:NE2	1:A:239:MET:H	1.95	0.63
1:I:150:ARG:NH1	4:I:1:G39:O10	2.32	0.63
1:M:104:GLY:O	1:M:138:GLN:NE2	2.31	0.63
1:A:183:HIS:CD2	1:A:185:GLY:H	2.17	0.63
1:B:277:CYS:HB3	1:B:289:CYS:HB3	1.80	0.63
1:I:225:GLN:HE21	1:I:239:MET:N	1.96	0.63
1:G:193:VAL:HG11	1:G:222:LEU:O	1.99	0.63
1:P:150:ARG:NH1	4:P:1:G39:O10	2.28	0.63
1:L:225:GLN:HE21	1:L:239:MET:H	1.45	0.63
1:M:449:MET:HE1	1:P:203:LYS:HB3	1.81	0.63
1:J:277:CYS:HB3	1:J:289:CYS:HB3	1.81	0.63
1:O:277:CYS:HB3	1:O:289:CYS:HB3	1.81	0.63
1:G:81:THR:HG22	1:G:184:ASP:C	2.24	0.62
1:G:223:ARG:HD2	4:G:1:G39:H912	1.80	0.62
1:B:203:LYS:HB3	1:C:449:MET:HE1	1.80	0.62
1:B:225:GLN:HE21	1:B:239:MET:N	1.97	0.62
1:M:221:ILE:O	1:M:223:ARG:HD3	1.99	0.62
1:C:81:THR:HG22	1:C:184:ASP:C	2.25	0.62
1:E:225:GLN:NE2	1:E:239:MET:H	1.97	0.62
1:L:183:HIS:CD2	1:L:185:GLY:H	2.16	0.62
1:C:225:GLN:HE21	1:C:239:MET:N	1.95	0.62
1:F:221:ILE:O	1:F:223:ARG:HD3	1.99	0.62
1:G:198:ASN:HD22	1:G:198:ASN:N	1.98	0.62
1:I:183:HIS:CD2	1:I:185:GLY:H	2.18	0.62
1:I:277:CYS:HB3	1:I:289:CYS:HB3	1.80	0.62
1:M:193:VAL:HG11	1:M:222:LEU:O	1.99	0.62
1:E:221:ILE:O	1:E:223:ARG:HD3	1.99	0.62
1:B:223:ARG:HD2	4:B:1:G39:H912	1.81	0.62
1:D:294:ASN:ND2	4:D:1:G39:H821	2.15	0.62
1:K:277:CYS:HB3	1:K:289:CYS:HB3	1.82	0.62
1:O:193:VAL:HG11	1:O:222:LEU:O	1.99	0.62
1:F:239:MET:HE1	6:F:2009:HOH:O	2.01	0.61
1:K:183:HIS:CD2	1:K:185:GLY:H	2.19	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:81:THR:HG22	1:L:184:ASP:C	2.26	0.61
1:J:183:HIS:CD2	1:J:185:GLY:H	2.16	0.61
1:D:239:MET:HE1	6:D:2009:HOH:O	1.99	0.61
1:E:277:CYS:HB3	1:E:289:CYS:HB3	1.82	0.61
1:M:117:GLU:OE2	4:M:1:G39:N4	2.34	0.61
1:A:203:LYS:HB3	1:B:449:MET:HE1	1.83	0.61
1:K:239:MET:HE1	6:K:2009:HOH:O	2.01	0.61
1:M:225:GLN:HE21	1:M:239:MET:N	1.98	0.61
1:B:81:THR:HG22	1:B:184:ASP:C	2.24	0.60
1:I:81:THR:HG22	1:I:184:ASP:C	2.26	0.60
1:J:315:ARG:HG3	1:J:388:TRP:CD2	2.35	0.60
1:D:277:CYS:HB3	1:D:289:CYS:HB3	1.84	0.60
1:E:223:ARG:HD2	4:E:1:G39:H912	1.83	0.60
1:P:225:GLN:HE21	1:P:239:MET:N	1.91	0.60
1:F:193:VAL:HG11	1:F:222:LEU:O	2.01	0.60
1:F:277:CYS:HB3	1:F:289:CYS:HB3	1.83	0.60
1:D:81:THR:HG22	1:D:184:ASP:C	2.25	0.60
1:G:117:GLU:OE2	4:G:1:G39:N4	2.34	0.60
1:E:449:MET:HE1	1:H:203:LYS:HB3	1.84	0.60
1:H:104:GLY:O	1:H:138:GLN:NE2	2.35	0.60
1:M:183:HIS:CD2	1:M:185:GLY:H	2.19	0.60
1:J:313:GLU:OE2	1:J:315:ARG:NH2	2.29	0.60
1:N:221:ILE:O	1:N:223:ARG:HD3	2.02	0.60
1:O:198:ASN:HD22	1:O:198:ASN:N	1.95	0.60
1:F:101:HIS:C	1:F:103:PHE:H	2.09	0.60
1:O:104:GLY:O	1:O:138:GLN:NE2	2.35	0.60
1:L:223:ARG:HD2	4:L:1:G39:H912	1.82	0.59
1:O:81:THR:HG22	1:O:184:ASP:C	2.27	0.59
1:A:231:CYS:O	6:A:2047:HOH:O	2.17	0.59
1:E:225:GLN:NE2	1:E:238:LEU:HD12	2.18	0.59
1:P:239:MET:HE1	6:P:2009:HOH:O	2.02	0.59
1:B:193:VAL:HG11	1:B:222:LEU:O	2.02	0.59
1:E:101:HIS:C	1:E:103:PHE:H	2.11	0.59
1:L:277:CYS:HB3	1:L:289:CYS:HB3	1.84	0.59
1:J:223:ARG:CD	4:J:1:G39:H912	2.32	0.59
1:F:225:GLN:HE21	1:F:239:MET:N	1.97	0.58
1:J:225:GLN:HE21	1:J:239:MET:N	1.98	0.58
1:A:101:HIS:C	1:A:103:PHE:H	2.11	0.58
1:E:225:GLN:HE21	1:E:239:MET:N	2.01	0.58
1:E:409:TYR:HB2	1:E:428:GLU:OE1	2.03	0.58
1:O:239:MET:HE1	6:O:2009:HOH:O	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:221:ILE:O	1:H:223:ARG:HD3	2.02	0.58
1:H:277:CYS:HB3	1:H:289:CYS:HB3	1.85	0.58
1:D:315:ARG:HG3	1:D:388:TRP:CD2	2.38	0.58
1:D:183:HIS:CD2	1:D:185:GLY:H	2.19	0.58
1:M:187:GLU:HG3	1:M:188:TRP:N	2.18	0.58
1:O:183:HIS:CD2	1:O:185:GLY:H	2.21	0.58
1:G:369:MET:HB2	1:G:376:GLY:HA3	1.86	0.57
1:M:277:CYS:HB3	1:M:289:CYS:HB3	1.86	0.57
1:H:409:TYR:HB2	1:H:428:GLU:OE1	2.03	0.57
1:K:223:ARG:HD2	4:K:1:G39:H912	1.86	0.57
1:E:297:THR:OG1	1:E:340:ASN:O	2.13	0.57
1:H:193:VAL:HG11	1:H:222:LEU:O	2.03	0.57
1:O:225:GLN:HE21	1:O:239:MET:N	2.01	0.57
1:D:373:LYS:HE3	1:L:433:GLY:CA	2.23	0.57
1:E:149:ASP:CG	4:E:1:G39:N4	2.62	0.57
1:B:315:ARG:NH2	1:E:217:TYR:O	2.33	0.57
1:E:203:LYS:HB3	1:F:449:MET:HE1	1.86	0.57
1:A:104:GLY:O	1:A:138:GLN:NE2	2.37	0.57
1:L:225:GLN:NE2	1:L:239:MET:H	2.02	0.57
1:O:150:ARG:NH1	4:O:1:G39:O10	2.36	0.57
1:K:81:THR:HG22	1:K:184:ASP:C	2.30	0.57
1:B:203:LYS:HB3	1:C:449:MET:CE	2.34	0.56
1:C:101:HIS:C	1:C:103:PHE:H	2.13	0.56
1:C:313:GLU:OE2	1:C:315:ARG:NH2	2.33	0.56
1:E:139:PRO:HA	1:E:143:TYR:HH	1.71	0.56
1:F:343:LYS:HG2	1:N:465:ALA:HB2	1.88	0.56
1:G:409:TYR:HB2	1:G:428:GLU:OE1	2.05	0.56
1:I:149:ASP:CG	4:I:1:G39:N4	2.64	0.56
1:N:203:LYS:HB3	1:O:449:MET:CE	2.36	0.56
1:D:372:THR:HG23	1:L:436:GLU:HB2	1.88	0.56
1:G:203:LYS:HB3	1:H:449:MET:HE1	1.87	0.56
1:D:432:ASP:O	1:L:373:LYS:HE2	2.06	0.56
1:F:81:THR:HG22	1:F:184:ASP:C	2.31	0.56
1:O:369:MET:HB2	1:O:376:GLY:HA3	1.88	0.56
1:F:203:LYS:HB3	1:G:449:MET:HE1	1.88	0.56
1:B:302:PHE:HB2	1:B:317:MET:HG3	1.89	0.55
1:F:139:PRO:HA	1:F:143:TYR:OH	2.07	0.55
1:P:101:HIS:C	1:P:103:PHE:H	2.13	0.55
1:P:369:MET:HB2	1:P:376:GLY:HA3	1.89	0.55
1:C:104:GLY:O	1:C:138:GLN:NE2	2.39	0.55
1:E:193:VAL:HG11	1:E:222:LEU:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:315:ARG:HG3	1:K:388:TRP:CD2	2.41	0.55
1:M:81:THR:HG22	1:M:184:ASP:C	2.32	0.55
1:C:117:GLU:OE2	4:C:1:G39:N4	2.39	0.55
1:F:139:PRO:HA	1:F:143:TYR:HH	1.71	0.55
1:K:225:GLN:HE21	1:K:239:MET:N	1.97	0.55
1:G:225:GLN:HE21	1:G:239:MET:N	1.97	0.55
1:N:409:TYR:HB2	1:N:428:GLU:OE1	2.06	0.55
1:P:409:TYR:HB2	1:P:428:GLU:OE1	2.07	0.55
1:H:101:HIS:C	1:H:103:PHE:H	2.14	0.54
1:L:315:ARG:HG3	1:L:388:TRP:CD2	2.42	0.54
1:F:297:THR:OG1	1:F:340:ASN:O	2.20	0.54
1:C:198:ASN:HD22	1:C:198:ASN:N	2.03	0.54
1:D:294:ASN:CG	4:D:1:G39:H821	2.33	0.54
4:F:1:G39:H7	4:F:1:G39:H811	1.88	0.54
1:M:449:MET:CE	1:P:203:LYS:HB3	2.38	0.54
1:N:81:THR:HG22	1:N:184:ASP:C	2.32	0.54
1:A:315:ARG:HG3	1:A:388:TRP:CD2	2.43	0.53
1:F:409:TYR:HB2	1:F:428:GLU:OE1	2.08	0.53
1:J:297:THR:OG1	1:J:340:ASN:O	2.19	0.53
1:L:315:ARG:HB3	6:L:2033:HOH:O	2.08	0.53
1:G:239:MET:HE1	6:G:2009:HOH:O	2.09	0.53
1:P:198:ASN:HD22	1:P:198:ASN:N	1.96	0.53
1:P:315:ARG:HG3	1:P:388:TRP:CD2	2.44	0.53
1:F:343:LYS:HG2	1:N:465:ALA:CB	2.38	0.53
1:G:292:ARG:NH2	4:G:1:G39:O1B	2.40	0.53
1:H:223:ARG:CD	4:H:1:G39:H912	2.36	0.53
1:M:101:HIS:C	1:M:103:PHE:H	2.16	0.53
1:B:117:GLU:OE2	4:B:1:G39:N4	2.42	0.53
1:B:382:LYS:HD2	6:B:2013:HOH:O	2.09	0.53
1:G:139:PRO:HA	1:G:143:TYR:OH	2.08	0.53
1:D:302:PHE:HB2	1:D:317:MET:HG3	1.91	0.53
1:G:315:ARG:HG3	1:G:388:TRP:CD2	2.44	0.53
1:E:295:SER:HB2	1:E:296:TYR:CD2	2.44	0.53
1:G:295:SER:HB2	1:G:296:TYR:CD2	2.44	0.53
1:P:198:ASN:H	1:P:198:ASN:ND2	2.01	0.53
1:L:194:ASP:OD1	1:L:203:LYS:NZ	2.42	0.53
1:P:370:SER:HB2	1:P:403:MET:SD	2.48	0.53
1:E:198:ASN:HD22	1:E:198:ASN:N	2.07	0.52
1:G:101:HIS:C	1:G:103:PHE:H	2.17	0.52
1:I:449:MET:HE1	1:L:203:LYS:HB3	1.91	0.52
1:K:139:PRO:HA	1:K:143:TYR:HH	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:372:THR:HG22	1:N:372:THR:O	2.10	0.52
1:E:239:MET:HE1	6:E:2009:HOH:O	2.10	0.52
1:M:409:TYR:HB2	1:M:428:GLU:OE1	2.09	0.52
1:O:101:HIS:C	1:O:103:PHE:H	2.16	0.52
1:H:81:THR:HG22	1:H:184:ASP:C	2.35	0.52
1:N:187:GLU:HG3	1:N:188:TRP:N	2.24	0.52
1:B:219:ASN:OD1	1:F:360:LYS:NZ	2.37	0.52
1:M:315:ARG:HB2	1:M:388:TRP:CD1	2.45	0.52
1:O:370:SER:HB2	1:O:403:MET:SD	2.50	0.52
1:A:81:THR:HG22	1:A:184:ASP:C	2.34	0.52
1:B:338:GLU:HG3	1:E:266:PHE:CD1	2.44	0.52
1:C:315:ARG:HG3	1:C:388:TRP:CD2	2.44	0.52
1:E:369:MET:HB2	1:E:376:GLY:HA3	1.92	0.52
1:H:139:PRO:HA	1:H:143:TYR:HH	1.74	0.52
1:M:431:HIS:HB3	1:M:464:MET:SD	2.49	0.52
1:O:139:PRO:HA	1:O:143:TYR:HH	1.73	0.52
1:H:239:MET:HE1	6:H:2009:HOH:O	2.10	0.52
1:A:369:MET:HB2	1:A:376:GLY:HA3	1.92	0.51
1:G:139:PRO:HA	1:G:143:TYR:HH	1.75	0.51
1:J:198:ASN:HD22	1:J:198:ASN:N	2.01	0.51
1:P:139:PRO:HA	1:P:143:TYR:OH	2.10	0.51
1:F:372:THR:O	1:F:372:THR:HG22	2.11	0.51
1:F:465:ALA:HB2	1:N:343:LYS:HG2	1.92	0.51
1:H:198:ASN:H	1:H:198:ASN:ND2	2.00	0.51
1:E:187:GLU:HG3	1:E:188:TRP:N	2.25	0.51
1:A:203:LYS:HB3	1:B:449:MET:CE	2.39	0.51
1:M:369:MET:HB2	1:M:376:GLY:HA3	1.93	0.51
4:H:1:G39:C7	4:H:1:G39:H811	2.41	0.51
1:K:203:LYS:HB3	1:L:449:MET:CE	2.41	0.51
1:L:112:PRO:HD2	1:L:138:GLN:O	2.11	0.51
1:N:104:GLY:O	1:N:138:GLN:NE2	2.43	0.51
1:E:230:ASN:HB3	1:E:281:PHE:CE2	2.46	0.51
1:H:139:PRO:HA	1:H:143:TYR:OH	2.11	0.51
1:M:302:PHE:HB2	1:M:317:MET:HG3	1.93	0.51
1:K:313:GLU:HB3	1:K:388:TRP:HH2	1.76	0.51
1:M:239:MET:HE1	6:M:2009:HOH:O	2.11	0.51
1:N:302:PHE:HB2	1:N:317:MET:HG3	1.92	0.51
1:N:370:SER:HB2	1:N:403:MET:SD	2.50	0.51
1:A:225:GLN:HE21	1:A:239:MET:N	2.04	0.51
1:B:315:ARG:HG3	1:B:388:TRP:CD2	2.45	0.51
1:E:430:VAL:HG22	1:E:441:ALA:HB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:139:PRO:HA	1:M:143:TYR:HH	1.75	0.51
1:M:139:PRO:HA	1:M:143:TYR:OH	2.11	0.51
1:N:239:MET:HE1	6:N:2009:HOH:O	2.11	0.50
1:D:373:LYS:NZ	1:L:433:GLY:HA2	2.25	0.50
1:L:225:GLN:HE21	1:L:239:MET:N	2.09	0.50
1:J:104:GLY:O	1:J:138:GLN:NE2	2.45	0.50
1:M:315:ARG:HG3	1:M:388:TRP:CD2	2.47	0.50
1:M:430:VAL:HG22	1:M:441:ALA:HB2	1.93	0.50
1:E:117:GLU:OE2	4:E:1:G39:N4	2.45	0.50
1:H:198:ASN:HD22	1:H:198:ASN:N	1.93	0.50
1:N:101:HIS:C	1:N:103:PHE:H	2.20	0.50
1:E:372:THR:HG22	1:E:372:THR:O	2.12	0.50
1:I:101:HIS:C	1:I:103:PHE:H	2.20	0.50
1:K:302:PHE:HB2	1:K:317:MET:HG3	1.94	0.50
1:P:154:ARG:HG2	1:P:177:TRP:HA	1.94	0.50
1:K:203:LYS:HB3	1:L:449:MET:HE1	1.94	0.50
1:O:430:VAL:HG22	1:O:441:ALA:HB2	1.93	0.50
1:F:465:ALA:CB	1:N:343:LYS:HG2	2.42	0.50
1:D:433:GLY:HA2	1:L:373:LYS:NZ	2.26	0.49
1:E:449:MET:CE	1:H:203:LYS:HB3	2.42	0.49
1:G:372:THR:HG22	1:G:372:THR:O	2.12	0.49
1:L:372:THR:HG22	1:L:372:THR:O	2.12	0.49
1:A:372:THR:O	1:A:372:THR:HG22	2.12	0.49
1:L:193:VAL:HG11	1:L:222:LEU:O	2.12	0.49
1:P:81:THR:HG22	1:P:184:ASP:C	2.37	0.49
1:F:315:ARG:HG3	1:F:388:TRP:CD2	2.48	0.49
1:C:203:LYS:HB3	1:D:449:MET:HE1	1.94	0.49
1:D:193:VAL:HG11	1:D:222:LEU:O	2.12	0.49
1:N:139:PRO:HA	1:N:143:TYR:OH	2.13	0.49
1:B:401:VAL:CG1	1:B:405:GLU:HB2	2.43	0.49
1:D:433:GLY:CA	1:L:373:LYS:HE3	2.24	0.49
1:I:203:LYS:HB3	1:J:449:MET:HE1	1.95	0.49
1:A:370:SER:HB2	1:A:403:MET:SD	2.53	0.48
1:F:325:THR:HG1	1:F:368:THR:HG1	1.61	0.48
4:F:1:G39:H811	4:F:1:G39:C7	2.42	0.48
1:I:302:PHE:HB2	1:I:317:MET:HG3	1.95	0.48
1:J:139:PRO:HA	1:J:143:TYR:HH	1.78	0.48
1:K:139:PRO:HA	1:K:143:TYR:OH	2.13	0.48
1:H:183:HIS:HD2	1:H:185:GLY:N	2.00	0.48
1:H:370:SER:HB2	1:H:403:MET:SD	2.53	0.48
1:L:369:MET:HB2	1:L:376:GLY:HA3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:436:GLU:HB2	1:L:372:THR:HG23	1.94	0.48
1:H:315:ARG:HG3	1:H:388:TRP:CD2	2.49	0.48
1:N:315:ARG:HG3	1:N:388:TRP:CD2	2.49	0.48
1:D:315:ARG:HB3	6:D:2033:HOH:O	2.13	0.48
1:J:193:VAL:HG11	1:J:222:LEU:O	2.13	0.48
1:D:245:ALA:HB1	4:D:1:G39:H822	1.96	0.48
1:G:430:VAL:HG22	1:G:441:ALA:HB2	1.95	0.48
1:H:302:PHE:HB2	1:H:317:MET:HG3	1.95	0.48
1:I:139:PRO:HA	1:I:143:TYR:HH	1.79	0.48
1:I:449:MET:CE	1:L:203:LYS:HB3	2.44	0.48
1:K:372:THR:HG22	1:K:372:THR:O	2.13	0.48
1:F:203:LYS:HB3	1:G:449:MET:CE	2.44	0.48
1:I:230:ASN:HB3	1:I:281:PHE:CE2	2.49	0.48
1:I:313:GLU:HB3	1:I:388:TRP:HH2	1.79	0.48
1:F:343:LYS:CG	1:N:465:ALA:CB	2.92	0.48
1:K:101:HIS:C	1:K:103:PHE:H	2.22	0.48
1:K:118:PRO:O	1:K:119:PHE:HB3	2.14	0.48
1:B:112:PRO:HD2	1:B:138:GLN:O	2.14	0.48
1:C:295:SER:HB2	1:C:296:TYR:CD2	2.49	0.48
1:D:369:MET:HB2	1:D:376:GLY:HA3	1.94	0.48
1:F:101:HIS:C	1:F:103:PHE:N	2.68	0.48
1:N:313:GLU:HB3	1:N:388:TRP:HH2	1.79	0.48
1:P:313:GLU:HB3	1:P:388:TRP:HH2	1.79	0.48
1:A:101:HIS:C	1:A:103:PHE:N	2.71	0.47
1:A:223:ARG:HD2	4:A:1:G39:H912	1.94	0.47
1:E:302:PHE:HB2	1:E:317:MET:HG3	1.94	0.47
1:F:225:GLN:O	1:F:226:GLU:HB2	2.14	0.47
1:J:313:GLU:HB3	1:J:388:TRP:HH2	1.78	0.47
1:B:104:GLY:O	1:B:138:GLN:NE2	2.47	0.47
1:K:230:ASN:HB3	1:K:281:PHE:CE2	2.49	0.47
1:L:409:TYR:HB2	1:L:428:GLU:OE1	2.14	0.47
1:M:100:PRO:HB3	1:M:164:ILE:HG23	1.95	0.47
1:O:187:GLU:HG3	1:O:188:TRP:N	2.29	0.47
1:J:224:THR:OG1	1:J:225:GLN:N	2.47	0.47
1:N:369:MET:HB2	1:N:376:GLY:HA3	1.97	0.47
1:P:430:VAL:HG22	1:P:441:ALA:HB2	1.96	0.47
1:C:300:ARG:HG3	1:C:323:LEU:HB2	1.94	0.47
1:L:92:PHE:HB2	1:L:379:LEU:CD2	2.44	0.47
1:G:159:VAL:HG11	1:G:165:PRO:HA	1.97	0.47
1:H:276:GLU:HB3	1:H:349:LYS:HG3	1.96	0.47
1:I:223:ARG:HD2	4:I:1:G39:H912	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:223:ARG:CG	4:O:1:G39:H112	2.44	0.47
1:B:369:MET:HB2	1:B:376:GLY:HA3	1.95	0.47
1:L:147:ARG:HG2	1:L:439:HIS:CD2	2.50	0.47
1:N:297:THR:OG1	1:N:340:ASN:O	2.21	0.47
1:A:149:ASP:CG	4:A:1:G39:N4	2.73	0.47
1:C:409:TYR:HB2	1:C:428:GLU:OE1	2.14	0.47
1:D:101:HIS:C	1:D:103:PHE:H	2.21	0.47
1:G:225:GLN:NE2	1:G:238:LEU:HD12	2.29	0.47
1:I:314:ILE:C	1:I:315:ARG:HG2	2.39	0.47
1:N:139:PRO:HA	1:N:143:TYR:HH	1.79	0.47
1:O:315:ARG:HG3	1:O:388:TRP:CD2	2.50	0.47
1:A:187:GLU:HG3	1:A:188:TRP:N	2.30	0.47
1:J:203:LYS:HB3	1:K:449:MET:HE1	1.97	0.47
1:P:223:ARG:HD2	4:P:1:G39:H912	1.97	0.47
1:A:153:LEU:HD13	1:B:102:ARG:CZ	2.45	0.47
1:J:409:TYR:HB2	1:J:428:GLU:OE1	2.15	0.47
1:L:104:GLY:O	1:L:138:GLN:NE2	2.48	0.47
1:P:187:GLU:HG3	1:P:188:TRP:N	2.30	0.47
1:N:293:ASP:OD1	1:N:293:ASP:C	2.58	0.47
1:P:101:HIS:C	1:P:103:PHE:N	2.72	0.47
1:A:139:PRO:HA	1:A:143:TYR:HH	1.79	0.46
1:G:104:GLY:O	1:G:138:GLN:NE2	2.47	0.46
1:L:315:ARG:HG3	1:L:388:TRP:CE2	2.50	0.46
1:E:101:HIS:C	1:E:103:PHE:N	2.71	0.46
1:O:139:PRO:HA	1:O:143:TYR:OH	2.15	0.46
1:F:313:GLU:HB3	1:F:388:TRP:HH2	1.81	0.46
1:J:322:TYR:O	1:J:367:ARG:NH1	2.39	0.46
1:A:112:PRO:HD2	1:A:138:GLN:O	2.15	0.46
1:D:92:PHE:HB2	1:D:379:LEU:CD2	2.45	0.46
1:D:372:THR:CG2	1:L:433:GLY:O	2.63	0.46
1:M:370:SER:HB2	1:M:403:MET:SD	2.55	0.46
1:N:154:ARG:HG2	1:N:177:TRP:HA	1.98	0.46
1:F:369:MET:HB2	1:F:376:GLY:HA3	1.97	0.46
1:F:430:VAL:HG22	1:F:441:ALA:HB2	1.97	0.46
1:H:147:ARG:HD2	1:H:434:GLY:C	2.41	0.46
1:J:139:PRO:HA	1:J:143:TYR:OH	2.16	0.46
1:L:313:GLU:HB3	1:L:388:TRP:HH2	1.80	0.46
1:P:147:ARG:HG2	1:P:439:HIS:CD2	2.50	0.46
1:G:315:ARG:HB2	1:G:388:TRP:CD1	2.49	0.46
1:H:187:GLU:HG3	1:H:188:TRP:N	2.30	0.46
1:L:225:GLN:O	1:L:226:GLU:HB2	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:149:ASP:O	1:P:154:ARG:HD3	2.15	0.46
1:B:409:TYR:HB2	1:B:428:GLU:OE1	2.16	0.46
1:D:433:GLY:O	1:L:372:THR:CG2	2.64	0.46
1:F:302:PHE:HB2	1:F:317:MET:HG3	1.97	0.46
1:J:243:GLY:HA3	1:J:249:SER:HA	1.97	0.46
1:O:431:HIS:HB3	1:O:464:MET:SD	2.55	0.46
1:P:372:THR:HG22	1:P:372:THR:O	2.15	0.46
1:H:225:GLN:O	1:H:226:GLU:HB2	2.16	0.46
1:L:139:PRO:HA	1:L:143:TYR:OH	2.16	0.46
1:M:372:THR:O	1:M:372:THR:HG22	2.16	0.46
1:P:302:PHE:HB2	1:P:317:MET:HG3	1.97	0.46
1:B:223:ARG:CG	4:B:1:G39:H112	2.46	0.46
1:E:430:VAL:HA	1:E:441:ALA:HA	1.98	0.46
1:H:372:THR:O	1:H:372:THR:HG22	2.15	0.46
1:O:315:ARG:HB2	1:O:388:TRP:CD1	2.51	0.46
1:A:210:TYR:CZ	1:B:95:ALA:HB1	2.51	0.46
1:J:112:PRO:HD2	1:J:138:GLN:O	2.16	0.46
1:A:224:THR:OG1	1:A:225:GLN:N	2.48	0.45
1:A:295:SER:HB2	1:A:296:TYR:CD2	2.51	0.45
1:G:203:LYS:HB3	1:H:449:MET:CE	2.46	0.45
1:B:322:TYR:O	1:B:367:ARG:NH1	2.38	0.45
1:E:431:HIS:HB3	1:E:464:MET:SD	2.56	0.45
1:G:313:GLU:HB3	1:G:388:TRP:HH2	1.81	0.45
1:G:340:ASN:CB	1:G:341:GLY:HA2	2.46	0.45
1:H:224:THR:OG1	1:H:225:GLN:N	2.49	0.45
1:J:147:ARG:HG2	1:J:439:HIS:CD2	2.52	0.45
1:A:430:VAL:HA	1:A:441:ALA:HA	1.97	0.45
1:E:203:LYS:HB3	1:F:449:MET:CE	2.47	0.45
1:I:149:ASP:OD1	4:I:1:G39:N4	2.49	0.45
1:O:340:ASN:CB	1:O:341:GLY:HA2	2.46	0.45
1:E:139:PRO:HA	1:E:143:TYR:OH	2.15	0.45
1:K:198:ASN:HD22	1:K:198:ASN:N	2.04	0.45
1:N:198:ASN:HD22	1:N:198:ASN:N	2.00	0.45
1:O:150:ARG:HG2	1:O:177:TRP:CD2	2.52	0.45
1:P:104:GLY:O	1:P:138:GLN:NE2	2.49	0.45
1:A:92:PHE:HB2	1:A:379:LEU:CD2	2.47	0.45
1:B:150:ARG:HG2	1:B:177:TRP:CD2	2.51	0.45
1:C:372:THR:O	1:C:372:THR:HG22	2.16	0.45
1:D:401:VAL:CG1	1:D:405:GLU:HB2	2.46	0.45
1:E:313:GLU:HB3	1:E:388:TRP:HH2	1.81	0.45
1:F:198:ASN:H	1:F:198:ASN:ND2	2.01	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:275:GLU:OE2	4:H:1:G39:H812	2.17	0.45
1:L:230:ASN:HB3	1:L:281:PHE:CE2	2.52	0.45
1:D:104:GLY:O	1:D:138:GLN:NE2	2.50	0.45
1:I:203:LYS:HB3	1:J:449:MET:CE	2.47	0.45
1:J:430:VAL:HG22	1:J:441:ALA:HB2	1.99	0.45
1:M:225:GLN:O	1:M:226:GLU:HB2	2.16	0.45
1:C:369:MET:HB2	1:C:376:GLY:HA3	1.98	0.45
1:I:104:GLY:O	1:I:138:GLN:NE2	2.50	0.45
1:I:198:ASN:HD22	1:I:198:ASN:N	2.03	0.45
1:M:198:ASN:HD22	1:M:198:ASN:N	1.98	0.45
1:B:295:SER:HB2	1:B:296:TYR:CD2	2.52	0.45
1:C:101:HIS:C	1:C:103:PHE:N	2.74	0.45
1:I:187:GLU:HG3	1:I:188:TRP:N	2.30	0.45
1:I:340:ASN:CB	1:I:341:GLY:HA2	2.47	0.45
1:J:150:ARG:HG2	1:J:177:TRP:CD2	2.52	0.45
1:D:409:TYR:HB2	1:D:428:GLU:OE1	2.17	0.45
4:F:1:G39:H822	4:F:1:G39:H91	1.68	0.45
1:O:409:TYR:HB2	1:O:428:GLU:OE1	2.17	0.45
1:A:149:ASP:CG	4:A:1:G39:HN41	2.24	0.44
1:D:372:THR:HG21	1:L:433:GLY:O	2.17	0.44
1:F:230:ASN:HB3	1:F:281:PHE:CE2	2.52	0.44
1:G:100:PRO:HB3	1:G:164:ILE:HG23	1.98	0.44
1:I:92:PHE:HB2	1:I:379:LEU:CD2	2.48	0.44
1:K:104:GLY:O	1:K:138:GLN:NE2	2.51	0.44
1:E:150:ARG:HG2	1:E:177:TRP:CD2	2.51	0.44
1:F:411:PHE:CZ	1:F:426:GLY:HA3	2.53	0.44
1:F:465:ALA:CB	1:N:343:LYS:CG	2.96	0.44
1:H:101:HIS:C	1:H:103:PHE:N	2.71	0.44
1:A:409:TYR:HB2	1:A:428:GLU:OE1	2.16	0.44
1:E:159:VAL:HG11	1:E:165:PRO:HA	2.00	0.44
4:J:1:G39:H822	4:J:1:G39:H91	1.71	0.44
1:L:150:ARG:HG2	1:L:177:TRP:CD2	2.52	0.44
1:L:187:GLU:HG3	1:L:188:TRP:N	2.32	0.44
1:E:370:SER:HB2	1:E:403:MET:SD	2.58	0.44
1:H:297:THR:OG1	1:H:340:ASN:O	2.23	0.44
1:J:230:ASN:HB3	1:J:281:PHE:CE2	2.53	0.44
1:K:92:PHE:HB2	1:K:379:LEU:CD2	2.48	0.44
1:L:101:HIS:C	1:L:103:PHE:H	2.25	0.44
1:O:313:GLU:HB3	1:O:388:TRP:HH2	1.83	0.44
1:P:100:PRO:HB3	1:P:164:ILE:HG23	2.00	0.44
1:I:150:ARG:HG2	1:I:177:TRP:CD2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:119:PHE:HA	1:P:411:PHE:CZ	2.53	0.44
1:C:230:ASN:HB3	1:C:281:PHE:CE2	2.53	0.44
1:D:198:ASN:HD22	1:D:198:ASN:N	2.06	0.44
1:E:223:ARG:CD	4:E:1:G39:H912	2.48	0.44
1:E:224:THR:OG1	1:E:225:GLN:N	2.50	0.44
1:G:230:ASN:HB3	1:G:281:PHE:CE2	2.53	0.44
1:J:302:PHE:HB2	1:J:317:MET:HG3	1.99	0.44
1:K:150:ARG:HG2	1:K:177:TRP:CD2	2.53	0.44
1:E:340:ASN:CB	1:E:341:GLY:HA2	2.47	0.44
1:E:429:MET:HE2	1:E:460:THR:HG23	1.99	0.44
1:G:224:THR:OG1	1:G:225:GLN:N	2.50	0.44
1:J:177:TRP:CE2	1:J:194:ASP:HA	2.53	0.44
1:L:302:PHE:HB2	1:L:317:MET:HG3	1.98	0.44
1:N:401:VAL:CG1	1:N:405:GLU:HB2	2.48	0.44
1:O:297:THR:OG1	1:O:340:ASN:O	2.27	0.44
1:D:373:LYS:HE2	1:L:432:ASP:O	2.16	0.44
1:K:193:VAL:HG11	1:K:222:LEU:O	2.17	0.44
4:M:1:G39:H822	4:M:1:G39:H91	1.60	0.44
1:A:193:VAL:HG11	1:A:222:LEU:O	2.17	0.43
1:A:376:GLY:HA2	1:A:401:VAL:O	2.18	0.43
1:B:292:ARG:NH1	1:B:409:TYR:OH	2.50	0.43
1:B:370:SER:HB2	1:B:403:MET:SD	2.58	0.43
1:G:370:SER:HB2	1:G:403:MET:SD	2.58	0.43
1:J:92:PHE:HB2	1:J:379:LEU:CD2	2.48	0.43
1:J:340:ASN:CB	1:J:341:GLY:HA2	2.47	0.43
1:K:314:ILE:C	1:K:315:ARG:HG2	2.43	0.43
1:M:295:SER:HB2	1:M:296:TYR:CD2	2.53	0.43
1:C:340:ASN:CB	1:C:341:GLY:HA2	2.48	0.43
1:D:101:HIS:C	1:D:103:PHE:N	2.76	0.43
1:F:92:PHE:HB2	1:F:379:LEU:CD2	2.48	0.43
1:J:292:ARG:NH1	1:J:409:TYR:OH	2.50	0.43
1:O:401:VAL:CG1	1:O:405:GLU:HB2	2.47	0.43
1:C:92:PHE:HB2	1:C:379:LEU:CD2	2.48	0.43
1:C:370:SER:HB2	1:C:403:MET:SD	2.58	0.43
4:H:1:G39:H91	4:H:1:G39:H822	1.77	0.43
1:L:154:ARG:HG2	1:L:177:TRP:HA	2.00	0.43
1:L:430:VAL:HG22	1:L:441:ALA:HB2	2.01	0.43
1:O:101:HIS:C	1:O:103:PHE:N	2.77	0.43
1:A:198:ASN:HD22	1:A:198:ASN:N	2.02	0.43
1:B:293:ASP:OD1	1:B:293:ASP:C	2.61	0.43
1:D:272:LYS:HG2	1:D:296:TYR:CE2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:381:VAL:HG22	1:L:382:LYS:N	2.33	0.43
1:D:230:ASN:HB3	1:D:281:PHE:CE2	2.52	0.43
1:J:203:LYS:HB3	1:K:449:MET:CE	2.49	0.43
1:K:149:ASP:CG	4:K:1:G39:HN41	2.26	0.43
1:M:150:ARG:HG2	1:M:177:TRP:CD2	2.54	0.43
1:M:230:ASN:HB3	1:M:281:PHE:CE2	2.54	0.43
1:B:230:ASN:HB3	1:B:281:PHE:CE2	2.53	0.43
1:C:173:HIS:CE1	1:C:190:TYR:CE1	3.07	0.43
1:D:275:GLU:OE2	4:D:1:G39:H812	2.19	0.43
1:G:292:ARG:NH1	4:G:1:G39:O1B	2.49	0.43
1:K:272:LYS:HG2	1:K:296:TYR:CE2	2.54	0.43
1:A:300:ARG:HG3	1:A:323:LEU:HB2	2.00	0.43
1:C:139:PRO:HA	1:C:143:TYR:HH	1.83	0.43
4:C:1:G39:H822	4:C:1:G39:H92	1.75	0.43
1:I:293:ASP:OD1	1:I:293:ASP:C	2.61	0.43
1:K:177:TRP:CE2	1:K:194:ASP:HA	2.53	0.43
1:M:101:HIS:C	1:M:103:PHE:N	2.77	0.43
1:D:232:ILE:HB	1:D:281:PHE:CZ	2.54	0.43
1:H:149:ASP:CG	4:H:1:G39:N4	2.77	0.43
1:K:300:ARG:HG3	1:K:323:LEU:HB2	1.99	0.43
1:N:101:HIS:C	1:N:103:PHE:N	2.77	0.43
1:A:92:PHE:HB2	1:A:379:LEU:HD21	2.01	0.43
1:B:225:GLN:O	1:B:226:GLU:HB2	2.18	0.43
1:E:214:TYR:OH	1:E:264:GLU:OE1	2.29	0.43
1:E:315:ARG:HG3	1:E:388:TRP:CD2	2.54	0.43
1:H:92:PHE:HB2	1:H:379:LEU:CD2	2.49	0.43
1:K:315:ARG:HG3	1:K:388:TRP:CE2	2.54	0.43
1:L:159:VAL:HG11	1:L:165:PRO:HA	2.01	0.43
1:N:177:TRP:CE2	1:N:194:ASP:HA	2.53	0.43
1:P:401:VAL:CG1	1:P:405:GLU:HB2	2.49	0.43
1:A:117:GLU:OE2	4:A:1:G39:N4	2.52	0.43
1:C:193:VAL:HG11	1:C:222:LEU:O	2.19	0.43
1:E:104:GLY:O	1:E:138:GLN:NE2	2.51	0.43
1:G:92:PHE:HB2	1:G:379:LEU:CD2	2.48	0.43
1:I:370:SER:HB2	1:I:403:MET:SD	2.59	0.43
1:L:225:GLN:NE2	1:L:238:LEU:HD12	2.34	0.43
1:M:172:PHE:N	1:M:172:PHE:CD2	2.87	0.43
1:M:340:ASN:CB	1:M:341:GLY:HA2	2.49	0.43
1:P:300:ARG:NH2	6:P:2015:HOH:O	2.29	0.43
1:D:112:PRO:HD2	1:D:138:GLN:O	2.18	0.42
1:D:172:PHE:N	1:D:172:PHE:CD2	2.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:232:ILE:HB	1:E:281:PHE:CZ	2.54	0.42
1:J:223:ARG:HD2	4:J:1:G39:C91	2.43	0.42
1:J:315:ARG:HG3	1:J:388:TRP:CE2	2.54	0.42
1:J:401:VAL:CG1	1:J:405:GLU:HB2	2.49	0.42
1:L:136:ALA:HB1	6:L:2019:HOH:O	2.19	0.42
1:D:154:ARG:HG2	1:D:177:TRP:HA	1.99	0.42
1:J:198:ASN:H	1:J:198:ASN:ND2	2.07	0.42
1:L:224:THR:OG1	1:L:225:GLN:N	2.51	0.42
1:L:401:VAL:CG1	1:L:405:GLU:HB2	2.49	0.42
1:N:211:THR:HG22	1:O:417:ASP:OD2	2.18	0.42
1:A:449:MET:HE2	1:D:203:LYS:HB3	2.00	0.42
1:E:198:ASN:H	1:E:198:ASN:ND2	2.12	0.42
1:E:213:THR:HG22	1:F:449:MET:HE2	2.02	0.42
1:I:313:GLU:OE2	1:I:315:ARG:NH2	2.20	0.42
1:J:101:HIS:C	1:J:103:PHE:H	2.27	0.42
1:N:92:PHE:HB2	1:N:379:LEU:CD2	2.50	0.42
1:A:225:GLN:O	1:A:226:GLU:HB2	2.19	0.42
1:A:230:ASN:HB3	1:A:281:PHE:CE2	2.55	0.42
1:B:92:PHE:HB2	1:B:379:LEU:CD2	2.49	0.42
1:D:372:THR:HG22	1:D:372:THR:O	2.19	0.42
1:E:92:PHE:HB2	1:E:379:LEU:CD2	2.49	0.42
1:E:142:TYR:CZ	1:F:466:LEU:HD12	2.53	0.42
1:F:370:SER:HB2	1:F:403:MET:SD	2.59	0.42
1:I:369:MET:HB2	1:I:376:GLY:HA3	2.00	0.42
1:J:295:SER:HB2	1:J:296:TYR:CD2	2.54	0.42
1:K:430:VAL:HG22	1:K:441:ALA:HB2	2.01	0.42
1:M:139:PRO:HD2	6:M:2027:HOH:O	2.18	0.42
1:N:401:VAL:HG12	1:N:405:GLU:HB2	2.01	0.42
1:O:302:PHE:HB2	1:O:317:MET:HG3	2.00	0.42
1:A:232:ILE:HB	1:A:281:PHE:CZ	2.54	0.42
1:G:118:PRO:O	1:G:119:PHE:HB3	2.19	0.42
1:H:401:VAL:CG1	1:H:405:GLU:HB2	2.49	0.42
1:L:293:ASP:OD1	1:L:293:ASP:C	2.63	0.42
1:M:92:PHE:HB2	1:M:379:LEU:CD2	2.49	0.42
1:N:368:THR:HA	1:N:376:GLY:O	2.18	0.42
1:N:430:VAL:HA	1:N:441:ALA:HA	2.02	0.42
1:F:381:VAL:HG22	1:F:382:LYS:N	2.33	0.42
1:I:295:SER:HB2	1:I:296:TYR:CD2	2.55	0.42
1:M:232:ILE:HB	1:M:281:PHE:CZ	2.55	0.42
1:N:230:ASN:HB3	1:N:281:PHE:CE2	2.55	0.42
1:A:225:GLN:NE2	1:A:238:LEU:HD12	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:203:LYS:HB3	1:D:449:MET:CE	2.49	0.42
1:D:139:PRO:HA	1:D:143:TYR:OH	2.20	0.42
1:F:315:ARG:HB2	1:F:388:TRP:CD1	2.54	0.42
1:F:401:VAL:CG1	1:F:405:GLU:HB2	2.50	0.42
1:H:430:VAL:HG22	1:H:441:ALA:HB2	2.01	0.42
1:K:224:THR:OG1	1:K:225:GLN:N	2.53	0.42
1:M:414:GLU:HA	1:M:422:VAL:O	2.19	0.42
1:O:177:TRP:CE2	1:O:194:ASP:HA	2.55	0.42
1:O:225:GLN:NE2	1:O:238:LEU:HD12	2.34	0.42
1:P:293:ASP:OD1	1:P:293:ASP:C	2.63	0.42
1:P:401:VAL:HG12	1:P:405:GLU:HB2	2.01	0.42
1:C:139:PRO:HA	1:C:143:TYR:OH	2.20	0.42
1:D:430:VAL:HG22	1:D:441:ALA:HB2	2.02	0.42
1:G:302:PHE:HB2	1:G:317:MET:HG3	2.00	0.42
1:K:369:MET:HB2	1:K:376:GLY:HA3	2.01	0.42
1:J:411:PHE:CZ	1:J:426:GLY:HA3	2.54	0.42
1:M:401:VAL:CG1	1:M:405:GLU:HB2	2.50	0.42
1:C:210:TYR:CZ	1:D:95:ALA:HB1	2.55	0.42
1:D:300:ARG:HG3	1:D:323:LEU:HB2	2.02	0.42
1:E:401:VAL:CG1	1:E:405:GLU:HB2	2.50	0.42
1:L:198:ASN:H	1:L:198:ASN:ND2	2.03	0.42
1:C:142:TYR:CZ	1:D:466:LEU:HD12	2.55	0.41
1:C:302:PHE:HB2	1:C:317:MET:HG3	2.02	0.41
1:D:100:PRO:HB3	1:D:164:ILE:HG23	2.01	0.41
1:H:313:GLU:HB3	1:H:388:TRP:HH2	1.85	0.41
1:I:224:THR:OG1	1:I:225:GLN:N	2.53	0.41
1:J:368:THR:HA	1:J:376:GLY:O	2.20	0.41
1:N:147:ARG:HG2	1:N:439:HIS:CD2	2.55	0.41
1:N:183:HIS:HD2	1:N:185:GLY:N	2.07	0.41
1:C:277:CYS:HB3	1:C:289:CYS:CB	2.47	0.41
1:D:373:LYS:HE3	1:L:432:ASP:O	2.18	0.41
1:D:381:VAL:HG22	1:D:382:LYS:N	2.35	0.41
1:G:401:VAL:CG1	1:G:405:GLU:HB2	2.50	0.41
1:B:430:VAL:HG22	1:B:441:ALA:HB2	2.02	0.41
1:C:118:PRO:O	1:C:119:PHE:HB3	2.20	0.41
1:D:291:CYS:SG	1:D:303:VAL:HG23	2.60	0.41
1:F:409:TYR:OH	4:F:1:G39:C2	2.68	0.41
1:I:198:ASN:H	1:I:198:ASN:ND2	2.11	0.41
1:J:372:THR:O	1:J:372:THR:HG22	2.20	0.41
1:L:313:GLU:OE2	1:L:315:ARG:NH2	2.34	0.41
1:M:313:GLU:HB3	1:M:388:TRP:HH2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:292:ARG:NH1	1:N:409:TYR:OH	2.52	0.41
1:O:300:ARG:HG3	1:O:323:LEU:HB2	2.03	0.41
1:B:101:HIS:C	1:B:103:PHE:H	2.27	0.41
1:B:382:LYS:CD	6:B:2013:HOH:O	2.67	0.41
1:D:225:GLN:O	1:D:226:GLU:HB2	2.19	0.41
1:J:369:MET:HB2	1:J:376:GLY:HA3	2.02	0.41
1:O:230:ASN:HB3	1:O:281:PHE:CE2	2.56	0.41
1:O:372:THR:O	1:O:372:THR:HG22	2.20	0.41
1:D:177:TRP:CE2	1:D:194:ASP:HA	2.55	0.41
1:I:118:PRO:O	1:I:119:PHE:HB3	2.21	0.41
1:J:225:GLN:O	1:J:226:GLU:HB2	2.20	0.41
1:P:428:GLU:HG2	1:P:430:VAL:HG23	2.03	0.41
1:A:302:PHE:HB2	1:A:317:MET:HG3	2.03	0.41
1:B:372:THR:O	1:B:372:THR:HG22	2.20	0.41
1:C:224:THR:OG1	1:C:225:GLN:N	2.54	0.41
1:D:243:GLY:HA3	1:D:249:SER:HA	2.02	0.41
1:G:101:HIS:C	1:G:103:PHE:N	2.76	0.41
1:G:381:VAL:HG22	1:G:382:LYS:N	2.34	0.41
1:I:210:TYR:CZ	1:J:95:ALA:HB1	2.56	0.41
1:I:215:HIS:NE2	1:J:451:SER:O	2.50	0.41
1:I:275:GLU:OE2	4:I:1:G39:H812	2.21	0.41
1:M:115:ILE:O	1:M:440:SER:HA	2.21	0.41
1:M:180:SER:OG	1:M:227:SER:O	2.36	0.41
1:A:315:ARG:HB2	1:A:388:TRP:CD1	2.56	0.41
1:B:225:GLN:NE2	1:B:238:LEU:HD12	2.36	0.41
1:B:340:ASN:CB	1:B:341:GLY:HA2	2.50	0.41
1:F:147:ARG:HG2	1:F:439:HIS:CD2	2.56	0.41
1:I:177:TRP:CE2	1:I:194:ASP:HA	2.55	0.41
1:I:193:VAL:CG2	1:I:202:LEU:HD12	2.50	0.41
1:J:428:GLU:HG2	1:J:430:VAL:HG23	2.03	0.41
1:K:159:VAL:HG11	1:K:165:PRO:HA	2.03	0.41
1:M:224:THR:OG1	1:M:225:GLN:N	2.52	0.41
1:O:147:ARG:HD2	1:O:434:GLY:C	2.45	0.41
1:O:159:VAL:HG11	1:O:165:PRO:HA	2.03	0.41
1:O:198:ASN:H	1:O:198:ASN:ND2	2.01	0.41
1:B:194:ASP:OD1	1:B:203:LYS:NZ	2.54	0.41
1:D:315:ARG:HG3	1:D:388:TRP:CE2	2.56	0.41
1:G:118:PRO:HA	1:G:130:PHE:O	2.20	0.41
1:H:369:MET:HB2	1:H:376:GLY:HA3	2.02	0.41
1:N:198:ASN:H	1:N:198:ASN:ND2	2.06	0.41
1:A:150:ARG:HG2	1:A:177:TRP:CD2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:414:GLU:HA	1:A:422:VAL:O	2.21	0.41
1:D:150:ARG:HG2	1:D:177:TRP:CD2	2.55	0.41
1:D:224:THR:OG1	1:D:225:GLN:N	2.52	0.41
1:E:100:PRO:HG3	1:E:165:PRO:HD2	2.01	0.41
1:E:357:MET:O	1:E:358:ALA:C	2.64	0.41
1:F:263:LYS:NZ	1:F:310:ASP:OD2	2.47	0.41
1:G:150:ARG:HG2	1:G:177:TRP:CD2	2.55	0.41
1:H:100:PRO:HB3	1:H:164:ILE:HG23	2.03	0.41
1:J:232:ILE:HB	1:J:281:PHE:CZ	2.56	0.41
1:K:150:ARG:NH1	4:K:1:G39:O10	2.50	0.41
1:K:340:ASN:CB	1:K:341:GLY:HA2	2.51	0.41
1:L:272:LYS:HG2	1:L:296:TYR:CE2	2.56	0.41
1:M:147:ARG:HD2	1:M:434:GLY:C	2.46	0.41
1:N:300:ARG:HG3	1:N:323:LEU:HB2	2.03	0.41
1:N:351:GLY:N	1:N:410:SER:OG	2.53	0.41
1:O:178:SER:HB3	1:O:193:VAL:HB	2.03	0.41
1:D:149:ASP:CG	4:D:1:G39:N4	2.79	0.41
1:D:295:SER:HB2	1:D:296:TYR:CD2	2.56	0.41
1:D:370:SER:HB2	1:D:403:MET:SD	2.61	0.41
1:D:433:GLY:O	1:L:372:THR:HG21	2.21	0.41
1:E:115:ILE:H	1:E:440:SER:HG	1.69	0.41
1:E:245:ALA:HB1	4:E:1:G39:H822	2.02	0.41
1:H:430:VAL:HA	1:H:441:ALA:HA	2.03	0.41
1:I:300:ARG:HG3	1:I:323:LEU:HB2	2.03	0.41
1:J:381:VAL:HG22	1:J:382:LYS:N	2.36	0.41
1:L:177:TRP:CE2	1:L:194:ASP:HA	2.56	0.41
1:N:149:ASP:O	1:N:154:ARG:HD3	2.20	0.41
1:O:172:PHE:CD2	1:O:172:PHE:N	2.89	0.41
1:D:322:TYR:O	1:D:367:ARG:NH1	2.42	0.40
1:G:172:PHE:N	1:G:172:PHE:CD2	2.89	0.40
1:G:232:ILE:HB	1:G:281:PHE:CZ	2.56	0.40
1:M:430:VAL:HA	1:M:441:ALA:HA	2.02	0.40
1:A:139:PRO:HA	1:A:143:TYR:OH	2.22	0.40
1:A:401:VAL:CG1	1:A:405:GLU:HB2	2.51	0.40
1:B:314:ILE:C	1:B:315:ARG:HG2	2.45	0.40
1:C:232:ILE:HB	1:C:281:PHE:CZ	2.56	0.40
1:I:155:HIS:CE1	1:J:97:LEU:HB3	2.57	0.40
1:N:225:GLN:O	1:N:226:GLU:HB2	2.20	0.40
1:N:295:SER:HB2	1:N:296:TYR:CD2	2.56	0.40
1:A:300:ARG:NH2	6:A:2015:HOH:O	2.25	0.40
1:C:153:LEU:HD13	1:D:102:ARG:CZ	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:112:PRO:HD2	1:F:138:GLN:O	2.21	0.40
1:I:193:VAL:HG11	1:I:222:LEU:O	2.21	0.40
1:O:232:ILE:HB	1:O:281:PHE:CZ	2.57	0.40
1:P:225:GLN:O	1:P:226:GLU:HB2	2.20	0.40
1:A:177:TRP:CE2	1:A:194:ASP:HA	2.57	0.40
1:B:272:LYS:HG2	1:B:296:TYR:CE2	2.57	0.40
1:C:155:HIS:CE1	1:D:97:LEU:HB3	2.57	0.40
1:G:147:ARG:HD2	1:G:434:GLY:C	2.46	0.40
1:H:315:ARG:HB2	1:H:388:TRP:CD1	2.56	0.40
1:K:295:SER:HB2	1:K:296:TYR:CD2	2.56	0.40
1:L:243:GLY:HA3	1:L:249:SER:HA	2.04	0.40
1:L:295:SER:HB2	1:L:296:TYR:CD2	2.56	0.40
1:L:429:MET:HE2	1:L:460:THR:HG23	2.02	0.40
1:P:381:VAL:HG22	1:P:382:LYS:N	2.36	0.40
1:B:118:PRO:HA	1:B:130:PHE:O	2.21	0.40
1:B:177:TRP:CE2	1:B:194:ASP:HA	2.56	0.40
1:C:149:ASP:O	1:C:154:ARG:HD3	2.22	0.40
1:E:325:THR:HG1	1:E:368:THR:HG1	1.69	0.40
1:F:300:ARG:HG3	1:F:323:LEU:HB2	2.04	0.40
1:F:430:VAL:HA	1:F:441:ALA:HA	2.04	0.40
1:I:260:ARG:HH21	1:J:87:CYS:HB3	1.86	0.40
1:L:431:HIS:HB3	1:L:464:MET:SD	2.60	0.40
4:L:1:G39:H822	4:L:1:G39:H91	1.66	0.40
1:M:95:ALA:HB1	1:P:210:TYR:CZ	2.57	0.40
1:N:150:ARG:HG2	1:N:177:TRP:CD2	2.55	0.40
1:O:154:ARG:HG2	1:O:177:TRP:HA	2.03	0.40
1:O:295:SER:HB2	1:O:296:TYR:CD2	2.57	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:B:343:LYS:NZ	1:J:436:GLU:O[1_554]	1.80	0.40
1:B:436:GLU:O	1:J:343:LYS:NZ[1_554]	1.86	0.34
1:C:315:ARG:NH2	1:H:217:TYR:O[1_556]	1.99	0.21
1:D:315:ARG:NH2	1:G:217:TYR:O[1_546]	2.04	0.16
1:I:315:ARG:NH2	1:N:217:TYR:O[1_446]	2.11	0.09
1:A:315:ARG:NH2	1:F:217:TYR:O[1_545]	2.12	0.08
1:J:315:ARG:NH2	1:M:217:TYR:O[1_456]	2.15	0.05
1:K:315:ARG:NH2	1:P:217:TYR:O[1_455]	2.15	0.05
1:L:315:ARG:NH2	1:O:217:TYR:O[1_445]	2.16	0.04

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	387/397 (98%)	359 (93%)	25 (6%)	3 (1%)	16	34
1	B	387/397 (98%)	360 (93%)	24 (6%)	3 (1%)	16	34
1	C	387/397 (98%)	358 (92%)	27 (7%)	2 (0%)	24	46
1	D	387/397 (98%)	361 (93%)	23 (6%)	3 (1%)	16	34
1	E	387/397 (98%)	359 (93%)	24 (6%)	4 (1%)	12	28
1	F	387/397 (98%)	361 (93%)	23 (6%)	3 (1%)	16	34
1	G	387/397 (98%)	363 (94%)	20 (5%)	4 (1%)	12	28
1	H	387/397 (98%)	359 (93%)	25 (6%)	3 (1%)	16	34
1	I	387/397 (98%)	361 (93%)	24 (6%)	2 (0%)	24	46
1	J	387/397 (98%)	357 (92%)	29 (8%)	1 (0%)	36	58
1	K	387/397 (98%)	361 (93%)	24 (6%)	2 (0%)	24	46
1	L	387/397 (98%)	359 (93%)	25 (6%)	3 (1%)	16	34
1	M	387/397 (98%)	362 (94%)	23 (6%)	2 (0%)	24	46
1	N	387/397 (98%)	359 (93%)	27 (7%)	1 (0%)	36	58
1	O	387/397 (98%)	361 (93%)	23 (6%)	3 (1%)	16	34
1	P	387/397 (98%)	363 (94%)	23 (6%)	1 (0%)	36	58
All	All	6192/6352 (98%)	5763 (93%)	389 (6%)	40 (1%)	21	42

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	199	ASN
1	B	199	ASN
1	B	219	ASN
1	D	199	ASN
1	E	219	ASN
1	F	199	ASN

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Mol	Chain	Res	Type
1	F	219	ASN
1	G	199	ASN
1	O	219	ASN
1	A	384	ASP
1	C	384	ASP
1	D	219	ASN
1	E	199	ASN
1	G	219	ASN
1	H	199	ASN
1	I	199	ASN
1	M	199	ASN
1	E	352	PHE
1	G	200	ALA
1	J	403	MET
1	K	199	ASN
1	K	340	ASN
1	L	199	ASN
1	L	384	ASP
1	O	199	ASN
1	A	199	ASN
1	H	200	ALA
1	N	221	ILE
1	B	221	ILE
1	D	221	ILE
1	E	221	ILE
1	F	221	ILE
1	H	221	ILE
1	M	221	ILE
1	A	221	ILE
1	G	221	ILE
1	I	221	ILE
1	L	221	ILE
1	O	221	ILE
1	P	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	320/329 (97%)	304 (95%)	16 (5%)	22	46
1	B	320/329 (97%)	304 (95%)	16 (5%)	22	46
1	C	320/329 (97%)	304 (95%)	16 (5%)	22	46
1	D	320/329 (97%)	303 (95%)	17 (5%)	20	43
1	E	320/329 (97%)	304 (95%)	16 (5%)	22	46
1	F	320/329 (97%)	302 (94%)	18 (6%)	19	40
1	G	320/329 (97%)	303 (95%)	17 (5%)	20	43
1	H	320/329 (97%)	303 (95%)	17 (5%)	20	43
1	I	320/329 (97%)	303 (95%)	17 (5%)	20	43
1	J	320/329 (97%)	303 (95%)	17 (5%)	20	43
1	K	320/329 (97%)	302 (94%)	18 (6%)	19	40
1	L	320/329 (97%)	302 (94%)	18 (6%)	19	40
1	M	320/329 (97%)	304 (95%)	16 (5%)	22	46
1	N	320/329 (97%)	303 (95%)	17 (5%)	20	43
1	O	320/329 (97%)	302 (94%)	18 (6%)	19	40
1	P	320/329 (97%)	303 (95%)	17 (5%)	20	43
All	All	5120/5264 (97%)	4849 (95%)	271 (5%)	20	43

All (271) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	84	ARG
1	A	85	LEU
1	A	106	THR
1	A	125	LYS
1	A	135	TYR
1	A	147	ARG
1	A	198	ASN
1	A	239	MET
1	A	241	THR
1	A	338	GLU
1	A	369	MET
1	A	382	LYS
1	A	394	LEU
1	A	416	LYS
1	A	455	LEU
1	A	456	TRP

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Mol	Chain	Res	Type
1	B	84	ARG
1	B	85	LEU
1	B	106	THR
1	B	125	LYS
1	B	135	TYR
1	B	198	ASN
1	B	229	CYS
1	B	239	MET
1	B	241	THR
1	B	338	GLU
1	B	369	MET
1	B	382	LYS
1	B	394	LEU
1	B	416	LYS
1	B	455	LEU
1	B	456	TRP
1	C	84	ARG
1	C	85	LEU
1	C	106	THR
1	C	125	LYS
1	C	135	TYR
1	C	147	ARG
1	C	198	ASN
1	C	239	MET
1	C	241	THR
1	C	338	GLU
1	C	369	MET
1	C	382	LYS
1	C	394	LEU
1	C	416	LYS
1	C	455	LEU
1	C	456	TRP
1	D	84	ARG
1	D	85	LEU
1	D	106	THR
1	D	125	LYS
1	D	135	TYR
1	D	147	ARG
1	D	198	ASN
1	D	229	CYS
1	D	239	MET
1	D	241	THR

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Mol	Chain	Res	Type
1	D	338	GLU
1	D	369	MET
1	D	382	LYS
1	D	394	LEU
1	D	416	LYS
1	D	455	LEU
1	D	456	TRP
1	E	84	ARG
1	E	85	LEU
1	E	106	THR
1	E	125	LYS
1	E	135	TYR
1	E	147	ARG
1	E	198	ASN
1	E	239	MET
1	E	241	THR
1	E	338	GLU
1	E	369	MET
1	E	382	LYS
1	E	394	LEU
1	E	416	LYS
1	E	455	LEU
1	E	456	TRP
1	F	84	ARG
1	F	85	LEU
1	F	106	THR
1	F	125	LYS
1	F	135	TYR
1	F	147	ARG
1	F	191	ILE
1	F	198	ASN
1	F	229	CYS
1	F	239	MET
1	F	241	THR
1	F	338	GLU
1	F	369	MET
1	F	382	LYS
1	F	394	LEU
1	F	416	LYS
1	F	455	LEU
1	F	456	TRP
1	G	84	ARG

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Mol	Chain	Res	Type
1	G	85	LEU
1	G	106	THR
1	G	125	LYS
1	G	135	TYR
1	G	198	ASN
1	G	226	GLU
1	G	229	CYS
1	G	239	MET
1	G	241	THR
1	G	338	GLU
1	G	369	MET
1	G	382	LYS
1	G	394	LEU
1	G	416	LYS
1	G	455	LEU
1	G	456	TRP
1	H	84	ARG
1	H	85	LEU
1	H	106	THR
1	H	125	LYS
1	H	135	TYR
1	H	147	ARG
1	H	198	ASN
1	H	229	CYS
1	H	239	MET
1	H	241	THR
1	H	338	GLU
1	H	369	MET
1	H	382	LYS
1	H	394	LEU
1	H	416	LYS
1	H	455	LEU
1	H	456	TRP
1	I	84	ARG
1	I	85	LEU
1	I	106	THR
1	I	125	LYS
1	I	135	TYR
1	I	147	ARG
1	I	198	ASN
1	I	229	CYS
1	I	239	MET

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Mol	Chain	Res	Type
1	I	241	THR
1	I	338	GLU
1	I	369	MET
1	I	382	LYS
1	I	394	LEU
1	I	416	LYS
1	I	455	LEU
1	I	456	TRP
1	J	84	ARG
1	J	85	LEU
1	J	106	THR
1	J	125	LYS
1	J	135	TYR
1	J	147	ARG
1	J	198	ASN
1	J	229	CYS
1	J	239	MET
1	J	241	THR
1	J	338	GLU
1	J	369	MET
1	J	382	LYS
1	J	394	LEU
1	J	416	LYS
1	J	455	LEU
1	J	456	TRP
1	K	84	ARG
1	K	85	LEU
1	K	106	THR
1	K	115	ILE
1	K	125	LYS
1	K	135	TYR
1	K	147	ARG
1	K	198	ASN
1	K	229	CYS
1	K	239	MET
1	K	241	THR
1	K	338	GLU
1	K	369	MET
1	K	382	LYS
1	K	394	LEU
1	K	416	LYS
1	K	455	LEU

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Mol	Chain	Res	Type
1	K	456	TRP
1	L	84	ARG
1	L	85	LEU
1	L	106	THR
1	L	125	LYS
1	L	135	TYR
1	L	147	ARG
1	L	191	ILE
1	L	198	ASN
1	L	229	CYS
1	L	239	MET
1	L	241	THR
1	L	338	GLU
1	L	369	MET
1	L	382	LYS
1	L	394	LEU
1	L	416	LYS
1	L	455	LEU
1	L	456	TRP
1	M	84	ARG
1	M	85	LEU
1	M	106	THR
1	M	125	LYS
1	M	135	TYR
1	M	198	ASN
1	M	239	MET
1	M	241	THR
1	M	246	SER
1	M	338	GLU
1	M	369	MET
1	M	382	LYS
1	M	394	LEU
1	M	416	LYS
1	M	455	LEU
1	M	456	TRP
1	N	84	ARG
1	N	85	LEU
1	N	106	THR
1	N	125	LYS
1	N	135	TYR
1	N	147	ARG
1	N	191	ILE

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Mol	Chain	Res	Type
1	N	198	ASN
1	N	239	MET
1	N	241	THR
1	N	338	GLU
1	N	369	MET
1	N	382	LYS
1	N	394	LEU
1	N	416	LYS
1	N	455	LEU
1	N	456	TRP
1	O	84	ARG
1	O	85	LEU
1	O	106	THR
1	O	125	LYS
1	O	135	TYR
1	O	147	ARG
1	O	191	ILE
1	O	198	ASN
1	O	229	CYS
1	O	239	MET
1	O	241	THR
1	O	338	GLU
1	O	369	MET
1	O	382	LYS
1	O	394	LEU
1	O	416	LYS
1	O	455	LEU
1	O	456	TRP
1	P	84	ARG
1	P	85	LEU
1	P	106	THR
1	P	125	LYS
1	P	135	TYR
1	P	154	ARG
1	P	191	ILE
1	P	198	ASN
1	P	239	MET
1	P	241	THR
1	P	338	GLU
1	P	369	MET
1	P	382	LYS
1	P	394	LEU

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Mol	Chain	Res	Type
1	P	416	LYS
1	P	455	LEU
1	P	456	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (71) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	183	HIS
1	A	198	ASN
1	A	225	GLN
1	A	340	ASN
1	B	183	HIS
1	B	198	ASN
1	B	225	GLN
1	C	129	HIS
1	C	183	HIS
1	C	198	ASN
1	C	225	GLN
1	C	340	ASN
1	D	183	HIS
1	D	198	ASN
1	D	225	GLN
1	E	183	HIS
1	E	198	ASN
1	E	225	GLN
1	E	439	HIS
1	F	183	HIS
1	F	198	ASN
1	F	225	GLN
1	F	439	HIS
1	G	183	HIS
1	G	198	ASN
1	G	225	GLN
1	G	439	HIS
1	H	129	HIS
1	H	183	HIS
1	H	198	ASN
1	H	225	GLN
1	H	340	ASN
1	H	439	HIS
1	I	138	GLN
1	I	183	HIS

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Mol	Chain	Res	Type
1	I	198	ASN
1	I	225	GLN
1	I	235	ASN
1	J	183	HIS
1	J	198	ASN
1	J	225	GLN
1	J	439	HIS
1	K	129	HIS
1	K	183	HIS
1	K	198	ASN
1	K	225	GLN
1	L	138	GLN
1	L	183	HIS
1	L	198	ASN
1	L	225	GLN
1	L	235	ASN
1	L	439	HIS
1	M	183	HIS
1	M	198	ASN
1	M	225	GLN
1	M	439	HIS
1	N	129	HIS
1	N	183	HIS
1	N	198	ASN
1	N	225	GLN
1	N	439	HIS
1	O	138	GLN
1	O	183	HIS
1	O	198	ASN
1	O	225	GLN
1	O	439	HIS
1	P	129	HIS
1	P	183	HIS
1	P	198	ASN
1	P	225	GLN
1	P	439	HIS

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	$\# Z > 2$
4	G39	B	1	-	19,20,20	2.59	5 (26%)	20,27,27	4.37	10 (50%)
2	NAG	B	900	1	14,14,15	0.61	0	17,19,21	1.50	2 (11%)
4	G39	J	1	-	19,20,20	2.95	5 (26%)	20,27,27	3.93	11 (55%)
2	NAG	P	900	1	14,14,15	0.82	1 (7%)	17,19,21	1.73	2 (11%)
2	NAG	C	900	1	14,14,15	0.57	0	17,19,21	1.22	2 (11%)
4	G39	G	1	-	19,20,20	1.43	2 (10%)	20,27,27	3.65	9 (45%)
2	NAG	H	900	1	14,14,15	0.65	0	17,19,21	1.68	2 (11%)
2	NAG	I	900	1	14,14,15	0.69	0	17,19,21	1.50	3 (17%)
2	NAG	J	900	1	14,14,15	0.42	0	17,19,21	1.11	1 (5%)
2	NAG	K	900	1	14,14,15	0.62	0	17,19,21	1.34	2 (11%)
4	G39	C	1	-	19,20,20	1.49	2 (10%)	20,27,27	3.00	8 (40%)
2	NAG	G	900	1	14,14,15	0.64	0	17,19,21	1.80	3 (17%)
4	G39	A	1	-	19,20,20	2.01	2 (10%)	20,27,27	3.02	6 (30%)
4	G39	F	1	-	19,20,20	1.08	1 (5%)	20,27,27	4.38	10 (50%)
2	NAG	O	900	1	14,14,15	0.50	0	17,19,21	1.57	2 (11%)
4	G39	M	1	-	19,20,20	1.44	1 (5%)	20,27,27	3.44	6 (30%)
4	G39	K	1	-	19,20,20	3.18	10 (52%)	20,27,27	3.17	6 (30%)
2	NAG	L	900	1	14,14,15	0.54	0	17,19,21	1.46	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	D	900	1	14,14,15	0.49	0	17,19,21	1.49	2 (11%)
4	G39	D	1	-	19,20,20	1.62	2 (10%)	20,27,27	3.75	12 (60%)
2	NAG	A	900	1	14,14,15	0.63	0	17,19,21	1.66	3 (17%)
4	G39	E	1	-	19,20,20	2.70	5 (26%)	20,27,27	4.07	7 (35%)
4	G39	H	1	-	19,20,20	2.23	5 (26%)	20,27,27	5.36	11 (55%)
4	G39	I	1	-	19,20,20	2.08	3 (15%)	20,27,27	2.27	6 (30%)
4	G39	O	1	-	19,20,20	1.92	2 (10%)	20,27,27	3.01	7 (35%)
2	NAG	E	900	1	14,14,15	0.51	0	17,19,21	1.85	3 (17%)
4	G39	L	1	-	19,20,20	2.62	3 (15%)	20,27,27	3.96	9 (45%)
2	NAG	F	900	1	14,14,15	0.76	0	17,19,21	1.61	2 (11%)
4	G39	P	1	-	19,20,20	1.42	3 (15%)	20,27,27	2.92	8 (40%)
4	G39	N	1	-	19,20,20	1.56	2 (10%)	20,27,27	2.85	10 (50%)
2	NAG	N	900	1	14,14,15	0.88	1 (7%)	17,19,21	1.73	2 (11%)
2	NAG	M	900	1	14,14,15	0.54	0	17,19,21	1.75	2 (11%)

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	G39	B	1	-	-	2/16/32/32	0/1/1/1
2	NAG	B	900	1	-	0/6/23/26	0/1/1/1
4	G39	J	1	-	-	3/16/32/32	0/1/1/1
2	NAG	P	900	1	-	0/6/23/26	0/1/1/1
2	NAG	C	900	1	-	0/6/23/26	0/1/1/1
4	G39	G	1	-	-	4/16/32/32	0/1/1/1
2	NAG	H	900	1	-	0/6/23/26	0/1/1/1
2	NAG	I	900	1	-	0/6/23/26	0/1/1/1
2	NAG	J	900	1	-	0/6/23/26	0/1/1/1
2	NAG	K	900	1	-	0/6/23/26	0/1/1/1
4	G39	C	1	-	-	4/16/32/32	0/1/1/1
2	NAG	G	900	1	-	0/6/23/26	0/1/1/1
4	G39	A	1	-	-	0/16/32/32	0/1/1/1
4	G39	F	1	-	-	2/16/32/32	0/1/1/1
2	NAG	O	900	1	-	0/6/23/26	0/1/1/1
4	G39	M	1	-	-	2/16/32/32	0/1/1/1
4	G39	K	1	-	-	5/16/32/32	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	L	900	1	-	0/6/23/26	0/1/1/1
2	NAG	D	900	1	-	0/6/23/26	0/1/1/1
4	G39	D	1	-	-	5/16/32/32	0/1/1/1
2	NAG	A	900	1	-	0/6/23/26	0/1/1/1
4	G39	E	1	-	-	2/16/32/32	0/1/1/1
4	G39	H	1	-	-	0/16/32/32	0/1/1/1
4	G39	I	1	-	-	0/16/32/32	0/1/1/1
4	G39	O	1	-	-	2/16/32/32	0/1/1/1
2	NAG	E	900	1	-	0/6/23/26	0/1/1/1
4	G39	L	1	-	-	1/16/32/32	0/1/1/1
2	NAG	F	900	1	-	0/6/23/26	0/1/1/1
4	G39	P	1	-	-	4/16/32/32	0/1/1/1
4	G39	N	1	-	-	6/16/32/32	0/1/1/1
2	NAG	N	900	1	-	0/6/23/26	0/1/1/1
2	NAG	M	900	1	-	0/6/23/26	0/1/1/1

All (55) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	J	1	G39	C1-C2	-9.15	1.28	1.49
4	L	1	G39	C1-C2	-9.01	1.28	1.49
4	B	1	G39	C1-C2	-8.59	1.29	1.49
4	H	1	G39	C1-C2	-7.73	1.31	1.49
4	J	1	G39	C6-C7	7.34	1.60	1.50
4	K	1	G39	C5-N5	-7.29	1.34	1.45
4	I	1	G39	C1-C2	-7.08	1.33	1.49
4	A	1	G39	C1-C2	-7.01	1.33	1.49
4	E	1	G39	C1-C2	-6.90	1.33	1.49
4	O	1	G39	C1-C2	-6.83	1.33	1.49
4	K	1	G39	C1-C2	-6.23	1.35	1.49
4	E	1	G39	O1B-C1	-5.70	1.15	1.30
4	N	1	G39	C4-C5	-5.49	1.46	1.53
4	E	1	G39	C4-C5	-5.27	1.46	1.53
4	D	1	G39	C6-C7	5.21	1.57	1.50
4	L	1	G39	C6-C7	5.17	1.57	1.50
4	C	1	G39	C1-C2	-5.09	1.37	1.49
4	G	1	G39	C1-C2	-4.60	1.38	1.49
4	M	1	G39	C1-C2	-4.49	1.39	1.49
4	K	1	G39	C3-C4	4.40	1.61	1.54
4	B	1	G39	O1B-C1	-3.96	1.19	1.30
4	B	1	G39	C6-C7	3.82	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	P	1	G39	C4-C5	-3.76	1.48	1.53
4	D	1	G39	C1-C2	-3.75	1.40	1.49
4	K	1	G39	C3-C2	3.68	1.57	1.51
4	K	1	G39	O1B-C1	-3.58	1.20	1.30
4	I	1	G39	O1B-C1	-3.43	1.21	1.30
4	O	1	G39	O1B-C1	-3.38	1.21	1.30
4	P	1	G39	C1-C2	-3.33	1.41	1.49
4	K	1	G39	O7-C6	3.28	1.50	1.44
4	K	1	G39	C10-N5	3.26	1.44	1.34
4	A	1	G39	O1B-C1	-3.25	1.21	1.30
4	B	1	G39	C3-C4	3.16	1.59	1.54
4	E	1	G39	C3-C2	-3.13	1.46	1.51
4	K	1	G39	O10-C10	3.08	1.30	1.23
4	H	1	G39	C6-C7	3.05	1.54	1.50
4	E	1	G39	C3-C4	-3.03	1.49	1.54
4	K	1	G39	C4-C5	-2.97	1.49	1.53
4	B	1	G39	O7-C6	2.69	1.49	1.44
4	F	1	G39	C1-C2	-2.64	1.43	1.49
4	J	1	G39	O7-C6	2.60	1.49	1.44
2	N	900	NAG	C1-C2	2.49	1.55	1.52
4	K	1	G39	O1A-C1	-2.46	1.16	1.22
4	N	1	G39	O1B-C1	-2.35	1.24	1.30
4	G	1	G39	C4-C5	-2.35	1.50	1.53
4	H	1	G39	C4-C5	2.32	1.55	1.53
4	H	1	G39	O7-C6	2.31	1.48	1.44
4	P	1	G39	O1B-C1	-2.30	1.24	1.30
4	J	1	G39	O1B-C1	-2.25	1.24	1.30
4	L	1	G39	C10-N5	2.21	1.41	1.34
2	P	900	NAG	C1-C2	2.13	1.55	1.52
4	J	1	G39	C3-C4	2.09	1.57	1.54
4	I	1	G39	C6-C7	2.08	1.53	1.50
4	C	1	G39	C11-C10	2.05	1.54	1.50
4	H	1	G39	O1B-C1	-2.05	1.25	1.30

All (172) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	1	G39	C6-C5-N5	-14.56	94.79	111.13
4	H	1	G39	C3-C2-C7	13.84	139.31	122.25
4	E	1	G39	C3-C2-C7	12.59	137.77	122.25
4	J	1	G39	O1A-C1-C2	-9.79	104.48	121.64
4	D	1	G39	C7-C2-C1	-9.48	107.03	119.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	1	G39	C7-C2-C1	-9.37	107.18	119.99
4	M	1	G39	O1B-C1-C2	9.25	134.96	115.43
4	H	1	G39	C6-C5-N5	-9.24	100.77	111.13
4	M	1	G39	O1A-C1-C2	-8.90	106.03	121.64
4	L	1	G39	O1A-C1-C2	-8.82	106.18	121.64
4	G	1	G39	C3-C2-C7	8.67	132.94	122.25
4	B	1	G39	C3-C2-C7	-8.55	111.71	122.25
4	L	1	G39	O1B-C1-O1A	8.10	143.20	123.90
4	K	1	G39	C5-N5-C10	8.10	142.07	123.11
4	H	1	G39	O1B-C1-O1A	8.02	142.99	123.90
4	B	1	G39	C4-C3-C2	7.95	118.72	109.72
4	O	1	G39	O1A-C1-C2	-7.93	107.75	121.64
4	J	1	G39	O1B-C1-O1A	7.71	142.25	123.90
4	A	1	G39	C3-C2-C7	7.63	131.66	122.25
4	B	1	G39	O1B-C1-C2	-7.48	99.63	115.43
4	H	1	G39	O1A-C1-C2	-7.21	109.00	121.64
4	J	1	G39	C6-C5-N5	-7.20	103.06	111.13
4	C	1	G39	C3-C2-C7	7.03	130.92	122.25
4	L	1	G39	C5-N5-C10	6.98	139.45	123.11
4	B	1	G39	O1B-C1-O1A	6.92	140.39	123.90
4	L	1	G39	C3-C4-N4	-6.80	97.30	110.76
4	A	1	G39	C5-N5-C10	6.74	138.88	123.11
4	F	1	G39	O1B-C1-C2	6.69	129.56	115.43
4	P	1	G39	O1A-C1-C2	-6.62	110.03	121.64
4	G	1	G39	C7-C2-C1	-6.58	110.98	119.99
4	K	1	G39	O10-C10-N5	6.58	133.60	121.98
4	H	1	G39	C6-C7-C2	-6.51	112.53	122.66
4	E	1	G39	C6-C7-C2	-6.49	112.57	122.66
4	O	1	G39	O1B-C1-C2	6.38	128.92	115.43
4	G	1	G39	O1A-C1-C2	-6.38	110.46	121.64
4	F	1	G39	O1A-C1-C2	-6.27	110.65	121.64
4	D	1	G39	C5-N5-C10	6.27	137.79	123.11
4	P	1	G39	C3-C2-C7	6.20	129.89	122.25
4	I	1	G39	C3-C4-N4	-6.07	98.76	110.76
4	E	1	G39	C6-C5-N5	-6.06	104.33	111.13
4	K	1	G39	O10-C10-C11	-6.03	111.32	122.05
4	C	1	G39	O1A-C1-C2	-5.98	111.15	121.64
4	B	1	G39	C6-C5-N5	-5.84	104.58	111.13
4	G	1	G39	C6-C5-N5	-5.82	104.60	111.13
4	C	1	G39	C6-C7-C2	-5.80	113.63	122.66
2	E	900	NAG	C1-O5-C5	5.75	119.89	112.19
4	N	1	G39	O1B-C1-C2	5.69	127.45	115.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1	G39	C3-C2-C7	5.63	129.19	122.25
4	N	1	G39	O1A-C1-C2	-5.60	111.82	121.64
2	M	900	NAG	C1-O5-C5	5.49	119.54	112.19
4	G	1	G39	C6-C7-C2	-5.49	114.13	122.66
4	B	1	G39	C5-N5-C10	5.39	135.73	123.11
2	G	900	NAG	C1-O5-C5	5.34	119.35	112.19
4	O	1	G39	C4-C3-C2	5.33	115.75	109.72
4	L	1	G39	C7-C2-C1	-5.31	112.73	119.99
4	A	1	G39	C7-C2-C1	-5.26	112.80	119.99
4	E	1	G39	C7-C2-C1	-5.24	112.82	119.99
4	P	1	G39	C3-C4-N4	-5.20	100.46	110.76
4	M	1	G39	C3-C2-C7	5.19	128.65	122.25
2	P	900	NAG	C1-O5-C5	5.06	118.96	112.19
4	J	1	G39	C4-C3-C2	5.04	115.42	109.72
4	D	1	G39	C6-C5-N5	-5.00	105.53	111.13
4	D	1	G39	C3-C4-N4	-4.95	100.96	110.76
4	E	1	G39	C3-C2-C1	-4.95	107.90	116.99
4	N	1	G39	C4-C3-C2	4.92	115.29	109.72
4	B	1	G39	C11-C10-N5	-4.82	108.12	116.12
2	H	900	NAG	C1-O5-C5	4.75	118.55	112.19
4	B	1	G39	O10-C10-N5	4.69	130.27	121.98
2	O	900	NAG	C1-O5-C5	4.66	118.43	112.19
2	N	900	NAG	C1-O5-C5	4.63	118.39	112.19
4	K	1	G39	C7-C2-C1	-4.61	113.69	119.99
4	J	1	G39	C5-N5-C10	4.58	133.84	123.11
4	O	1	G39	C3-C2-C7	4.58	127.89	122.25
4	B	1	G39	C7-C2-C1	4.48	126.12	119.99
4	E	1	G39	C5-N5-C10	4.46	133.55	123.11
2	F	900	NAG	C1-O5-C5	4.41	118.09	112.19
4	N	1	G39	C6-C7-C2	-4.33	115.92	122.66
4	P	1	G39	O1B-C1-C2	4.20	124.31	115.43
4	P	1	G39	C4-C3-C2	-4.17	104.99	109.72
2	I	900	NAG	C1-O5-C5	4.14	117.74	112.19
2	A	900	NAG	C1-O5-C5	4.07	117.65	112.19
4	F	1	G39	C3-C2-C7	4.05	127.24	122.25
4	A	1	G39	O1A-C1-C2	-3.96	114.71	121.64
4	D	1	G39	O10-C10-N5	3.93	128.92	121.98
4	J	1	G39	O10-C10-N5	3.85	128.79	121.98
2	B	900	NAG	C1-O5-C5	3.84	117.34	112.19
4	I	1	G39	C6-C7-C2	-3.82	116.72	122.66
4	H	1	G39	O1B-C1-C2	-3.80	107.40	115.43
4	L	1	G39	O10-C10-C11	-3.79	115.31	122.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	1	G39	O7-C6-C7	3.73	117.86	109.19
4	D	1	G39	O1A-C1-C2	-3.72	115.13	121.64
2	A	900	NAG	C1-C2-N2	-3.71	104.58	110.43
2	L	900	NAG	C1-O5-C5	3.71	117.16	112.19
4	I	1	G39	O1B-C1-C2	3.70	123.25	115.43
4	M	1	G39	C6-C7-C2	-3.67	116.95	122.66
4	F	1	G39	C11-C10-N5	-3.66	110.05	116.12
4	E	1	G39	O1B-C1-C2	-3.64	107.75	115.43
4	C	1	G39	O1B-C1-O1A	3.55	132.35	123.90
4	C	1	G39	C5-N5-C10	3.51	131.32	123.11
4	A	1	G39	O7-C6-C7	3.48	117.28	109.19
2	D	900	NAG	C1-O5-C5	3.48	116.85	112.19
2	K	900	NAG	C1-O5-C5	3.44	116.80	112.19
4	P	1	G39	C5-N5-C10	3.40	131.06	123.11
4	H	1	G39	C4-C3-C2	-3.38	105.89	109.72
4	C	1	G39	C7-C2-C1	-3.37	115.38	119.99
4	D	1	G39	O7-C6-C7	3.34	116.96	109.19
4	K	1	G39	O7-C6-C7	3.31	116.89	109.19
4	M	1	G39	C3-C2-C1	-3.25	111.03	116.99
4	L	1	G39	O10-C10-N5	3.24	127.71	121.98
4	F	1	G39	C6-C7-C2	-3.17	117.73	122.66
4	G	1	G39	O1B-C1-O1A	3.09	131.26	123.90
4	F	1	G39	C5-N5-C10	3.08	130.31	123.11
4	G	1	G39	C5-N5-C10	3.07	130.29	123.11
2	N	900	NAG	C1-C2-N2	-3.04	105.64	110.43
2	L	900	NAG	C1-C2-N2	-3.03	105.66	110.43
4	F	1	G39	C7-C2-C1	-3.01	115.87	119.99
4	C	1	G39	O7-C8-C81	3.01	121.34	108.87
4	F	1	G39	O7-C6-C7	2.96	116.08	109.19
4	I	1	G39	O1B-C1-O1A	-2.96	116.86	123.90
2	J	900	NAG	C1-O5-C5	2.95	116.14	112.19
4	J	1	G39	O1B-C1-C2	-2.95	109.20	115.43
4	N	1	G39	O7-C6-C7	2.95	116.04	109.19
2	B	900	NAG	C1-C2-N2	-2.90	105.86	110.43
4	J	1	G39	O10-C10-C11	-2.88	116.93	122.05
4	N	1	G39	C3-C2-C1	-2.85	111.75	116.99
4	K	1	G39	C3-C2-C7	2.83	125.73	122.25
4	N	1	G39	O7-C8-C81	2.82	120.57	108.87
4	F	1	G39	O7-C8-C9	2.80	120.49	108.87
2	I	900	NAG	C1-C2-N2	-2.79	106.04	110.43
4	N	1	G39	C5-N5-C10	2.78	129.62	123.11
2	H	900	NAG	C1-C2-N2	-2.77	106.06	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	N	1	G39	C7-C2-C1	2.75	123.74	119.99
4	N	1	G39	C6-C5-N5	2.73	114.20	111.13
4	D	1	G39	C6-C7-C2	-2.72	118.43	122.66
4	L	1	G39	O1B-C1-C2	-2.71	109.71	115.43
2	C	900	NAG	C1-C2-N2	-2.70	106.18	110.43
4	M	1	G39	O1B-C1-O1A	-2.68	117.52	123.90
2	D	900	NAG	C1-C2-N2	-2.67	106.22	110.43
2	E	900	NAG	C1-C2-N2	-2.66	106.25	110.43
4	H	1	G39	C3-C2-C1	-2.66	112.11	116.99
2	G	900	NAG	C1-C2-N2	-2.51	106.47	110.43
4	H	1	G39	C5-N5-C10	2.48	128.91	123.11
2	K	900	NAG	C1-C2-N2	-2.48	106.53	110.43
2	F	900	NAG	C1-C2-N2	-2.45	106.57	110.43
4	D	1	G39	O10-C10-C11	-2.45	117.69	122.05
4	D	1	G39	O7-C8-C81	2.45	119.02	108.87
2	M	900	NAG	C1-C2-N2	-2.44	106.58	110.43
4	G	1	G39	C4-C3-C2	-2.44	106.95	109.72
4	C	1	G39	C3-C2-C1	-2.42	112.54	116.99
2	P	900	NAG	C1-C2-N2	-2.40	106.66	110.43
2	C	900	NAG	C1-O5-C5	2.29	115.26	112.19
4	I	1	G39	O7-C6-C7	-2.28	103.88	109.19
4	L	1	G39	O7-C6-C7	2.28	114.49	109.19
4	A	1	G39	O10-C10-C11	-2.26	118.04	122.05
2	A	900	NAG	C6-C5-C4	-2.25	107.50	113.02
4	P	1	G39	C3-C2-C1	-2.25	112.86	116.99
2	I	900	NAG	O4-C4-C5	2.22	114.80	109.32
4	O	1	G39	C3-C2-C1	-2.20	112.96	116.99
2	O	900	NAG	C1-C2-N2	-2.18	107.00	110.43
2	L	900	NAG	C6-C5-C4	-2.17	107.68	113.02
4	J	1	G39	C3-C4-N4	-2.17	106.47	110.76
4	O	1	G39	C6-C7-C2	-2.15	119.31	122.66
4	J	1	G39	O7-C6-C7	2.15	114.19	109.19
4	H	1	G39	O7-C6-C7	2.15	114.18	109.19
4	I	1	G39	C6-C5-N5	-2.14	108.73	111.13
4	J	1	G39	C7-C2-C1	-2.14	117.06	119.99
4	D	1	G39	C3-C2-C1	2.12	120.87	116.99
4	B	1	G39	C3-C2-C1	2.09	120.83	116.99
4	O	1	G39	C11-C10-N5	-2.06	112.70	116.12
2	G	900	NAG	O4-C4-C5	2.06	114.40	109.32
2	E	900	NAG	O4-C4-C5	2.06	114.40	109.32
4	P	1	G39	C7-C2-C1	-2.01	117.24	119.99

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	G	1	G39	C9-C8-C81-C82
4	N	1	G39	O10-C10-N5-C5
4	N	1	G39	C7-C6-O7-C8
4	N	1	G39	C11-C10-N5-C5
4	N	1	G39	C9-C8-C81-C82
4	P	1	G39	C11-C10-N5-C5
4	K	1	G39	O7-C8-C9-C91
4	P	1	G39	O10-C10-N5-C5
4	F	1	G39	O7-C8-C9-C91
4	M	1	G39	O7-C8-C9-C91
4	D	1	G39	C9-C8-C81-C82
4	K	1	G39	C11-C10-N5-C5
4	G	1	G39	O7-C8-C81-C82
4	N	1	G39	O7-C8-C81-C82
4	C	1	G39	C9-C8-C81-C82
4	P	1	G39	C9-C8-C81-C82
4	J	1	G39	O1A-C1-C2-C7
4	B	1	G39	O10-C10-N5-C5
4	B	1	G39	C11-C10-N5-C5
4	C	1	G39	C81-C8-C9-C91
4	M	1	G39	C81-C8-C9-C91
4	C	1	G39	C81-C8-O7-C6
4	D	1	G39	C81-C8-O7-C6
4	G	1	G39	C81-C8-O7-C6
4	K	1	G39	C81-C8-O7-C6
4	L	1	G39	C81-C8-O7-C6
4	N	1	G39	C81-C8-O7-C6
4	D	1	G39	O7-C8-C81-C82
4	D	1	G39	C81-C8-C9-C91
4	P	1	G39	O7-C8-C81-C82
4	F	1	G39	C81-C8-C9-C91
4	K	1	G39	C81-C8-C9-C91
4	O	1	G39	O10-C10-N5-C5
4	E	1	G39	C9-C8-C81-C82
4	D	1	G39	O1B-C1-C2-C3
4	E	1	G39	O10-C10-N5-C5
4	O	1	G39	C11-C10-N5-C5
4	K	1	G39	O10-C10-N5-C5
4	J	1	G39	C81-C8-O7-C6
4	C	1	G39	C5-C6-O7-C8
4	G	1	G39	C5-C6-O7-C8
4	J	1	G39	O7-C8-C9-C91

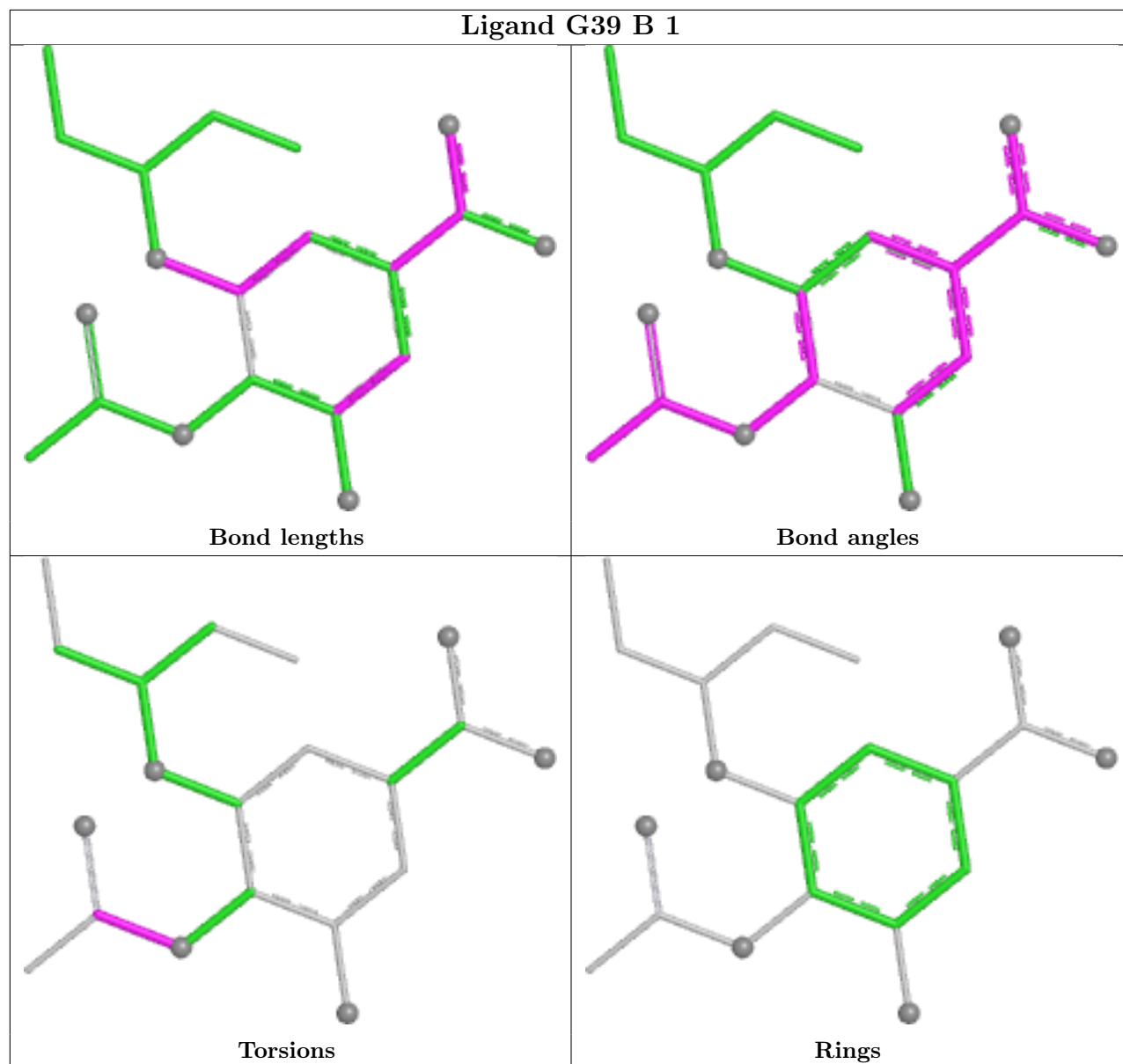
There are no ring outliers.

16 monomers are involved in 73 short contacts:

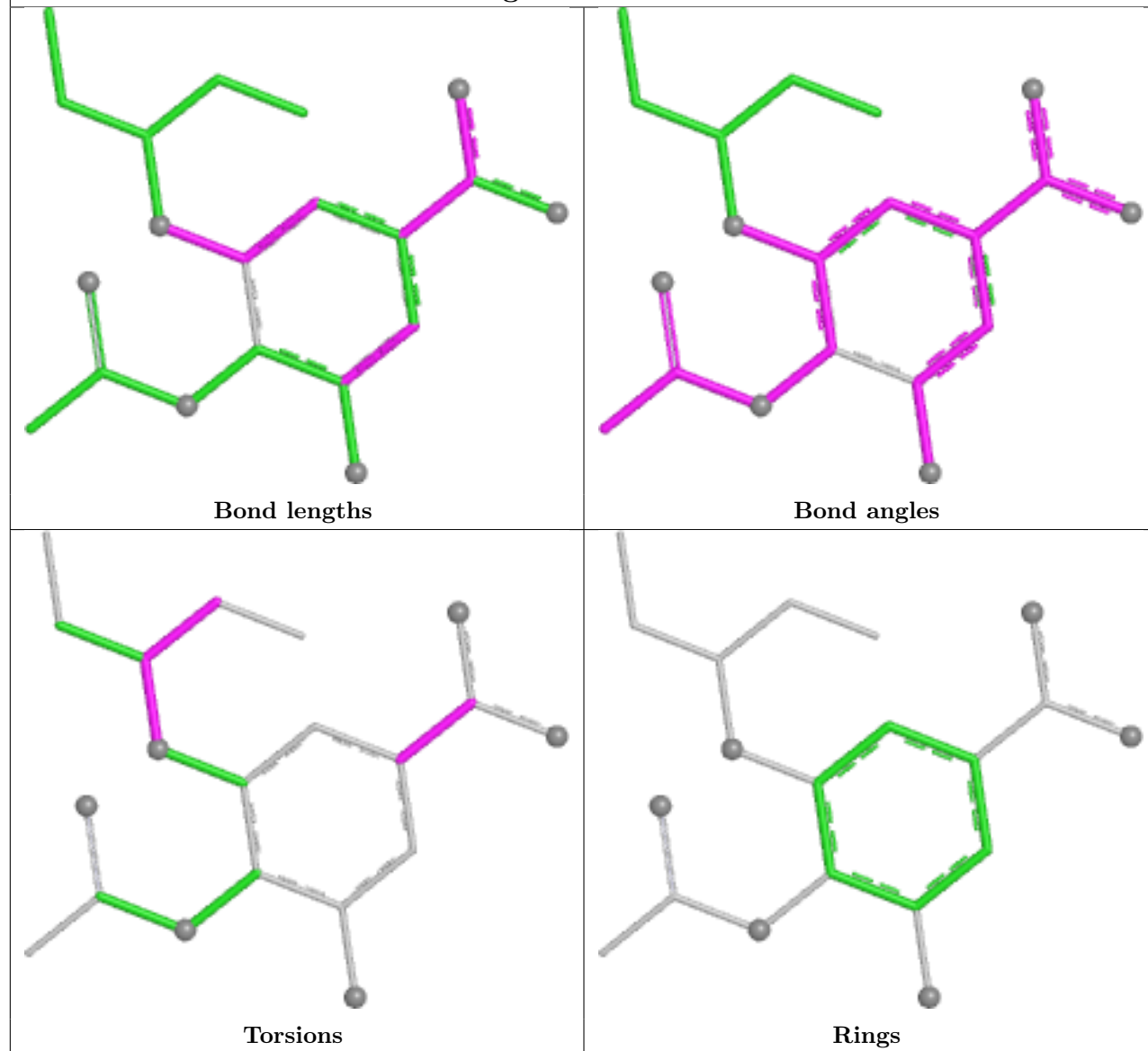
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1	G39	3	0
4	J	1	G39	5	0
4	G	1	G39	6	0
4	C	1	G39	3	0
4	A	1	G39	4	0
4	F	1	G39	7	0
4	M	1	G39	2	0
4	K	1	G39	3	0
4	D	1	G39	6	0
4	E	1	G39	6	0
4	H	1	G39	7	0
4	I	1	G39	6	0
4	O	1	G39	3	0
4	L	1	G39	4	0
4	P	1	G39	5	0
4	N	1	G39	3	0

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.

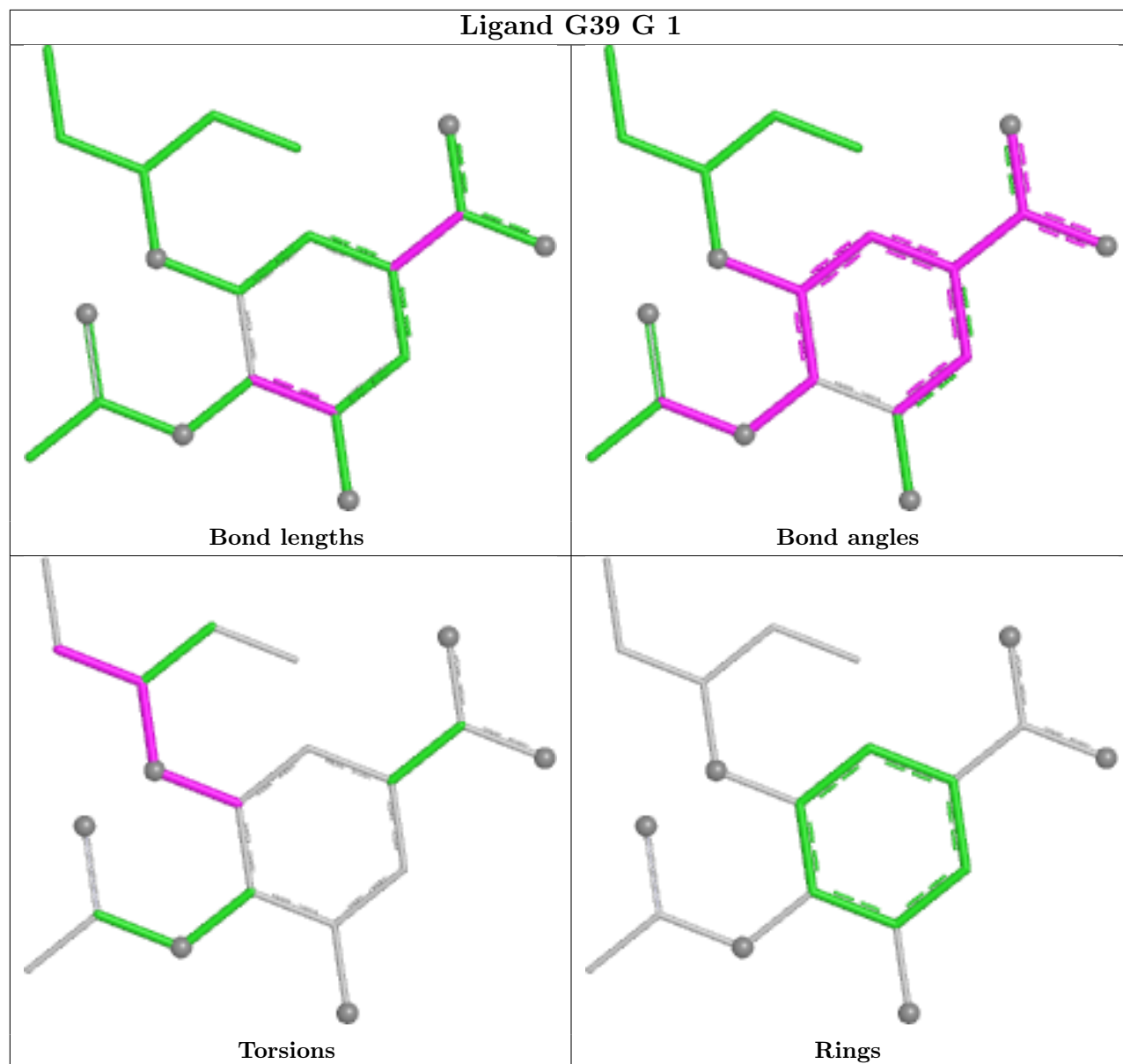
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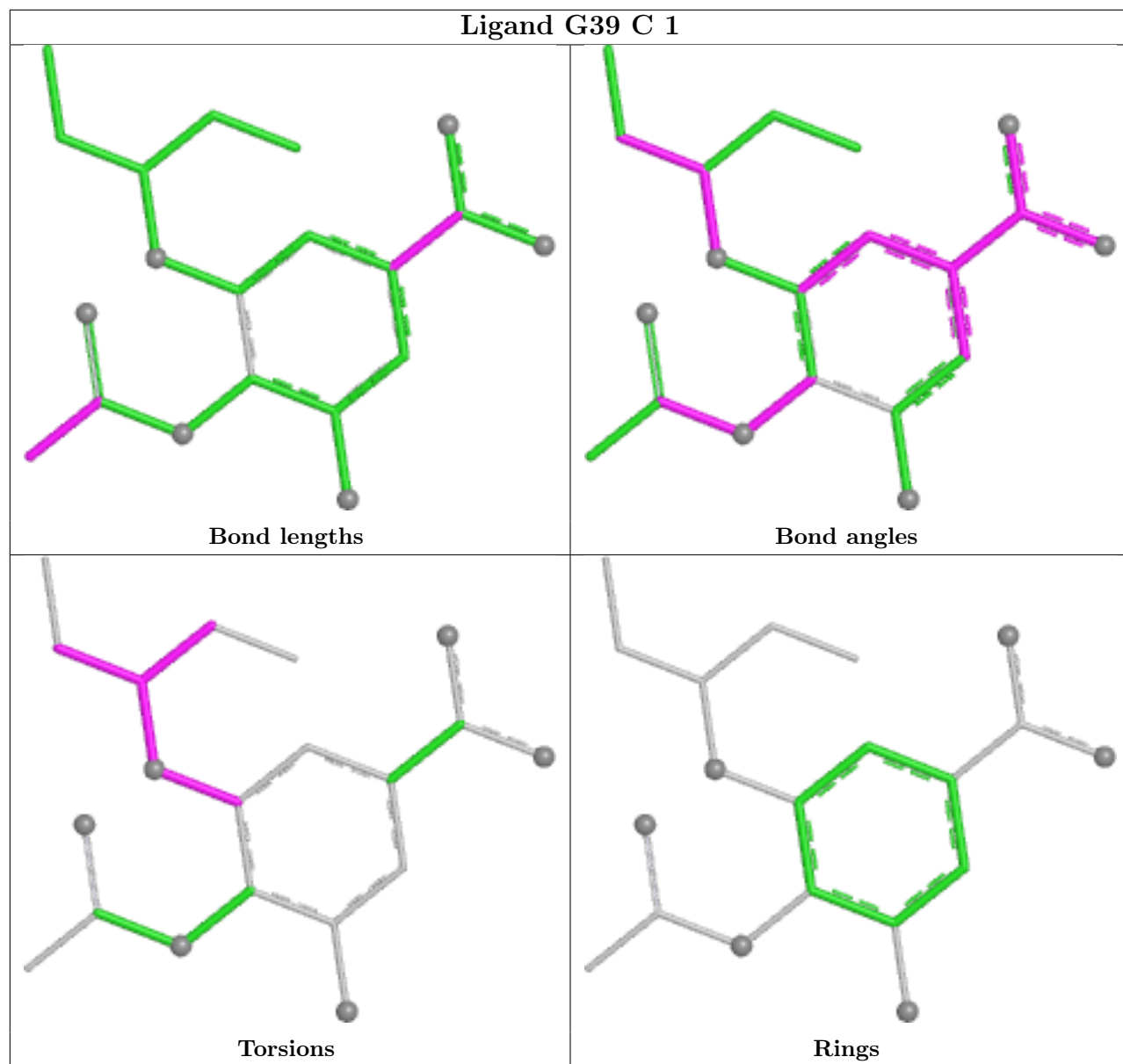
Ligand G39 J 1



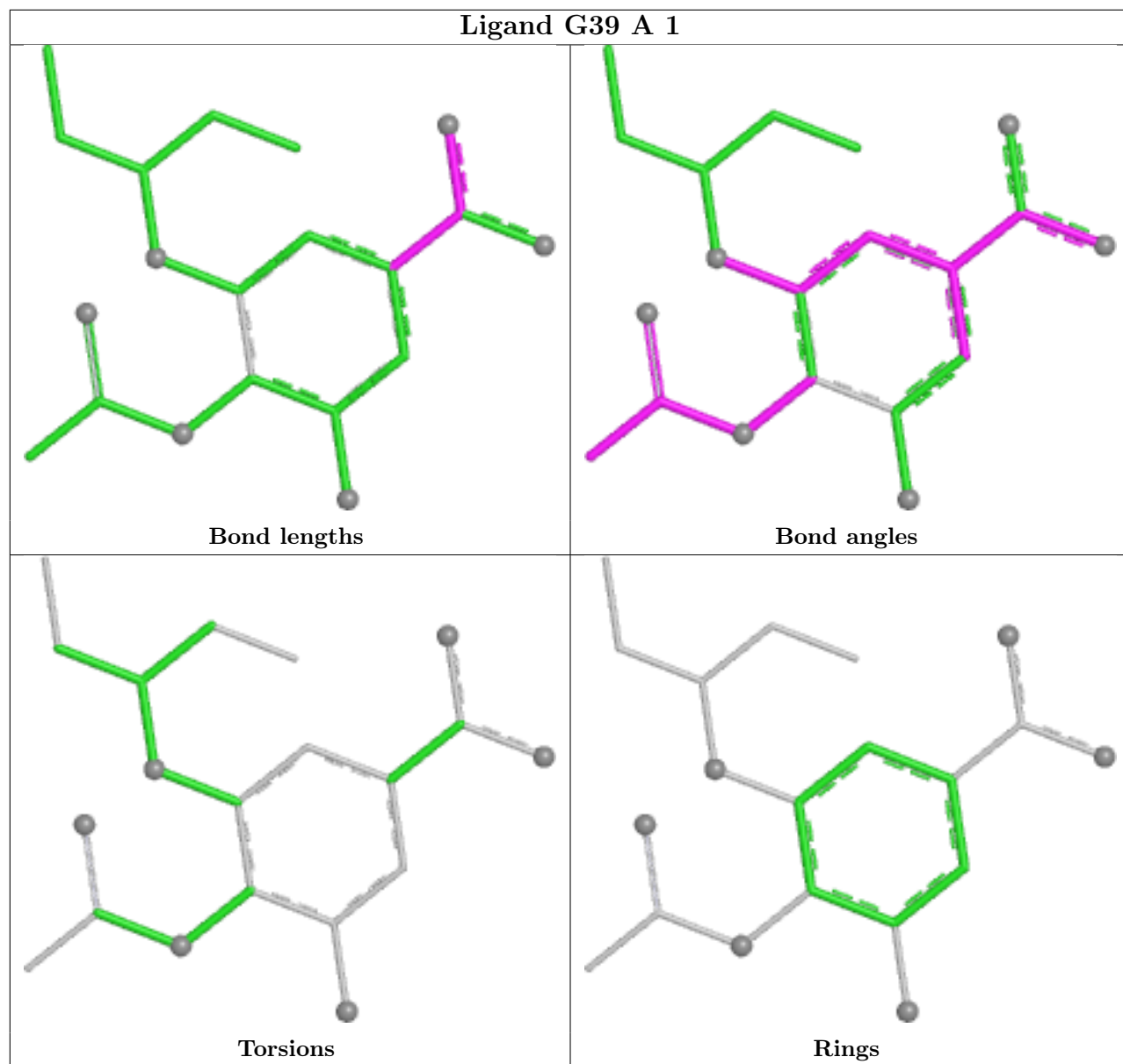
Ligand G39 G 1



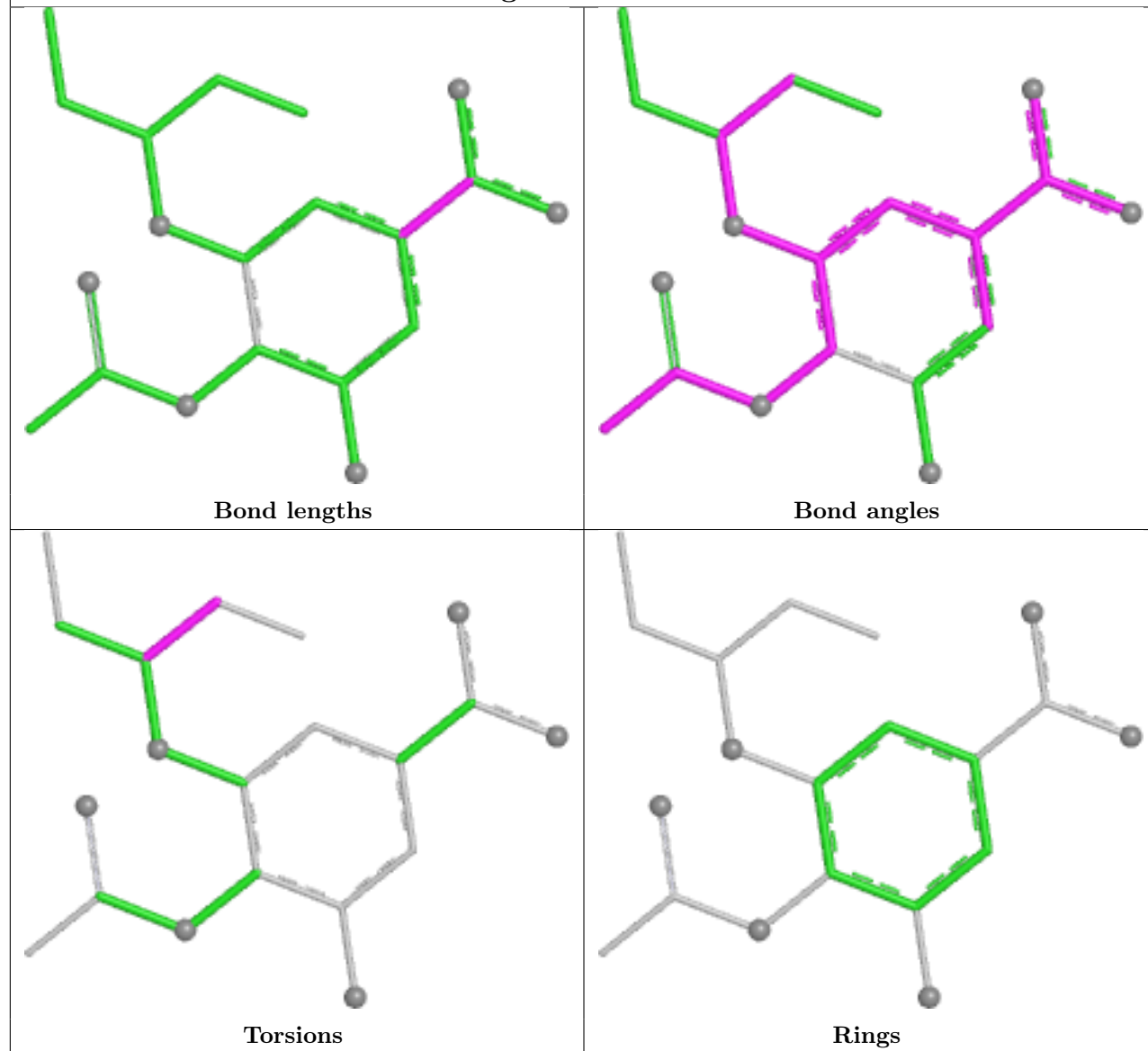
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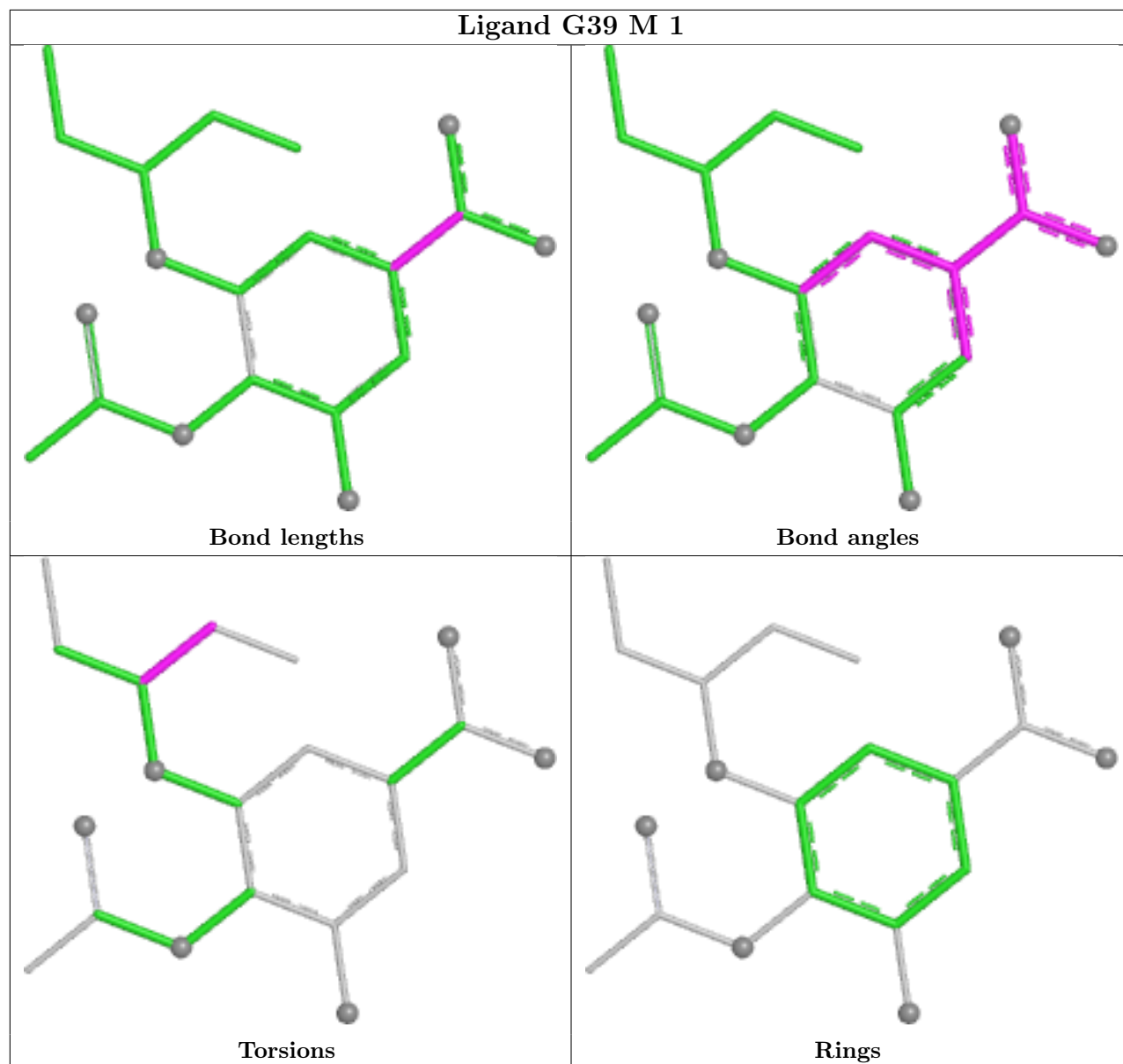
Ligand G39 A 1



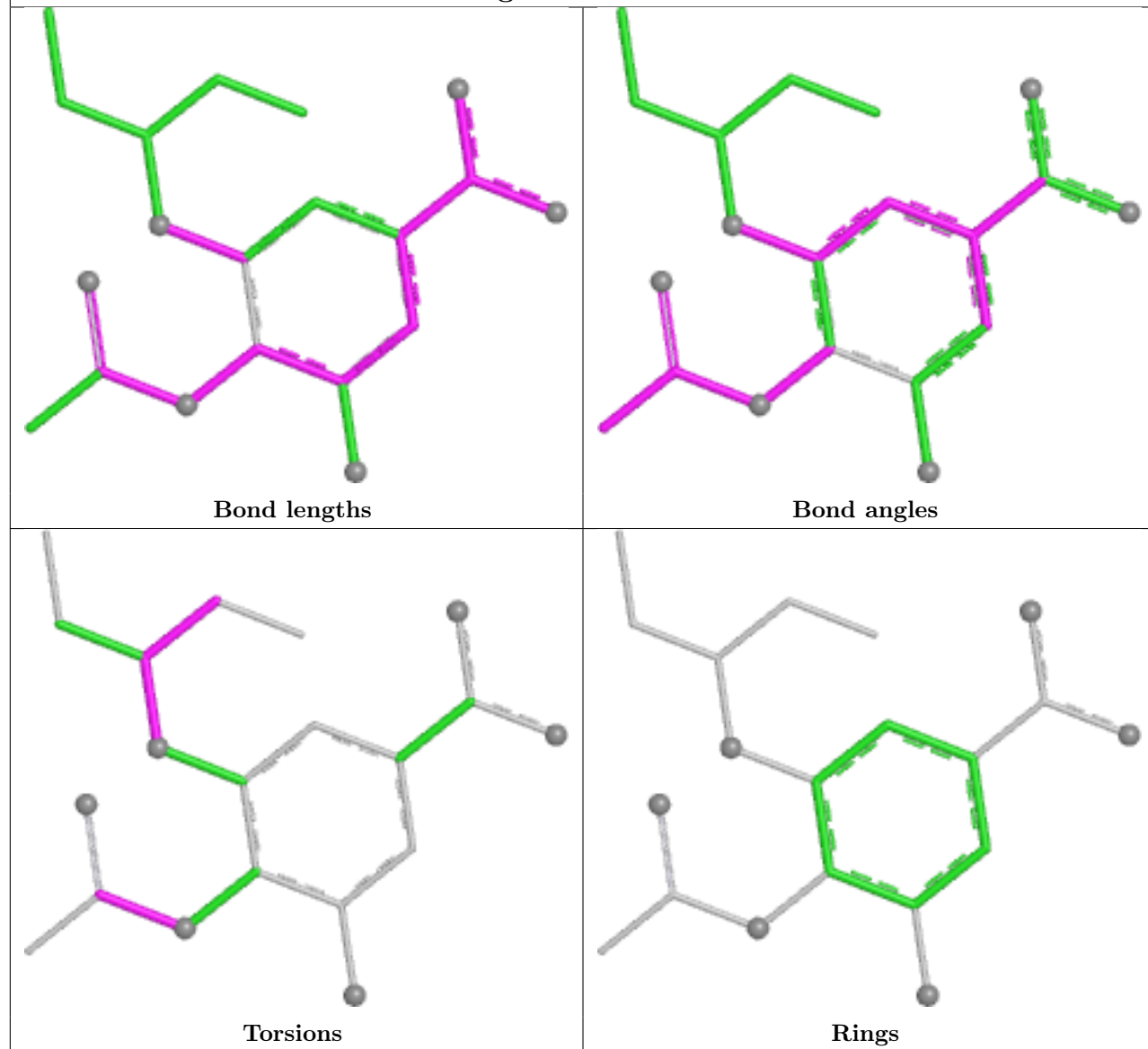
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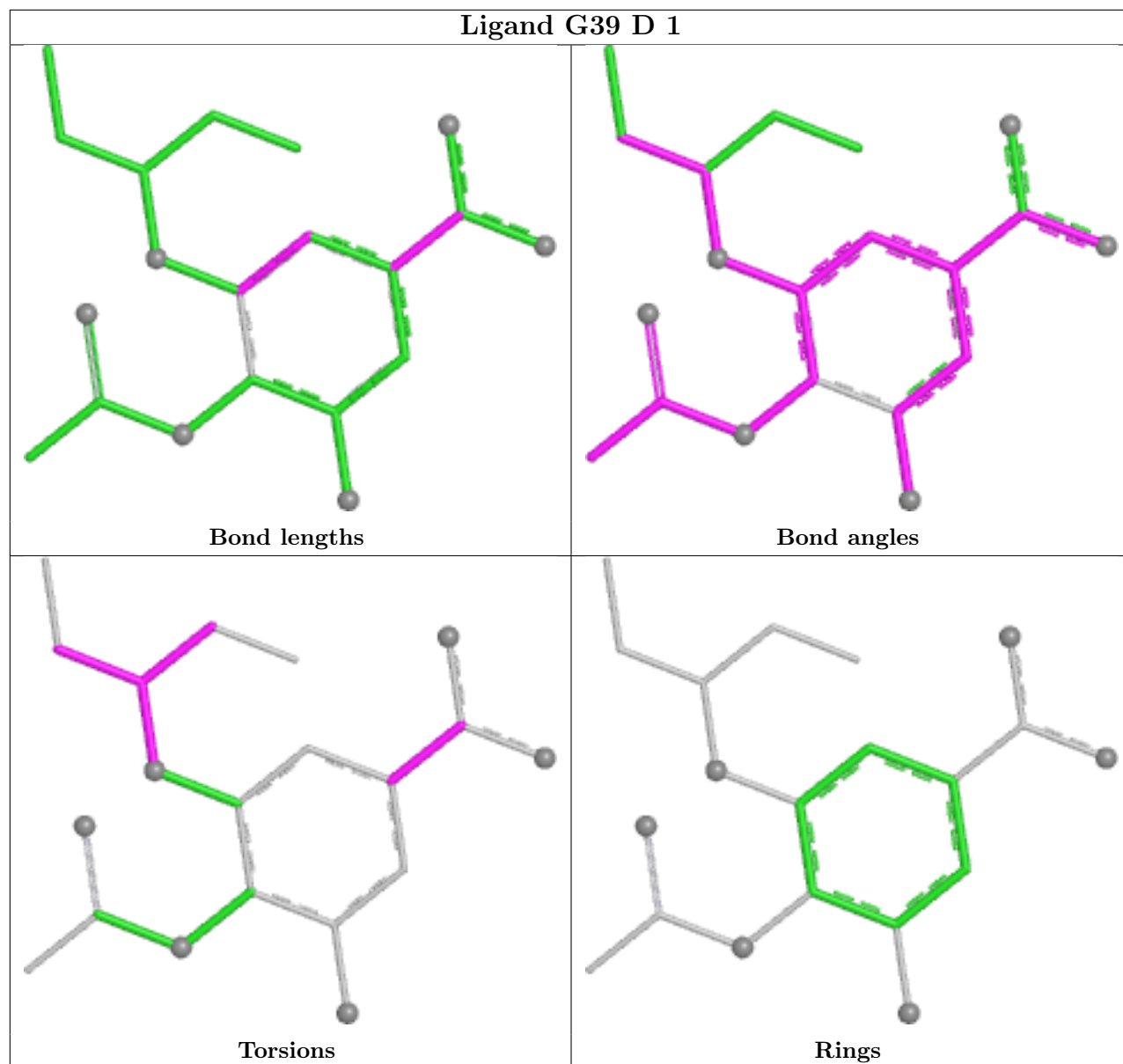
Ligand G39 M 1



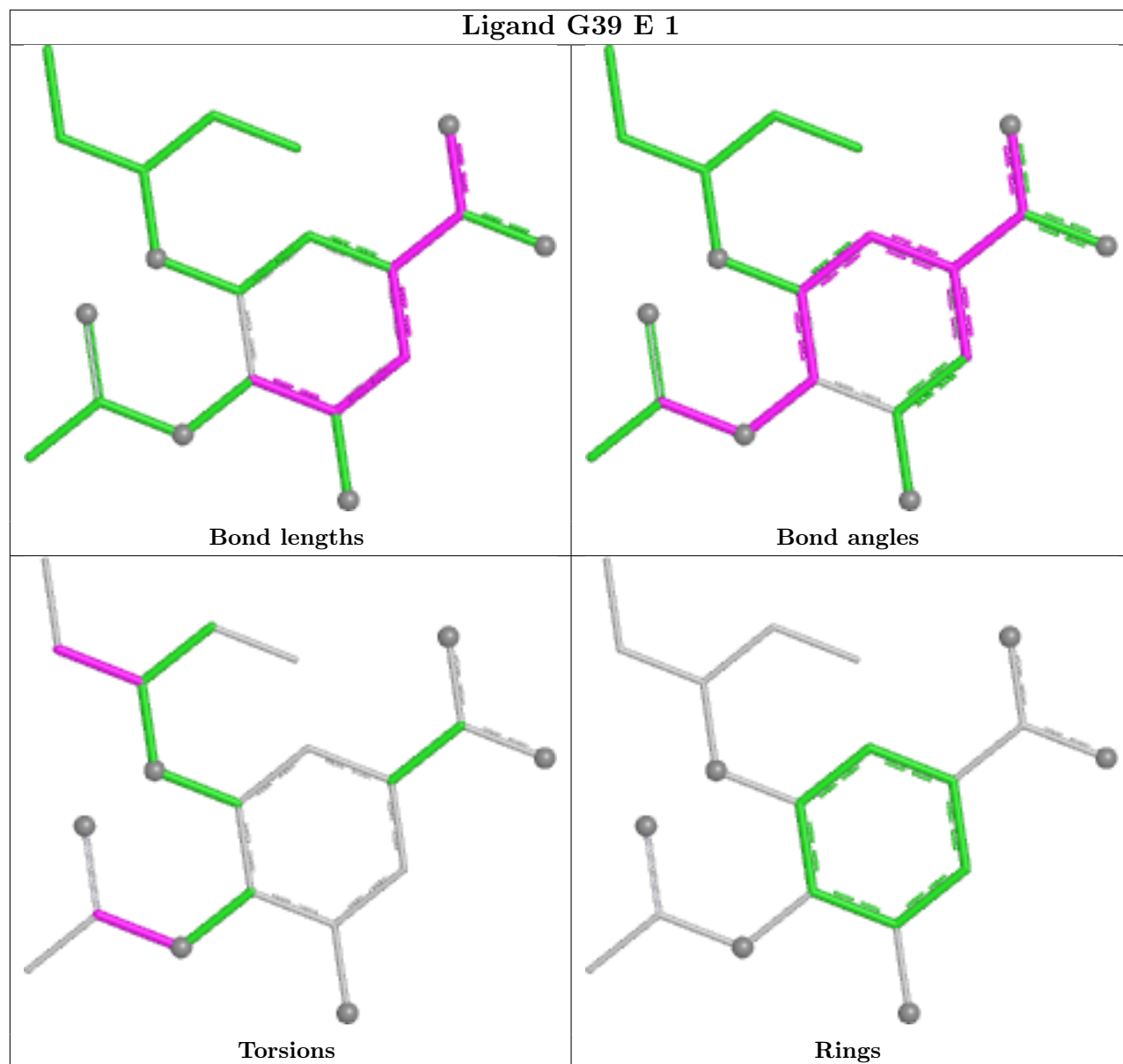
Ligand G39 K 1



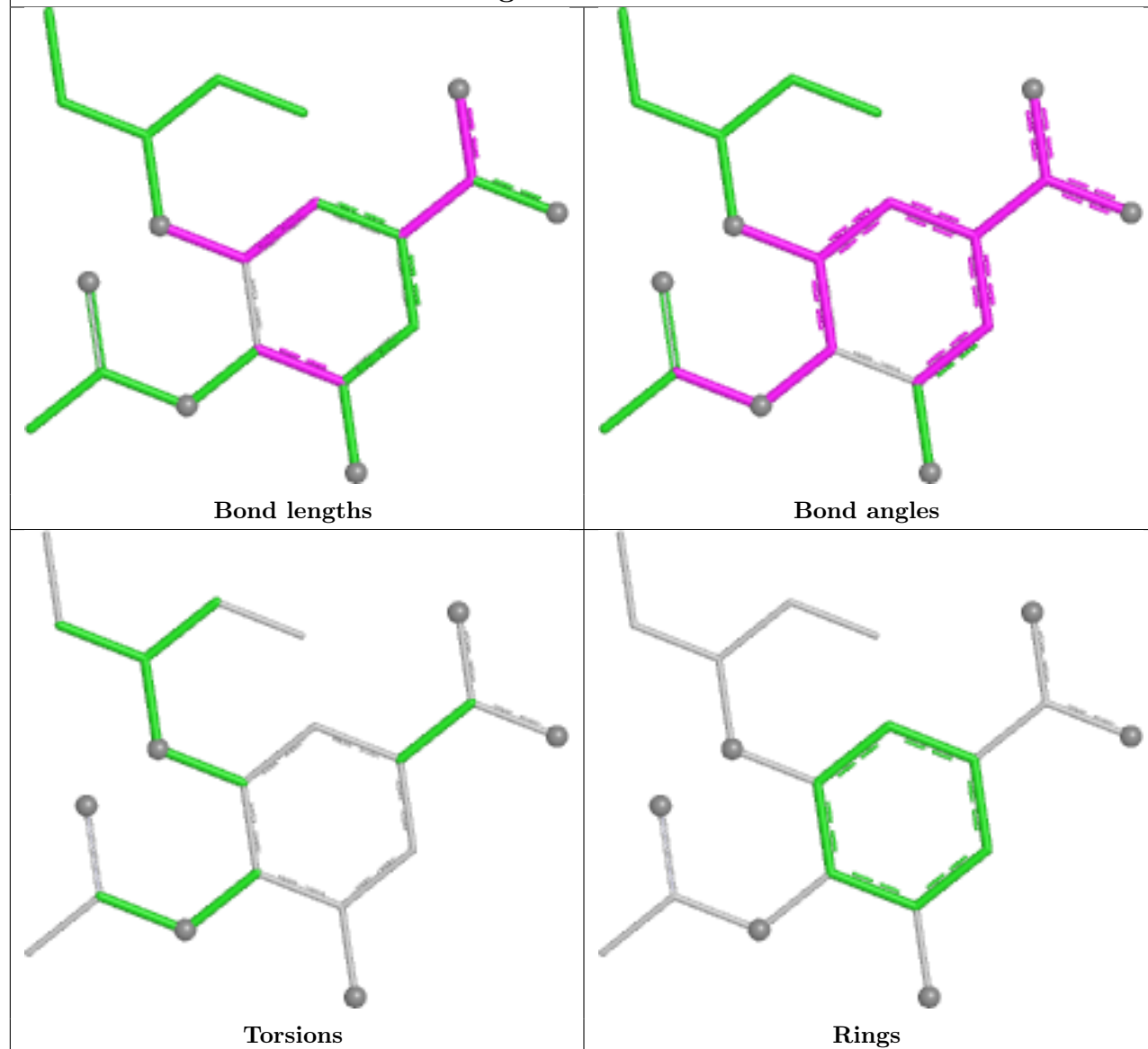
Ligand G39 D 1



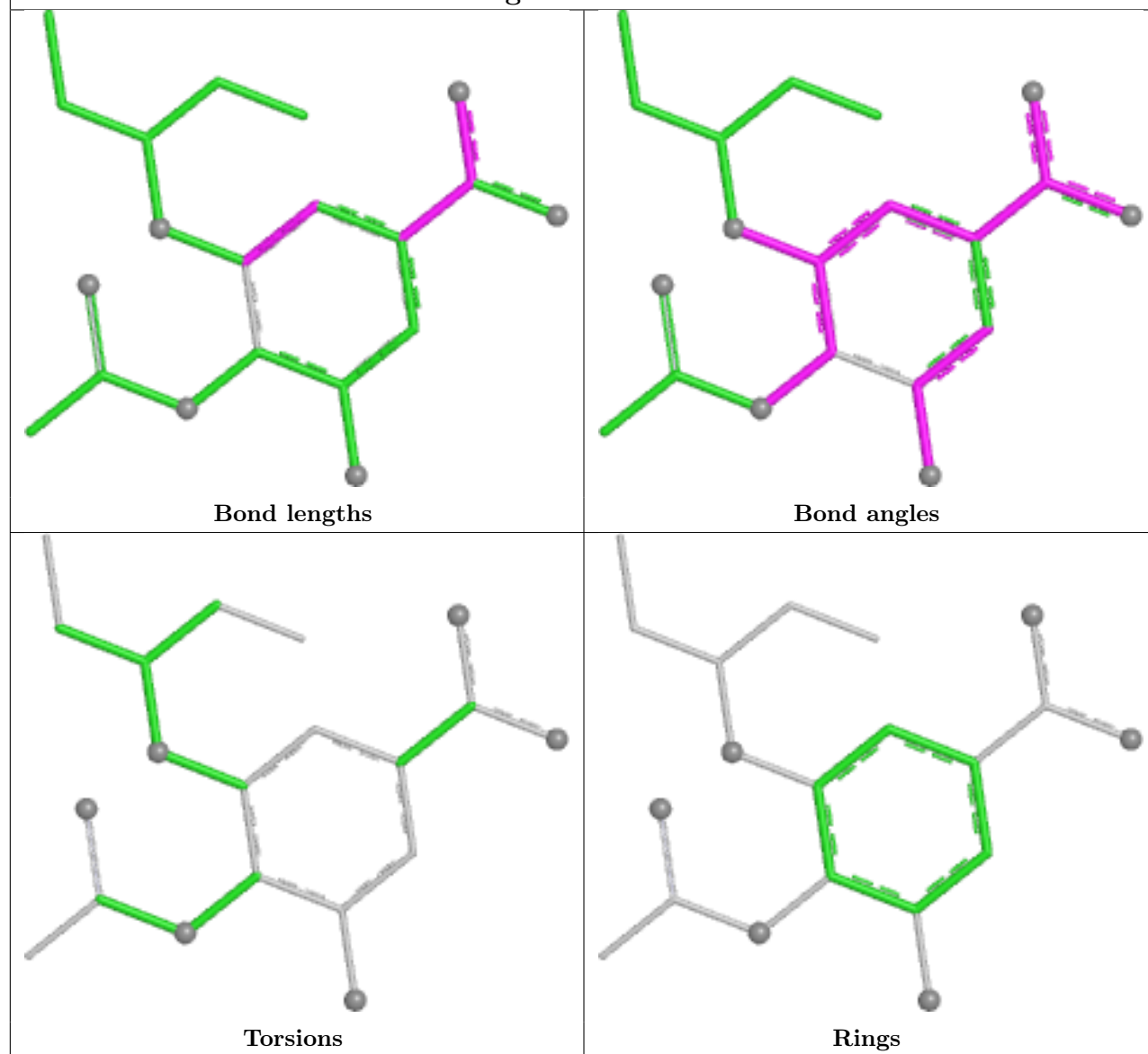
Ligand G39 E 1

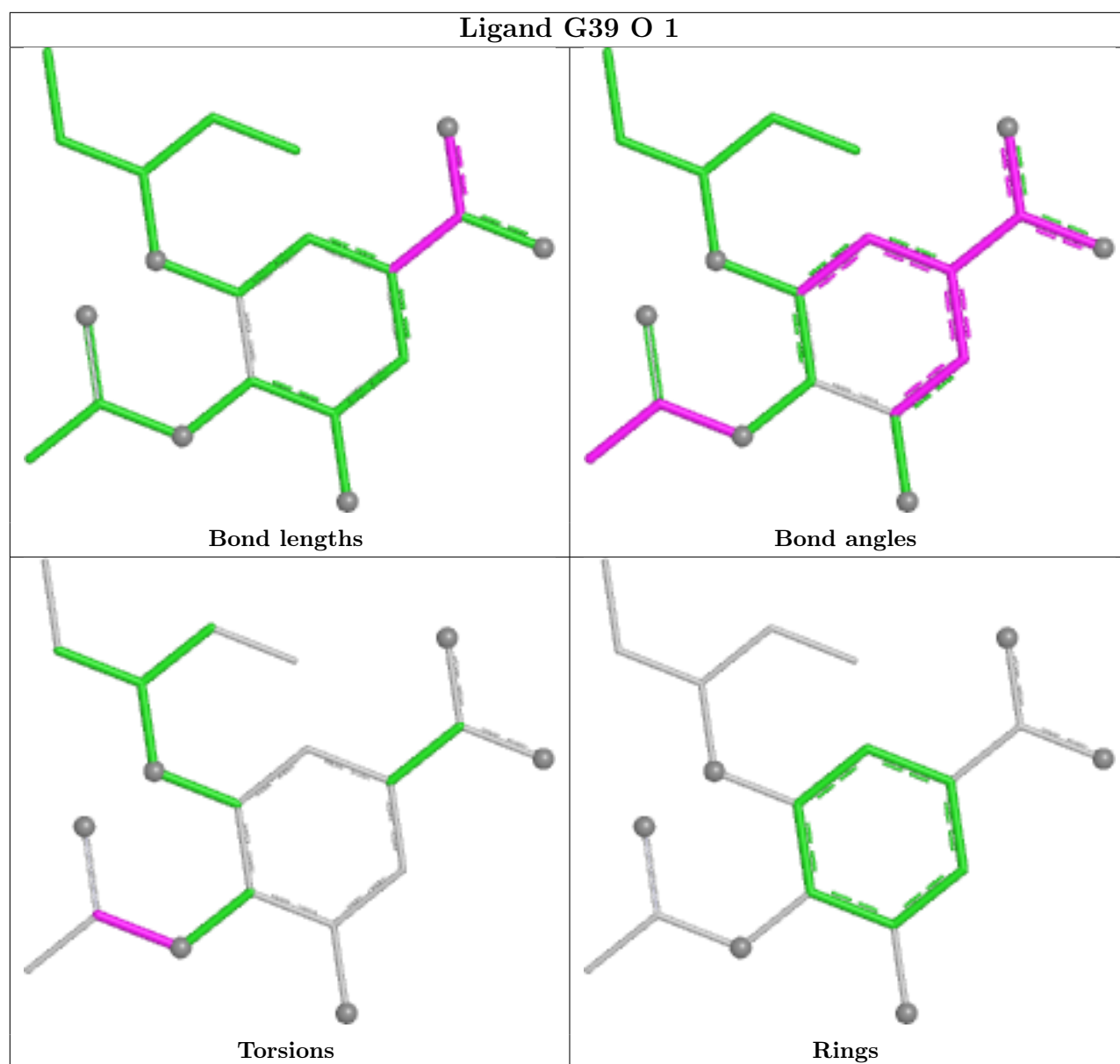


Ligand G39 H 1

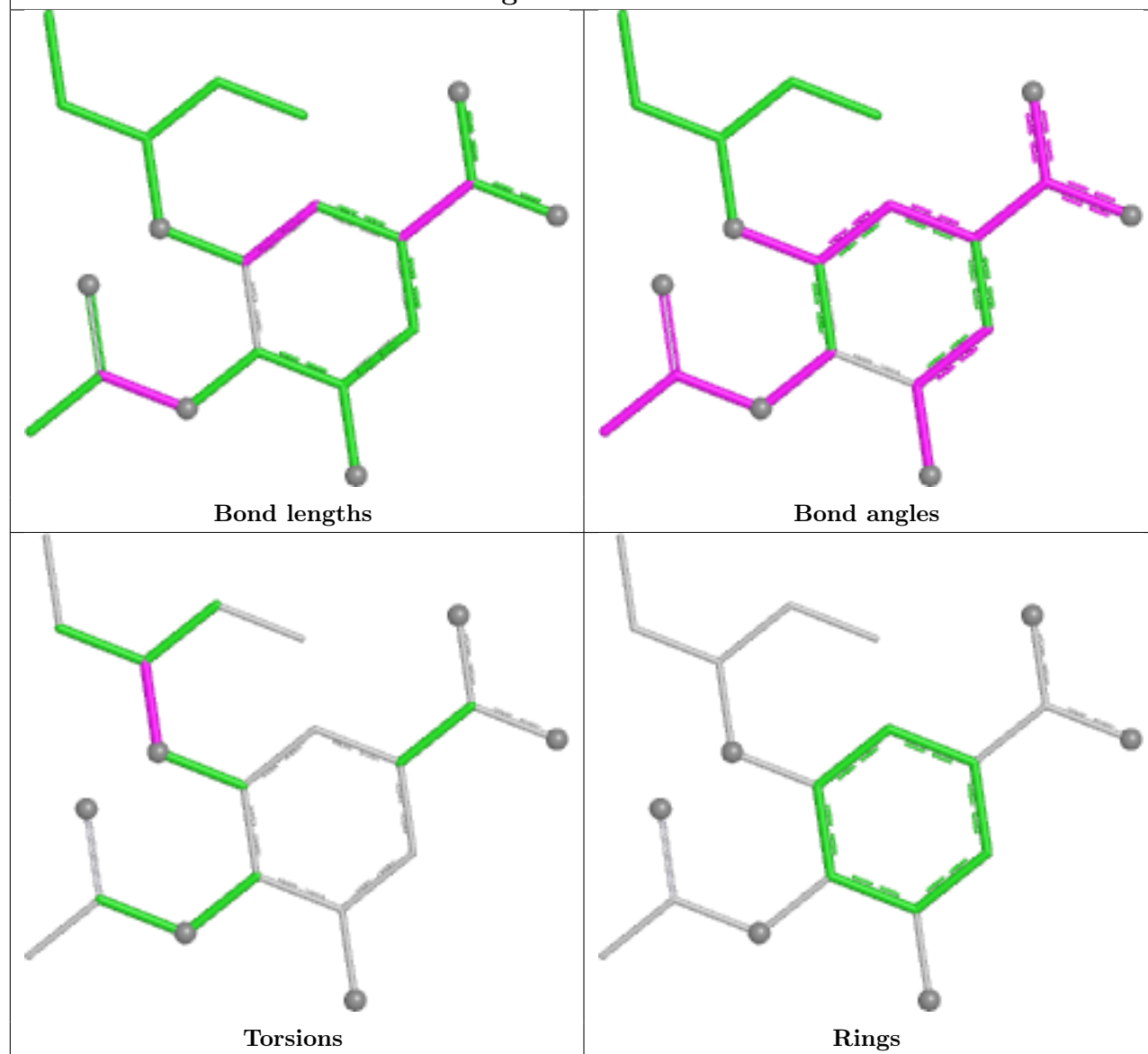


Ligand G39 I 1

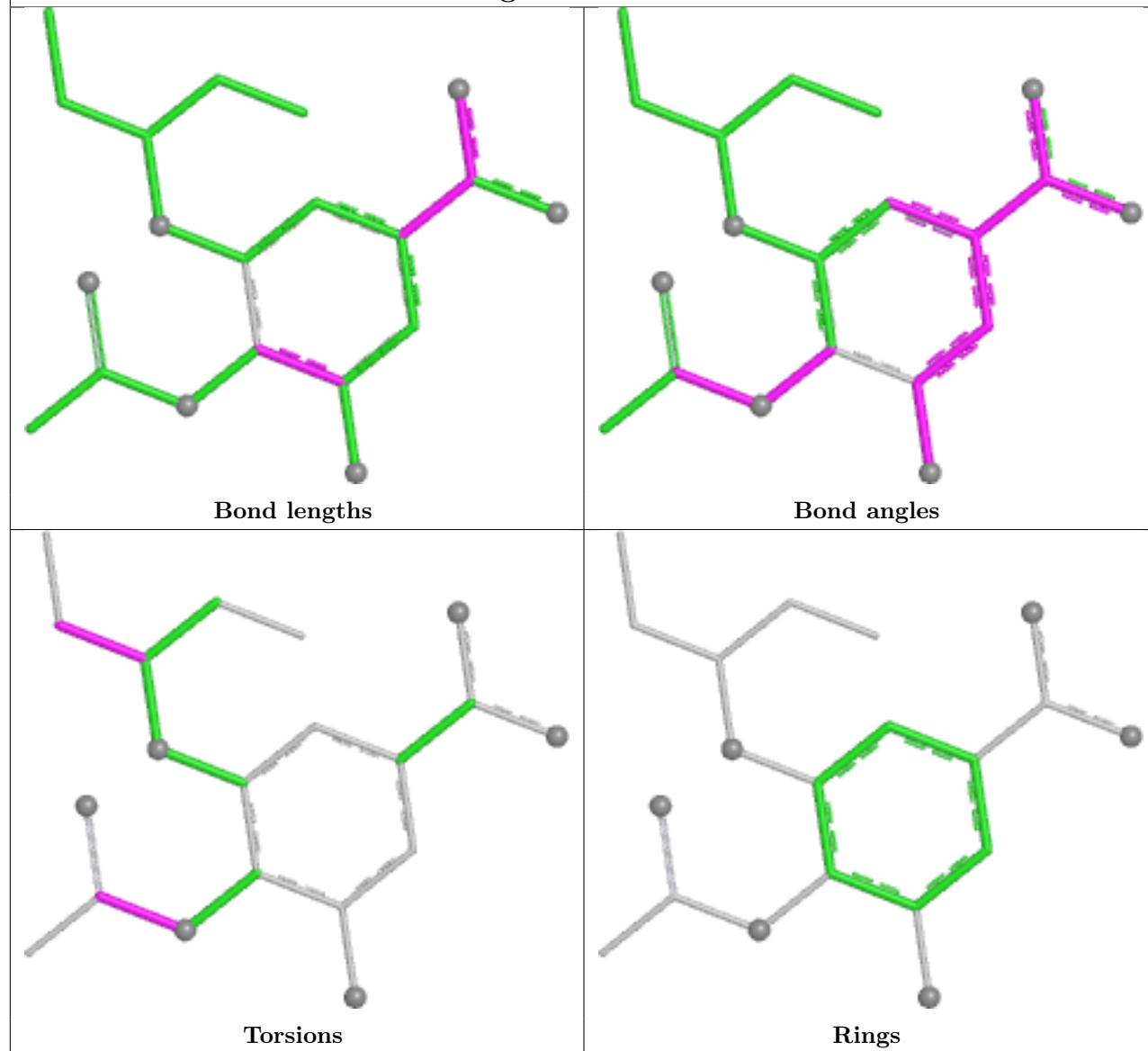


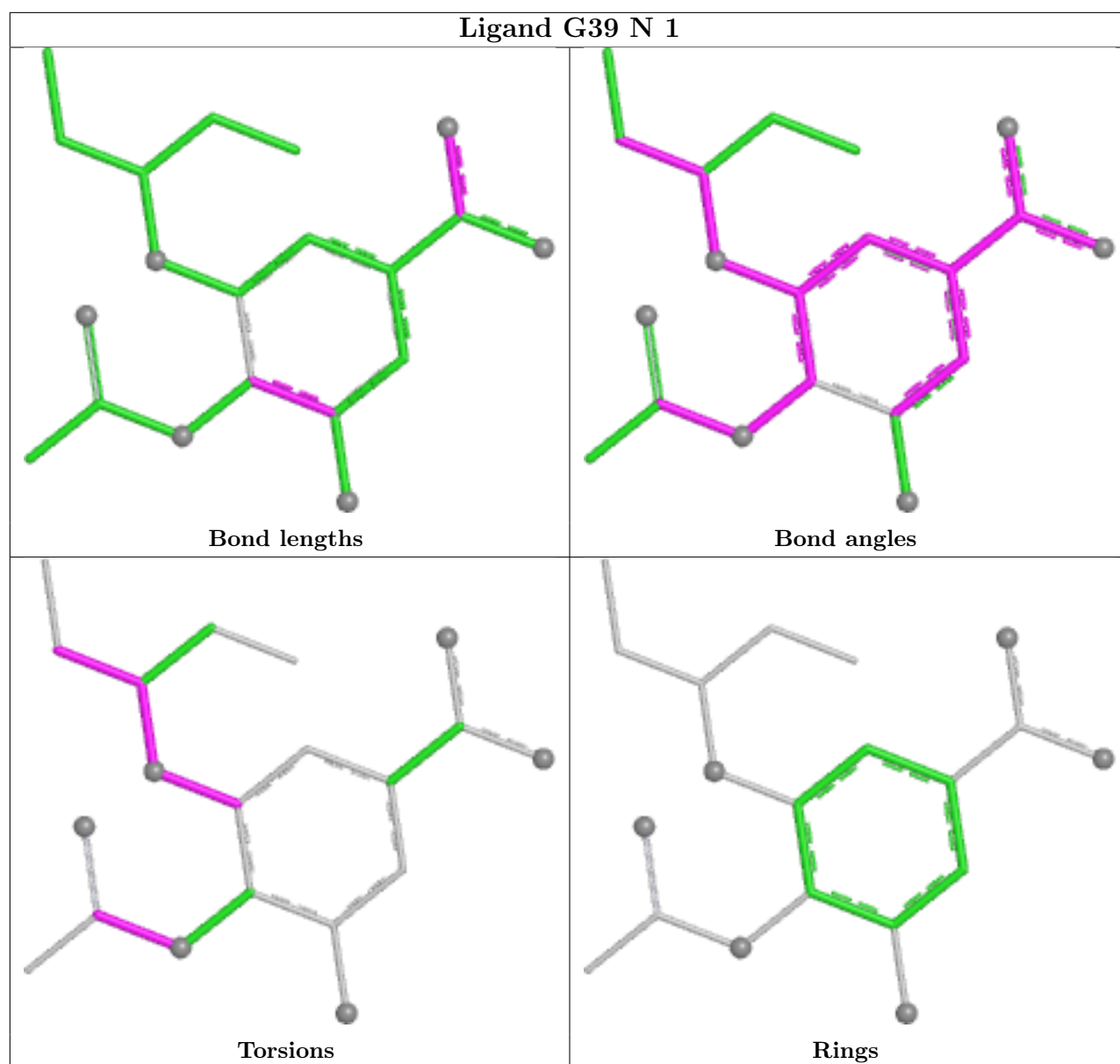


Ligand G39 L 1



Ligand G39 P 1





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%)	1.39	62 (15%) 5 4	27, 40, 43, 46	1 (0%)
1	B	389/397 (97%)	1.42	69 (17%) 4 3	27, 40, 43, 46	1 (0%)
1	C	389/397 (97%)	1.39	60 (15%) 5 4	27, 40, 43, 46	1 (0%)
1	D	389/397 (97%)	1.43	70 (17%) 3 3	27, 40, 43, 46	1 (0%)
1	E	389/397 (97%)	1.41	67 (17%) 4 3	27, 40, 43, 46	1 (0%)
1	F	389/397 (97%)	1.41	71 (18%) 3 3	27, 40, 43, 46	1 (0%)
1	G	389/397 (97%)	1.45	78 (20%) 3 2	27, 40, 43, 46	1 (0%)
1	H	389/397 (97%)	1.44	73 (18%) 3 2	27, 40, 43, 46	1 (0%)
1	I	389/397 (97%)	1.33	59 (15%) 5 4	27, 40, 43, 46	1 (0%)
1	J	389/397 (97%)	1.34	63 (16%) 4 3	27, 40, 43, 46	1 (0%)
1	K	389/397 (97%)	1.35	47 (12%) 8 6	27, 40, 43, 46	1 (0%)
1	L	389/397 (97%)	1.34	66 (16%) 4 3	27, 40, 43, 46	1 (0%)
1	M	389/397 (97%)	1.38	67 (17%) 4 3	27, 40, 43, 46	1 (0%)
1	N	389/397 (97%)	1.38	63 (16%) 4 3	27, 40, 43, 46	1 (0%)
1	O	389/397 (97%)	1.39	72 (18%) 3 3	27, 40, 43, 46	1 (0%)
1	P	389/397 (97%)	1.43	71 (18%) 3 3	27, 40, 43, 46	1 (0%)
All	All	6224/6352 (97%)	1.39	1058 (16%) 4 3	27, 40, 43, 46	16 (0%)

All (1058) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	337	CYS	5.1
1	C	315	ARG	4.9
1	B	315	ARG	4.9
1	I	315	ARG	4.9
1	N	285	LYS	4.8

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Mol	Chain	Res	Type	RSRZ
1	B	337	CYS	4.6
1	D	285	LYS	4.5
1	K	315	ARG	4.4
1	C	358	ALA	4.4
1	F	285	LYS	4.3
1	P	285	LYS	4.3
1	F	434	GLY	4.2
1	I	358	ALA	4.2
1	C	451	SER	4.1
1	J	285	LYS	4.1
1	G	81	THR	4.1
1	D	315	ARG	4.1
1	K	285	LYS	4.1
1	G	195	GLY	4.0
1	L	337	CYS	4.0
1	H	285	LYS	4.0
1	K	340	ASN	4.0
1	I	451	SER	4.0
1	B	285	LYS	3.9
1	J	315	ARG	3.9
1	A	315	ARG	3.9
1	C	359	SER	3.9
1	K	136	ALA	3.8
1	L	285	LYS	3.8
1	N	340	ASN	3.8
1	N	95	ALA	3.8
1	G	179	GLY	3.8
1	E	388	TRP	3.7
1	E	336	PRO	3.7
1	J	341	GLY	3.7
1	A	81	THR	3.6
1	G	390	ASP	3.6
1	E	81	THR	3.6
1	A	451	SER	3.6
1	E	345	SER	3.6
1	C	341	GLY	3.6
1	O	344	GLY	3.6
1	L	95	ALA	3.6
1	N	434	GLY	3.6
1	H	392	ASP	3.6
1	P	95	ALA	3.6
1	H	120	ILE	3.6

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Mol	Chain	Res	Type	RSRZ
1	J	289	CYS	3.5
1	G	125	LYS	3.5
1	K	79	GLU	3.5
1	M	81	THR	3.5
1	A	337	CYS	3.5
1	H	277	CYS	3.5
1	K	451	SER	3.5
1	G	388	TRP	3.5
1	F	277	CYS	3.5
1	O	372	THR	3.5
1	K	341	GLY	3.5
1	F	388	TRP	3.5
1	J	79	GLU	3.5
1	M	318	CYS	3.5
1	K	358	ALA	3.5
1	O	388	TRP	3.5
1	I	79	GLU	3.4
1	E	85	LEU	3.4
1	L	234	GLY	3.4
1	P	192	GLY	3.4
1	A	285	LYS	3.4
1	N	261	ILE	3.4
1	C	79	GLU	3.4
1	L	441	ALA	3.4
1	F	451	SER	3.4
1	B	79	GLU	3.4
1	M	388	TRP	3.4
1	O	336	PRO	3.4
1	D	451	SER	3.4
1	J	392	ASP	3.4
1	G	285	LYS	3.3
1	D	341	GLY	3.3
1	D	337	CYS	3.3
1	H	85	LEU	3.3
1	A	358	ALA	3.3
1	G	115	ILE	3.3
1	G	277	CYS	3.3
1	M	195	GLY	3.3
1	O	436	GLU	3.3
1	B	234	GLY	3.3
1	D	247	GLY	3.3
1	A	340	ASN	3.2

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Mol	Chain	Res	Type	RSRZ
1	G	85	LEU	3.2
1	K	337	CYS	3.2
1	P	85	LEU	3.2
1	L	79	GLU	3.2
1	C	314	ILE	3.2
1	F	261	ILE	3.2
1	E	397	SER	3.2
1	P	200	ALA	3.2
1	B	390	ASP	3.2
1	E	285	LYS	3.2
1	N	106	THR	3.2
1	C	285	LYS	3.1
1	A	341	GLY	3.1
1	D	422	VAL	3.1
1	M	269	GLY	3.1
1	A	372	THR	3.1
1	E	245	ALA	3.1
1	F	282	ALA	3.1
1	J	337	CYS	3.1
1	B	177	TRP	3.1
1	F	359	SER	3.1
1	N	85	LEU	3.1
1	B	81	THR	3.1
1	A	209	ALA	3.1
1	B	245	ALA	3.1
1	H	337	CYS	3.1
1	M	125	LYS	3.1
1	O	85	LEU	3.1
1	H	388	TRP	3.1
1	M	340	ASN	3.1
1	H	344	GLY	3.1
1	J	233	GLY	3.1
1	L	209	ALA	3.1
1	K	392	ASP	3.1
1	C	340	ASN	3.1
1	L	315	ARG	3.1
1	F	191	ILE	3.1
1	E	372	THR	3.0
1	I	81	THR	3.0
1	B	117	GLU	3.0
1	P	451	SER	3.0
1	E	125	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	O	179	GLY	3.0
1	K	314	ILE	3.0
1	F	106	THR	3.0
1	D	209	ALA	3.0
1	E	95	ALA	3.0
1	C	149	ASP	3.0
1	I	289	CYS	3.0
1	A	314	ILE	3.0
1	H	282	ALA	3.0
1	J	451	SER	3.0
1	K	359	SER	3.0
1	O	81	THR	3.0
1	M	336	PRO	3.0
1	E	383	TYR	3.0
1	O	435	LYS	3.0
1	G	436	GLU	2.9
1	K	325	THR	2.9
1	P	389	THR	2.9
1	M	393	ALA	2.9
1	L	341	GLY	2.9
1	B	157	ILE	2.9
1	H	462	VAL	2.9
1	D	372	THR	2.9
1	B	95	ALA	2.9
1	I	285	LYS	2.9
1	B	341	GLY	2.9
1	E	294	ASN	2.9
1	B	248	ILE	2.9
1	D	221	ILE	2.9
1	G	337	CYS	2.9
1	H	251	CYS	2.9
1	C	136	ALA	2.9
1	M	95	ALA	2.9
1	K	85	LEU	2.9
1	D	149	ASP	2.9
1	O	190	TYR	2.9
1	A	79	GLU	2.9
1	A	169	ASN	2.9
1	D	79	GLU	2.9
1	E	451	SER	2.9
1	H	451	SER	2.9
1	M	451	SER	2.9

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Mol	Chain	Res	Type	RSRZ
1	J	248	ILE	2.9
1	L	248	ILE	2.9
1	N	159	VAL	2.9
1	M	435	LYS	2.9
1	A	95	ALA	2.9
1	B	267	PRO	2.9
1	D	81	THR	2.9
1	E	200	ALA	2.9
1	C	390	ASP	2.9
1	D	148	GLY	2.9
1	H	434	GLY	2.9
1	O	269	GLY	2.9
1	G	345	SER	2.8
1	O	115	ILE	2.8
1	F	81	THR	2.8
1	P	337	CYS	2.8
1	O	465	ALA	2.8
1	N	296	TYR	2.8
1	P	296	TYR	2.8
1	E	89	GLY	2.8
1	E	269	GLY	2.8
1	G	192	GLY	2.8
1	G	169	ASN	2.8
1	H	332	SER	2.8
1	K	295	SER	2.8
1	M	191	ILE	2.8
1	P	120	ILE	2.8
1	E	334	THR	2.8
1	J	441	ALA	2.8
1	P	466	LEU	2.8
1	N	79	GLU	2.8
1	H	192	GLY	2.8
1	H	296	TYR	2.8
1	K	385	GLY	2.8
1	P	269	GLY	2.8
1	P	434	GLY	2.8
1	A	248	ILE	2.8
1	B	427	ILE	2.8
1	O	246	SER	2.8
1	B	441	ALA	2.8
1	K	81	THR	2.8
1	M	245	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	P	106	THR	2.8
1	B	221	ILE	2.8
1	G	296	TYR	2.8
1	B	451	SER	2.8
1	M	345	SER	2.8
1	B	78	PRO	2.8
1	D	228	ALA	2.8
1	F	85	LEU	2.8
1	I	136	ALA	2.8
1	P	96	LEU	2.8
1	P	282	ALA	2.8
1	C	289	CYS	2.8
1	N	337	CYS	2.8
1	J	195	GLY	2.7
1	K	108	GLY	2.7
1	P	340	ASN	2.7
1	P	388	TRP	2.7
1	B	409	TYR	2.7
1	F	296	TYR	2.7
1	G	190	TYR	2.7
1	H	110	SER	2.7
1	H	295	SER	2.7
1	A	443	THR	2.7
1	K	323	LEU	2.7
1	B	442	ALA	2.7
1	D	121	ALA	2.7
1	G	228	ALA	2.7
1	G	393	ALA	2.7
1	P	81	THR	2.7
1	C	125	LYS	2.7
1	A	436	GLU	2.7
1	L	197	GLU	2.7
1	L	436	GLU	2.7
1	P	436	GLU	2.7
1	I	337	CYS	2.7
1	L	392	ASP	2.7
1	G	269	GLY	2.7
1	H	207	GLY	2.7
1	M	192	GLY	2.7
1	D	339	SER	2.7
1	N	388	TRP	2.7
1	C	85	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	H	238	LEU	2.7
1	L	394	LEU	2.7
1	D	136	ALA	2.7
1	N	435	LYS	2.7
1	B	392	ASP	2.7
1	M	179	GLY	2.7
1	P	195	GLY	2.7
1	C	221	ILE	2.7
1	O	78	PRO	2.7
1	D	295	SER	2.7
1	I	222	LEU	2.7
1	N	96	LEU	2.7
1	N	125	LYS	2.7
1	C	81	THR	2.7
1	F	200	ALA	2.7
1	G	458	THR	2.7
1	N	282	ALA	2.7
1	J	390	ASP	2.7
1	D	291	CYS	2.7
1	E	337	CYS	2.7
1	L	148	GLY	2.7
1	L	233	GLY	2.7
1	M	344	GLY	2.7
1	N	185	GLY	2.7
1	N	192	GLY	2.7
1	E	359	SER	2.7
1	N	430	VAL	2.7
1	H	200	ALA	2.7
1	J	81	THR	2.7
1	N	166	THR	2.7
1	P	465	ALA	2.7
1	H	149	ASP	2.6
1	L	108	GLY	2.6
1	N	269	GLY	2.6
1	B	328	PRO	2.6
1	D	87	CYS	2.6
1	D	267	PRO	2.6
1	G	336	PRO	2.6
1	O	87	CYS	2.6
1	M	85	LEU	2.6
1	P	422	VAL	2.6
1	B	359	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	G	397	SER	2.6
1	J	436	GLU	2.6
1	N	295	SER	2.6
1	C	209	ALA	2.6
1	C	453	GLN	2.6
1	E	206	TYR	2.6
1	O	106	THR	2.6
1	A	390	ASP	2.6
1	D	390	ASP	2.6
1	E	344	GLY	2.6
1	F	269	GLY	2.6
1	M	78	PRO	2.6
1	M	115	ILE	2.6
1	L	289	CYS	2.6
1	I	85	LEU	2.6
1	I	340	ASN	2.6
1	B	249	SER	2.6
1	A	442	ALA	2.6
1	B	372	THR	2.6
1	E	106	THR	2.6
1	I	209	ALA	2.6
1	J	225	GLN	2.6
1	I	392	ASP	2.6
1	M	390	ASP	2.6
1	N	341	GLY	2.6
1	A	455	LEU	2.6
1	O	153	LEU	2.6
1	M	294	ASN	2.6
1	P	359	SER	2.6
1	C	131	ALA	2.6
1	F	228	ALA	2.6
1	H	389	THR	2.6
1	J	95	ALA	2.6
1	J	245	ALA	2.6
1	H	206	TYR	2.6
1	G	344	GLY	2.6
1	G	392	ASP	2.6
1	I	314	ILE	2.6
1	D	305	LEU	2.6
1	E	153	LEU	2.6
1	F	436	GLU	2.6
1	K	153	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	K	436	GLU	2.6
1	B	159	VAL	2.6
1	O	236	CYS	2.6
1	A	295	SER	2.6
1	A	397	SER	2.6
1	G	395	ALA	2.6
1	J	339	SER	2.6
1	O	451	SER	2.6
1	G	435	LYS	2.6
1	B	148	GLY	2.5
1	J	234	GLY	2.5
1	M	341	GLY	2.5
1	O	192	GLY	2.5
1	P	350	GLY	2.5
1	E	157	ILE	2.5
1	L	221	ILE	2.5
1	P	240	ILE	2.5
1	E	394	LEU	2.5
1	F	271	VAL	2.5
1	O	159	VAL	2.5
1	O	340	ASN	2.5
1	F	111	ALA	2.5
1	H	444	ALA	2.5
1	N	290	ALA	2.5
1	H	81	THR	2.5
1	M	372	THR	2.5
1	D	234	GLY	2.5
1	I	341	GLY	2.5
1	I	342	ASP	2.5
1	M	145	GLY	2.5
1	F	333	ILE	2.5
1	L	364	TRP	2.5
1	J	340	ASN	2.5
1	L	144	ASN	2.5
1	A	441	ALA	2.5
1	G	465	ALA	2.5
1	F	410	SER	2.5
1	C	291	CYS	2.5
1	E	229	CYS	2.5
1	G	372	THR	2.5
1	J	359	SER	2.5
1	M	391	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	M	397	SER	2.5
1	P	318	CYS	2.5
1	F	89	GLY	2.5
1	J	108	GLY	2.5
1	A	392	ASP	2.5
1	E	436	GLU	2.5
1	O	463	ASP	2.5
1	G	114	ILE	2.5
1	G	191	ILE	2.5
1	F	188	TRP	2.5
1	F	130	PHE	2.5
1	I	352	PHE	2.5
1	J	96	LEU	2.5
1	H	125	LYS	2.5
1	O	285	LYS	2.5
1	C	442	ALA	2.5
1	G	290	ALA	2.5
1	H	121	ALA	2.5
1	J	393	ALA	2.5
1	M	315	ARG	2.5
1	B	295	SER	2.5
1	L	295	SER	2.5
1	D	289	CYS	2.5
1	L	291	CYS	2.5
1	M	289	CYS	2.5
1	P	87	CYS	2.5
1	D	117	GLU	2.5
1	I	436	GLU	2.5
1	D	392	ASP	2.5
1	E	342	ASP	2.5
1	L	149	ASP	2.5
1	D	394	LEU	2.5
1	O	253	PHE	2.5
1	D	144	ASN	2.5
1	K	169	ASN	2.5
1	A	136	ALA	2.5
1	D	245	ALA	2.5
1	E	218	ALA	2.5
1	E	444	ALA	2.5
1	G	312	ALA	2.5
1	E	332	SER	2.5
1	H	311	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	J	295	SER	2.5
1	J	325	THR	2.5
1	K	372	THR	2.5
1	N	110	SER	2.5
1	B	289	CYS	2.4
1	G	318	CYS	2.4
1	J	291	CYS	2.4
1	B	436	GLU	2.4
1	C	243	GLY	2.4
1	D	436	GLU	2.4
1	E	195	GLY	2.4
1	F	123	GLY	2.4
1	H	79	GLU	2.4
1	H	433	GLY	2.4
1	E	435	LYS	2.4
1	H	171	ILE	2.4
1	H	191	ILE	2.4
1	H	287	ILE	2.4
1	H	383	TYR	2.4
1	L	409	TYR	2.4
1	M	383	TYR	2.4
1	O	206	TYR	2.4
1	G	201	LEU	2.4
1	N	466	LEU	2.4
1	H	188	TRP	2.4
1	K	364	TRP	2.4
1	G	441	ALA	2.4
1	K	95	ALA	2.4
1	M	218	ALA	2.4
1	O	393	ALA	2.4
1	P	369	MET	2.4
1	P	91	THR	2.4
1	G	158	SER	2.4
1	N	451	SER	2.4
1	P	336	PRO	2.4
1	C	197	GLU	2.4
1	D	197	GLU	2.4
1	F	318	CYS	2.4
1	G	89	GLY	2.4
1	A	342	ASP	2.4
1	E	287	ILE	2.4
1	F	432	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	G	261	ILE	2.4
1	I	191	ILE	2.4
1	I	390	ASP	2.4
1	E	409	TYR	2.4
1	F	340	ASN	2.4
1	O	294	ASN	2.4
1	D	358	ALA	2.4
1	G	95	ALA	2.4
1	H	131	ALA	2.4
1	C	372	THR	2.4
1	F	372	THR	2.4
1	G	106	THR	2.4
1	O	334	THR	2.4
1	F	125	LYS	2.4
1	H	197	GLU	2.4
1	J	246	SER	2.4
1	O	339	SER	2.4
1	I	125	LYS	2.4
1	A	243	GLY	2.4
1	B	207	GLY	2.4
1	F	344	GLY	2.4
1	B	87	CYS	2.4
1	D	127	CYS	2.4
1	N	277	CYS	2.4
1	O	289	CYS	2.4
1	P	348	ILE	2.4
1	B	132	LEU	2.4
1	F	411	PHE	2.4
1	O	462	VAL	2.4
1	P	430	VAL	2.4
1	D	151	ASN	2.4
1	H	95	ALA	2.4
1	O	200	ALA	2.4
1	A	166	THR	2.4
1	C	325	THR	2.4
1	D	343	LYS	2.4
1	E	458	THR	2.4
1	G	146	THR	2.4
1	H	435	LYS	2.4
1	L	372	THR	2.4
1	M	334	THR	2.4
1	O	224	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	G	339	SER	2.4
1	O	240	ILE	2.4
1	E	149	ASP	2.4
1	J	305	LEU	2.4
1	M	342	ASP	2.4
1	O	342	ASP	2.4
1	L	87	CYS	2.4
1	N	352	PHE	2.4
1	D	198	ASN	2.4
1	C	441	ALA	2.4
1	D	441	ALA	2.4
1	J	197	GLU	2.4
1	M	436	GLU	2.4
1	G	166	THR	2.3
1	M	458	THR	2.3
1	I	339	SER	2.3
1	I	359	SER	2.3
1	L	246	SER	2.3
1	K	192	GLY	2.3
1	K	362	GLY	2.3
1	N	433	GLY	2.3
1	A	333	ILE	2.3
1	P	115	ILE	2.3
1	P	315	ARG	2.3
1	B	149	ASP	2.3
1	P	390	ASP	2.3
1	N	206	TYR	2.3
1	P	206	TYR	2.3
1	B	422	VAL	2.3
1	E	416	LYS	2.3
1	K	125	LYS	2.3
1	C	169	ASN	2.3
1	G	294	ASN	2.3
1	O	126	GLU	2.3
1	O	245	ALA	2.3
1	K	328	PRO	2.3
1	G	189	THR	2.3
1	L	81	THR	2.3
1	M	106	THR	2.3
1	N	80	TRP	2.3
1	F	332	SER	2.3
1	P	295	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	347	GLY	2.3
1	P	335	GLY	2.3
1	B	314	ILE	2.3
1	L	157	ILE	2.3
1	F	343	LYS	2.3
1	G	343	LYS	2.3
1	H	411	PHE	2.3
1	P	302	PHE	2.3
1	G	217	TYR	2.3
1	C	436	GLU	2.3
1	H	436	GLU	2.3
1	D	340	ASN	2.3
1	E	219	ASN	2.3
1	J	196	PRO	2.3
1	L	282	ALA	2.3
1	M	282	ALA	2.3
1	C	278	THR	2.3
1	H	106	THR	2.3
1	O	325	THR	2.3
1	D	177	TRP	2.3
1	D	362	GLY	2.3
1	D	364	TRP	2.3
1	I	233	GLY	2.3
1	J	345	SER	2.3
1	K	249	SER	2.3
1	L	450	GLY	2.3
1	N	359	SER	2.3
1	D	96	LEU	2.3
1	O	466	LEU	2.3
1	P	261	ILE	2.3
1	O	390	ASP	2.3
1	B	127	CYS	2.3
1	B	182	CYS	2.3
1	B	276	GLU	2.3
1	G	159	VAL	2.3
1	I	291	CYS	2.3
1	O	318	CYS	2.3
1	M	206	TYR	2.3
1	M	365	TYR	2.3
1	C	294	ASN	2.3
1	F	336	PRO	2.3
1	G	245	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	I	131	ALA	2.3
1	J	209	ALA	2.3
1	L	267	PRO	2.3
1	L	465	ALA	2.3
1	M	169	ASN	2.3
1	M	196	PRO	2.3
1	M	209	ALA	2.3
1	H	325	THR	2.3
1	C	351	GLY	2.3
1	I	453	GLN	2.3
1	A	332	SER	2.3
1	D	359	SER	2.3
1	F	295	SER	2.3
1	K	246	SER	2.3
1	L	451	SER	2.3
1	M	170	SER	2.3
1	A	80	TRP	2.3
1	B	438	TRP	2.3
1	L	314	ILE	2.3
1	E	390	ASP	2.3
1	P	125	LYS	2.3
1	K	208	GLU	2.3
1	K	352	PHE	2.3
1	N	436	GLU	2.3
1	P	119	PHE	2.3
1	P	253	PHE	2.3
1	K	459	VAL	2.3
1	G	196	PRO	2.3
1	B	383	TYR	2.3
1	D	298	ALA	2.2
1	E	465	ALA	2.2
1	G	200	ALA	2.2
1	G	206	TYR	2.3
1	K	289	CYS	2.3
1	H	395	ALA	2.2
1	I	95	ALA	2.2
1	J	442	ALA	2.2
1	J	465	ALA	2.2
1	K	294	ASN	2.2
1	L	340	ASN	2.2
1	M	200	ALA	2.2
1	M	409	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	N	393	ALA	2.2
1	D	104	GLY	2.2
1	G	341	GLY	2.2
1	L	195	GLY	2.2
1	O	346	GLY	2.2
1	P	453	GLN	2.2
1	A	249	SER	2.2
1	B	323	LEU	2.2
1	D	132	LEU	2.2
1	D	248	ILE	2.2
1	F	466	LEU	2.2
1	K	248	ILE	2.2
1	M	466	LEU	2.2
1	N	339	SER	2.2
1	O	96	LEU	2.2
1	O	345	SER	2.2
1	O	397	SER	2.2
1	C	80	TRP	2.2
1	C	364	TRP	2.2
1	H	390	ASP	2.2
1	J	188	TRP	2.2
1	J	103	PHE	2.2
1	N	119	PHE	2.2
1	B	223	ARG	2.2
1	C	267	PRO	2.2
1	E	78	PRO	2.2
1	F	303	VAL	2.2
1	G	423	PRO	2.2
1	H	271	VAL	2.2
1	L	430	VAL	2.2
1	N	336	PRO	2.2
1	B	209	ALA	2.2
1	F	393	ALA	2.2
1	L	228	ALA	2.2
1	A	318	CYS	2.2
1	C	277	CYS	2.2
1	E	277	CYS	2.2
1	O	409	TYR	2.2
1	G	224	THR	2.2
1	I	325	THR	2.2
1	G	331	GLY	2.2
1	H	350	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	I	243	GLY	2.2
1	K	141	GLY	2.2
1	M	89	GLY	2.2
1	N	369	MET	2.2
1	P	89	GLY	2.2
1	P	233	GLY	2.2
1	A	153	LEU	2.2
1	C	466	LEU	2.2
1	I	455	LEU	2.2
1	C	227	SER	2.2
1	E	191	ILE	2.2
1	G	246	SER	2.2
1	K	90	SER	2.2
1	F	392	ASP	2.2
1	I	242	ASP	2.2
1	F	276	GLU	2.2
1	G	79	GLU	2.2
1	H	208	GLU	2.2
1	F	266	PHE	2.2
1	H	302	PHE	2.2
1	J	352	PHE	2.2
1	A	78	PRO	2.2
1	A	303	VAL	2.2
1	E	307	VAL	2.2
1	I	328	PRO	2.2
1	B	121	ALA	2.2
1	F	95	ALA	2.2
1	G	282	ALA	2.2
1	I	294	ASN	2.2
1	L	151	ASN	2.2
1	M	298	ALA	2.2
1	B	125	LYS	2.2
1	A	251	CYS	2.2
1	A	380	TYR	2.2
1	C	106	THR	2.2
1	C	225	GLN	2.2
1	C	334	THR	2.2
1	E	190	TYR	2.2
1	H	343	LYS	2.2
1	F	251	CYS	2.2
1	F	389	THR	2.2
1	G	289	CYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	H	409	TYR	2.2
1	M	285	LYS	2.2
1	P	217	TYR	2.2
1	A	351	GLY	2.2
1	B	96	LEU	2.2
1	D	192	GLY	2.2
1	D	233	GLY	2.2
1	F	341	GLY	2.2
1	I	385	GLY	2.2
1	N	398	GLY	2.2
1	F	171	ILE	2.2
1	G	120	ILE	2.2
1	O	261	ILE	2.2
1	C	342	ASP	2.2
1	E	80	TRP	2.2
1	J	364	TRP	2.2
1	L	456	TRP	2.2
1	N	456	TRP	2.2
1	E	411	PHE	2.2
1	G	411	PHE	2.2
1	P	411	PHE	2.2
1	N	271	VAL	2.2
1	N	462	VAL	2.2
1	O	399	VAL	2.2
1	O	422	VAL	2.2
1	B	358	ALA	2.2
1	C	360	LYS	2.2
1	J	181	ALA	2.2
1	L	198	ASN	2.2
1	L	444	ALA	2.2
1	N	395	ALA	2.2
1	P	121	ALA	2.2
1	P	435	LYS	2.2
1	D	169	ASN	2.2
1	D	294	ASN	2.2
1	E	393	ALA	2.2
1	C	357	MET	2.2
1	H	166	THR	2.2
1	H	321	THR	2.2
1	A	291	CYS	2.2
1	A	323	LEU	2.2
1	B	104	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	113	LEU	2.2
1	B	305	LEU	2.2
1	B	396	LEU	2.2
1	C	135	TYR	2.2
1	C	455	LEU	2.2
1	D	243	GLY	2.2
1	E	179	GLY	2.2
1	F	350	GLY	2.2
1	F	383	TYR	2.2
1	J	106	THR	2.2
1	G	394	LEU	2.2
1	H	466	LEU	2.2
1	I	82	TYR	2.2
1	I	277	CYS	2.2
1	J	87	CYS	2.2
1	J	145	GLY	2.2
1	L	323	LEU	2.2
1	M	434	GLY	2.2
1	N	217	TYR	2.2
1	O	217	TYR	2.2
1	O	341	GLY	2.2
1	P	289	CYS	2.2
1	B	114	ILE	2.2
1	A	359	SER	2.2
1	A	197	GLU	2.2
1	C	313	GLU	2.2
1	E	392	ASP	2.2
1	F	404	GLU	2.2
1	G	250	GLU	2.2
1	L	390	ASP	2.2
1	M	250	GLU	2.2
1	F	80	TRP	2.2
1	M	456	TRP	2.2
1	N	408	TRP	2.2
1	O	456	TRP	2.2
1	B	92	PHE	2.2
1	F	435	LYS	2.2
1	N	103	PHE	2.2
1	O	125	LYS	2.2
1	F	159	VAL	2.1
1	I	381	VAL	2.1
1	A	199	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	245	ALA	2.1
1	A	294	ASN	2.1
1	H	393	ALA	2.1
1	M	465	ALA	2.1
1	O	95	ALA	2.1
1	A	148	GLY	2.1
1	B	192	GLY	2.1
1	B	233	GLY	2.1
1	B	344	GLY	2.1
1	B	394	LEU	2.1
1	D	443	THR	2.1
1	E	305	LEU	2.1
1	F	316	LEU	2.1
1	G	238	LEU	2.1
1	H	316	LEU	2.1
1	I	211	THR	2.1
1	F	135	TYR	2.1
1	H	190	TYR	2.1
1	H	265	ILE	2.1
1	L	427	ILE	2.1
1	M	240	ILE	2.1
1	N	427	ILE	2.1
1	O	383	TYR	2.1
1	I	182	CYS	2.1
1	J	122	CYS	2.1
1	K	291	CYS	2.1
1	O	337	CYS	2.1
1	J	117	GLU	2.1
1	K	313	GLU	2.1
1	G	451	SER	2.1
1	I	246	SER	2.1
1	L	147	ARG	2.1
1	N	315	ARG	2.1
1	K	390	ASP	2.1
1	O	392	ASP	2.1
1	P	170	SER	2.1
1	A	125	LYS	2.1
1	I	373	LYS	2.1
1	I	382	LYS	2.1
1	O	112	PRO	2.1
1	A	399	VAL	2.1
1	C	422	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	177	TRP	2.1
1	F	302	PHE	2.1
1	F	408	TRP	2.1
1	L	130	PHE	2.1
1	G	193	VAL	2.1
1	L	438	TRP	2.1
1	P	80	TRP	2.1
1	J	358	ALA	2.1
1	K	441	ALA	2.1
1	M	312	ALA	2.1
1	A	385	GLY	2.1
1	B	455	LEU	2.1
1	C	452	GLY	2.1
1	D	146	THR	2.1
1	E	145	GLY	2.1
1	F	91	THR	2.1
1	F	224	THR	2.1
1	G	346	GLY	2.1
1	J	466	LEU	2.1
1	L	305	LEU	2.1
1	N	179	GLY	2.1
1	P	321	THR	2.1
1	N	191	ILE	2.1
1	A	210	TYR	2.1
1	E	126	GLU	2.1
1	J	383	TYR	2.1
1	O	250	GLU	2.1
1	E	318	CYS	2.1
1	L	182	CYS	2.1
1	N	229	CYS	2.1
1	G	391	SER	2.1
1	H	178	SER	2.1
1	H	384	ASP	2.1
1	P	160	LYS	2.1
1	C	78	PRO	2.1
1	H	139	PRO	2.1
1	P	78	PRO	2.1
1	C	173	HIS	2.1
1	L	352	PHE	2.1
1	M	411	PHE	2.1
1	O	369	MET	2.1
1	G	399	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	L	422	VAL	2.1
1	B	218	ALA	2.1
1	D	175	ALA	2.1
1	A	145	GLY	2.1
1	E	316	LEU	2.1
1	G	153	LEU	2.1
1	G	305	LEU	2.1
1	I	108	GLY	2.1
1	I	153	LEU	2.1
1	J	140	GLY	2.1
1	J	394	LEU	2.1
1	L	153	LEU	2.1
1	L	222	LEU	2.1
1	M	153	LEU	2.1
1	B	278	THR	2.1
1	E	241	THR	2.1
1	J	372	THR	2.1
1	P	166	THR	2.1
1	P	311	THR	2.1
1	F	315	ARG	2.1
1	B	126	GLU	2.1
1	E	114	ILE	2.1
1	F	208	GLU	2.1
1	N	232	ILE	2.1
1	P	208	GLU	2.1
1	P	275	GLU	2.1
1	A	322	TYR	2.1
1	E	217	TYR	2.1
1	F	206	TYR	2.1
1	A	90	SER	2.1
1	D	246	SER	2.1
1	F	457	ASP	2.1
1	G	87	CYS	2.1
1	H	359	SER	2.1
1	I	90	SER	2.1
1	M	246	SER	2.1
1	N	392	ASP	2.1
1	E	139	PRO	2.1
1	H	78	PRO	2.1
1	L	78	PRO	2.1
1	L	326	PRO	2.1
1	P	273	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	303	VAL	2.1
1	F	167	VAL	2.1
1	F	459	VAL	2.1
1	M	119	PHE	2.1
1	N	302	PHE	2.1
1	P	159	VAL	2.1
1	P	172	PHE	2.1
1	D	111	ALA	2.1
1	H	465	ALA	2.1
1	I	312	ALA	2.1
1	B	466	LEU	2.1
1	D	388	TRP	2.1
1	G	188	TRP	2.1
1	G	340	ASN	2.1
1	H	80	TRP	2.1
1	H	340	ASN	2.1
1	I	396	LEU	2.1
1	N	238	LEU	2.1
1	P	153	LEU	2.1
1	P	219	ASN	2.1
1	A	89	GLY	2.1
1	D	123	GLY	2.1
1	D	344	GLY	2.1
1	E	433	GLY	2.1
1	J	247	GLY	2.1
1	L	223	ARG	2.1
1	O	434	GLY	2.1
1	E	274	THR	2.1
1	I	208	GLU	2.1
1	L	286	THR	2.1
1	H	261	ILE	2.1
1	M	157	ILE	2.1
1	N	240	ILE	2.1
1	I	380	TYR	2.1
1	O	322	TYR	2.1
1	P	383	TYR	2.1
1	C	391	SER	2.1
1	K	339	SER	2.1
1	A	301	PRO	2.1
1	B	139	PRO	2.1
1	N	78	PRO	2.1
1	P	277	CYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	453	GLN	2.0
1	A	413	PHE	2.0
1	G	307	VAL	2.0
1	H	119	PHE	2.0
1	J	411	PHE	2.0
1	F	395	ALA	2.0
1	L	393	ALA	2.0
1	M	395	ALA	2.0
1	O	209	ALA	2.0
1	A	85	LEU	2.0
1	C	199	ASN	2.0
1	E	466	LEU	2.0
1	N	153	LEU	2.0
1	B	195	GLY	2.0
1	E	341	GLY	2.0
1	D	325	THR	2.0
1	D	438	TRP	2.0
1	K	140	GLY	2.0
1	K	145	GLY	2.0
1	L	280	GLY	2.0
1	I	268	THR	2.0
1	O	348	ILE	2.0
1	P	224	THR	2.0
1	P	438	TRP	2.0
1	E	204	ILE	2.0
1	F	287	ILE	2.0
1	J	314	ILE	2.0
1	J	382	LYS	2.0
1	M	107	LYS	2.0
1	O	255	LYS	2.0
1	O	272	LYS	2.0
1	B	196	PRO	2.0
1	H	217	TYR	2.0
1	I	322	TYR	2.0
1	J	118	PRO	2.0
1	L	196	PRO	2.0
1	M	217	TYR	2.0
1	F	170	SER	2.0
1	H	410	SER	2.0
1	A	231	CYS	2.0
1	H	130	PHE	2.0
1	J	147	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
1	J	223	ARG	2.0
1	J	422	VAL	2.0
1	M	159	VAL	2.0
1	O	307	VAL	2.0
1	A	396	LEU	2.0
1	D	466	LEU	2.0
1	F	250	GLU	2.0
1	G	316	LEU	2.0
1	I	197	GLU	2.0
1	I	201	LEU	2.0
1	I	466	LEU	2.0
1	L	442	ALA	2.0
1	O	323	LEU	2.0
1	B	144	ASN	2.0
1	C	109	ASN	2.0
1	C	148	GLY	2.0
1	D	89	GLY	2.0
1	D	179	GLY	2.0
1	O	169	ASN	2.0
1	A	106	THR	2.0
1	A	146	THR	2.0
1	C	240	ILE	2.0
1	H	240	ILE	2.0
1	I	287	ILE	2.0
1	I	443	THR	2.0
1	I	460	THR	2.0
1	J	268	THR	2.0
1	L	106	THR	2.0
1	L	191	ILE	2.0
1	N	311	THR	2.0
1	O	120	ILE	2.0
1	P	445	ILE	2.0
1	C	196	PRO	2.0
1	C	328	PRO	2.0
1	F	267	PRO	2.0
1	J	78	PRO	2.0
1	J	149	ASP	2.0
1	N	390	ASP	2.0
1	C	249	SER	2.0
1	D	143	TYR	2.0
1	K	380	TYR	2.0
1	M	237	TYR	2.0

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Mol	Chain	Res	Type	RSRZ
1	M	322	TYR	2.0
1	N	86	SER	2.0
1	N	190	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	F	900	14/15	0.63	0.17	43,45,46,47	0
2	NAG	A	900	14/15	0.64	0.17	43,45,46,47	0
2	NAG	D	900	14/15	0.65	0.17	43,45,47,47	0
2	NAG	B	900	14/15	0.65	0.17	43,45,46,47	0
2	NAG	C	900	14/15	0.66	0.15	43,45,47,47	0
2	NAG	I	900	14/15	0.66	0.16	43,45,46,46	0
2	NAG	H	900	14/15	0.67	0.17	43,45,46,46	0
2	NAG	L	900	14/15	0.67	0.16	43,45,46,47	0
2	NAG	N	900	14/15	0.68	0.16	43,45,46,46	0
2	NAG	P	900	14/15	0.69	0.15	43,45,46,46	0
2	NAG	O	900	14/15	0.71	0.16	43,45,47,47	0
2	NAG	K	900	14/15	0.72	0.17	43,45,46,46	0
2	NAG	J	900	14/15	0.75	0.15	43,45,46,47	0
2	NAG	M	900	14/15	0.78	0.15	43,45,46,46	0
2	NAG	E	900	14/15	0.80	0.15	43,45,46,46	0
2	NAG	G	900	14/15	0.82	0.14	43,45,47,47	0
3	CA	F	1000	1/1	0.83	0.16	58,58,58,58	0
3	CA	D	1000	1/1	0.85	0.11	57,57,57,57	0
3	CA	M	1000	1/1	0.87	0.17	58,58,58,58	0
4	G39	I	1	20/20	0.88	0.16	2,18,36,38	0

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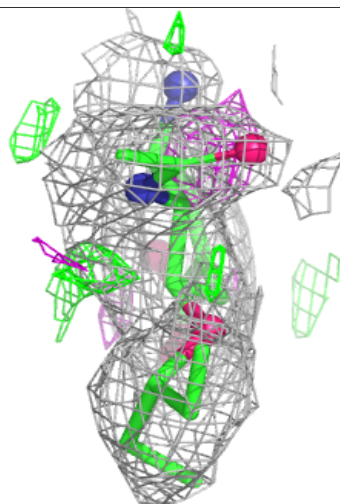
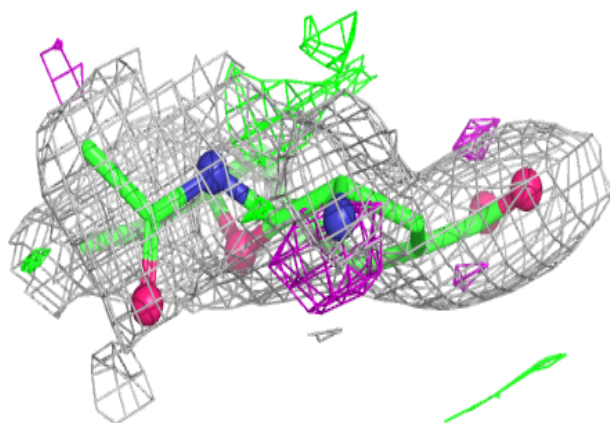
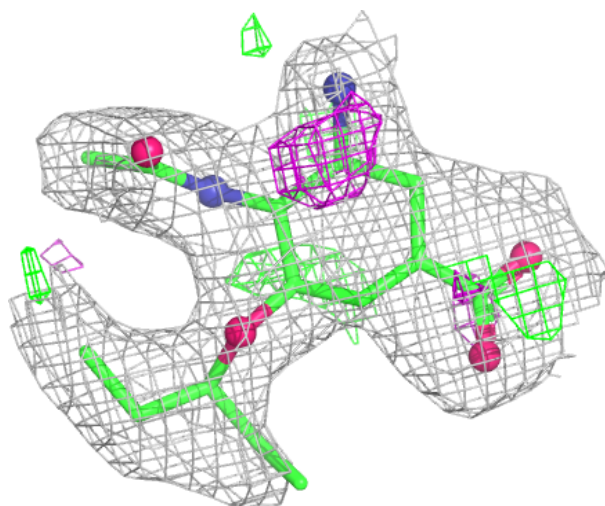
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	G39	M	1	20/20	0.88	0.14	2,18,30,34	0
4	G39	C	1	20/20	0.89	0.13	2,16,28,33	0
4	G39	G	1	20/20	0.89	0.13	2,13,27,32	0
3	CA	N	1000	1/1	0.90	0.09	57,57,57,57	0
3	CA	O	1000	1/1	0.90	0.15	58,58,58,58	0
3	CA	C	1000	1/1	0.90	0.10	57,57,57,57	0
4	G39	N	1	20/20	0.90	0.12	2,16,31,36	0
4	G39	F	1	20/20	0.91	0.13	2,21,35,40	0
3	CA	A	1000	1/1	0.91	0.11	57,57,57,57	0
3	CA	G	1000	1/1	0.91	0.12	58,58,58,58	0
3	CA	B	1000	1/1	0.91	0.09	57,57,57,57	0
4	G39	E	1	20/20	0.91	0.12	2,9,26,29	0
4	G39	O	1	20/20	0.91	0.11	2,11,29,30	0
4	G39	H	1	20/20	0.92	0.12	2,10,28,33	0
4	G39	D	1	20/20	0.92	0.11	2,6,30,32	0
4	G39	K	1	20/20	0.92	0.14	2,2,21,22	0
3	CA	P	1000	1/1	0.92	0.11	57,57,57,57	0
4	G39	A	1	20/20	0.92	0.14	2,2,27,30	0
3	CA	H	1000	1/1	0.92	0.11	57,57,57,57	0
4	G39	P	1	20/20	0.92	0.11	2,13,30,31	0
3	CA	L	1000	1/1	0.93	0.08	57,57,57,57	0
4	G39	J	1	20/20	0.93	0.14	2,2,28,29	0
4	G39	B	1	20/20	0.93	0.10	2,6,26,29	0
4	G39	L	1	20/20	0.93	0.12	2,2,22,23	0
3	CA	K	1000	1/1	0.94	0.10	57,57,57,57	0
3	CA	I	1000	1/1	0.94	0.09	57,57,57,57	0
3	CA	J	1000	1/1	0.95	0.06	57,57,57,57	0
3	CA	E	1000	1/1	0.96	0.12	57,57,57,57	0
5	YT3	P	4	1/1	0.96	0.07	51,51,51,51	0
5	YT3	E	2	1/1	0.97	0.06	46,46,46,46	0
5	YT3	J	3	1/1	0.98	0.04	50,50,50,50	0
5	YT3	A	467	1/1	0.99	0.04	50,50,50,50	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.

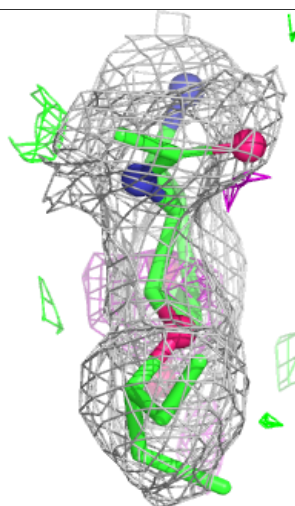
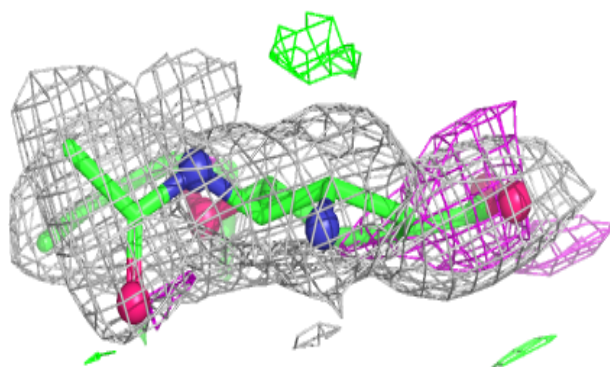
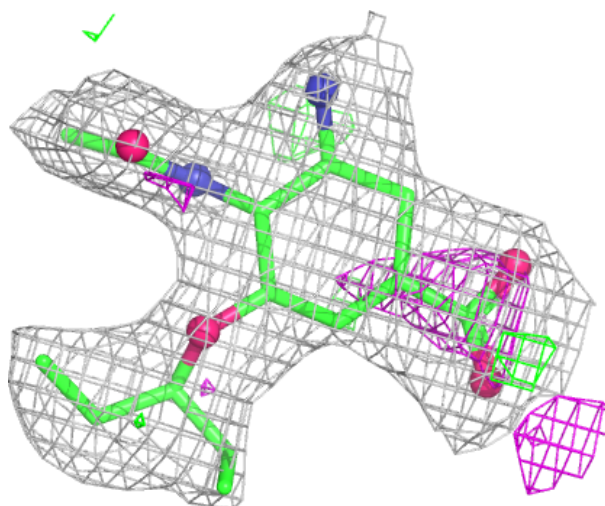
Electron density around G39 I 1:

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



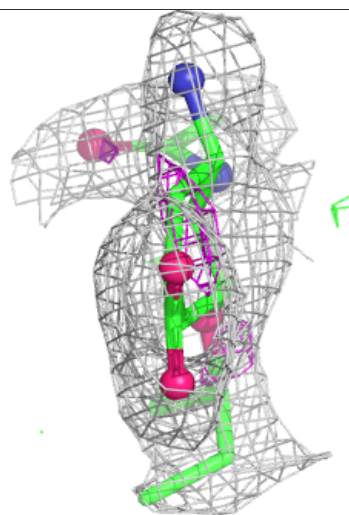
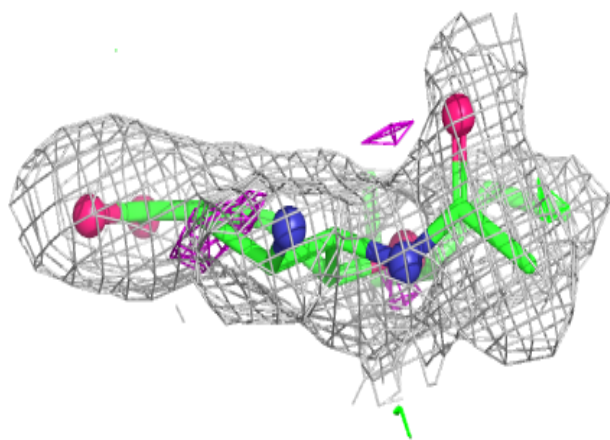
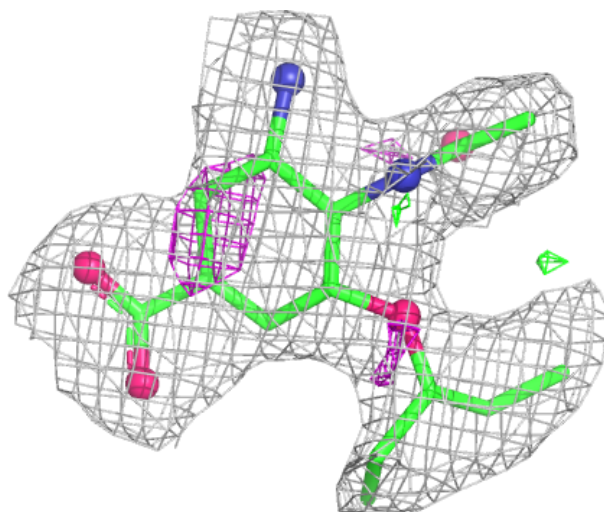
Electron density around G39 M 1:

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and green (positive)



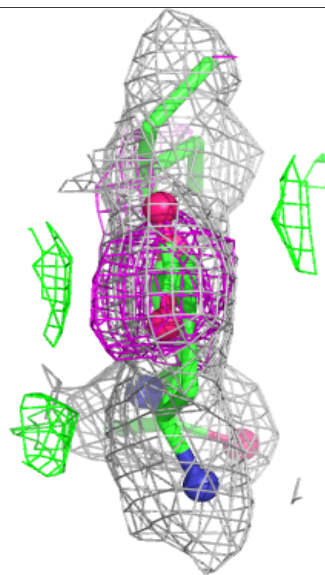
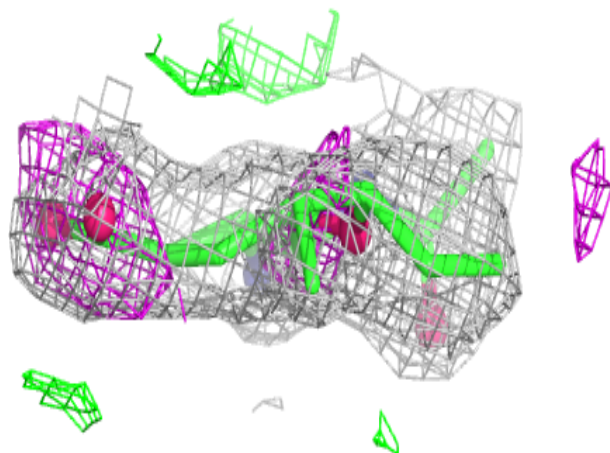
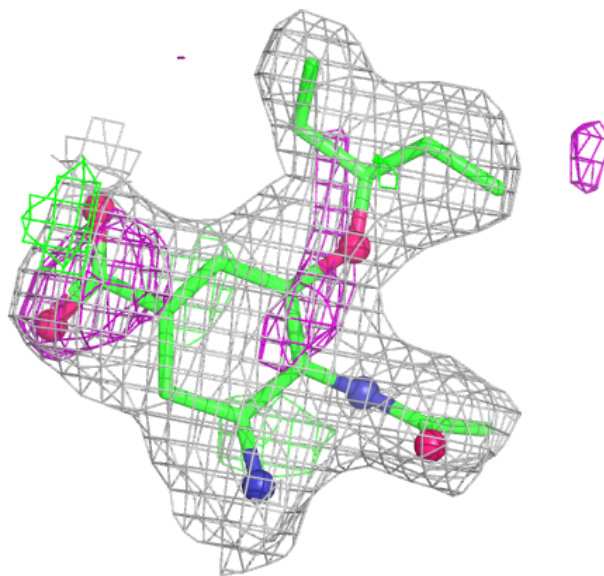
Electron density around G39 C 1:

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



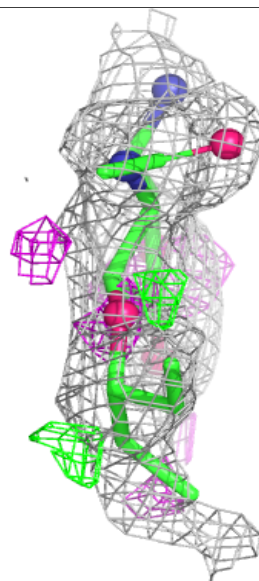
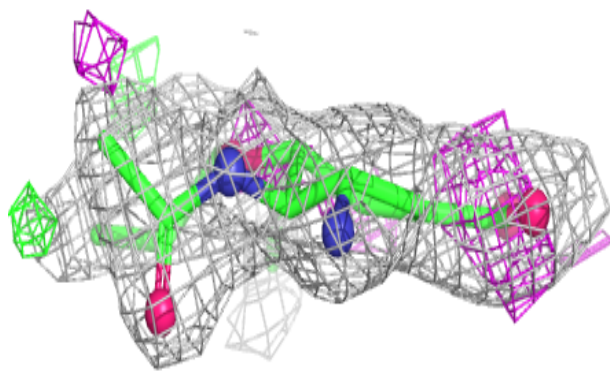
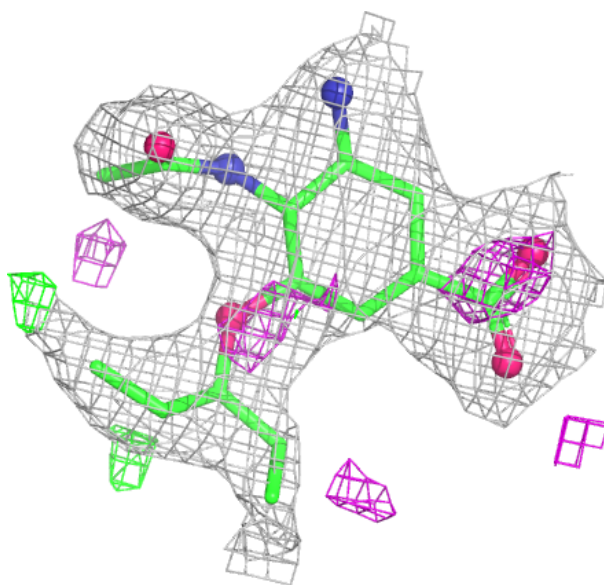
Electron density around G39 G 1:

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



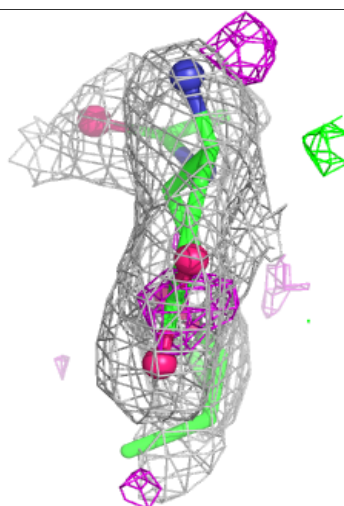
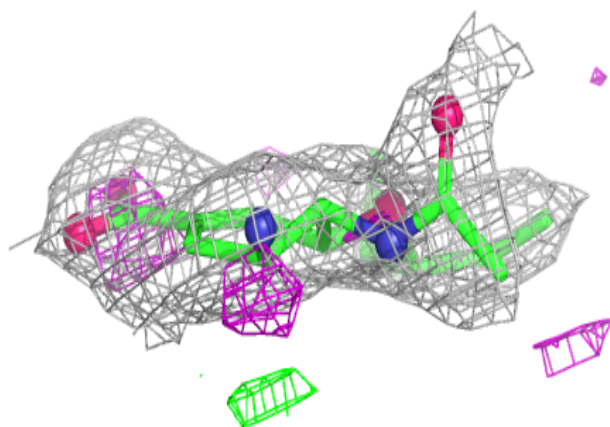
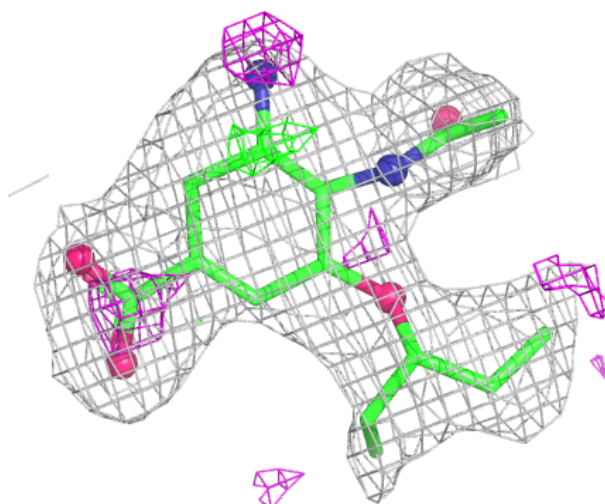
Electron density around G39 N 1:

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and green (positive)



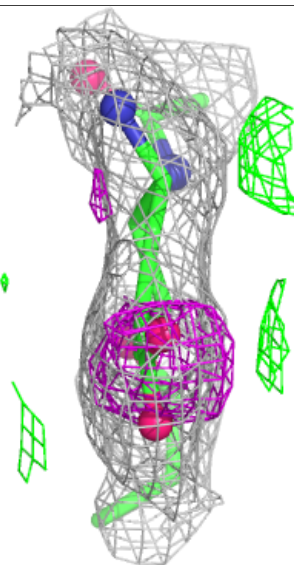
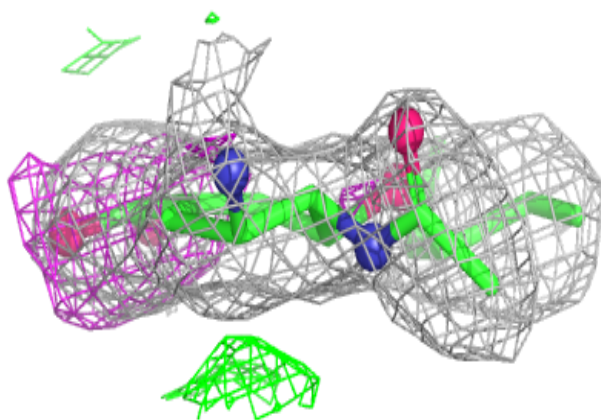
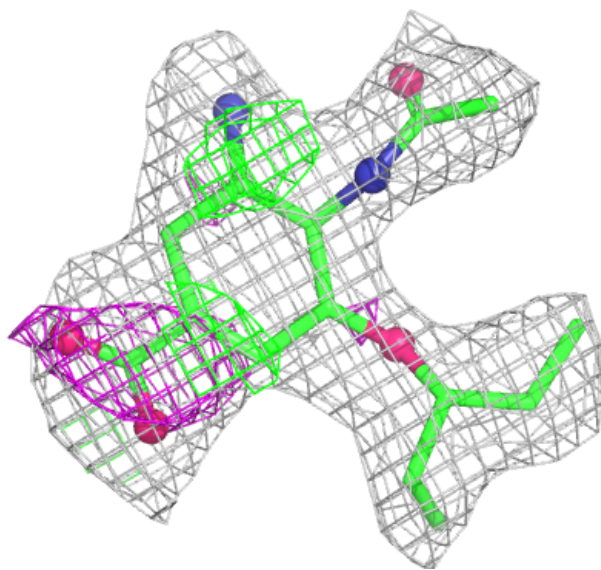
Electron density around G39 F 1:

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and green (positive)



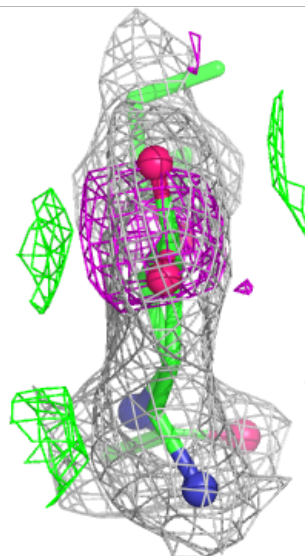
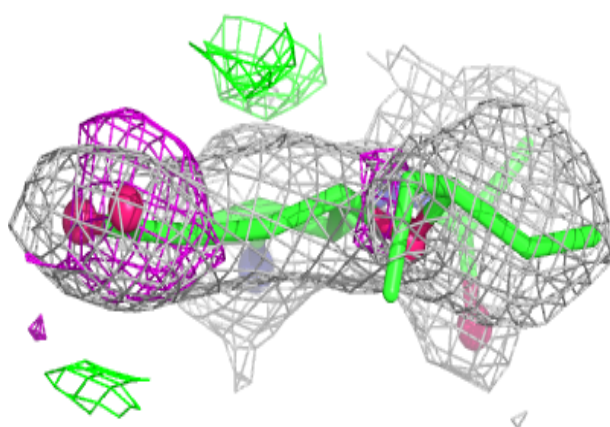
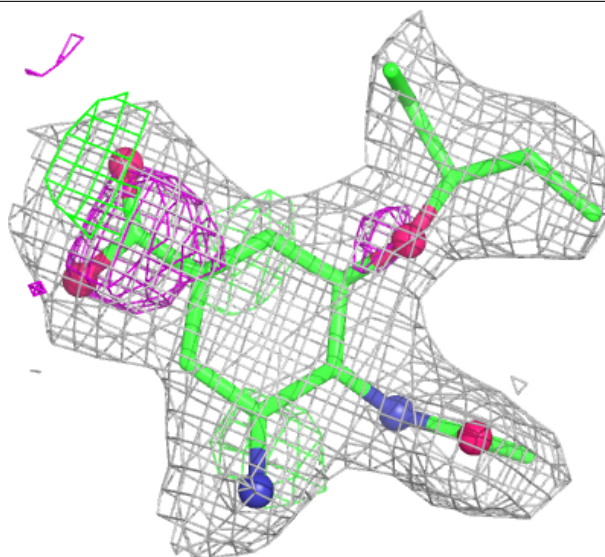
Electron density around G39 E 1:

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



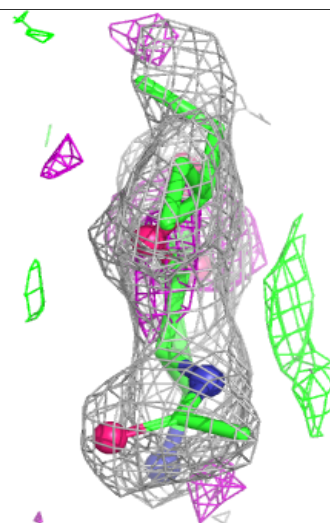
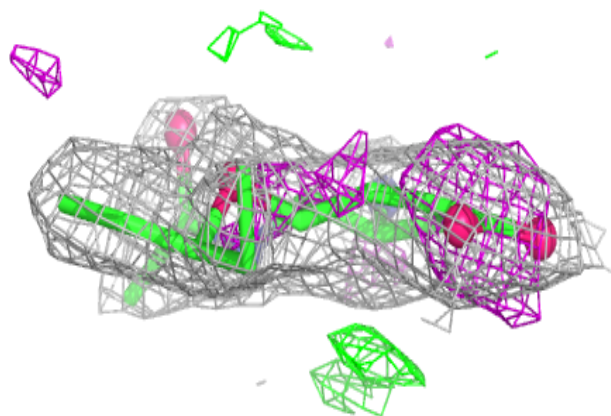
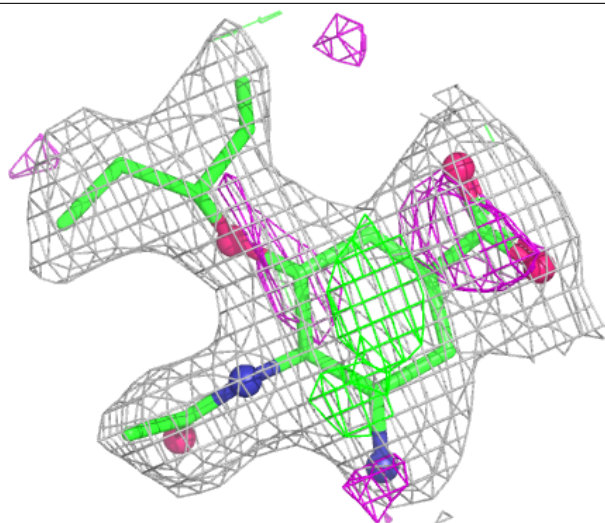
Electron density around G39 O 1:

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and green (positive)



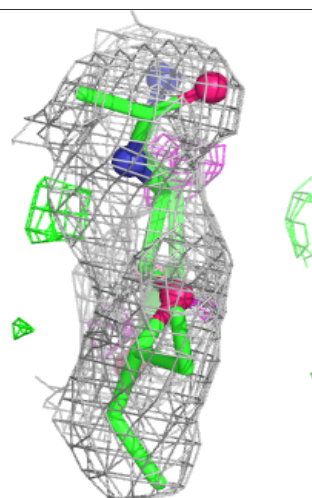
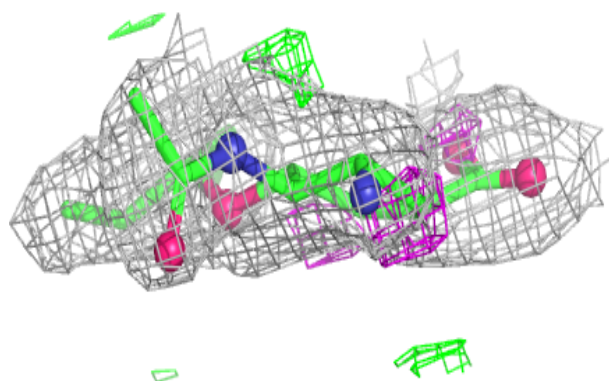
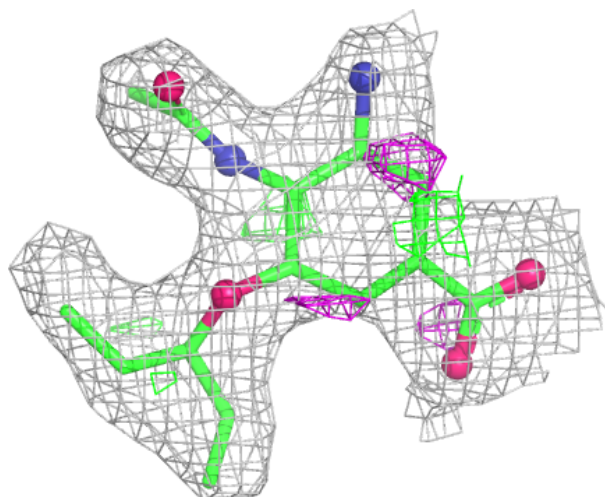
Electron density around G39 H 1:

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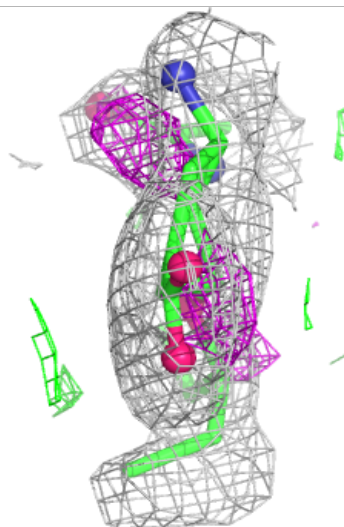
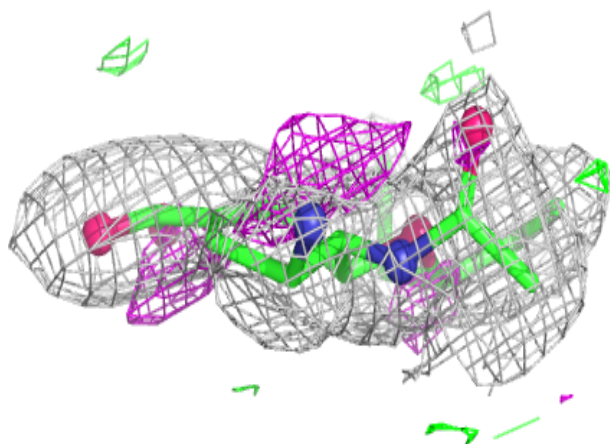
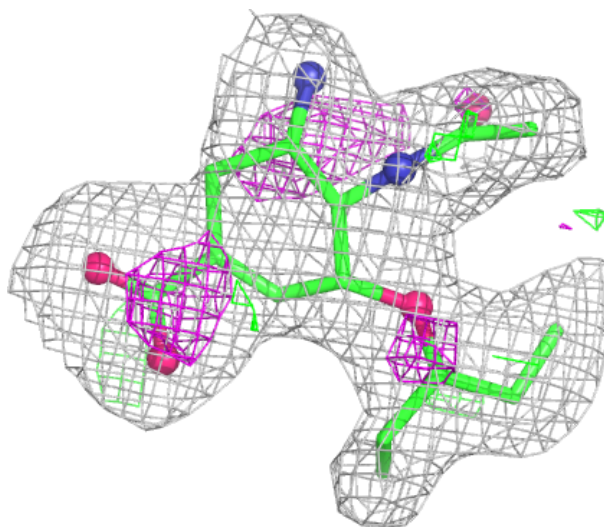
Electron density around G39 D 1:

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



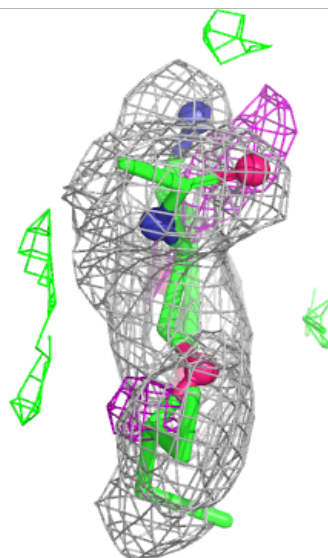
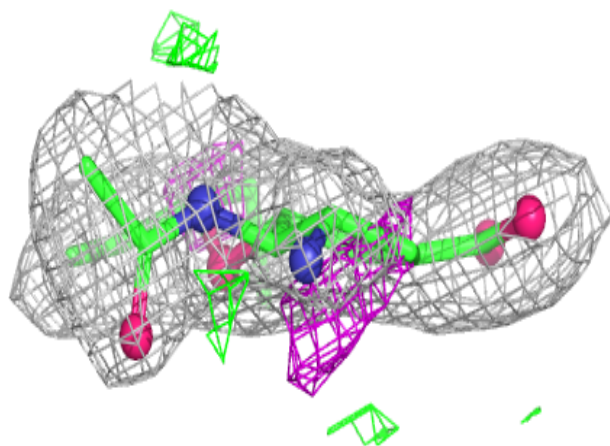
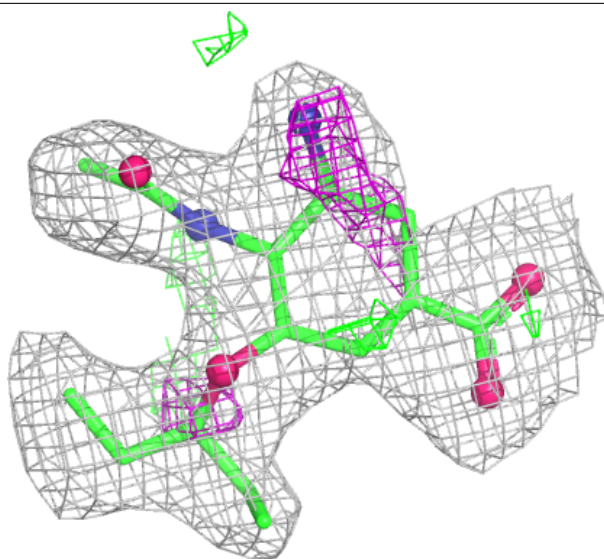
Electron density around G39 K 1:

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



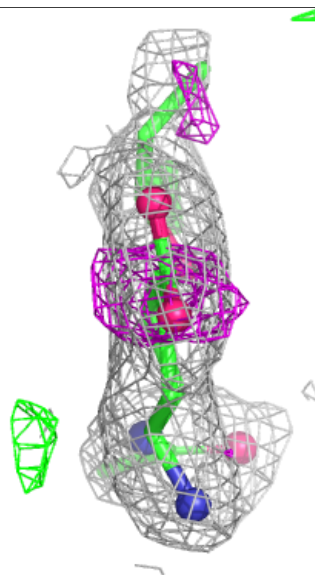
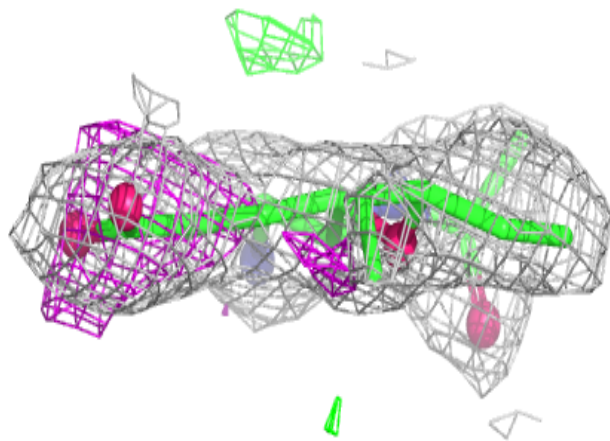
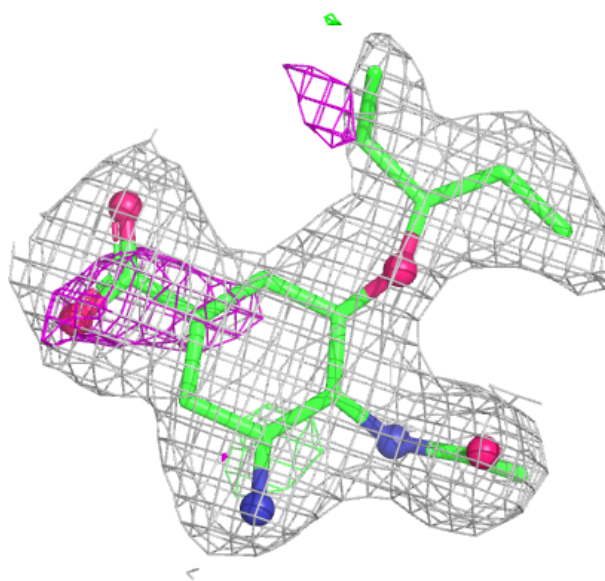
Electron density around G39 A 1:

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and green (positive)



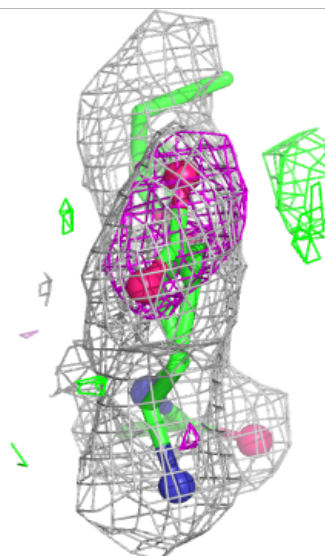
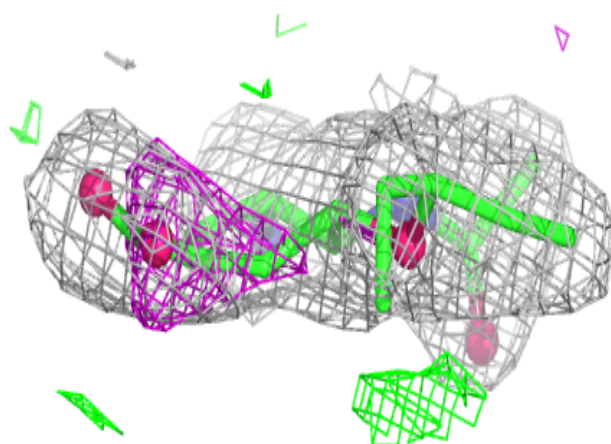
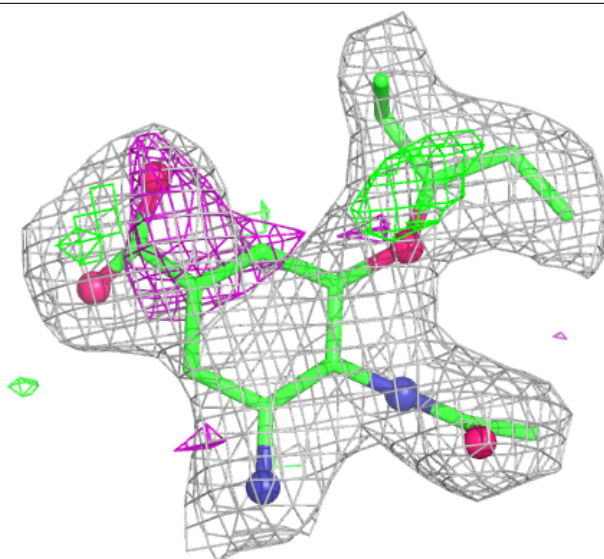
Electron density around G39 P 1:

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and green (positive)



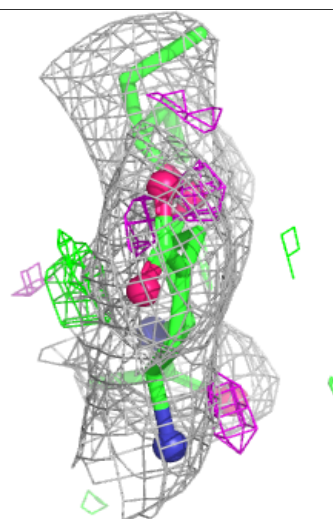
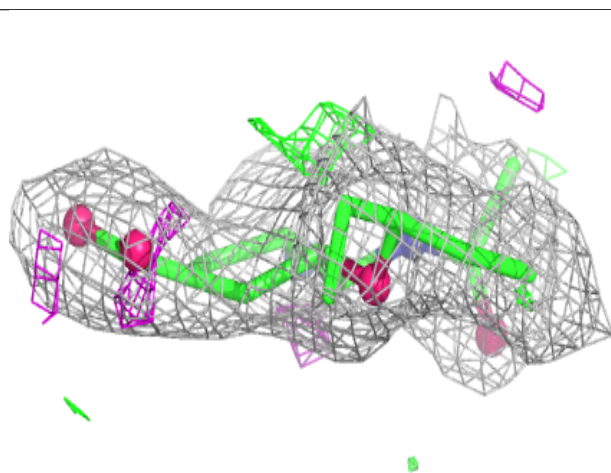
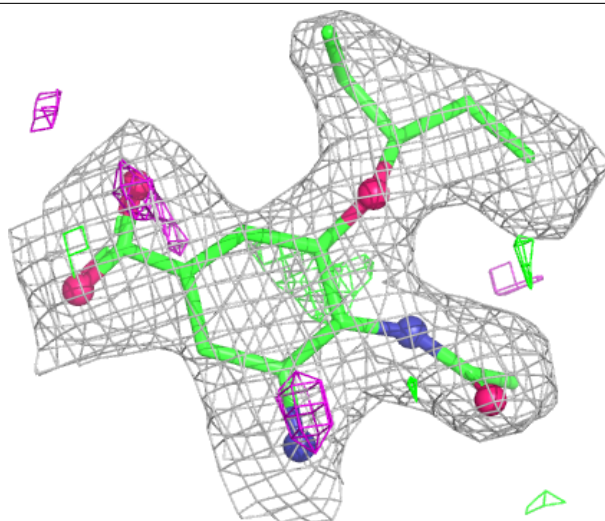
Electron density around G39 J 1:

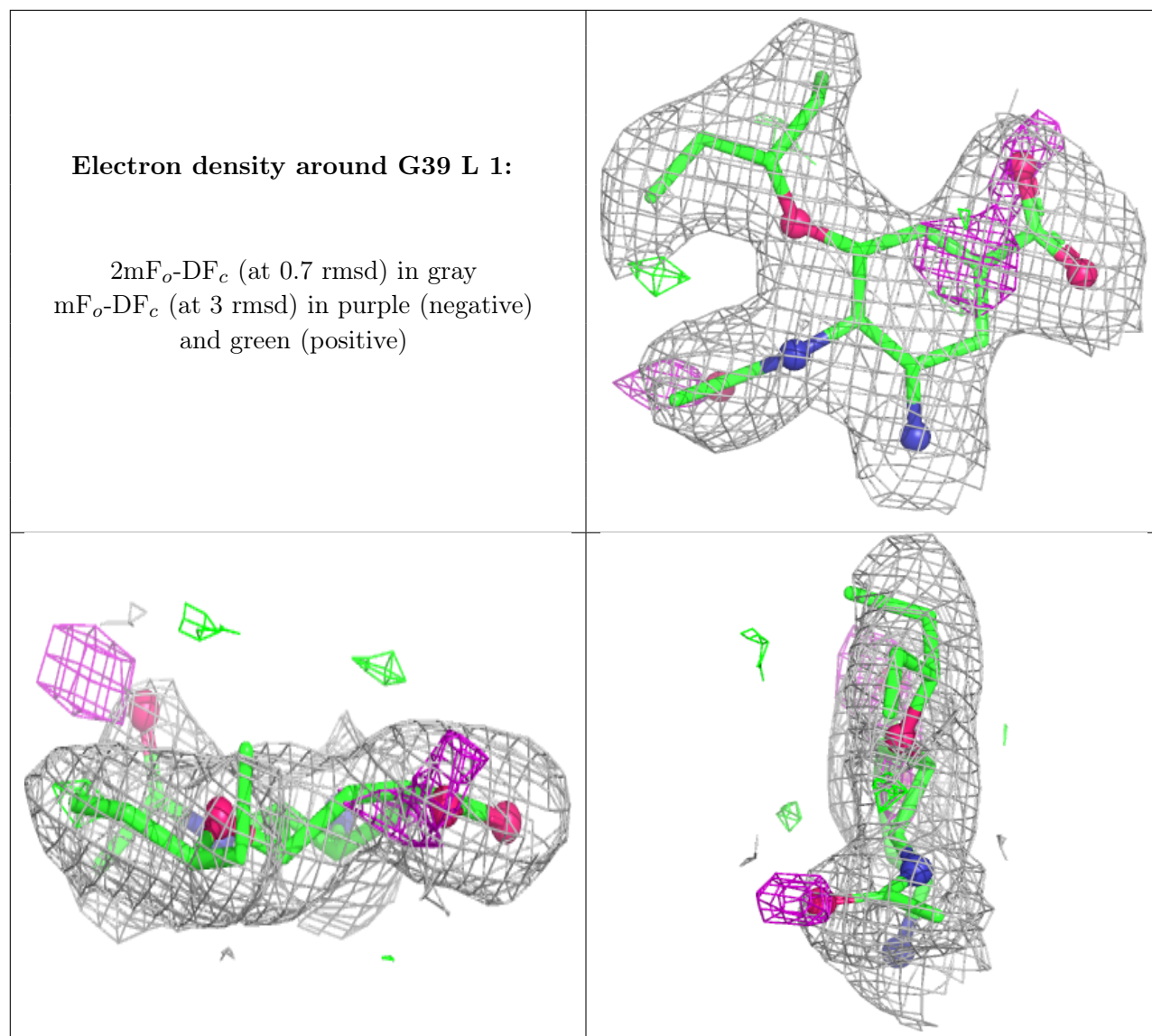
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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around G39 B 1:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.