



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:56 PM UTC

PDB ID : 3N87 / pdb_00003n87
Title : Crystal structure of 3-dehydroquinate dehydratase from Mycobacterium tuberculosis in complex with inhibitor 3
Authors : Dias, M.V.B.; Snee, W.C.; Bromfield, K.M.; Payne, R.; Palaninathan, S.K.; Ciulli, A.; Howard, N.I.; Abell, C.; Sacchettini, J.C.; Blundell, T.L.
Deposited on : 2010-05-27
Resolution : 2.40 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:

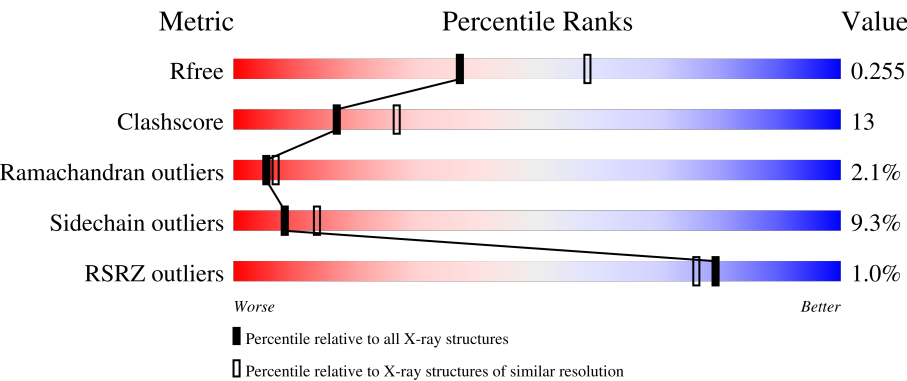
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	147	% 73%19% . .
1	B	147	78%14% . .
1	C	147	3% 70%20%5% . .
1	D	147	2% 69%21%5% . .

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Mol	Chain	Length	Quality of chain
1	E	147	 2% 67% 22% 6% . .
1	F	147	 % 74% 16% 5% .
1	G	147	 59% 32% 5% . .
1	H	147	 71% 18% 5% . .
1	I	147	 % 73% 16% 6% . .
1	J	147	 % 67% 23% 5% . .
1	K	147	 % 68% 22% 5% . .
1	L	147	 % 71% 22% . .
1	M	147	 % 68% 22% 6% .
1	N	147	 % 68% 22% 5% . .
1	O	147	 % 73% 18% . . .
1	P	147	 64% 22% 9% . .
1	Q	147	 % 71% 21% . . .
1	R	147	 % 65% 27% . . .
1	S	147	 % 68% 22% . . .
1	T	147	 79% 14% . . .
1	U	147	 % 73% 18% . . .
1	V	147	 63% 20% 12% . .
1	W	147	 % 73% 19% . . .
1	X	147	 % 71% 19% . . .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 27701 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 3-dehydroquinate dehydratase.

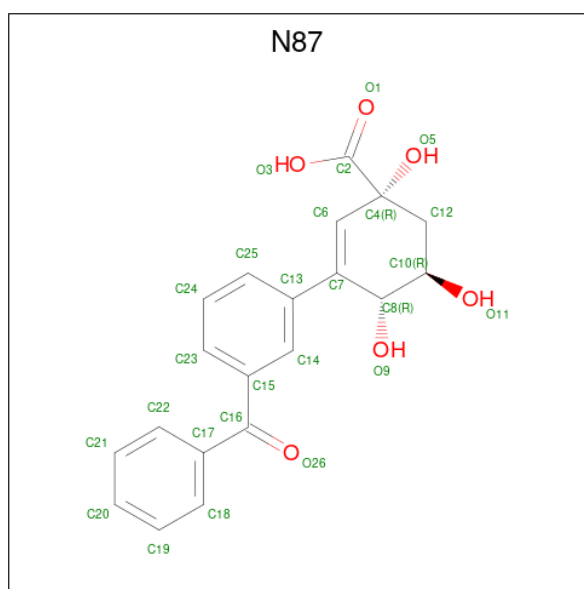
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	141	Total	C	N	O	S	0	0	0
			1065	671	193	200	1			
1	B	141	Total	C	N	O	S	0	0	0
			1071	674	196	200	1			
1	C	141	Total	C	N	O	S	0	0	0
			1065	670	196	198	1			
1	D	141	Total	C	N	O	S	0	0	0
			1069	672	196	200	1			
1	E	141	Total	C	N	O	S	0	0	0
			1071	674	196	200	1			
1	F	141	Total	C	N	O	S	0	1	0
			1071	675	195	200	1			
1	G	141	Total	C	N	O	S	0	0	0
			1071	674	196	200	1			
1	H	141	Total	C	N	O	S	0	0	0
			1071	674	196	200	1			
1	I	141	Total	C	N	O	S	0	0	0
			1071	674	196	200	1			
1	J	141	Total	C	N	O	S	0	0	0
			1065	670	196	198	1			
1	K	141	Total	C	N	O	S	0	0	0
			1061	669	193	198	1			
1	L	141	Total	C	N	O	S	0	0	0
			1071	674	196	200	1			
1	M	141	Total	C	N	O	S	0	0	0
			1071	674	196	200	1			
1	N	141	Total	C	N	O	S	0	1	0
			1077	678	198	200	1			
1	O	141	Total	C	N	O	S	0	0	0
			1071	674	196	200	1			
1	P	141	Total	C	N	O	S	0	0	0
			1071	674	196	200	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	141	Total	C	N	O	S	0	0	0
			1065	671	193	200	1			
1	R	141	Total	C	N	O	S	0	0	0
			1059	667	193	198	1			
1	S	141	Total	C	N	O	S	0	0	0
			1071	674	196	200	1			
1	T	141	Total	C	N	O	S	0	0	0
			1071	674	196	200	1			
1	U	141	Total	C	N	O	S	0	0	0
			1071	674	196	200	1			
1	V	141	Total	C	N	O	S	0	0	0
			1067	672	196	198	1			
1	W	141	Total	C	N	O	S	0	0	0
			1065	671	193	200	1			
1	X	141	Total	C	N	O	S	0	0	0
			1061	669	193	198	1			

- Molecule 2 is (1R,4R,5R)-1,4,5-trihydroxy-3-[3-(phenylcarbonyl)phenyl]cyclohex-2-ene-1-carboxylic acid (CCD ID: N87) (formula: C₂₀H₁₈O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			26	20	6		
2	B	1	Total	C	O	0	0
			26	20	6		
2	C	1	Total	C	O	0	0
			26	20	6		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	D	1	Total	C	O	0	0
			26	20	6		
2	E	1	Total	C	O	0	0
			26	20	6		
2	F	1	Total	C	O	0	0
			26	20	6		
2	G	1	Total	C	O	0	0
			26	20	6		
2	H	1	Total	C	O	0	0
			26	20	6		
2	I	1	Total	C	O	0	0
			26	20	6		
2	J	1	Total	C	O	0	0
			26	20	6		
2	K	1	Total	C	O	0	0
			26	20	6		
2	L	1	Total	C	O	0	0
			26	20	6		
2	M	1	Total	C	O	0	0
			26	20	6		
2	N	1	Total	C	O	0	0
			26	20	6		
2	O	1	Total	C	O	0	0
			26	20	6		
2	P	1	Total	C	O	0	0
			26	20	6		
2	Q	1	Total	C	O	0	0
			26	20	6		
2	R	1	Total	C	O	0	0
			26	20	6		
2	S	1	Total	C	O	0	0
			26	20	6		
2	T	1	Total	C	O	0	0
			26	20	6		
2	U	1	Total	C	O	0	0
			26	20	6		
2	V	1	Total	C	O	0	0
			26	20	6		
2	W	1	Total	C	O	0	0
			26	20	6		
2	X	1	Total	C	O	0	0
			26	20	6		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	53	Total O 53 53	0	0
3	B	90	Total O 90 90	0	0
3	C	59	Total O 59 59	0	0
3	D	54	Total O 54 54	0	0
3	E	78	Total O 78 78	0	0
3	F	60	Total O 60 60	0	0
3	G	66	Total O 66 66	0	0
3	H	59	Total O 59 59	0	0
3	I	48	Total O 48 48	0	0
3	J	70	Total O 70 70	0	0
3	K	55	Total O 55 55	0	0
3	L	49	Total O 49 49	0	0
3	M	57	Total O 57 57	0	0
3	N	54	Total O 54 54	0	0
3	O	53	Total O 53 53	0	0
3	P	67	Total O 67 67	0	0
3	Q	50	Total O 50 50	0	0
3	R	63	Total O 63 63	0	0
3	S	66	Total O 66 66	0	0
3	T	73	Total O 73 73	0	0
3	U	59	Total O 59 59	0	0

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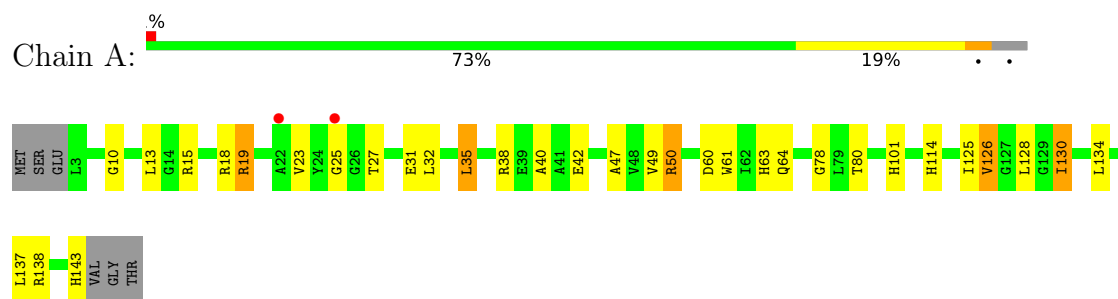
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	V	61	Total 61	O 61	0	0
3	W	43	Total 43	O 43	0	0
3	X	48	Total 48	O 48	0	0

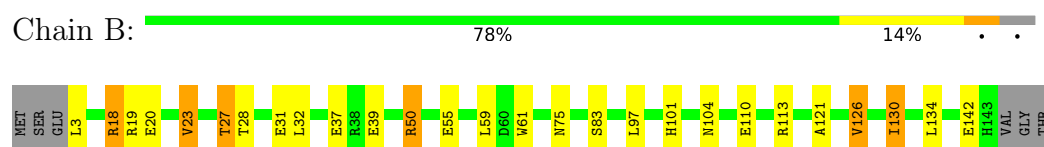
3 Residue-property plots [i](#)

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.

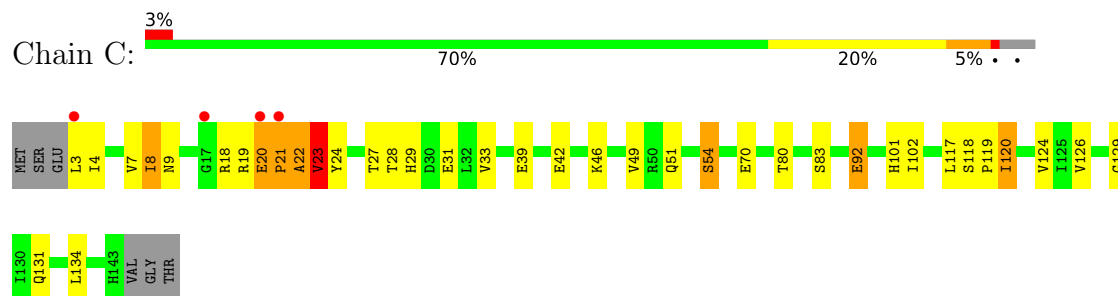
- Molecule 1: 3-dehydroquinate dehydratase



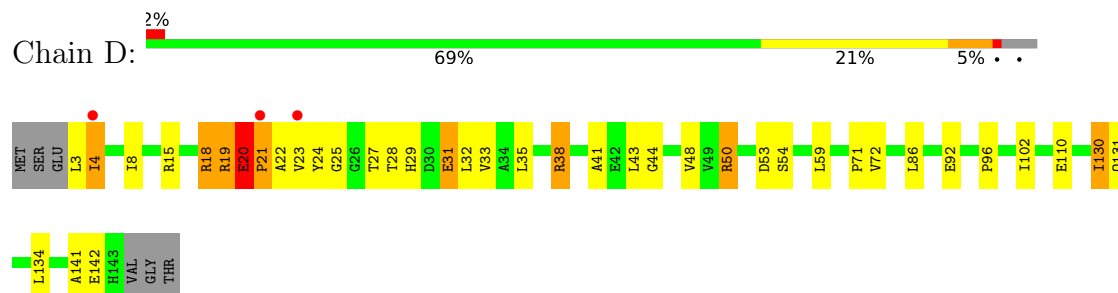
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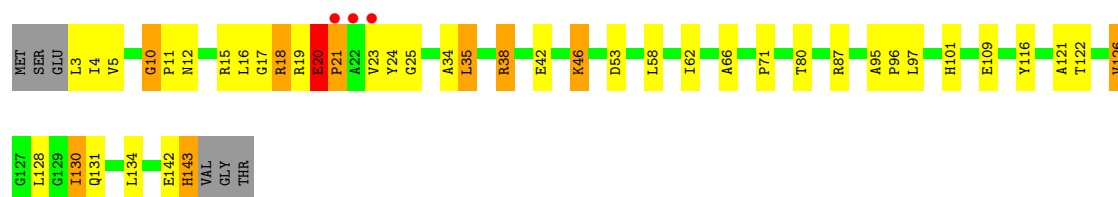
- Molecule 1: 3-dehydroquinate dehydratase



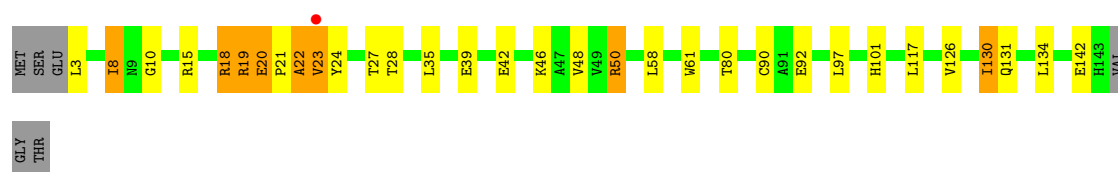
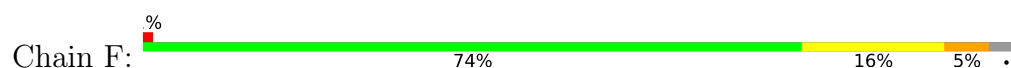
- Molecule 1: 3-dehydroquinate dehydratase



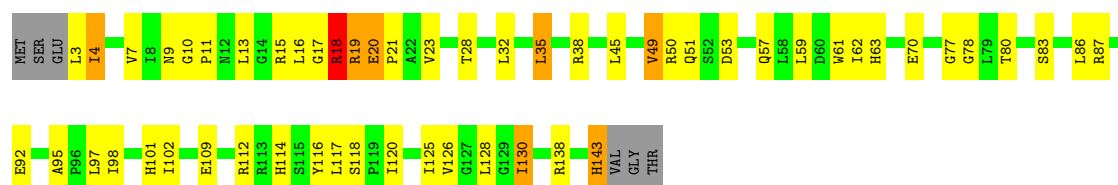
- Molecule 1: 3-dehydroquinate dehydratase



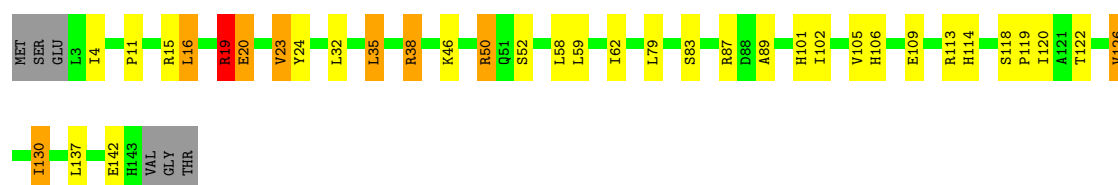
- Molecule 1: 3-dehydroquinate dehydratase



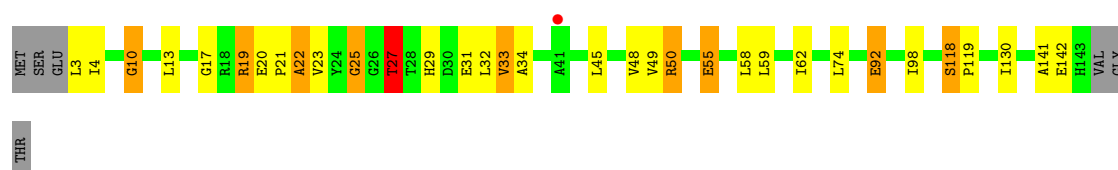
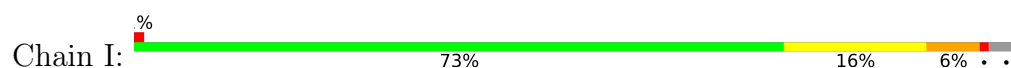
- Molecule 1: 3-dehydroquinate dehydratase



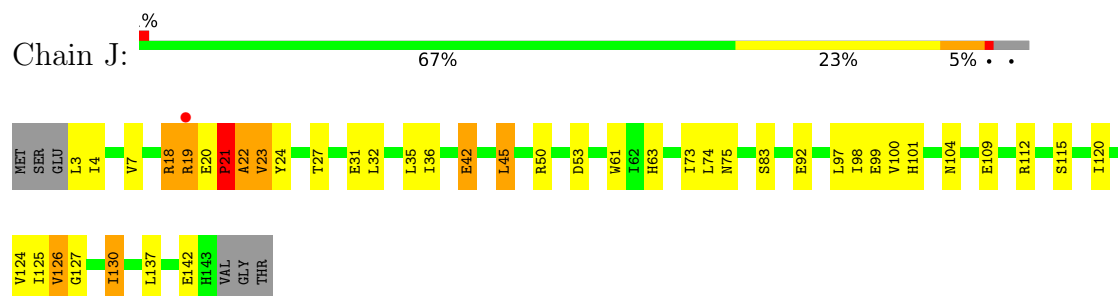
- Molecule 1: 3-dehydroquinate dehydratase



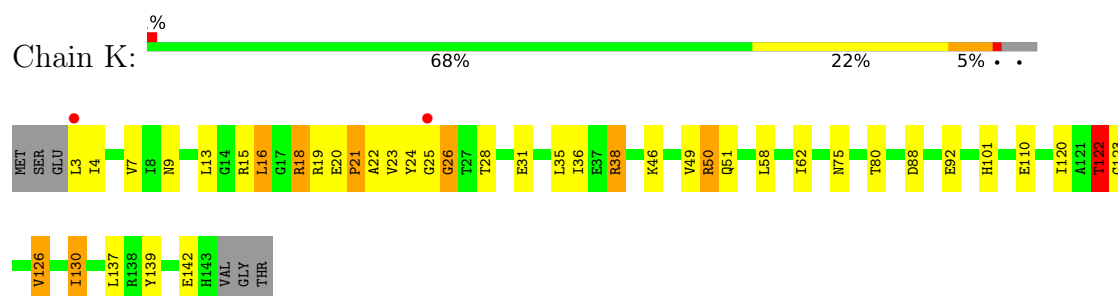
- Molecule 1: 3-dehydroquinate dehydratase



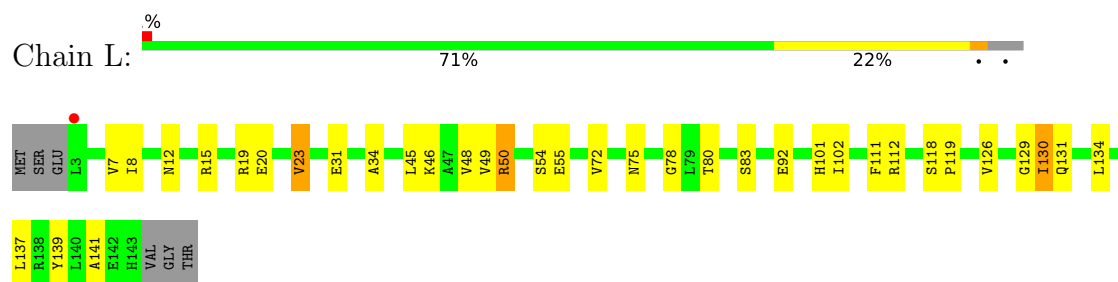
- Molecule 1: 3-dehydroquinase dehydratase



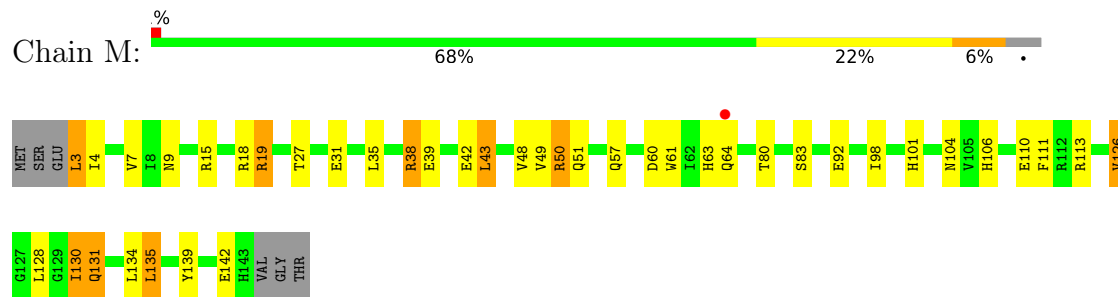
- Molecule 1: 3-dehydroquinase dehydratase



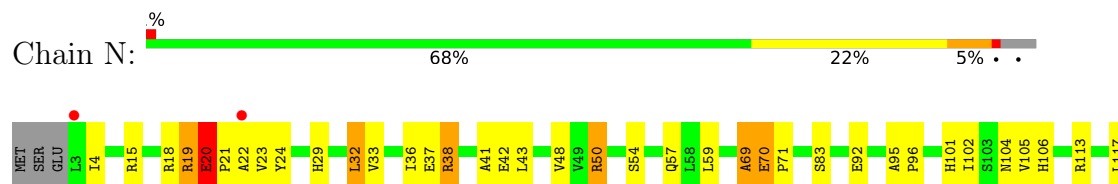
- Molecule 1: 3-dehydroquinase dehydratase



- Molecule 1: 3-dehydroquinase dehydratase

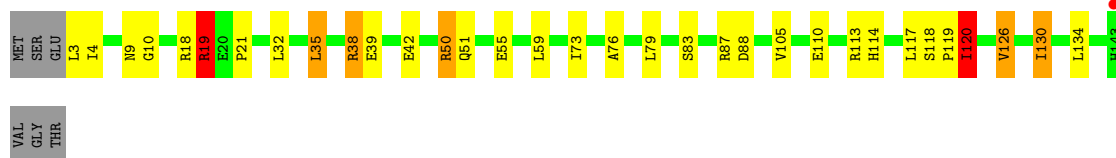
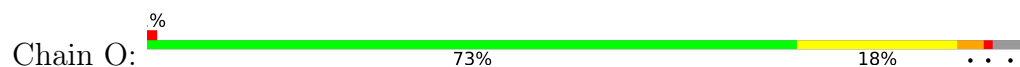


- Molecule 1: 3-dehydroquinase dehydratase

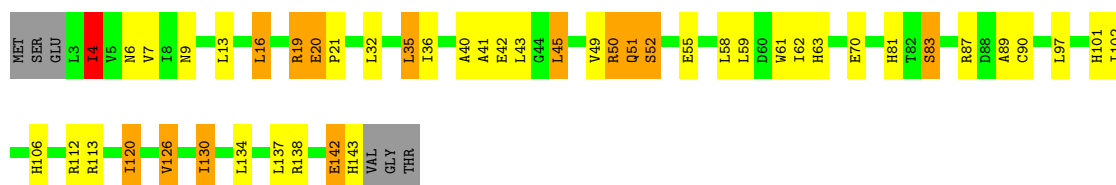




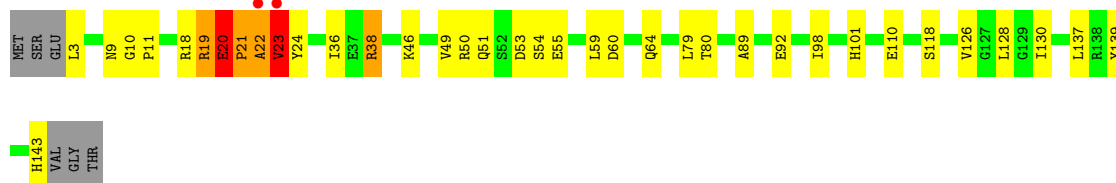
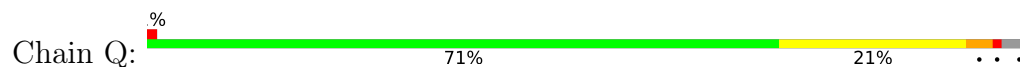
- Molecule 1: 3-dehydroquinate dehydratase



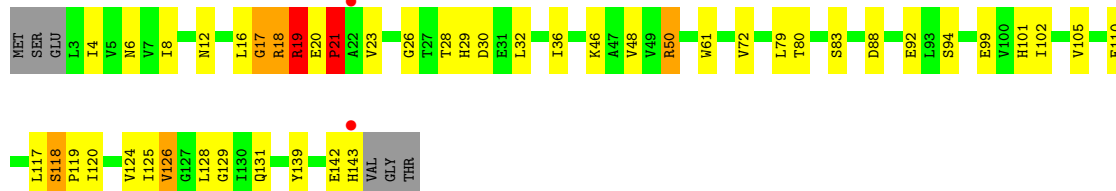
- Molecule 1: 3-dehydroquinate dehydratase



- Molecule 1: 3-dehydroquinate dehydratase

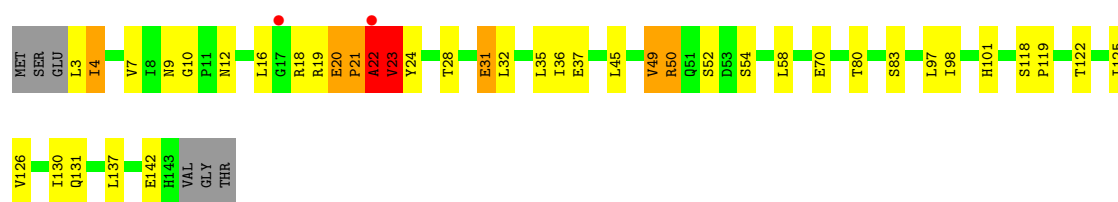


- Molecule 1: 3-dehydroquinate dehydratase



- Molecule 1: 3-dehydroquinate dehydratase





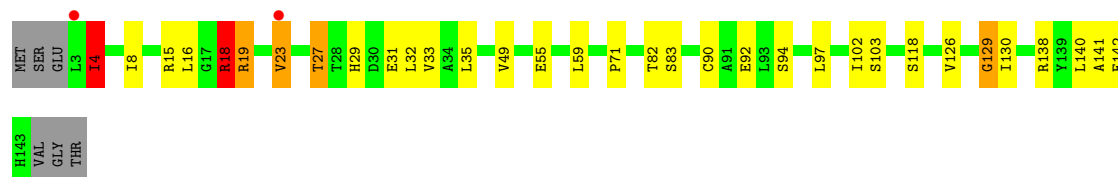
- Molecule 1: 3-dehydroquinate dehydratase

Chain T: 79% 14% . . .



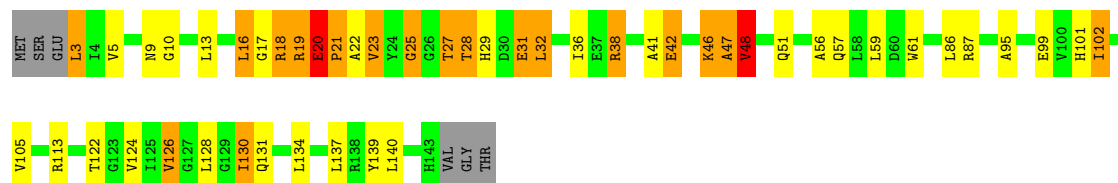
- Molecule 1: 3-dehydroquinate dehydratase

Chain U: 73% 18% . . .



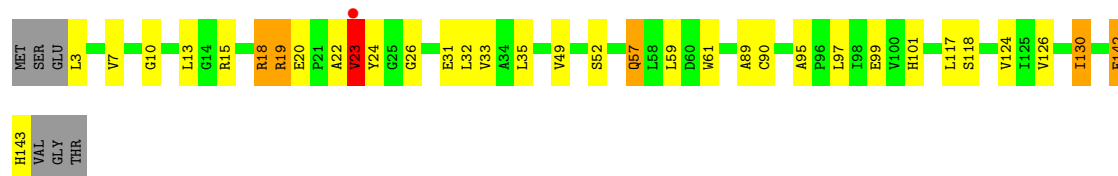
- Molecule 1: 3-dehydroquinate dehydratase

Chain V: 63% 20% 12% . . .



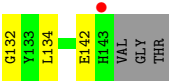
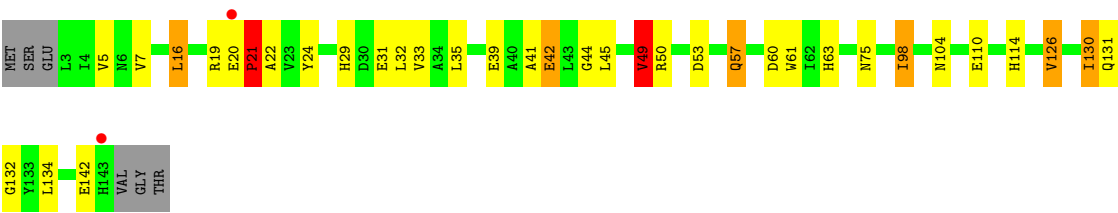
- Molecule 1: 3-dehydroquinate dehydratase

Chain W: 73% 19% . . .



- Molecule 1: 3-dehydroquinate dehydratase

Chain X: 71% 19% . . .



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	91.02Å 96.78Å 128.11Å 78.36° 81.24° 78.58°	Depositor
Resolution (Å)	36.22 – 2.40 36.22 – 2.40	Depositor EDS
% Data completeness (in resolution range)	95.4 (36.22-2.40) 95.4 (36.22-2.40)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.23 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.191 , 0.274 (Not available) , 0.255	Depositor DCC
R_{free} test set	7761 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	31.9	Xtriage
Anisotropy	0.154	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 58.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	27701	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.46% 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: N87

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	0.90	0/1083	1.07	1/1476 (0.1%)
1	B	1.05	0/1089	1.18	1/1483 (0.1%)
1	C	0.98	0/1082	1.19	4/1473 (0.3%)
1	D	0.98	0/1087	1.15	5/1480 (0.3%)
1	E	0.97	0/1089	1.24	7/1483 (0.5%)
1	F	0.99	0/1094	1.15	2/1491 (0.1%)
1	G	1.07	1/1089 (0.1%)	1.20	10/1483 (0.7%)
1	H	1.03	1/1089 (0.1%)	1.23	6/1483 (0.4%)
1	I	0.93	0/1089	1.15	6/1483 (0.4%)
1	J	1.12	0/1082	1.24	11/1473 (0.7%)
1	K	0.94	0/1079	1.16	3/1471 (0.2%)
1	L	0.93	0/1089	1.05	1/1483 (0.1%)
1	M	1.01	0/1089	1.13	1/1483 (0.1%)
1	N	0.97	1/1100 (0.1%)	1.14	2/1498 (0.1%)
1	O	0.99	2/1089 (0.2%)	1.13	3/1483 (0.2%)
1	P	1.12	4/1089 (0.4%)	1.22	5/1483 (0.3%)
1	Q	1.04	2/1083 (0.2%)	1.23	9/1476 (0.6%)
1	R	1.00	0/1076	1.29	8/1466 (0.5%)
1	S	1.11	1/1089 (0.1%)	1.24	8/1483 (0.5%)
1	T	1.06	1/1089 (0.1%)	1.21	4/1483 (0.3%)
1	U	1.08	1/1089 (0.1%)	1.14	4/1483 (0.3%)
1	V	1.14	2/1085 (0.2%)	1.26	6/1478 (0.4%)
1	W	0.98	1/1083 (0.1%)	1.14	5/1476 (0.3%)
1	X	0.96	1/1079 (0.1%)	1.13	2/1471 (0.1%)
All	All	1.02	18/26081 (0.1%)	1.18	114/35525 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	E	0	2
1	H	0	1
1	I	0	2
1	Q	0	2
1	U	0	1
1	V	0	1
1	X	0	1
All	All	0	11

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	W	23	VAL	CA-CB	7.50	1.64	1.54
1	P	51	GLN	CA-C	6.50	1.58	1.52
1	O	120	ILE	CA-CB	6.26	1.62	1.54
1	X	49	VAL	CA-CB	5.95	1.61	1.54
1	G	80	THR	CA-CB	5.91	1.62	1.53
1	Q	23	VAL	CA-C	5.86	1.60	1.52
1	V	9	ASN	CA-C	5.77	1.59	1.52
1	O	73	ILE	CA-CB	5.70	1.61	1.54
1	U	82	THR	C-O	-5.53	1.17	1.24
1	T	100	VAL	CA-C	5.51	1.59	1.52
1	P	20	GLU	C-O	-5.51	1.21	1.23
1	Q	23	VAL	CA-CB	5.48	1.61	1.54
1	V	56	ALA	CA-CB	5.46	1.61	1.53
1	H	20	GLU	C-O	-5.44	1.18	1.24
1	P	120	ILE	CA-CB	5.26	1.61	1.54
1	S	9	ASN	CA-C	5.20	1.59	1.52
1	N	69	ALA	CA-C	5.16	1.59	1.52
1	P	52	SER	N-CA	5.01	1.52	1.46

All (114) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	19	ARG	CA-C-N	-8.44	112.45	123.34
1	H	19	ARG	C-N-CA	-8.44	112.45	123.34
1	R	21	PRO	N-CA-CB	8.32	111.75	102.60
1	P	52	SER	N-CA-C	8.06	127.96	110.80
1	P	51	GLN	N-CA-C	8.05	122.91	112.12
1	J	21	PRO	N-CA-CB	8.04	111.69	103.25
1	U	4	ILE	N-CA-C	7.72	119.97	108.54
1	R	26	GLY	N-CA-C	-7.66	102.47	115.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	24	TYR	N-CA-C	-7.59	105.19	114.75
1	I	118	SER	CA-C-N	-7.49	111.93	119.56
1	I	118	SER	C-N-CA	-7.49	111.93	119.56
1	H	19	ARG	N-CA-C	7.42	122.80	112.93
1	K	25	GLY	N-CA-C	7.32	119.92	111.36
1	Q	49	VAL	N-CA-C	7.21	119.26	108.23
1	Q	20	GLU	CA-C-N	7.17	128.81	119.84
1	Q	20	GLU	C-N-CA	7.17	128.81	119.84
1	E	20	GLU	CA-C-N	-7.16	110.89	119.84
1	E	20	GLU	C-N-CA	-7.16	110.89	119.84
1	D	24	TYR	N-CA-C	7.09	122.06	113.41
1	G	70	GLU	CA-C-N	6.61	127.00	119.92
1	G	70	GLU	C-N-CA	6.61	127.00	119.92
1	P	4	ILE	N-CA-C	6.59	118.89	108.87
1	R	83	SER	N-CA-C	6.54	119.57	107.99
1	E	66	ALA	N-CA-C	-6.53	104.24	111.36
1	O	10	GLY	CA-C-N	6.49	126.52	119.90
1	O	10	GLY	C-N-CA	6.49	126.52	119.90
1	W	26	GLY	N-CA-C	-6.45	107.57	114.67
1	Q	10	GLY	CA-C-N	6.42	127.87	119.84
1	Q	10	GLY	C-N-CA	6.42	127.87	119.84
1	R	19	ARG	CA-C-N	6.38	133.18	121.70
1	R	19	ARG	C-N-CA	6.38	133.18	121.70
1	J	20	GLU	CA-C-N	6.35	127.78	119.84
1	J	20	GLU	C-N-CA	6.35	127.78	119.84
1	C	92	GLU	N-CA-C	-6.34	105.70	113.50
1	P	19	ARG	N-CA-C	6.24	119.18	109.52
1	R	8	ILE	N-CA-C	6.21	116.86	108.17
1	A	49	VAL	N-CA-C	6.16	115.60	106.85
1	F	10	GLY	CA-C-N	6.14	126.08	119.76
1	F	10	GLY	C-N-CA	6.14	126.08	119.76
1	X	22	ALA	N-CA-C	-6.13	105.39	112.92
1	D	20	GLU	CA-C-N	-6.11	112.20	119.84
1	D	20	GLU	C-N-CA	-6.11	112.20	119.84
1	S	22	ALA	CA-C-N	6.02	132.54	121.70
1	S	22	ALA	C-N-CA	6.02	132.54	121.70
1	C	83	SER	N-CA-C	6.00	118.61	107.99
1	K	26	GLY	N-CA-C	5.99	127.39	113.18
1	E	62	ILE	N-CA-C	5.97	116.63	110.36
1	C	21	PRO	N-CA-CB	5.96	109.51	103.25
1	W	95	ALA	CA-C-N	-5.86	113.93	119.85
1	W	95	ALA	C-N-CA	-5.86	113.93	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	10	GLY	CA-C-N	5.85	125.80	119.78
1	I	10	GLY	C-N-CA	5.85	125.80	119.78
1	V	22	ALA	CA-C-N	5.80	132.14	121.70
1	V	22	ALA	C-N-CA	5.80	132.14	121.70
1	J	53	ASP	N-CA-C	-5.78	105.56	113.30
1	J	83	SER	N-CA-C	5.75	117.89	108.52
1	K	122	THR	N-CA-C	-5.74	105.11	111.36
1	G	80	THR	CB-CA-C	-5.73	101.64	110.81
1	I	23	VAL	N-CA-C	-5.71	104.77	111.00
1	N	4	ILE	CB-CA-C	-5.69	103.78	111.63
1	J	100	VAL	N-CA-C	5.67	116.29	108.12
1	S	125	ILE	N-CA-C	5.58	115.90	107.75
1	U	118	SER	CA-C-N	-5.58	113.14	119.28
1	U	118	SER	C-N-CA	-5.58	113.14	119.28
1	R	118	SER	CA-C-N	-5.52	113.21	119.28
1	R	118	SER	C-N-CA	-5.52	113.21	119.28
1	B	27	THR	CB-CA-C	-5.51	101.57	109.84
1	G	95	ALA	CA-C-N	-5.43	114.65	120.03
1	G	95	ALA	C-N-CA	-5.43	114.65	120.03
1	D	8	ILE	N-CA-C	5.43	115.35	106.72
1	M	83	SER	N-CA-C	5.41	117.81	107.75
1	V	47	ALA	N-CA-C	5.39	118.19	111.24
1	V	122	THR	N-CA-C	-5.38	105.42	111.28
1	G	83	SER	N-CA-C	5.37	117.49	108.73
1	J	73	ILE	N-CA-C	-5.37	100.01	107.80
1	L	83	SER	N-CA-C	5.37	117.38	108.20
1	O	83	SER	N-CA-C	5.35	117.03	108.41
1	W	23	VAL	CA-C-N	5.35	131.33	121.70
1	W	23	VAL	C-N-CA	5.35	131.33	121.70
1	N	83	SER	N-CA-C	5.33	117.31	108.20
1	S	24	TYR	N-CA-C	5.33	119.77	113.16
1	H	122	THR	N-CA-C	-5.32	104.91	111.40
1	P	83	SER	N-CA-C	5.32	118.37	107.69
1	S	23	VAL	N-CA-C	5.25	125.71	111.00
1	Q	50	ARG	N-CA-C	5.25	117.98	109.06
1	G	23	VAL	N-CA-C	5.24	115.35	110.42
1	T	130	ILE	CB-CG1-CD1	-5.24	102.80	113.80
1	U	83	SER	N-CA-C	5.24	117.16	108.20
1	S	142	GLU	N-CA-C	5.22	119.64	113.12
1	C	54	SER	N-CA-C	5.20	117.00	108.52
1	E	10	GLY	CA-C-N	5.18	125.18	119.90
1	E	10	GLY	C-N-CA	5.18	125.18	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	74	LEU	N-CA-C	5.18	117.34	108.90
1	Q	118	SER	CA-C-N	-5.16	114.50	119.87
1	Q	118	SER	C-N-CA	-5.16	114.50	119.87
1	H	4	ILE	N-CA-C	5.13	116.09	108.23
1	S	122	THR	N-CA-C	-5.13	105.60	111.14
1	T	98	ILE	N-CA-C	5.13	114.96	107.37
1	X	53	ASP	N-CA-C	-5.13	107.02	113.28
1	E	122	THR	N-CA-C	-5.12	105.69	111.28
1	S	83	SER	N-CA-C	5.12	116.65	108.41
1	I	74	LEU	N-CA-C	5.10	116.72	108.41
1	J	127	GLY	N-CA-C	5.08	122.72	114.90
1	D	72	VAL	N-CA-C	5.07	115.27	107.77
1	G	118	SER	CA-C-N	-5.07	114.60	119.87
1	G	118	SER	C-N-CA	-5.07	114.60	119.87
1	J	125	ILE	N-CA-C	5.04	115.17	108.11
1	V	95	ALA	CA-C-N	-5.03	114.73	119.76
1	V	95	ALA	C-N-CA	-5.03	114.73	119.76
1	H	83	SER	N-CA-C	5.02	116.79	108.20
1	J	20	GLU	N-CA-C	5.02	118.41	110.58
1	G	18	ARG	N-CA-C	-5.01	100.13	110.80
1	T	59	LEU	CA-C-N	5.00	127.29	120.54
1	T	59	LEU	C-N-CA	5.00	127.29	120.54

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	25	GLY	Peptide
1	E	16	LEU	Peptide
1	E	25	GLY	Peptide
1	H	142	GLU	Peptide
1	I	22	ALA	Peptide
1	I	25	GLY	Peptide
1	Q	22	ALA	Peptide
1	Q	23	VAL	Peptide
1	U	23	VAL	Peptide
1	V	20	GLU	Peptide
1	X	21	PRO	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1065	0	1068	21	0
1	B	1071	0	1079	18	0
1	C	1065	0	1069	20	0
1	D	1069	0	1072	39	0
1	E	1071	0	1079	44	0
1	F	1071	0	1071	25	0
1	G	1071	0	1079	39	0
1	H	1071	0	1079	27	0
1	I	1071	0	1079	21	0
1	J	1065	0	1069	38	0
1	K	1061	0	1064	33	0
1	L	1071	0	1079	22	0
1	M	1071	0	1079	24	0
1	N	1077	0	1082	32	0
1	O	1071	0	1079	30	0
1	P	1071	0	1079	26	0
1	Q	1065	0	1068	19	0
1	R	1059	0	1058	34	0
1	S	1071	0	1079	29	0
1	T	1071	0	1079	12	0
1	U	1071	0	1079	24	0
1	V	1067	0	1075	40	0
1	W	1065	0	1068	17	0
1	X	1061	0	1064	28	0
2	A	26	0	17	1	0
2	B	26	0	17	1	0
2	C	26	0	17	4	0
2	D	26	0	17	0	0
2	E	26	0	17	3	0
2	F	26	0	17	1	0
2	G	26	0	17	7	0
2	H	26	0	17	0	0
2	I	26	0	17	5	0
2	J	26	0	17	2	0
2	K	26	0	17	1	0
2	L	26	0	17	8	0
2	M	26	0	17	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	N	26	0	17	2	0
2	O	26	0	17	3	0
2	P	26	0	17	0	0
2	Q	26	0	17	3	0
2	R	26	0	17	3	0
2	S	26	0	17	5	0
2	T	26	0	17	0	0
2	U	26	0	17	5	0
2	V	26	0	17	4	0
2	W	26	0	17	2	0
2	X	26	0	17	0	0
3	A	53	0	0	2	0
3	B	90	0	0	7	0
3	C	59	0	0	1	0
3	D	54	0	0	2	0
3	E	78	0	0	2	0
3	F	60	0	0	3	0
3	G	66	0	0	5	0
3	H	59	0	0	2	0
3	I	48	0	0	0	0
3	J	70	0	0	10	0
3	K	55	0	0	3	0
3	L	49	0	0	1	0
3	M	57	0	0	0	0
3	N	54	0	0	2	0
3	O	53	0	0	7	0
3	P	67	0	0	2	0
3	Q	50	0	0	2	0
3	R	63	0	0	1	0
3	S	66	0	0	3	0
3	T	73	0	0	0	0
3	U	59	0	0	1	0
3	V	61	0	0	1	0
3	W	43	0	0	1	0
3	X	48	0	0	3	0
All	All	27701	0	26184	668	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (668) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:21:PRO:HA	1:F:22:ALA:O	1.46	1.13
2:I:147:N87:H22	2:I:147:N87:H23	1.19	1.12
2:M:147:N87:H22	2:M:147:N87:H23	1.13	1.11
1:Q:38:ARG:HH11	1:Q:38:ARG:HG2	1.11	1.10
1:J:18:ARG:HH11	1:J:18:ARG:HG3	0.93	1.10
2:C:147:N87:H22	2:C:147:N87:H23	1.31	1.08
1:O:3:LEU:HA	3:O:808:HOH:O	1.52	1.08
1:J:21:PRO:HA	1:J:22:ALA:HB3	1.30	1.06
2:G:147:N87:H22	2:G:147:N87:H23	1.32	1.05
2:V:147:N87:H22	2:V:147:N87:H23	1.37	1.01
1:R:20:GLU:HA	1:R:21:PRO:CB	1.89	1.01
1:F:92:GLU:HG3	1:G:19:ARG:HG3	1.44	0.98
1:J:18:ARG:HH11	1:J:18:ARG:CG	1.75	0.98
1:J:18:ARG:HG3	1:J:18:ARG:NH1	1.67	0.98
1:D:20:GLU:HB2	1:D:21:PRO:HD3	1.44	0.98
1:M:19:ARG:HB2	2:M:147:N87:H20	1.45	0.97
2:M:147:N87:H22	2:M:147:N87:C23	1.91	0.96
1:R:19:ARG:CB	1:R:20:GLU:CB	2.45	0.95
1:O:50:ARG:HG3	1:O:50:ARG:HH11	1.32	0.95
2:R:147:N87:H22	2:R:147:N87:H23	1.48	0.94
1:D:48:VAL:HG12	1:D:50:ARG:HD2	1.48	0.94
2:G:147:N87:H22	2:G:147:N87:C23	1.96	0.93
2:U:147:N87:H23	2:U:147:N87:H18	1.52	0.92
2:M:147:N87:H23	2:M:147:N87:C22	2.00	0.91
1:R:20:GLU:CA	1:R:21:PRO:CB	2.47	0.91
1:N:18:ARG:O	1:N:19:ARG:HB2	1.71	0.91
1:D:38:ARG:HG2	1:D:38:ARG:HH11	1.33	0.91
1:J:3:LEU:HD23	1:J:45:LEU:CD2	2.02	0.90
1:O:19:ARG:HB3	2:O:147:N87:H20	1.53	0.89
1:X:19:ARG:C	1:X:21:PRO:HD3	1.98	0.89
1:U:18:ARG:HG3	1:U:18:ARG:HH11	1.38	0.89
1:D:20:GLU:HB2	1:D:21:PRO:CD	2.03	0.88
2:C:147:N87:H22	2:C:147:N87:C23	2.02	0.88
1:I:21:PRO:HB3	1:I:25:GLY:O	1.73	0.88
1:J:3:LEU:HD23	1:J:45:LEU:HD23	1.56	0.88
1:V:28:THR:HG23	1:V:31:GLU:HB2	1.58	0.85
1:J:21:PRO:HA	1:J:22:ALA:CB	2.06	0.85
1:H:105:VAL:HG22	1:H:126:VAL:HG21	1.60	0.84
1:Q:38:ARG:HG2	1:Q:38:ARG:NH1	1.89	0.84
1:I:17:GLY:HA2	1:I:25:GLY:HA3	1.61	0.83
1:H:50:ARG:HB2	1:H:50:ARG:HH11	1.43	0.83
2:I:147:N87:H22	2:I:147:N87:C23	2.04	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:19:ARG:HG3	1:V:20:GLU:N	1.92	0.82
1:G:17:GLY:O	1:G:18:ARG:HG3	1.81	0.80
1:R:17:GLY:O	1:R:18:ARG:HB2	1.81	0.80
1:R:28:THR:HG22	1:R:30:ASP:N	1.96	0.80
1:K:122:THR:HG23	3:K:501:HOH:O	1.81	0.80
1:U:94:SER:HB3	1:V:19:ARG:HH22	1.46	0.79
2:U:147:N87:H23	2:U:147:N87:C18	2.12	0.79
1:C:19:ARG:HG3	1:C:20:GLU:O	1.82	0.79
1:Q:38:ARG:HH11	1:Q:38:ARG:CG	1.95	0.79
1:K:21:PRO:O	1:K:23:VAL:N	2.15	0.78
1:R:20:GLU:CB	1:R:21:PRO:CB	2.62	0.78
1:V:46:LYS:HB3	3:V:983:HOH:O	1.83	0.78
2:C:147:N87:H23	2:C:147:N87:C22	2.14	0.77
1:M:39:GLU:O	1:M:43:LEU:HD23	1.85	0.77
1:O:105:VAL:HG22	1:O:126:VAL:HG21	1.67	0.76
1:D:38:ARG:HH11	1:D:38:ARG:CG	1.99	0.76
1:W:57:GLN:NE2	1:W:61:TRP:CZ2	2.54	0.75
1:E:17:GLY:HA2	1:E:19:ARG:H	1.52	0.75
1:X:114:HIS:HB2	3:X:294:HOH:O	1.84	0.75
1:F:21:PRO:HB3	1:F:24:TYR:O	1.89	0.73
1:E:46:LYS:HB2	1:E:46:LYS:NZ	2.03	0.73
1:O:113:ARG:HD2	3:O:1245:HOH:O	1.86	0.73
1:P:9:ASN:O	1:P:51:GLN:O	2.06	0.73
1:O:19:ARG:CB	2:O:147:N87:H20	2.19	0.73
1:L:19:ARG:HB3	2:L:147:N87:H20	1.70	0.73
1:V:38:ARG:NH2	1:V:42:GLU:HG3	2.04	0.73
1:G:38:ARG:HD3	3:G:347:HOH:O	1.87	0.73
1:F:21:PRO:CA	1:F:22:ALA:O	2.34	0.72
1:L:102:ILE:HG23	1:L:129:GLY:HA2	1.71	0.72
1:O:50:ARG:HG3	1:O:50:ARG:NH1	2.02	0.72
1:I:17:GLY:HA3	1:I:27:THR:O	1.89	0.72
1:H:114:HIS:HB2	3:H:181:HOH:O	1.90	0.72
1:K:28:THR:OG1	1:K:31:GLU:HG3	1.89	0.72
1:J:50:ARG:HB3	1:J:61:TRP:CH2	2.24	0.71
1:D:21:PRO:O	1:D:25:GLY:HA2	1.90	0.71
2:I:147:N87:H23	2:I:147:N87:C22	2.07	0.71
1:L:19:ARG:CB	2:L:147:N87:H20	2.21	0.71
1:D:21:PRO:O	1:D:25:GLY:CA	2.39	0.71
1:R:92:GLU:OE1	1:S:19:ARG:NH2	2.23	0.70
1:D:15:ARG:HH21	1:D:19:ARG:HH12	1.37	0.70
1:D:21:PRO:HG2	1:D:22:ALA:H	1.55	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:71:PRO:HB3	1:N:96:PRO:HD2	1.73	0.70
1:S:28:THR:OG1	1:S:31:GLU:HG2	1.93	0.69
1:T:109:GLU:OE1	1:T:112:ARG:NE	2.21	0.69
1:J:3:LEU:CD2	1:J:45:LEU:CD2	2.70	0.69
1:N:19:ARG:HD2	2:N:147:N87:H20	1.73	0.69
1:X:57:GLN:HE21	1:X:57:GLN:HA	1.58	0.69
1:I:21:PRO:CB	1:I:25:GLY:O	2.41	0.68
1:A:114:HIS:HB2	3:A:1050:HOH:O	1.93	0.68
2:G:147:N87:H23	2:G:147:N87:C22	2.18	0.68
1:H:19:ARG:CG	1:H:19:ARG:HH11	2.06	0.68
1:H:19:ARG:HH11	1:H:19:ARG:HG3	1.58	0.68
1:B:101:HIS:HB2	1:B:126:VAL:HG22	1.75	0.68
1:W:32:LEU:HD13	1:W:130:ILE:HG12	1.77	0.67
1:O:19:ARG:HB3	2:O:147:N87:C20	2.25	0.67
1:O:19:ARG:O	1:O:21:PRO:HD3	1.95	0.67
1:D:21:PRO:CG	1:D:22:ALA:H	2.08	0.67
1:K:38:ARG:HH11	1:K:38:ARG:HG3	1.59	0.66
2:V:147:N87:H22	2:V:147:N87:C23	2.21	0.66
1:M:38:ARG:O	1:M:42:GLU:HG3	1.95	0.66
1:S:19:ARG:HB3	2:S:147:N87:H20	1.77	0.66
1:A:32:LEU:HD13	1:A:130:ILE:CG1	2.26	0.66
1:V:5:VAL:O	1:V:47:ALA:O	2.13	0.66
1:H:101:HIS:HB2	1:H:126:VAL:HG23	1.76	0.66
1:K:16:LEU:O	1:K:28:THR:HA	1.96	0.66
1:T:32:LEU:HD13	1:T:130:ILE:HD11	1.78	0.66
1:E:109:GLU:CD	1:E:109:GLU:H	2.04	0.65
2:L:147:N87:H22	2:L:147:N87:C23	2.25	0.65
1:V:20:GLU:O	1:V:21:PRO:O	2.14	0.65
1:E:95:ALA:HB1	1:E:96:PRO:CD	2.26	0.65
1:P:58:LEU:O	1:P:62:ILE:HG12	1.97	0.65
1:N:48:VAL:HG12	1:N:50:ARG:HD2	1.79	0.65
1:B:27:THR:HG22	1:B:28:THR:O	1.96	0.65
1:V:32:LEU:HD22	1:V:36:ILE:HD11	1.77	0.65
1:F:20:GLU:HB3	1:F:21:PRO:HA	1.78	0.65
1:O:35:LEU:HA	1:O:38:ARG:HH12	1.63	0.64
1:R:28:THR:HG21	3:R:675:HOH:O	1.97	0.64
2:R:147:N87:H22	2:R:147:N87:C23	2.26	0.64
1:S:7:VAL:HB	1:S:49:VAL:HB	1.78	0.64
1:O:32:LEU:HD13	1:O:130:ILE:HG13	1.77	0.64
2:S:147:N87:H22	2:S:147:N87:C23	2.28	0.64
1:R:125:ILE:HG23	1:R:128:LEU:HD12	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:29:HIS:O	1:D:33:VAL:HG23	1.98	0.64
1:G:19:ARG:C	1:G:21:PRO:HD3	2.23	0.64
1:S:20:GLU:N	1:S:21:PRO:HD3	2.13	0.64
1:D:15:ARG:NH2	1:D:19:ARG:HH12	1.96	0.64
1:S:4:ILE:HD12	1:S:70:GLU:OE2	1.97	0.63
1:O:88:ASP:HB3	2:Q:147:N87:O26	1.97	0.63
1:G:16:LEU:O	1:G:28:THR:HA	1.99	0.63
1:H:19:ARG:NE	1:J:92:GLU:OE2	2.31	0.63
1:M:3:LEU:HD23	1:M:4:ILE:H	1.63	0.63
1:D:4:ILE:HD12	1:D:4:ILE:H	1.64	0.63
1:U:18:ARG:HG3	1:U:18:ARG:NH1	2.12	0.63
1:X:20:GLU:N	1:X:21:PRO:HD3	2.14	0.63
1:M:19:ARG:HG2	1:M:19:ARG:HH11	1.63	0.63
1:D:23:VAL:O	1:D:102:ILE:HG22	2.00	0.62
1:V:16:LEU:O	1:V:27:THR:O	2.17	0.62
1:B:37:GLU:HB3	3:B:1026:HOH:O	1.99	0.62
1:B:113:ARG:HD2	3:B:1298:HOH:O	1.98	0.62
1:V:32:LEU:HD22	1:V:36:ILE:CD1	2.28	0.62
1:D:48:VAL:CG1	1:D:50:ARG:HD2	2.24	0.62
1:A:32:LEU:HD13	1:A:130:ILE:HG13	1.82	0.62
1:V:3:LEU:N	1:V:46:LYS:HZ2	1.98	0.62
1:R:32:LEU:O	1:R:36:ILE:HG12	1.99	0.62
2:V:147:N87:H23	2:V:147:N87:C22	2.23	0.62
1:G:20:GLU:N	1:G:21:PRO:HD3	2.15	0.62
1:I:17:GLY:HA2	1:I:25:GLY:CA	2.30	0.62
1:X:41:ALA:O	1:X:42:GLU:HB2	2.00	0.62
1:X:32:LEU:HD13	1:X:130:ILE:HG12	1.82	0.61
1:X:31:GLU:O	1:X:35:LEU:HG	2.00	0.61
1:W:33:VAL:HG13	1:W:49:VAL:HB	1.83	0.61
1:F:20:GLU:HG2	1:F:23:VAL:HB	1.81	0.61
1:S:20:GLU:O	1:S:22:ALA:N	2.34	0.61
1:J:3:LEU:HD12	3:J:1308:HOH:O	2.00	0.61
1:O:3:LEU:CA	3:O:808:HOH:O	2.28	0.61
1:B:20:GLU:HB3	1:B:23:VAL:HG13	1.82	0.61
1:Q:20:GLU:O	1:Q:21:PRO:O	2.18	0.61
1:Q:21:PRO:HB2	3:Q:920:HOH:O	2.01	0.61
1:R:28:THR:HG22	1:R:30:ASP:H	1.64	0.61
1:T:45:LEU:HD11	1:T:141:ALA:HB2	1.81	0.61
1:D:20:GLU:CB	1:D:21:PRO:CD	2.78	0.61
1:S:28:THR:OG1	1:S:31:GLU:CG	2.48	0.61
1:W:31:GLU:O	1:W:35:LEU:HD23	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:32:LEU:HD13	1:N:36:ILE:HD12	1.83	0.60
1:V:19:ARG:HG3	1:V:20:GLU:H	1.64	0.60
1:X:21:PRO:HB2	1:X:24:TYR:H	1.66	0.60
1:K:130:ILE:HD13	1:K:130:ILE:N	2.16	0.60
1:P:4:ILE:HG12	1:P:70:GLU:OE2	2.00	0.60
1:R:17:GLY:O	1:R:18:ARG:CB	2.50	0.60
1:B:20:GLU:HB3	1:B:23:VAL:CG1	2.31	0.60
1:I:45:LEU:HD11	1:I:141:ALA:HB2	1.83	0.60
1:M:57:GLN:NE2	1:M:61:TRP:CE2	2.70	0.60
1:J:19:ARG:HD3	3:J:472:HOH:O	2.02	0.60
1:W:7:VAL:HB	1:W:49:VAL:HG22	1.84	0.60
1:P:63:HIS:HE1	1:R:12:ASN:OD1	1.85	0.60
1:F:19:ARG:O	1:F:20:GLU:HB2	2.02	0.60
1:S:10:GLY:HA2	1:S:58:LEU:HD11	1.85	0.59
1:B:32:LEU:HD13	1:B:130:ILE:HG13	1.84	0.59
1:E:20:GLU:CB	1:E:21:PRO:HD3	2.31	0.59
1:I:92:GLU:HG2	2:J:147:N87:C19	2.33	0.59
1:I:29:HIS:O	1:I:33:VAL:HG23	2.03	0.59
2:Q:147:N87:H22	2:Q:147:N87:C23	2.32	0.59
1:F:39:GLU:HG2	1:F:134:LEU:HB3	1.85	0.59
1:D:18:ARG:HG2	1:D:18:ARG:HH11	1.68	0.59
1:L:75:ASN:HA	3:L:152:HOH:O	2.02	0.59
1:L:20:GLU:HB3	1:L:23:VAL:HG12	1.84	0.58
1:O:87:ARG:HG3	1:O:120:ILE:HD12	1.84	0.58
1:Q:110:GLU:OE2	1:Q:110:GLU:HA	2.03	0.58
1:G:7:VAL:HB	1:G:49:VAL:HB	1.85	0.58
1:U:27:THR:HG22	1:U:31:GLU:HB2	1.84	0.58
1:F:80:THR:HG21	1:F:101:HIS:CE1	2.37	0.58
1:U:18:ARG:HH11	1:U:18:ARG:CG	2.15	0.58
1:D:41:ALA:O	1:D:44:GLY:N	2.33	0.58
1:C:80:THR:HG21	1:C:101:HIS:CE1	2.38	0.58
1:N:117:LEU:O	1:N:120:ILE:HD13	2.04	0.58
1:E:17:GLY:CA	1:E:19:ARG:H	2.15	0.58
1:A:10:GLY:H	1:A:13:LEU:HD12	1.69	0.58
1:O:3:LEU:C	3:O:808:HOH:O	2.46	0.58
1:K:75:ASN:HA	3:K:152:HOH:O	2.04	0.57
1:X:29:HIS:O	1:X:33:VAL:HG23	2.04	0.57
1:Q:19:ARG:HA	1:Q:20:GLU:HG3	1.86	0.57
1:C:29:HIS:O	1:C:33:VAL:HG23	2.05	0.57
1:R:28:THR:HG21	1:R:30:ASP:HB2	1.86	0.57
1:E:46:LYS:HB2	1:E:46:LYS:HZ2	1.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:39:GLU:HG2	1:T:134:LEU:HB3	1.86	0.57
1:V:38:ARG:HH22	1:V:42:GLU:HG3	1.70	0.57
1:K:130:ILE:N	1:K:130:ILE:CD1	2.67	0.57
1:N:101:HIS:HB2	1:N:126:VAL:HG22	1.85	0.57
1:N:19:ARG:HD3	1:N:20:GLU:H	1.68	0.57
1:P:50:ARG:HB3	1:P:61:TRP:CZ3	2.39	0.57
1:K:130:ILE:CD1	1:K:130:ILE:H	2.18	0.57
1:M:3:LEU:CD2	1:M:4:ILE:H	2.17	0.57
1:B:19:ARG:HD3	3:B:1186:HOH:O	2.05	0.56
1:C:102:ILE:HG23	1:C:129:GLY:HA2	1.87	0.56
1:G:19:ARG:HB2	2:G:147:N87:H20	1.87	0.56
1:K:7:VAL:HB	1:K:49:VAL:HG22	1.85	0.56
1:O:3:LEU:HG	1:O:4:ILE:N	2.20	0.56
1:O:35:LEU:HA	1:O:38:ARG:NH1	2.19	0.56
2:R:147:N87:H23	2:R:147:N87:C22	2.30	0.56
1:V:20:GLU:C	1:V:21:PRO:O	2.48	0.56
1:O:3:LEU:HG	1:O:4:ILE:H	1.70	0.56
1:A:27:THR:HG23	1:A:31:GLU:HB3	1.88	0.56
1:E:143:HIS:N	1:E:143:HIS:CD2	2.73	0.56
2:G:147:N87:C23	2:G:147:N87:C22	2.73	0.56
1:S:4:ILE:HD12	1:S:70:GLU:HG2	1.87	0.56
1:E:11:PRO:O	1:E:12:ASN:HB2	2.07	0.55
1:N:24:TYR:HA	1:N:102:ILE:HG21	1.88	0.55
1:J:50:ARG:HD3	1:J:61:TRP:CE2	2.41	0.55
1:V:113:ARG:HH12	1:X:114:HIS:HD2	1.52	0.55
1:W:18:ARG:O	1:W:19:ARG:CB	2.54	0.55
1:S:131:GLN:HB2	3:S:149:HOH:O	2.06	0.55
1:L:12:ASN:HB2	2:L:147:N87:C24	2.36	0.55
1:R:125:ILE:CG2	1:R:128:LEU:HD12	2.37	0.55
1:I:20:GLU:N	1:I:21:PRO:HD3	2.22	0.54
1:M:98:ILE:HD11	1:M:139:TYR:CD2	2.43	0.54
1:U:55:GLU:O	1:U:59:LEU:HG	2.07	0.54
1:E:131:GLN:HE22	1:K:139:TYR:HA	1.72	0.54
1:O:87:ARG:NE	3:O:308:HOH:O	2.41	0.54
1:U:94:SER:HB3	1:V:19:ARG:NH2	2.19	0.54
1:J:50:ARG:HB3	1:J:61:TRP:CZ3	2.43	0.54
1:N:21:PRO:O	1:N:22:ALA:HB3	2.07	0.54
1:G:18:ARG:O	1:G:19:ARG:HB2	2.07	0.54
2:M:147:N87:C23	2:M:147:N87:C22	2.68	0.54
1:D:21:PRO:HD3	3:D:1062:HOH:O	2.07	0.54
1:X:32:LEU:HD13	1:X:130:ILE:CG1	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:24:TYR:HA	1:C:102:ILE:HG21	1.89	0.54
1:G:102:ILE:HD13	1:G:130:ILE:HD12	1.88	0.54
1:H:101:HIS:HB2	1:H:126:VAL:CG2	2.38	0.54
1:V:102:ILE:CD1	1:V:102:ILE:N	2.69	0.54
1:D:32:LEU:HD13	1:D:130:ILE:HG12	1.88	0.54
1:U:18:ARG:O	1:U:19:ARG:CB	2.55	0.54
1:J:101:HIS:HB2	1:J:126:VAL:HG22	1.90	0.54
1:K:88:ASP:OD1	1:L:112:ARG:NH2	2.34	0.54
1:L:31:GLU:O	1:L:34:ALA:HB3	2.08	0.54
1:E:17:GLY:HA2	1:E:19:ARG:N	2.22	0.54
1:F:50:ARG:HB3	1:F:61:TRP:CZ3	2.42	0.54
1:N:104:ASN:HA	1:N:126:VAL:HG13	1.89	0.53
1:U:33:VAL:HG22	1:U:49:VAL:HG11	1.90	0.53
1:X:20:GLU:N	1:X:21:PRO:CD	2.71	0.53
1:D:28:THR:OG1	1:D:31:GLU:HG2	2.09	0.53
1:J:109:GLU:CD	1:J:109:GLU:H	2.16	0.53
1:G:32:LEU:HD13	1:G:130:ILE:CG1	2.39	0.53
1:I:118:SER:HB2	1:I:119:PRO:HD3	1.90	0.53
1:G:117:LEU:O	1:G:120:ILE:HG13	2.07	0.53
1:R:102:ILE:HG23	1:R:129:GLY:HA2	1.90	0.53
1:E:21:PRO:HD2	1:E:23:VAL:HG12	1.91	0.53
1:G:19:ARG:HB3	2:G:147:N87:H19	1.89	0.53
1:I:19:ARG:HB3	2:I:147:N87:H20	1.90	0.53
1:U:32:LEU:CD1	1:U:130:ILE:HG23	2.39	0.53
1:G:35:LEU:HD23	3:G:173:HOH:O	2.08	0.53
1:F:21:PRO:HB2	1:F:22:ALA:HA	1.89	0.52
1:G:32:LEU:HD13	1:G:130:ILE:HG12	1.91	0.52
1:R:6:ASN:HB2	1:R:72:VAL:HG22	1.90	0.52
1:W:101:HIS:HB2	1:W:126:VAL:HG22	1.91	0.52
1:K:80:THR:HG21	1:K:101:HIS:CE1	2.45	0.52
1:S:22:ALA:HA	1:S:23:VAL:C	2.34	0.52
1:C:3:LEU:HD12	3:C:1231:HOH:O	2.09	0.52
1:H:109:GLU:CD	1:H:109:GLU:H	2.18	0.52
1:A:60:ASP:O	1:A:63:HIS:HB2	2.10	0.52
1:H:19:ARG:CD	1:J:92:GLU:OE2	2.58	0.52
1:J:19:ARG:CD	3:J:472:HOH:O	2.58	0.52
1:J:36:ILE:HG23	1:J:137:LEU:HD11	1.92	0.52
1:V:27:THR:CG2	1:V:31:GLU:HB3	2.39	0.52
2:W:147:N87:C23	2:W:147:N87:H18	2.39	0.52
1:J:42:GLU:HG2	3:J:153:HOH:O	2.09	0.52
1:J:63:HIS:HD2	3:J:1086:HOH:O	1.93	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:80:THR:HG21	1:L:101:HIS:CE1	2.45	0.52
1:P:55:GLU:OE2	1:P:83:SER:OG	2.28	0.52
1:S:32:LEU:HD13	1:S:130:ILE:HG23	1.91	0.52
1:W:143:HIS:CE1	3:W:1192:HOH:O	2.62	0.51
1:R:92:GLU:HG2	1:S:19:ARG:HD2	1.91	0.51
1:A:15:ARG:HE	1:L:92:GLU:CD	2.18	0.51
1:C:39:GLU:HG2	1:C:134:LEU:HD22	1.92	0.51
1:S:3:LEU:N	3:S:1279:HOH:O	2.44	0.51
1:A:63:HIS:HB3	1:K:15:ARG:NH1	2.24	0.51
1:D:21:PRO:CG	1:D:22:ALA:N	2.73	0.51
1:F:21:PRO:HA	1:F:22:ALA:C	2.29	0.51
1:O:39:GLU:HG2	1:O:134:LEU:HB3	1.92	0.51
1:X:7:VAL:HB	1:X:49:VAL:HB	1.92	0.51
1:E:71:PRO:HB3	1:E:96:PRO:HD2	1.93	0.51
1:M:39:GLU:O	1:M:43:LEU:CD2	2.58	0.51
1:M:19:ARG:CB	2:M:147:N87:H20	2.29	0.51
1:D:18:ARG:HG2	1:D:18:ARG:NH1	2.26	0.51
1:D:28:THR:OG1	1:D:31:GLU:CG	2.59	0.51
1:V:59:LEU:HD21	1:V:86:LEU:HA	1.93	0.51
1:J:99:GLU:HB3	1:J:124:VAL:HG13	1.92	0.51
1:V:29:HIS:CE1	1:V:51:GLN:HB2	2.46	0.51
2:B:147:N87:H22	2:B:147:N87:C23	2.42	0.50
1:J:18:ARG:NH1	1:J:18:ARG:CG	2.45	0.50
1:J:21:PRO:CB	1:J:23:VAL:H	2.25	0.50
1:P:81:HIS:CE1	1:P:112:ARG:HA	2.46	0.50
1:H:101:HIS:CE1	3:H:154:HOH:O	2.65	0.50
1:M:80:THR:HG21	1:M:101:HIS:CE1	2.46	0.50
1:X:39:GLU:O	1:X:42:GLU:HB3	2.11	0.50
1:F:20:GLU:HB3	1:F:21:PRO:CA	2.42	0.50
1:H:50:ARG:HB2	1:H:50:ARG:NH1	2.22	0.50
1:V:102:ILE:N	1:V:102:ILE:HD13	2.25	0.50
1:E:21:PRO:HD2	1:E:23:VAL:H	1.77	0.50
1:P:102:ILE:HG12	1:P:130:ILE:HD12	1.94	0.50
1:U:18:ARG:O	1:U:19:ARG:HB2	2.12	0.50
1:A:80:THR:HG21	1:A:101:HIS:CE1	2.47	0.50
1:J:3:LEU:CD2	1:J:45:LEU:HD22	2.42	0.50
1:E:19:ARG:O	1:E:20:GLU:HB2	2.12	0.50
1:H:58:LEU:O	1:H:62:ILE:HG12	2.12	0.50
1:N:18:ARG:O	1:N:18:ARG:HG2	2.11	0.50
1:C:42:GLU:O	1:C:42:GLU:HG3	2.12	0.49
1:R:101:HIS:HB2	1:R:126:VAL:HG22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:20:GLU:O	1:H:23:VAL:O	2.30	0.49
1:F:8:ILE:CG2	1:F:58:LEU:HD22	2.42	0.49
1:E:38:ARG:O	1:E:42:GLU:HG2	2.12	0.49
1:E:46:LYS:HB2	1:E:46:LYS:HZ3	1.77	0.49
1:M:7:VAL:HB	1:M:49:VAL:HG22	1.95	0.49
1:V:10:GLY:O	1:V:13:LEU:HD12	2.11	0.49
1:C:92:GLU:CD	2:E:147:N87:H19	2.38	0.49
1:D:43:LEU:HD13	1:D:141:ALA:HB2	1.94	0.49
1:F:27:THR:HB	1:F:130:ILE:CD1	2.42	0.49
1:E:18:ARG:HH11	1:E:18:ARG:CG	2.26	0.49
1:G:50:ARG:HD3	1:G:61:TRP:CE2	2.48	0.49
1:U:23:VAL:HG11	1:U:103:SER:HA	1.94	0.49
1:G:57:GLN:NE2	1:G:61:TRP:CE2	2.81	0.49
1:E:95:ALA:HB1	1:E:96:PRO:HD3	1.94	0.49
1:F:18:ARG:O	1:F:19:ARG:CB	2.60	0.49
2:L:147:N87:H22	2:L:147:N87:H23	1.93	0.49
1:V:102:ILE:HD13	1:V:102:ILE:H	1.76	0.49
1:C:33:VAL:HG13	1:C:49:VAL:HB	1.95	0.48
1:R:28:THR:CG2	1:R:29:HIS:N	2.76	0.48
1:L:19:ARG:HB2	2:L:147:N87:H20	1.94	0.48
1:J:104:ASN:HA	1:J:126:VAL:HG13	1.95	0.48
2:K:147:N87:H22	2:K:147:N87:H23	1.95	0.48
1:M:92:GLU:OE1	1:W:15:ARG:NH2	2.46	0.48
1:S:19:ARG:NH2	1:S:19:ARG:HB2	2.28	0.48
1:U:15:ARG:O	1:U:16:LEU:C	2.57	0.48
1:I:55:GLU:O	1:I:59:LEU:HG	2.14	0.48
2:I:147:N87:C23	2:I:147:N87:C22	2.75	0.48
1:J:50:ARG:HD2	3:J:300:HOH:O	2.12	0.48
1:H:35:LEU:HD22	1:H:35:LEU:O	2.13	0.48
1:K:75:ASN:C	1:K:75:ASN:OD1	2.55	0.48
1:K:101:HIS:HB2	1:K:126:VAL:HG22	1.95	0.48
1:L:8:ILE:HD12	1:L:72:VAL:HG13	1.95	0.48
1:X:131:GLN:O	1:X:134:LEU:N	2.46	0.48
1:G:15:ARG:O	1:G:16:LEU:C	2.56	0.48
1:J:75:ASN:HA	3:J:1394:HOH:O	2.13	0.48
1:K:38:ARG:HH11	1:K:38:ARG:CG	2.26	0.48
1:M:48:VAL:HG12	1:M:50:ARG:HD3	1.95	0.48
1:V:20:GLU:O	1:V:21:PRO:C	2.55	0.48
1:S:36:ILE:HG23	1:S:137:LEU:HD11	1.95	0.48
1:V:130:ILE:HD12	1:V:130:ILE:HA	1.58	0.48
1:L:48:VAL:HG12	1:L:50:ARG:HD2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:4:ILE:HG12	1:P:70:GLU:CD	2.38	0.48
1:Q:11:PRO:HA	1:Q:53:ASP:OD1	2.14	0.48
1:A:50:ARG:HB3	1:A:61:TRP:CZ3	2.49	0.48
1:D:131:GLN:O	1:D:134:LEU:HB2	2.14	0.48
1:N:15:ARG:NH2	1:Q:92:GLU:OE1	2.42	0.48
1:S:4:ILE:CD1	1:S:70:GLU:OE2	2.61	0.48
1:V:48:VAL:O	1:V:48:VAL:HG23	2.14	0.48
1:P:138:ARG:NH1	1:U:138:ARG:CZ	2.77	0.48
1:A:125:ILE:HG23	1:A:128:LEU:HD12	1.96	0.47
1:C:101:HIS:HB2	1:C:126:VAL:HG22	1.96	0.47
1:G:109:GLU:OE1	1:G:112:ARG:NE	2.46	0.47
1:P:13:LEU:O	1:P:16:LEU:HB2	2.13	0.47
1:D:92:GLU:OE1	1:F:15:ARG:NH2	2.46	0.47
1:O:117:LEU:O	1:O:120:ILE:HD13	2.14	0.47
1:P:36:ILE:HG23	1:P:137:LEU:HD11	1.95	0.47
1:Q:59:LEU:HD22	1:Q:89:ALA:HB2	1.96	0.47
1:W:142:GLU:O	1:W:143:HIS:HB2	2.14	0.47
1:E:20:GLU:HB3	1:E:21:PRO:HD3	1.96	0.47
1:F:90:CYS:HB3	1:F:97:LEU:HD22	1.96	0.47
1:U:29:HIS:O	1:U:33:VAL:HG23	2.14	0.47
1:M:106:HIS:HA	1:M:113:ARG:HG2	1.95	0.47
1:N:41:ALA:C	1:N:43:LEU:H	2.22	0.47
1:M:128:LEU:HD23	1:M:128:LEU:HA	1.56	0.47
1:C:124:VAL:HG12	1:C:126:VAL:HG23	1.97	0.47
1:D:38:ARG:CG	1:D:38:ARG:NH1	2.65	0.47
1:F:80:THR:HG23	1:F:117:LEU:HD12	1.96	0.47
1:I:32:LEU:HD13	1:I:130:ILE:HG23	1.96	0.47
1:K:18:ARG:H	1:K:18:ARG:HG2	1.59	0.47
1:N:22:ALA:HA	3:N:1407:HOH:O	2.15	0.47
2:Q:147:N87:H22	2:Q:147:N87:H23	1.96	0.47
1:S:80:THR:OG1	1:S:101:HIS:HE1	1.98	0.47
2:S:147:N87:H22	2:S:147:N87:H23	1.95	0.47
1:T:101:HIS:HB2	1:T:126:VAL:HG22	1.97	0.47
1:D:71:PRO:HB3	1:D:96:PRO:HD2	1.95	0.47
1:V:21:PRO:HA	1:V:25:GLY:HA3	1.97	0.47
1:A:63:HIS:HB3	1:K:15:ARG:HH11	1.80	0.47
1:F:3:LEU:HD12	3:F:590:HOH:O	2.15	0.47
1:I:92:GLU:HG2	2:J:147:N87:H19	1.97	0.47
1:V:137:LEU:HD23	1:V:137:LEU:HA	1.82	0.47
1:E:11:PRO:HA	1:E:53:ASP:OD1	2.15	0.47
1:N:41:ALA:O	1:N:43:LEU:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:35:LEU:HD13	1:P:134:LEU:HD21	1.97	0.47
1:R:28:THR:CG2	1:R:30:ASP:HB2	2.45	0.47
1:A:40:ALA:HB2	1:A:47:ALA:HB2	1.97	0.46
1:E:20:GLU:HG2	1:E:21:PRO:HD3	1.97	0.46
1:N:20:GLU:O	1:N:20:GLU:HG2	2.15	0.46
1:N:106:HIS:HA	1:N:113:ARG:HG2	1.97	0.46
1:K:13:LEU:O	1:K:16:LEU:HB2	2.16	0.46
1:P:142:GLU:O	1:P:143:HIS:O	2.33	0.46
1:X:98:ILE:N	1:X:98:ILE:CD1	2.78	0.46
1:B:50:ARG:HB3	1:B:61:TRP:CZ3	2.50	0.46
1:G:63:HIS:HD2	3:G:388:HOH:O	1.98	0.46
1:I:33:VAL:HG13	1:I:49:VAL:HB	1.96	0.46
1:P:113:ARG:NH2	3:P:1368:HOH:O	2.48	0.46
1:K:9:ASN:O	1:K:51:GLN:HA	2.15	0.46
1:S:4:ILE:HD12	1:S:70:GLU:CG	2.45	0.46
1:V:27:THR:HG22	1:V:31:GLU:HB3	1.98	0.46
1:N:38:ARG:HH11	1:N:38:ARG:HB3	1.79	0.46
1:R:50:ARG:HB3	1:R:61:TRP:CZ3	2.51	0.46
1:B:3:LEU:N	3:B:468:HOH:O	2.49	0.46
1:P:7:VAL:HB	1:P:49:VAL:HG22	1.96	0.46
1:P:20:GLU:N	1:P:21:PRO:HD3	2.31	0.46
1:R:80:THR:OG1	1:R:101:HIS:HE1	1.99	0.46
1:E:20:GLU:HB3	1:E:21:PRO:CD	2.46	0.46
1:N:24:TYR:HA	1:N:102:ILE:CG2	2.45	0.46
2:S:147:N87:C23	2:S:147:N87:C22	2.94	0.46
1:W:22:ALA:O	1:W:23:VAL:O	2.33	0.46
1:E:80:THR:OG1	1:E:101:HIS:HE1	1.98	0.46
1:I:21:PRO:HA	1:I:22:ALA:HA	1.65	0.46
1:L:20:GLU:HB3	1:L:23:VAL:CG1	2.45	0.46
1:O:76:ALA:O	1:O:79:LEU:HB2	2.16	0.46
1:D:22:ALA:CB	1:D:23:VAL:HA	2.41	0.45
1:E:10:GLY:HA2	1:E:58:LEU:HD11	1.98	0.45
1:E:131:GLN:NE2	1:K:139:TYR:HA	2.31	0.45
2:F:147:N87:C23	2:F:147:N87:H22	2.46	0.45
1:P:101:HIS:HB2	1:P:126:VAL:HG22	1.97	0.45
1:F:22:ALA:HB2	3:F:1383:HOH:O	2.17	0.45
1:J:3:LEU:N	3:J:1307:HOH:O	2.49	0.45
1:D:59:LEU:CD2	1:D:86:LEU:HA	2.45	0.45
1:E:35:LEU:HD22	3:E:1035:HOH:O	2.15	0.45
1:I:48:VAL:HG12	1:I:50:ARG:HD2	1.98	0.45
1:N:41:ALA:C	1:N:43:LEU:N	2.74	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:20:GLU:C	1:S:22:ALA:H	2.24	0.45
1:T:83:SER:OG	1:T:86:LEU:HB2	2.17	0.45
1:D:53:ASP:OD2	1:G:63:HIS:HE1	2.00	0.45
1:I:31:GLU:O	1:I:34:ALA:HB3	2.15	0.45
2:L:147:N87:C23	2:L:147:N87:C22	2.92	0.45
1:M:9:ASN:O	1:M:51:GLN:HA	2.15	0.45
1:R:4:ILE:HG12	1:R:46:LYS:HD3	1.98	0.45
1:T:130:ILE:HD12	1:T:130:ILE:HA	1.49	0.45
1:X:41:ALA:O	1:X:42:GLU:CB	2.62	0.45
1:J:22:ALA:HB2	3:J:819:HOH:O	2.16	0.45
1:T:130:ILE:HG23	1:T:131:GLN:N	2.31	0.45
1:U:140:LEU:C	1:U:142:GLU:N	2.75	0.45
1:E:34:ALA:HB2	3:E:734:HOH:O	2.16	0.45
1:H:118:SER:HB2	1:H:119:PRO:HD3	1.98	0.45
1:M:19:ARG:HG2	1:M:19:ARG:NH1	2.31	0.45
1:M:60:ASP:O	1:M:63:HIS:HB2	2.17	0.45
1:N:18:ARG:NH2	3:N:1329:HOH:O	2.49	0.45
1:R:16:LEU:HD23	1:R:16:LEU:HA	1.75	0.45
1:R:99:GLU:HB3	1:R:124:VAL:HG13	1.99	0.45
1:X:19:ARG:O	1:X:21:PRO:HD3	2.16	0.45
1:G:143:HIS:ND1	1:G:143:HIS:N	2.64	0.45
1:X:50:ARG:HB3	1:X:61:TRP:CH2	2.51	0.45
1:E:35:LEU:HD23	1:E:35:LEU:HA	1.72	0.45
1:H:19:ARG:HD3	1:J:92:GLU:OE2	2.16	0.45
1:J:7:VAL:HG11	1:J:36:ILE:HD13	1.99	0.45
1:M:39:GLU:HG3	1:M:43:LEU:CD2	2.46	0.45
1:P:59:LEU:HD22	1:P:89:ALA:HB2	1.99	0.45
1:E:101:HIS:HB2	1:E:126:VAL:HG22	1.99	0.45
1:Q:60:ASP:OD2	1:Q:64:GLN:NE2	2.49	0.45
1:U:15:ARG:HB2	2:U:147:N87:H19	1.99	0.45
1:B:27:THR:HG23	1:B:31:GLU:HB3	1.99	0.45
1:C:22:ALA:C	1:C:23:VAL:HG23	2.42	0.45
1:O:3:LEU:HD23	3:O:736:HOH:O	2.15	0.45
1:S:20:GLU:N	1:S:21:PRO:CD	2.79	0.45
1:S:50:ARG:HE	1:S:50:ARG:HB2	1.45	0.45
1:T:3:LEU:HG	1:T:4:ILE:N	2.32	0.45
1:D:22:ALA:HA	1:D:23:VAL:HA	1.56	0.44
1:B:55:GLU:OE2	1:B:83:SER:OG	2.22	0.44
1:D:27:THR:HG22	1:D:28:THR:O	2.17	0.44
1:H:24:TYR:HA	1:H:102:ILE:HG21	1.99	0.44
1:R:117:LEU:O	1:R:120:ILE:HG13	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:139:TYR:HA	1:X:131:GLN:HE22	1.82	0.44
1:E:24:TYR:OH	2:E:147:N87:H14	2.17	0.44
1:K:20:GLU:C	1:K:21:PRO:O	2.61	0.44
1:L:118:SER:N	1:L:119:PRO:CD	2.81	0.44
1:M:27:THR:HB	1:M:130:ILE:HD13	1.99	0.44
1:P:106:HIS:HA	1:P:113:ARG:HG2	1.99	0.44
1:T:8:ILE:HD13	1:T:62:ILE:HD12	2.00	0.44
1:A:18:ARG:O	1:A:19:ARG:CB	2.65	0.44
1:X:60:ASP:O	1:X:63:HIS:HB2	2.17	0.44
1:E:5:VAL:HG22	1:E:71:PRO:HG2	1.98	0.44
1:L:134:LEU:HA	1:L:137:LEU:HD12	1.99	0.44
1:R:28:THR:HG22	1:R:29:HIS:N	2.31	0.44
1:X:42:GLU:H	1:X:44:GLY:H	1.65	0.44
1:X:104:ASN:HA	1:X:126:VAL:HG13	1.99	0.44
1:B:75:ASN:HA	3:B:1025:HOH:O	2.17	0.44
1:J:63:HIS:CD2	3:J:1086:HOH:O	2.70	0.44
1:L:7:VAL:HB	1:L:49:VAL:HG22	1.97	0.44
1:R:118:SER:HB2	1:R:119:PRO:HD3	2.00	0.44
1:U:23:VAL:N	3:U:1417:HOH:O	2.51	0.44
2:U:147:N87:H18	2:U:147:N87:C23	2.36	0.44
1:E:142:GLU:C	1:E:143:HIS:CD2	2.96	0.44
1:T:32:LEU:HD13	1:T:130:ILE:CD1	2.47	0.44
1:H:32:LEU:HD13	1:H:130:ILE:HG12	2.00	0.44
1:K:58:LEU:O	1:K:62:ILE:HG12	2.17	0.44
1:H:87:ARG:HG3	1:H:120:ILE:HG12	2.00	0.43
1:M:104:ASN:HA	1:M:126:VAL:HG13	2.00	0.43
1:N:54:SER:HB3	1:N:57:GLN:HB3	2.00	0.43
1:N:70:GLU:H	1:N:70:GLU:HG2	1.65	0.43
1:W:90:CYS:HB3	1:W:97:LEU:HD22	2.00	0.43
1:F:48:VAL:HG12	1:F:50:ARG:HD2	2.00	0.43
1:G:101:HIS:HB3	2:G:147:N87:C2	2.49	0.43
1:K:50:ARG:NH2	3:K:1147:HOH:O	2.51	0.43
1:N:19:ARG:HB3	2:N:147:N87:H20	2.00	0.43
1:O:114:HIS:HB2	3:O:1097:HOH:O	2.17	0.43
1:P:40:ALA:HB1	1:P:45:LEU:HB2	2.00	0.43
2:C:147:N87:C23	2:C:147:N87:C22	2.77	0.43
1:U:23:VAL:CG1	1:U:103:SER:HA	2.47	0.43
1:A:143:HIS:HB3	3:A:950:HOH:O	2.18	0.43
1:J:109:GLU:OE2	1:J:112:ARG:NE	2.51	0.43
1:V:57:GLN:NE2	1:V:61:TRP:CE2	2.87	0.43
1:V:101:HIS:HB2	1:V:126:VAL:HG22	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:139:TYR:HD2	1:V:140:LEU:HD23	1.84	0.43
1:W:117:LEU:O	1:W:118:SER:C	2.61	0.43
1:E:35:LEU:HD13	1:E:134:LEU:HD11	2.01	0.43
2:W:147:N87:H18	2:W:147:N87:H23	1.99	0.43
1:B:18:ARG:NH2	3:B:332:HOH:O	2.51	0.43
1:V:128:LEU:HD23	1:V:128:LEU:HA	1.80	0.43
1:E:17:GLY:CA	1:E:19:ARG:N	2.79	0.43
1:M:131:GLN:O	1:M:135:LEU:HD22	2.18	0.43
1:O:55:GLU:O	1:O:59:LEU:HG	2.18	0.43
1:O:118:SER:HB2	1:O:119:PRO:HD3	2.00	0.43
1:P:41:ALA:C	1:P:43:LEU:H	2.26	0.43
1:D:19:ARG:HH11	1:G:92:GLU:CD	2.27	0.43
1:V:41:ALA:O	1:V:42:GLU:C	2.61	0.43
1:B:97:LEU:HD23	1:B:121:ALA:HA	2.01	0.43
1:D:53:ASP:HB3	1:G:59:LEU:HD12	2.01	0.43
1:N:92:GLU:HG2	1:O:19:ARG:NH1	2.34	0.43
1:S:97:LEU:HD12	1:S:98:ILE:H	1.84	0.43
1:G:3:LEU:N	3:G:1305:HOH:O	2.52	0.42
1:G:4:ILE:N	1:G:4:ILE:HD13	2.35	0.42
1:H:38:ARG:HE	1:H:38:ARG:HB3	1.36	0.42
2:U:147:N87:C18	2:U:147:N87:C23	2.88	0.42
1:C:117:LEU:O	1:C:120:ILE:HG13	2.18	0.42
1:K:36:ILE:HG23	1:K:137:LEU:HD11	2.00	0.42
1:L:80:THR:HG21	1:L:101:HIS:HE1	1.85	0.42
1:S:118:SER:HB2	1:S:119:PRO:HD3	2.00	0.42
1:D:38:ARG:NH1	1:D:38:ARG:HB3	2.33	0.42
1:G:9:ASN:O	1:G:51:GLN:HA	2.19	0.42
1:G:59:LEU:HD23	1:G:86:LEU:HD12	2.01	0.42
1:G:117:LEU:HD23	1:G:117:LEU:HA	1.87	0.42
1:L:139:TYR:CD2	1:L:139:TYR:C	2.96	0.42
1:R:21:PRO:CB	1:R:23:VAL:H	2.32	0.42
1:U:102:ILE:HG23	1:U:129:GLY:HA2	2.00	0.42
1:X:39:GLU:O	1:X:39:GLU:HG3	2.19	0.42
1:G:125:ILE:HG23	1:G:128:LEU:HD12	2.02	0.42
1:S:131:GLN:CB	3:S:149:HOH:O	2.67	0.42
1:W:99:GLU:HB3	1:W:124:VAL:HG22	2.01	0.42
1:A:35:LEU:HD12	1:A:38:ARG:HH21	1.83	0.42
1:G:11:PRO:HA	1:G:53:ASP:HA	2.01	0.42
1:K:92:GLU:OE1	1:L:15:ARG:NE	2.53	0.42
1:A:134:LEU:HA	1:A:137:LEU:HD12	2.01	0.42
1:E:3:LEU:C	1:E:3:LEU:HD12	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:4:ILE:O	1:U:71:PRO:HD2	2.18	0.42
1:N:38:ARG:HH11	1:N:38:ARG:CB	2.32	0.42
1:P:6:ASN:ND2	1:P:70:GLU:HB2	2.34	0.42
1:Q:55:GLU:HG3	1:Q:79:LEU:HD13	2.00	0.42
1:C:9:ASN:O	1:C:51:GLN:HA	2.19	0.42
1:C:23:VAL:HG12	1:C:24:TYR:CZ	2.55	0.42
1:E:15:ARG:O	1:E:18:ARG:HB2	2.20	0.42
1:R:79:LEU:O	1:R:80:THR:C	2.62	0.42
1:S:52:SER:HG	1:S:54:SER:H	1.67	0.42
1:V:48:VAL:O	1:V:48:VAL:CG2	2.68	0.42
1:B:39:GLU:HG2	1:B:134:LEU:HB3	2.02	0.42
1:B:104:ASN:OD1	1:B:104:ASN:C	2.60	0.42
1:J:23:VAL:HG12	1:J:24:TYR:CE1	2.55	0.42
1:K:21:PRO:C	1:K:23:VAL:N	2.78	0.42
1:O:9:ASN:O	1:O:51:GLN:HA	2.20	0.42
1:G:97:LEU:C	1:G:98:ILE:HD12	2.44	0.42
1:Q:9:ASN:O	1:Q:51:GLN:HA	2.20	0.42
1:R:88:ASP:OD2	2:S:147:N87:O9	2.29	0.42
1:D:21:PRO:HG3	3:D:1062:HOH:O	2.19	0.41
1:E:20:GLU:CB	1:E:21:PRO:CD	2.98	0.41
1:K:139:TYR:CD2	1:K:139:TYR:C	2.97	0.41
1:L:111:PHE:CE1	1:L:112:ARG:HG3	2.55	0.41
2:A:147:N87:H23	2:A:147:N87:H18	2.02	0.41
1:G:10:GLY:N	1:G:13:LEU:HD12	2.35	0.41
1:Q:98:ILE:HD11	1:Q:139:TYR:CD2	2.54	0.41
1:V:134:LEU:O	1:V:137:LEU:HB2	2.20	0.41
1:W:10:GLY:O	1:W:13:LEU:HB2	2.20	0.41
1:E:24:TYR:CD2	2:E:147:N87:H22	2.55	0.41
1:S:3:LEU:HB3	1:S:45:LEU:HD23	2.02	0.41
1:U:90:CYS:HB3	1:U:97:LEU:HD22	2.02	0.41
1:E:87:ARG:HG3	1:E:116:TYR:O	2.21	0.41
1:G:77:GLY:O	1:G:78:GLY:C	2.63	0.41
1:K:3:LEU:HD12	1:K:4:ILE:H	1.85	0.41
1:X:98:ILE:N	1:X:98:ILE:HD13	2.35	0.41
1:C:27:THR:HG22	1:C:28:THR:N	2.35	0.41
1:F:19:ARG:C	1:F:20:GLU:OE2	2.63	0.41
1:M:111:PHE:CD1	1:M:111:PHE:C	2.98	0.41
1:E:46:LYS:NZ	1:E:46:LYS:CB	2.77	0.41
1:E:97:LEU:HD23	1:E:121:ALA:HA	2.02	0.41
1:X:75:ASN:HA	3:X:1388:HOH:O	2.21	0.41
1:I:3:LEU:HD12	1:I:4:ILE:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:97:LEU:HD12	1:J:98:ILE:N	2.36	0.41
1:N:15:ARG:NH1	1:N:18:ARG:HH21	2.19	0.41
1:P:101:HIS:CE1	3:P:336:HOH:O	2.72	0.41
1:K:92:GLU:OE2	1:L:15:ARG:NH2	2.50	0.41
1:S:16:LEU:O	1:S:28:THR:HA	2.21	0.41
1:A:10:GLY:N	1:A:13:LEU:HD12	2.34	0.41
1:B:83:SER:HB2	3:B:270:HOH:O	2.21	0.41
1:E:128:LEU:CD2	1:K:123:GLY:HA3	2.51	0.41
1:G:114:HIS:HB2	3:G:321:HOH:O	2.20	0.41
1:H:16:LEU:HD11	1:H:130:ILE:HD11	2.03	0.41
1:H:19:ARG:HD3	1:J:92:GLU:CG	2.51	0.41
1:I:13:LEU:HD23	1:I:13:LEU:HA	1.90	0.41
1:P:32:LEU:HD13	1:P:130:ILE:HG12	2.03	0.41
1:Q:36:ILE:HG23	1:Q:137:LEU:HD11	2.03	0.41
1:U:92:GLU:HG3	1:V:19:ARG:HB3	2.03	0.41
1:V:99:GLU:HB3	1:V:124:VAL:HG22	2.02	0.41
1:W:13:LEU:HD23	1:W:13:LEU:HA	1.91	0.41
1:X:16:LEU:HD11	1:X:130:ILE:HD11	2.02	0.41
1:X:131:GLN:N	3:X:530:HOH:O	2.36	0.41
1:C:7:VAL:C	1:C:8:ILE:HG12	2.45	0.41
1:D:31:GLU:HG2	1:D:31:GLU:H	1.48	0.41
1:H:11:PRO:HG2	1:H:79:LEU:HG	2.02	0.41
1:H:59:LEU:HD22	1:H:89:ALA:HB2	2.02	0.41
1:H:137:LEU:HD23	1:H:137:LEU:HA	1.92	0.41
1:G:87:ARG:HD3	1:G:116:TYR:O	2.21	0.40
1:H:106:HIS:HA	1:H:113:ARG:HG2	2.04	0.40
1:O:134:LEU:HD23	1:O:134:LEU:N	2.36	0.40
1:R:48:VAL:HG12	1:R:50:ARG:HD2	2.03	0.40
1:F:50:ARG:NH2	1:F:61:TRP:CD1	2.89	0.40
1:N:135:LEU:HD11	1:R:139:TYR:HB2	2.03	0.40
1:A:35:LEU:HD12	1:A:38:ARG:NH2	2.36	0.40
1:A:101:HIS:HB2	1:A:126:VAL:HG22	2.03	0.40
1:A:138:ARG:NH2	1:G:138:ARG:NH1	2.69	0.40
1:F:46:LYS:HE2	3:F:804:HOH:O	2.21	0.40
1:I:10:GLY:HA2	1:I:58:LEU:HD11	2.03	0.40
1:N:29:HIS:O	1:N:33:VAL:HG23	2.21	0.40
1:T:92:GLU:OE2	1:U:15:ARG:NE	2.54	0.40
1:W:59:LEU:HD22	1:W:89:ALA:HB2	2.03	0.40
1:C:7:VAL:HB	1:C:49:VAL:HG22	2.02	0.40
1:C:118:SER:HB2	1:C:119:PRO:HD3	2.03	0.40
1:E:128:LEU:HD21	1:K:123:GLY:HA3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:19:ARG:C	1:G:21:PRO:CD	2.94	0.40
1:N:19:ARG:HD3	1:N:20:GLU:N	2.36	0.40
1:N:95:ALA:HB1	1:N:96:PRO:CD	2.52	0.40
1:V:19:ARG:HB3	2:V:147:N87:H20	2.02	0.40
1:J:27:THR:HG22	1:J:31:GLU:HB2	2.02	0.40
2:L:147:N87:H23	2:L:147:N87:C22	2.52	0.40
1:O:59:LEU:HD12	1:Q:53:ASP:HB3	2.04	0.40
1:P:90:CYS:HB3	1:P:97:LEU:HD22	2.03	0.40
1:Q:3:LEU:N	3:Q:846:HOH:O	2.55	0.40
1:Q:80:THR:OG1	1:Q:101:HIS:HE1	2.04	0.40
1:Q:128:LEU:HD23	1:Q:128:LEU:HA	1.82	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	139/147 (95%)	126 (91%)	11 (8%)	2 (1%)	9	13
1	B	139/147 (95%)	130 (94%)	9 (6%)	0	100	100
1	C	139/147 (95%)	128 (92%)	7 (5%)	4 (3%)	3	3
1	D	139/147 (95%)	128 (92%)	8 (6%)	3 (2%)	5	6
1	E	139/147 (95%)	127 (91%)	9 (6%)	3 (2%)	5	6
1	F	140/147 (95%)	132 (94%)	4 (3%)	4 (3%)	3	3
1	G	139/147 (95%)	131 (94%)	6 (4%)	2 (1%)	9	13
1	H	139/147 (95%)	132 (95%)	7 (5%)	0	100	100
1	I	139/147 (95%)	132 (95%)	6 (4%)	1 (1%)	18	28
1	J	139/147 (95%)	130 (94%)	5 (4%)	4 (3%)	3	3
1	K	139/147 (95%)	124 (89%)	11 (8%)	4 (3%)	3	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	139/147 (95%)	131 (94%)	5 (4%)	3 (2%)	5	6
1	M	139/147 (95%)	134 (96%)	5 (4%)	0	100	100
1	N	140/147 (95%)	122 (87%)	13 (9%)	5 (4%)	2	2
1	O	139/147 (95%)	126 (91%)	12 (9%)	1 (1%)	18	28
1	P	139/147 (95%)	130 (94%)	7 (5%)	2 (1%)	9	13
1	Q	139/147 (95%)	127 (91%)	8 (6%)	4 (3%)	3	3
1	R	139/147 (95%)	123 (88%)	11 (8%)	5 (4%)	2	2
1	S	139/147 (95%)	130 (94%)	5 (4%)	4 (3%)	3	3
1	T	139/147 (95%)	132 (95%)	6 (4%)	1 (1%)	18	28
1	U	139/147 (95%)	126 (91%)	9 (6%)	4 (3%)	3	3
1	V	139/147 (95%)	125 (90%)	6 (4%)	8 (6%)	1	0
1	W	139/147 (95%)	129 (93%)	8 (6%)	2 (1%)	9	13
1	X	139/147 (95%)	126 (91%)	10 (7%)	3 (2%)	5	6
All	All	3338/3528 (95%)	3081 (92%)	188 (6%)	69 (2%)	5	7

All (69) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	19	ARG
1	C	20	GLU
1	C	21	PRO
1	D	20	GLU
1	D	21	PRO
1	E	20	GLU
1	E	21	PRO
1	F	20	GLU
1	F	22	ALA
1	G	19	ARG
1	J	21	PRO
1	J	22	ALA
1	K	19	ARG
1	K	21	PRO
1	K	26	GLY
1	N	19	ARG
1	P	52	SER
1	Q	21	PRO
1	Q	22	ALA

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Mol	Chain	Res	Type
1	Q	23	VAL
1	R	18	ARG
1	R	19	ARG
1	R	21	PRO
1	S	22	ALA
1	S	23	VAL
1	U	18	ARG
1	U	19	ARG
1	U	141	ALA
1	V	18	ARG
1	V	20	GLU
1	V	21	PRO
1	V	25	GLY
1	W	19	ARG
1	W	23	VAL
1	X	21	PRO
1	C	22	ALA
1	F	19	ARG
1	F	23	VAL
1	J	130	ILE
1	L	130	ILE
1	P	42	GLU
1	R	17	GLY
1	V	23	VAL
1	V	27	THR
1	X	42	GLU
1	I	27	THR
1	L	78	GLY
1	L	141	ALA
1	N	42	GLU
1	N	69	ALA
1	V	48	VAL
1	C	23	VAL
1	D	18	ARG
1	J	19	ARG
1	K	22	ALA
1	N	130	ILE
1	R	105	VAL
1	S	12	ASN
1	V	17	GLY
1	A	78	GLY
1	G	20	GLU

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Mol	Chain	Res	Type
1	O	19	ARG
1	X	132	GLY
1	Q	19	ARG
1	S	21	PRO
1	E	130	ILE
1	N	20	GLU
1	T	130	ILE
1	U	129	GLY

5.3.2 Protein sidechains [i](#)

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	109/115 (95%)	102 (94%)	7 (6%)	16	28
1	B	110/115 (96%)	102 (93%)	8 (7%)	13	22
1	C	108/115 (94%)	98 (91%)	10 (9%)	8	14
1	D	109/115 (95%)	97 (89%)	12 (11%)	6	9
1	E	110/115 (96%)	102 (93%)	8 (7%)	13	22
1	F	110/115 (96%)	100 (91%)	10 (9%)	9	14
1	G	110/115 (96%)	101 (92%)	9 (8%)	10	18
1	H	110/115 (96%)	99 (90%)	11 (10%)	7	11
1	I	110/115 (96%)	101 (92%)	9 (8%)	10	18
1	J	108/115 (94%)	96 (89%)	12 (11%)	6	9
1	K	108/115 (94%)	95 (88%)	13 (12%)	5	7
1	L	110/115 (96%)	101 (92%)	9 (8%)	10	18
1	M	110/115 (96%)	93 (84%)	17 (16%)	2	3
1	N	111/115 (96%)	100 (90%)	11 (10%)	7	11
1	O	110/115 (96%)	100 (91%)	10 (9%)	9	14
1	P	110/115 (96%)	99 (90%)	11 (10%)	7	11
1	Q	109/115 (95%)	100 (92%)	9 (8%)	10	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	R	107/115 (93%)	100 (94%)	7 (6%)	15	27
1	S	110/115 (96%)	100 (91%)	10 (9%)	9	14
1	T	110/115 (96%)	101 (92%)	9 (8%)	10	18
1	U	110/115 (96%)	104 (94%)	6 (6%)	19	34
1	V	109/115 (95%)	91 (84%)	18 (16%)	2	3
1	W	109/115 (95%)	100 (92%)	9 (8%)	10	17
1	X	108/115 (94%)	98 (91%)	10 (9%)	8	14
All	All	2625/2760 (95%)	2380 (91%)	245 (9%)	8	14

All (245) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	VAL
1	A	35	LEU
1	A	42	GLU
1	A	50	ARG
1	A	64	GLN
1	A	126	VAL
1	A	130	ILE
1	B	18	ARG
1	B	23	VAL
1	B	50	ARG
1	B	59	LEU
1	B	110	GLU
1	B	126	VAL
1	B	130	ILE
1	B	142	GLU
1	C	4	ILE
1	C	8	ILE
1	C	18	ARG
1	C	23	VAL
1	C	31	GLU
1	C	46	LYS
1	C	54	SER
1	C	70	GLU
1	C	120	ILE
1	C	131	GLN
1	D	3	LEU
1	D	4	ILE
1	D	19	ARG

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Mol	Chain	Res	Type
1	D	20	GLU
1	D	31	GLU
1	D	35	LEU
1	D	38	ARG
1	D	50	ARG
1	D	54	SER
1	D	110	GLU
1	D	130	ILE
1	D	142	GLU
1	E	4	ILE
1	E	18	ARG
1	E	35	LEU
1	E	38	ARG
1	E	46	LYS
1	E	126	VAL
1	E	130	ILE
1	E	143	HIS
1	F	8	ILE
1	F	18	ARG
1	F	28	THR
1	F	35	LEU
1	F	42	GLU
1	F	50	ARG
1	F	126	VAL
1	F	130	ILE
1	F	131	GLN
1	F	142	GLU
1	G	4	ILE
1	G	18	ARG
1	G	35	LEU
1	G	45	LEU
1	G	49	VAL
1	G	62	ILE
1	G	126	VAL
1	G	130	ILE
1	G	143	HIS
1	H	15	ARG
1	H	16	LEU
1	H	19	ARG
1	H	23	VAL
1	H	35	LEU
1	H	38	ARG

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Mol	Chain	Res	Type
1	H	46	LYS
1	H	50	ARG
1	H	52	SER
1	H	126	VAL
1	H	130	ILE
1	I	19	ARG
1	I	27	THR
1	I	33	VAL
1	I	50	ARG
1	I	55	GLU
1	I	62	ILE
1	I	92	GLU
1	I	98	ILE
1	I	142	GLU
1	J	4	ILE
1	J	18	ARG
1	J	23	VAL
1	J	32	LEU
1	J	35	LEU
1	J	42	GLU
1	J	45	LEU
1	J	115	SER
1	J	120	ILE
1	J	126	VAL
1	J	130	ILE
1	J	142	GLU
1	K	16	LEU
1	K	18	ARG
1	K	24	TYR
1	K	35	LEU
1	K	38	ARG
1	K	46	LYS
1	K	50	ARG
1	K	110	GLU
1	K	120	ILE
1	K	122	THR
1	K	126	VAL
1	K	130	ILE
1	K	142	GLU
1	L	23	VAL
1	L	45	LEU
1	L	46	LYS

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Mol	Chain	Res	Type
1	L	50	ARG
1	L	54	SER
1	L	55	GLU
1	L	126	VAL
1	L	130	ILE
1	L	131	GLN
1	M	3	LEU
1	M	15	ARG
1	M	18	ARG
1	M	19	ARG
1	M	31	GLU
1	M	35	LEU
1	M	38	ARG
1	M	43	LEU
1	M	50	ARG
1	M	64	GLN
1	M	110	GLU
1	M	126	VAL
1	M	130	ILE
1	M	131	GLN
1	M	134	LEU
1	M	135	LEU
1	M	142	GLU
1	N	20	GLU
1	N	23	VAL
1	N	32	LEU
1	N	37	GLU
1	N	38	ARG
1	N	50	ARG
1	N	59	LEU
1	N	70	GLU
1	N	105	VAL
1	N	120	ILE
1	N	126	VAL
1	O	18	ARG
1	O	19	ARG
1	O	35	LEU
1	O	38	ARG
1	O	42	GLU
1	O	50	ARG
1	O	110	GLU
1	O	120	ILE

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Mol	Chain	Res	Type
1	O	126	VAL
1	O	130	ILE
1	P	4	ILE
1	P	16	LEU
1	P	19	ARG
1	P	35	LEU
1	P	45	LEU
1	P	50	ARG
1	P	87	ARG
1	P	120	ILE
1	P	126	VAL
1	P	130	ILE
1	P	142	GLU
1	Q	18	ARG
1	Q	20	GLU
1	Q	23	VAL
1	Q	38	ARG
1	Q	46	LYS
1	Q	54	SER
1	Q	126	VAL
1	Q	130	ILE
1	Q	143	HIS
1	R	50	ARG
1	R	94	SER
1	R	110	GLU
1	R	126	VAL
1	R	131	GLN
1	R	142	GLU
1	R	143	HIS
1	S	4	ILE
1	S	18	ARG
1	S	20	GLU
1	S	23	VAL
1	S	31	GLU
1	S	35	LEU
1	S	37	GLU
1	S	49	VAL
1	S	50	ARG
1	S	126	VAL
1	T	18	ARG
1	T	20	GLU
1	T	30	ASP

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Mol	Chain	Res	Type
1	T	45	LEU
1	T	59	LEU
1	T	62	ILE
1	T	120	ILE
1	T	126	VAL
1	T	130	ILE
1	U	4	ILE
1	U	8	ILE
1	U	18	ARG
1	U	27	THR
1	U	35	LEU
1	U	126	VAL
1	V	3	LEU
1	V	16	LEU
1	V	18	ARG
1	V	19	ARG
1	V	23	VAL
1	V	28	THR
1	V	31	GLU
1	V	32	LEU
1	V	38	ARG
1	V	42	GLU
1	V	46	LYS
1	V	48	VAL
1	V	87	ARG
1	V	102	ILE
1	V	105	VAL
1	V	126	VAL
1	V	130	ILE
1	V	131	GLN
1	W	3	LEU
1	W	18	ARG
1	W	20	GLU
1	W	23	VAL
1	W	24	TYR
1	W	52	SER
1	W	57	GLN
1	W	130	ILE
1	W	142	GLU
1	X	5	VAL
1	X	16	LEU
1	X	45	LEU

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Mol	Chain	Res	Type
1	X	49	VAL
1	X	57	GLN
1	X	98	ILE
1	X	110	GLU
1	X	126	VAL
1	X	130	ILE
1	X	142	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	64	GLN
1	B	131	GLN
1	C	51	GLN
1	C	63	HIS
1	C	64	GLN
1	C	131	GLN
1	D	63	HIS
1	D	106	HIS
1	E	131	GLN
1	E	143	HIS
1	F	57	GLN
1	F	63	HIS
1	F	131	GLN
1	H	57	GLN
1	H	63	HIS
1	I	51	GLN
1	I	57	GLN
1	I	63	HIS
1	I	131	GLN
1	J	114	HIS
1	K	114	HIS
1	K	131	GLN
1	L	6	ASN
1	M	57	GLN
1	M	64	GLN
1	O	63	HIS
1	O	131	GLN
1	P	63	HIS
1	Q	63	HIS
1	Q	64	GLN
1	R	6	ASN

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Mol	Chain	Res	Type
1	R	63	HIS
1	S	63	HIS
1	S	114	HIS
1	T	57	GLN
1	T	63	HIS
1	T	106	HIS
1	U	51	GLN
1	U	114	HIS
1	V	57	GLN
1	V	131	GLN
1	W	64	GLN
1	X	57	GLN
1	X	63	HIS
1	X	64	GLN
1	X	114	HIS
1	X	131	GLN
1	X	143	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

24 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	N87	Q	147	-	26,28,28	0.82	0	30,41,41	1.97	9 (30%)
2	N87	T	147	-	26,28,28	0.75	0	30,41,41	1.51	5 (16%)
2	N87	H	147	-	26,28,28	0.90	1 (3%)	30,41,41	1.88	8 (26%)
2	N87	N	147	-	26,28,28	1.27	4 (15%)	30,41,41	1.58	5 (16%)
2	N87	V	147	-	26,28,28	1.17	3 (11%)	30,41,41	1.65	8 (26%)
2	N87	R	147	-	26,28,28	1.02	0	30,41,41	1.50	5 (16%)
2	N87	X	147	-	26,28,28	1.30	3 (11%)	30,41,41	1.37	4 (13%)
2	N87	B	147	-	26,28,28	0.78	0	30,41,41	1.55	3 (10%)
2	N87	M	147	-	26,28,28	1.09	2 (7%)	30,41,41	1.09	3 (10%)
2	N87	D	147	-	26,28,28	1.58	4 (15%)	30,41,41	2.06	9 (30%)
2	N87	S	147	-	26,28,28	1.06	1 (3%)	30,41,41	1.19	2 (6%)
2	N87	U	147	-	26,28,28	1.07	1 (3%)	30,41,41	1.53	5 (16%)
2	N87	L	147	-	26,28,28	1.35	4 (15%)	30,41,41	1.03	0
2	N87	I	147	-	26,28,28	0.98	0	30,41,41	1.46	3 (10%)
2	N87	W	147	-	26,28,28	1.37	2 (7%)	30,41,41	1.35	3 (10%)
2	N87	G	147	-	26,28,28	0.71	0	30,41,41	1.61	3 (10%)
2	N87	K	147	-	26,28,28	1.35	4 (15%)	30,41,41	1.60	6 (20%)
2	N87	F	147	-	26,28,28	1.11	1 (3%)	30,41,41	1.03	1 (3%)
2	N87	P	147	-	26,28,28	1.13	1 (3%)	30,41,41	2.07	11 (36%)
2	N87	A	147	-	26,28,28	0.90	0	30,41,41	1.49	4 (13%)
2	N87	C	147	-	26,28,28	1.17	2 (7%)	30,41,41	1.39	4 (13%)
2	N87	J	147	-	26,28,28	1.09	1 (3%)	30,41,41	1.01	1 (3%)
2	N87	E	147	-	26,28,28	0.84	0	30,41,41	1.33	2 (6%)
2	N87	O	147	-	26,28,28	1.19	2 (7%)	30,41,41	1.38	3 (10%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	N87	Q	147	-	-	2/18/36/36	0/3/3/3
2	N87	T	147	-	-	3/18/36/36	0/3/3/3
2	N87	H	147	-	-	2/18/36/36	0/3/3/3
2	N87	N	147	-	-	3/18/36/36	0/3/3/3
2	N87	V	147	-	-	2/18/36/36	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	N87	R	147	-	-	3/18/36/36	0/3/3/3
2	N87	X	147	-	-	1/18/36/36	0/3/3/3
2	N87	B	147	-	-	3/18/36/36	0/3/3/3
2	N87	M	147	-	-	1/18/36/36	0/3/3/3
2	N87	D	147	-	-	1/18/36/36	0/3/3/3
2	N87	S	147	-	-	3/18/36/36	0/3/3/3
2	N87	U	147	-	-	1/18/36/36	0/3/3/3
2	N87	L	147	-	-	2/18/36/36	0/3/3/3
2	N87	I	147	-	-	2/18/36/36	0/3/3/3
2	N87	W	147	-	-	3/18/36/36	0/3/3/3
2	N87	G	147	-	-	3/18/36/36	0/3/3/3
2	N87	K	147	-	-	3/18/36/36	0/3/3/3
2	N87	F	147	-	-	2/18/36/36	0/3/3/3
2	N87	P	147	-	-	3/18/36/36	0/3/3/3
2	N87	A	147	-	-	3/18/36/36	0/3/3/3
2	N87	C	147	-	-	1/18/36/36	0/3/3/3
2	N87	J	147	-	-	2/18/36/36	0/3/3/3
2	N87	E	147	-	-	8/18/36/36	0/3/3/3
2	N87	O	147	-	-	2/18/36/36	0/3/3/3

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	W	147	N87	C13-C7	4.81	1.54	1.48
2	D	147	N87	C6-C7	4.12	1.37	1.34
2	D	147	N87	C13-C7	3.53	1.53	1.48
2	L	147	N87	C6-C7	3.49	1.37	1.34
2	J	147	N87	C6-C7	3.38	1.37	1.34
2	L	147	N87	C13-C7	2.91	1.52	1.48
2	F	147	N87	C13-C7	2.88	1.52	1.48
2	V	147	N87	C6-C7	2.84	1.36	1.34
2	X	147	N87	C13-C7	2.84	1.52	1.48
2	W	147	N87	C6-C7	2.76	1.36	1.34
2	M	147	N87	C6-C7	2.71	1.36	1.34
2	K	147	N87	C6-C7	2.69	1.36	1.34
2	K	147	N87	C13-C7	2.68	1.52	1.48
2	O	147	N87	C10-C8	2.62	1.55	1.52
2	C	147	N87	C6-C7	2.53	1.36	1.34
2	N	147	N87	C10-C8	2.41	1.55	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	147	N87	C18-C17	2.41	1.43	1.39
2	X	147	N87	C6-C7	2.40	1.36	1.34
2	K	147	N87	O5-C4	2.40	1.46	1.42
2	N	147	N87	O5-C4	2.38	1.46	1.42
2	V	147	N87	C13-C7	2.34	1.51	1.48
2	N	147	N87	C13-C7	2.33	1.51	1.48
2	S	147	N87	C6-C7	2.32	1.36	1.34
2	L	147	N87	C4-C6	2.32	1.54	1.50
2	P	147	N87	C13-C7	2.29	1.51	1.48
2	D	147	N87	C15-C16	2.15	1.53	1.49
2	L	147	N87	O5-C4	2.14	1.46	1.42
2	U	147	N87	C6-C7	2.11	1.35	1.34
2	H	147	N87	C6-C7	2.07	1.35	1.34
2	C	147	N87	C17-C16	2.06	1.52	1.49
2	N	147	N87	C6-C7	2.05	1.35	1.34
2	X	147	N87	C4-C6	2.05	1.54	1.50
2	K	147	N87	C18-C17	2.04	1.42	1.39
2	M	147	N87	C13-C7	2.02	1.51	1.48
2	V	147	N87	C12-C10	2.01	1.56	1.53
2	O	147	N87	C6-C7	2.00	1.35	1.34

All (107) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	147	N87	C17-C16-C15	6.04	131.58	120.18
2	G	147	N87	C13-C7-C6	-5.94	112.55	123.05
2	I	147	N87	C13-C7-C6	-5.32	113.64	123.05
2	D	147	N87	O26-C16-C17	-5.26	111.73	120.15
2	Q	147	N87	C13-C7-C6	-4.80	114.56	123.05
2	B	147	N87	C13-C7-C6	-4.68	114.77	123.05
2	C	147	N87	C13-C7-C6	-4.61	114.90	123.05
2	P	147	N87	O26-C16-C17	-4.46	113.01	120.15
2	U	147	N87	C13-C7-C6	-4.40	115.26	123.05
2	E	147	N87	C13-C7-C6	-4.35	115.35	123.05
2	O	147	N87	C13-C7-C6	-4.27	115.50	123.05
2	Q	147	N87	C25-C13-C7	-4.09	117.11	121.11
2	S	147	N87	C13-C7-C6	-4.04	115.90	123.05
2	P	147	N87	O11-C10-C12	3.98	119.22	109.97
2	N	147	N87	C13-C7-C6	-3.88	116.19	123.05
2	H	147	N87	O26-C16-C17	-3.84	114.00	120.15
2	R	147	N87	O9-C8-C10	-3.81	103.92	110.34
2	P	147	N87	O9-C8-C10	-3.79	103.96	110.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	147	N87	C17-C16-C15	3.76	127.28	120.18
2	P	147	N87	O5-C4-C2	3.70	115.81	108.52
2	U	147	N87	C25-C13-C7	-3.66	117.53	121.11
2	R	147	N87	C13-C7-C6	-3.65	116.59	123.05
2	K	147	N87	C17-C16-C15	3.64	127.06	120.18
2	J	147	N87	C13-C7-C6	-3.59	116.71	123.05
2	B	147	N87	C12-C4-C2	3.52	118.19	110.70
2	P	147	N87	C13-C7-C6	-3.43	116.98	123.05
2	V	147	N87	C12-C4-C2	3.36	117.85	110.70
2	A	147	N87	O26-C16-C17	-3.31	114.85	120.15
2	R	147	N87	C25-C13-C7	-3.28	117.91	121.11
2	Q	147	N87	C22-C17-C18	3.27	122.73	118.57
2	X	147	N87	C17-C16-C15	3.21	126.23	120.18
2	A	147	N87	C13-C7-C6	-3.18	117.42	123.05
2	H	147	N87	O5-C4-C6	-3.15	102.21	109.10
2	H	147	N87	C13-C7-C6	-3.12	117.53	123.05
2	H	147	N87	O11-C10-C12	3.12	117.22	109.97
2	T	147	N87	C13-C7-C6	-3.10	117.58	123.05
2	H	147	N87	C22-C17-C18	3.03	122.42	118.57
2	T	147	N87	C17-C16-C15	3.02	125.89	120.18
2	T	147	N87	O26-C16-C17	-2.99	115.37	120.15
2	P	147	N87	C22-C17-C18	2.99	122.36	118.57
2	V	147	N87	O11-C10-C12	2.97	116.88	109.97
2	U	147	N87	C12-C4-C2	2.97	117.00	110.70
2	D	147	N87	O9-C8-C10	-2.96	105.36	110.34
2	Q	147	N87	O5-C4-C2	2.92	114.27	108.52
2	W	147	N87	C13-C7-C6	-2.88	117.95	123.05
2	Q	147	N87	C20-C21-C22	-2.87	116.69	120.24
2	V	147	N87	C21-C20-C19	2.82	123.73	119.87
2	D	147	N87	C20-C19-C18	-2.82	116.75	120.24
2	Q	147	N87	C25-C13-C14	2.81	122.50	119.25
2	I	147	N87	C25-C13-C7	-2.79	118.38	121.11
2	H	147	N87	C25-C13-C7	2.79	123.84	121.11
2	D	147	N87	C21-C22-C17	-2.78	117.63	120.36
2	K	147	N87	O26-C16-C15	-2.76	115.73	120.15
2	R	147	N87	C17-C16-C15	2.72	125.31	120.18
2	S	147	N87	C12-C4-C2	2.69	116.43	110.70
2	H	147	N87	C21-C22-C17	-2.69	117.72	120.36
2	I	147	N87	O11-C10-C8	2.68	114.30	109.80
2	M	147	N87	C20-C21-C22	-2.68	116.93	120.24
2	Q	147	N87	C21-C20-C19	2.68	123.53	119.87
2	B	147	N87	C24-C25-C13	-2.63	117.78	120.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Q	147	N87	C19-C18-C17	-2.63	117.78	120.36
2	V	147	N87	C22-C17-C18	2.63	121.91	118.57
2	N	147	N87	C22-C17-C18	2.62	121.90	118.57
2	X	147	N87	O26-C16-C15	-2.60	115.98	120.15
2	H	147	N87	O9-C8-C10	-2.58	105.99	110.34
2	O	147	N87	C17-C16-C15	2.58	125.05	120.18
2	D	147	N87	C19-C18-C17	2.56	122.89	120.36
2	K	147	N87	O9-C8-C10	-2.55	106.04	110.34
2	F	147	N87	C13-C7-C6	-2.52	118.58	123.05
2	N	147	N87	C17-C16-C15	2.51	124.93	120.18
2	P	147	N87	O26-C16-C15	2.46	124.08	120.15
2	W	147	N87	C25-C13-C14	-2.45	116.41	119.25
2	C	147	N87	C12-C4-C2	2.42	115.84	110.70
2	V	147	N87	O11-C10-C8	-2.41	105.77	109.80
2	X	147	N87	O9-C8-C10	-2.41	106.28	110.34
2	P	147	N87	O11-C10-C8	2.40	113.82	109.80
2	A	147	N87	O5-C4-C6	-2.40	103.85	109.10
2	C	147	N87	C25-C13-C7	-2.38	118.78	121.11
2	V	147	N87	C25-C13-C7	2.36	123.42	121.11
2	U	147	N87	C24-C23-C15	2.30	122.62	120.36
2	M	147	N87	C21-C20-C19	2.28	122.99	119.87
2	W	147	N87	C24-C25-C13	2.28	122.60	120.36
2	G	147	N87	O5-C4-C6	-2.25	104.17	109.10
2	Q	147	N87	O5-C4-C6	-2.23	104.22	109.10
2	K	147	N87	C21-C22-C17	-2.23	118.18	120.36
2	T	147	N87	C23-C15-C16	2.22	125.43	120.55
2	D	147	N87	O11-C10-C12	2.20	115.08	109.97
2	P	147	N87	C21-C20-C19	2.20	122.88	119.87
2	K	147	N87	C25-C13-C7	2.19	123.26	121.11
2	N	147	N87	C14-C15-C16	-2.19	115.11	119.98
2	X	147	N87	C15-C14-C13	2.19	122.96	120.43
2	D	147	N87	O26-C16-C15	-2.17	116.68	120.15
2	G	147	N87	C19-C18-C17	-2.16	118.24	120.36
2	K	147	N87	C13-C7-C6	-2.16	119.23	123.05
2	C	147	N87	O5-C4-C2	-2.15	104.28	108.52
2	V	147	N87	C13-C7-C6	-2.15	119.25	123.05
2	D	147	N87	C18-C17-C16	-2.14	115.83	120.55
2	V	147	N87	C20-C19-C18	-2.13	117.62	120.24
2	T	147	N87	C14-C15-C16	-2.11	115.30	119.98
2	E	147	N87	O26-C16-C17	2.11	123.51	120.15
2	P	147	N87	O5-C4-C6	-2.08	104.55	109.10
2	M	147	N87	C12-C4-C2	2.08	115.11	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	147	N87	O26-C16-C15	-2.06	116.85	120.15
2	U	147	N87	C25-C24-C23	-2.06	117.60	120.24
2	R	147	N87	O26-C16-C17	-2.03	116.90	120.15
2	P	147	N87	C19-C18-C17	-2.01	118.39	120.36
2	N	147	N87	C24-C23-C15	-2.01	118.39	120.36

There are no chirality outliers.

All (59) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	147	N87	O1-C2-C4-C6
2	E	147	N87	O3-C2-C4-O5
2	K	147	N87	O1-C2-C4-C12
2	N	147	N87	O1-C2-C4-C6
2	P	147	N87	O1-C2-C4-C6
2	R	147	N87	O1-C2-C4-C6
2	S	147	N87	O3-C2-C4-O5
2	T	147	N87	O1-C2-C4-C6
2	W	147	N87	O1-C2-C4-C6
2	E	147	N87	O26-C16-C17-C18
2	E	147	N87	C15-C16-C17-C18
2	E	147	N87	O26-C16-C17-C22
2	E	147	N87	C15-C16-C17-C22
2	S	147	N87	O1-C2-C4-C6
2	A	147	N87	O1-C2-C4-O5
2	E	147	N87	O3-C2-C4-C12
2	G	147	N87	O1-C2-C4-O5
2	H	147	N87	O1-C2-C4-O5
2	N	147	N87	O1-C2-C4-O5
2	O	147	N87	O1-C2-C4-O5
2	P	147	N87	O1-C2-C4-O5
2	R	147	N87	O1-C2-C4-O5
2	S	147	N87	O1-C2-C4-O5
2	T	147	N87	O1-C2-C4-O5
2	W	147	N87	O1-C2-C4-O5
2	B	147	N87	C14-C13-C7-C8
2	A	147	N87	O3-C2-C4-O5
2	B	147	N87	O3-C2-C4-O5
2	C	147	N87	O3-C2-C4-O5
2	F	147	N87	O3-C2-C4-O5
2	G	147	N87	O3-C2-C4-O5
2	H	147	N87	O3-C2-C4-O5

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Mol	Chain	Res	Type	Atoms
2	I	147	N87	O3-C2-C4-O5
2	J	147	N87	O3-C2-C4-O5
2	K	147	N87	O3-C2-C4-O5
2	L	147	N87	O3-C2-C4-O5
2	M	147	N87	O3-C2-C4-O5
2	N	147	N87	O3-C2-C4-O5
2	O	147	N87	O3-C2-C4-O5
2	P	147	N87	O3-C2-C4-O5
2	Q	147	N87	O3-C2-C4-O5
2	R	147	N87	O3-C2-C4-O5
2	T	147	N87	O3-C2-C4-O5
2	U	147	N87	O3-C2-C4-O5
2	V	147	N87	O3-C2-C4-O5
2	W	147	N87	O3-C2-C4-O5
2	X	147	N87	O3-C2-C4-O5
2	B	147	N87	O3-C2-C4-C6
2	I	147	N87	O3-C2-C4-C6
2	Q	147	N87	C14-C15-C16-C17
2	G	147	N87	C14-C13-C7-C6
2	D	147	N87	O1-C2-C4-O5
2	E	147	N87	O1-C2-C4-O5
2	E	147	N87	O1-C2-C4-C12
2	F	147	N87	O1-C2-C4-O5
2	J	147	N87	O1-C2-C4-O5
2	K	147	N87	O3-C2-C4-C12
2	L	147	N87	O1-C2-C4-O5
2	V	147	N87	O1-C2-C4-O5

There are no ring outliers.

19 monomers are involved in 66 short contacts:

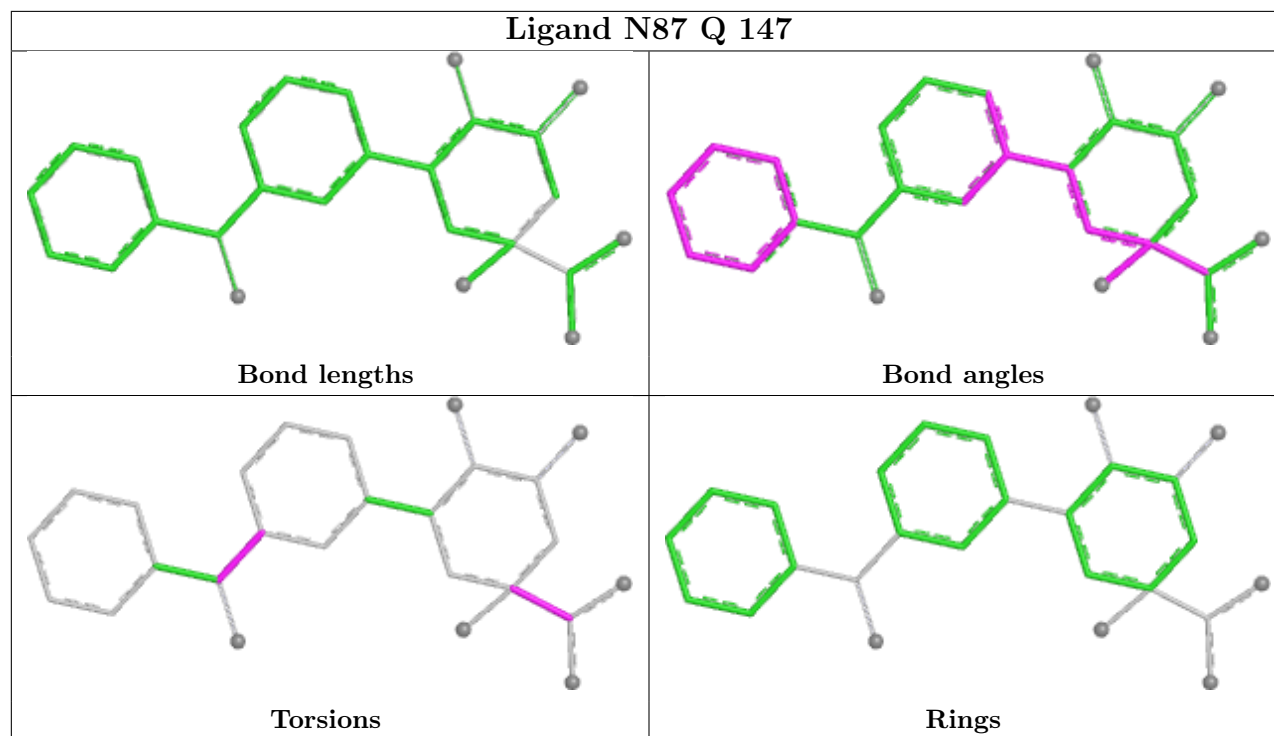
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	Q	147	N87	3	0
2	N	147	N87	2	0
2	V	147	N87	4	0
2	R	147	N87	3	0
2	B	147	N87	1	0
2	M	147	N87	6	0
2	S	147	N87	5	0
2	U	147	N87	5	0
2	L	147	N87	8	0
2	I	147	N87	5	0

Continued on next page...

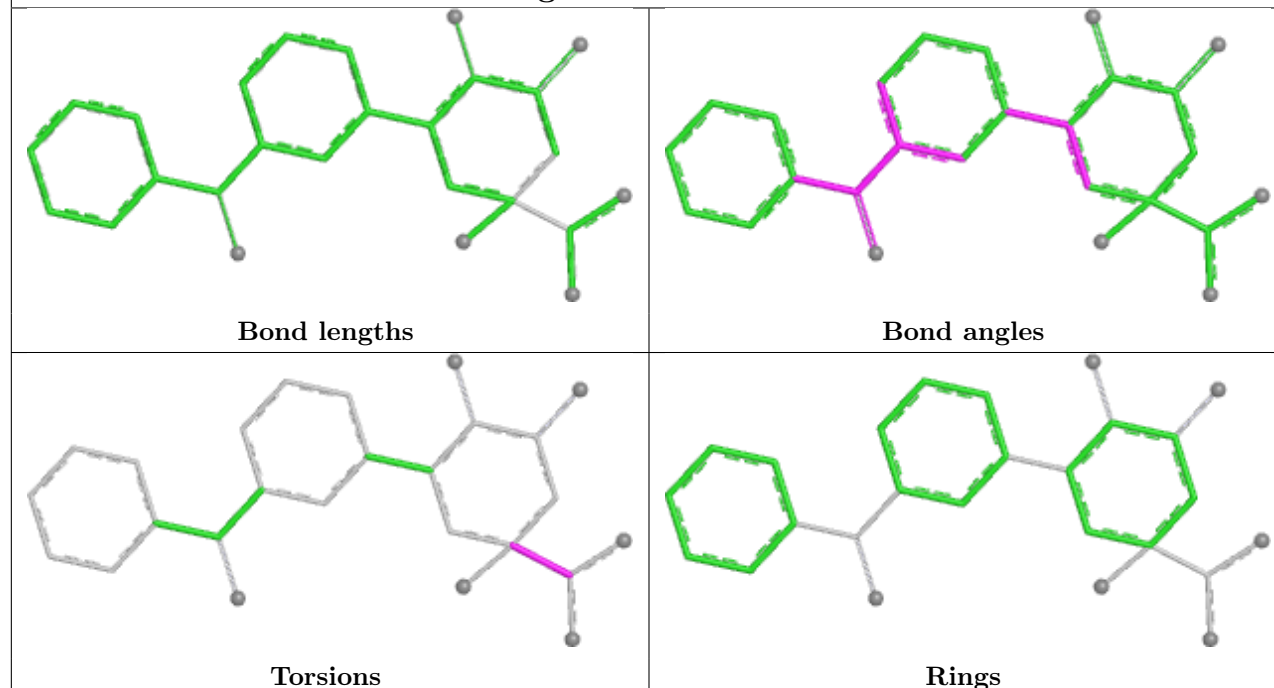
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	W	147	N87	2	0
2	G	147	N87	7	0
2	K	147	N87	1	0
2	F	147	N87	1	0
2	A	147	N87	1	0
2	C	147	N87	4	0
2	J	147	N87	2	0
2	E	147	N87	3	0
2	O	147	N87	3	0

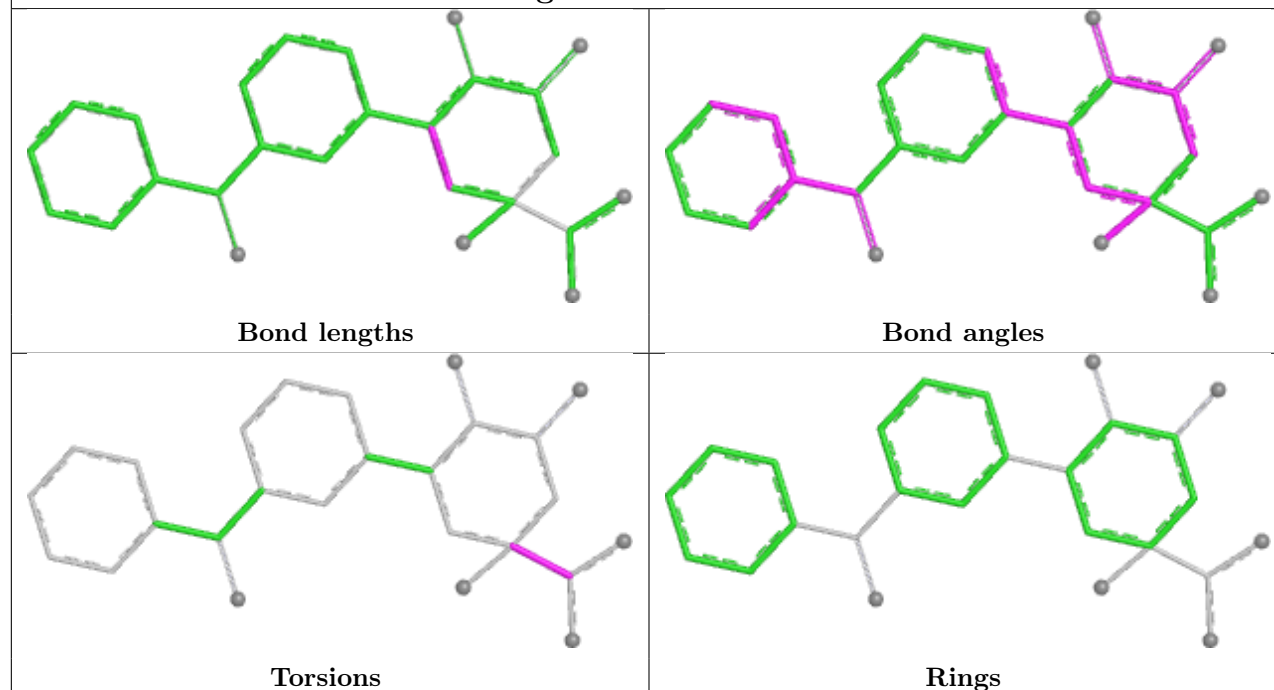
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



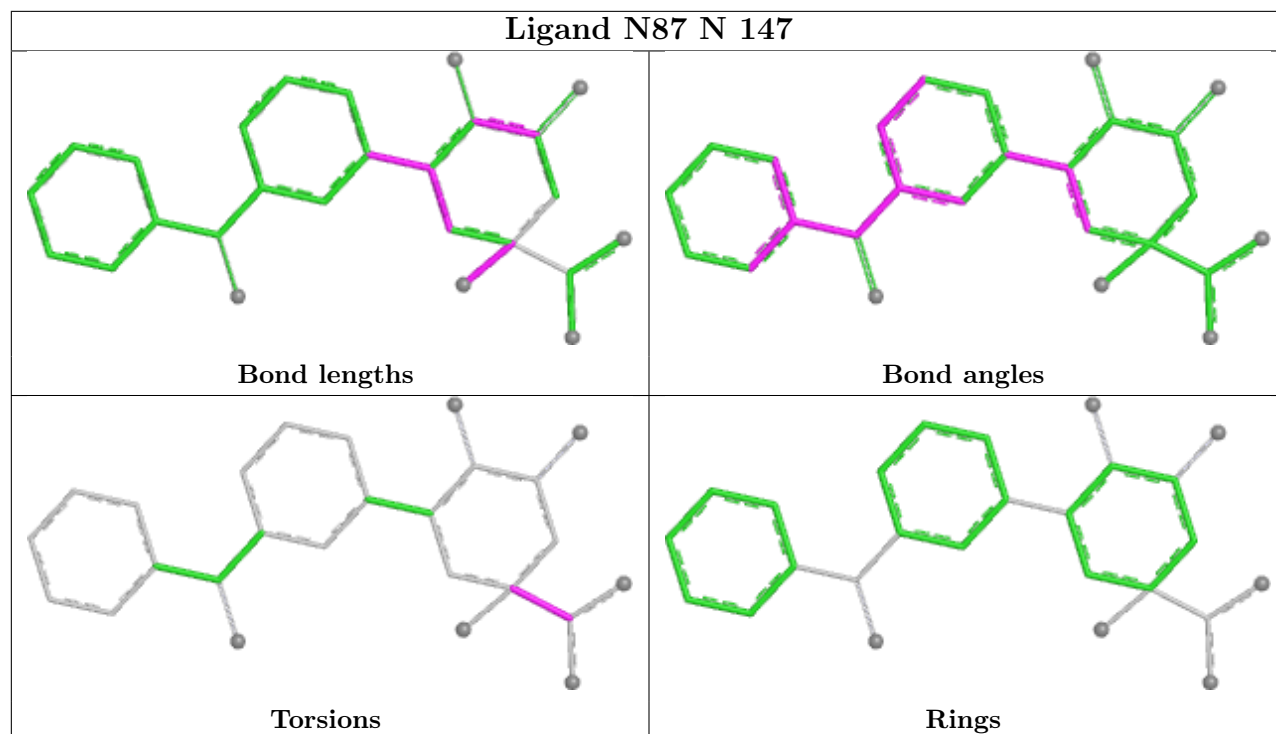
Ligand N87 T 147



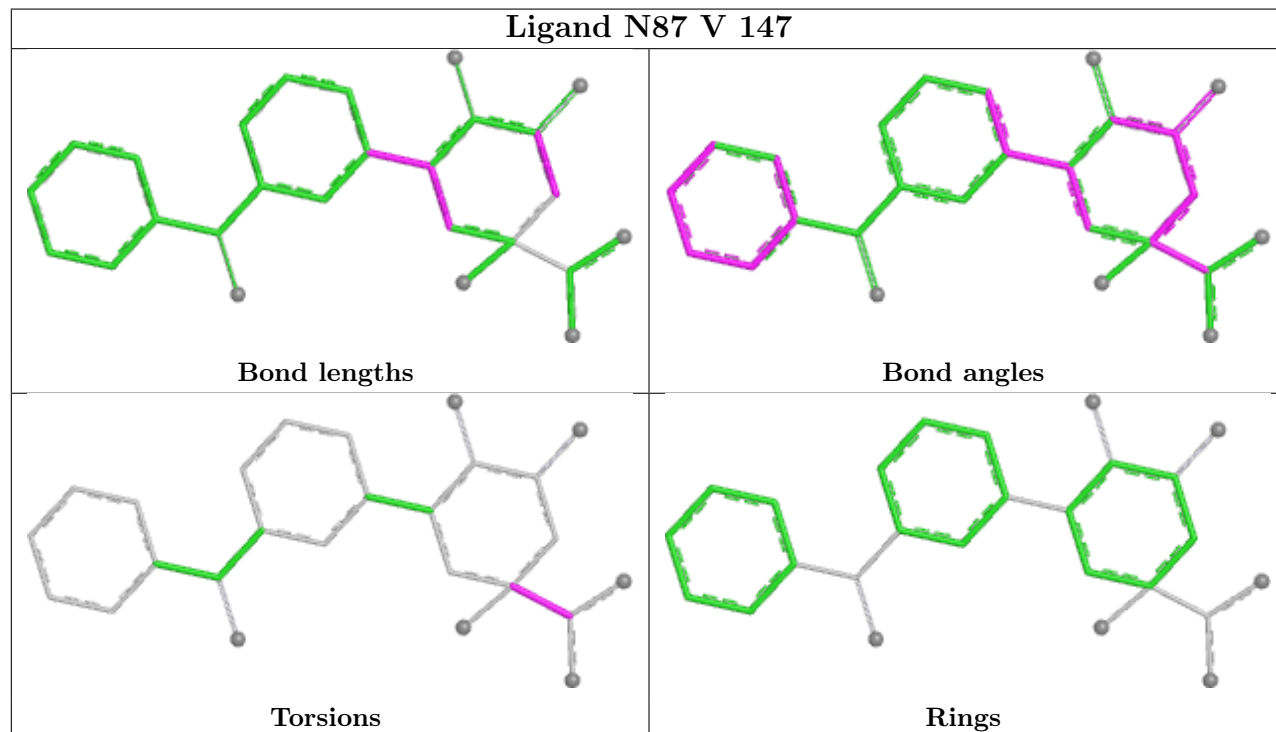
Ligand N87 H 147



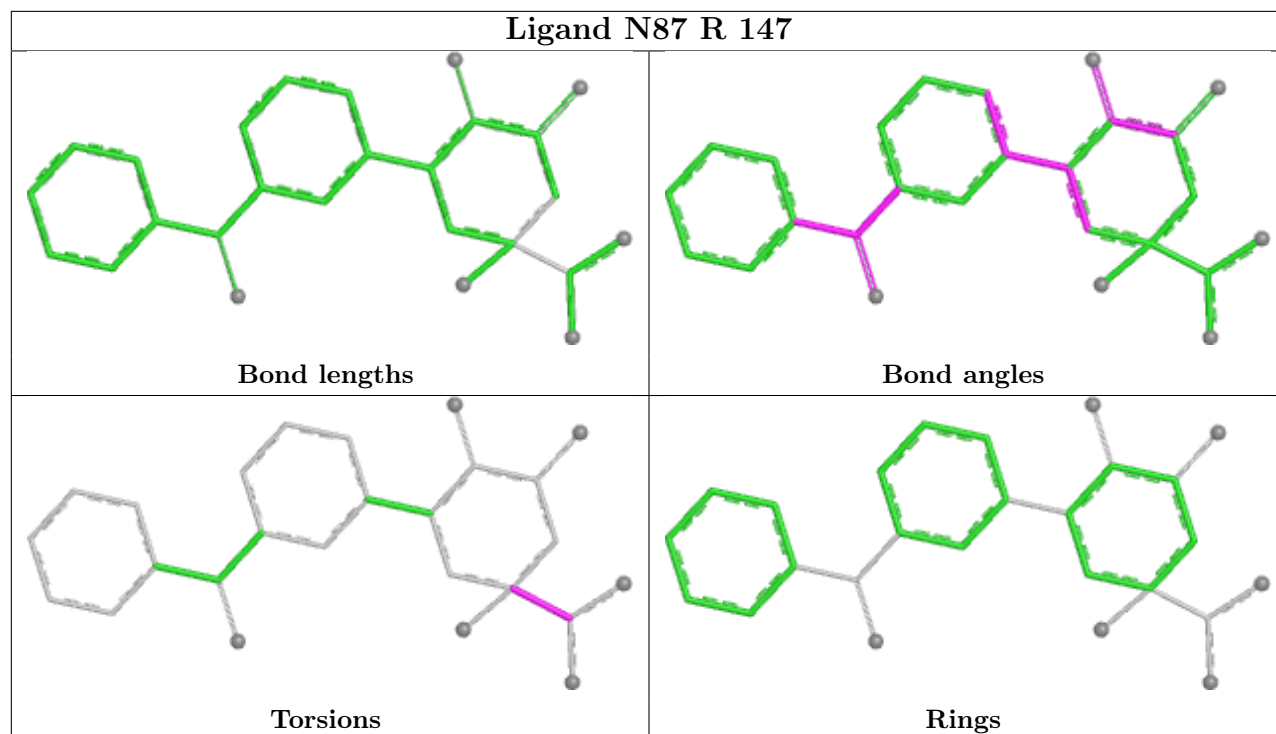
Ligand N87 N 147



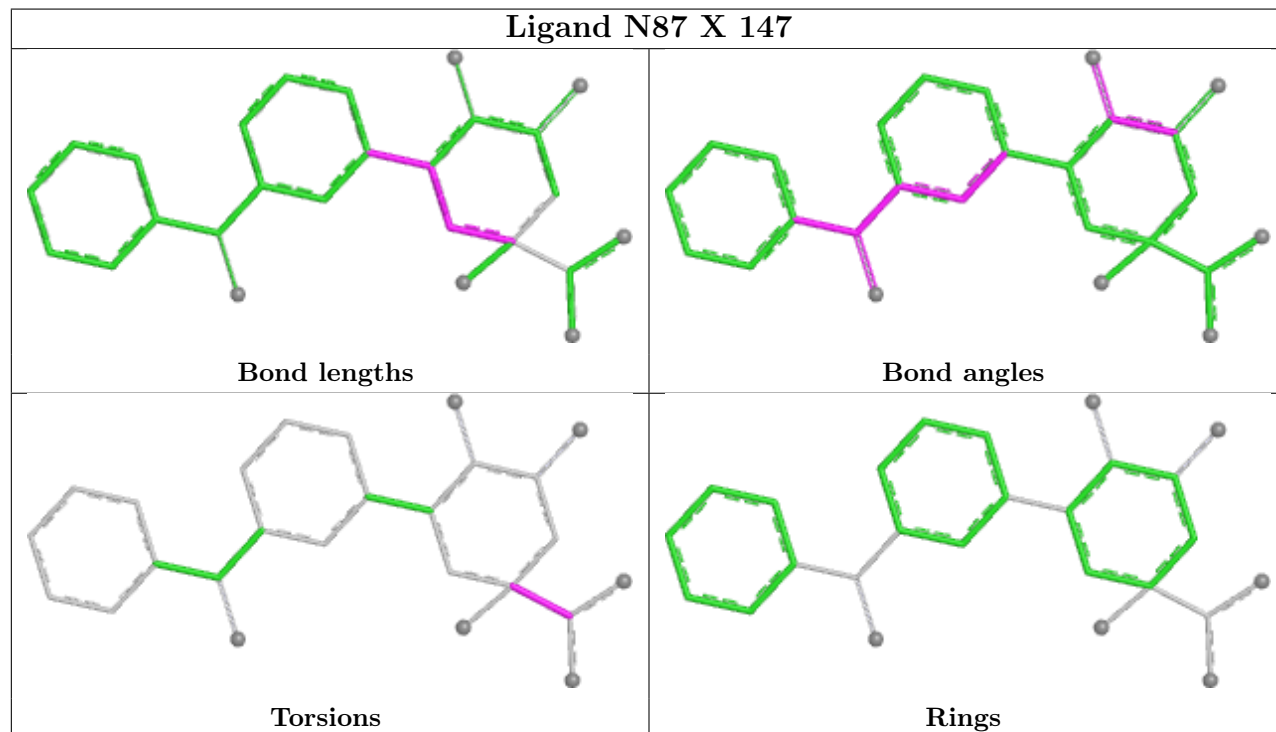
Ligand N87 V 147



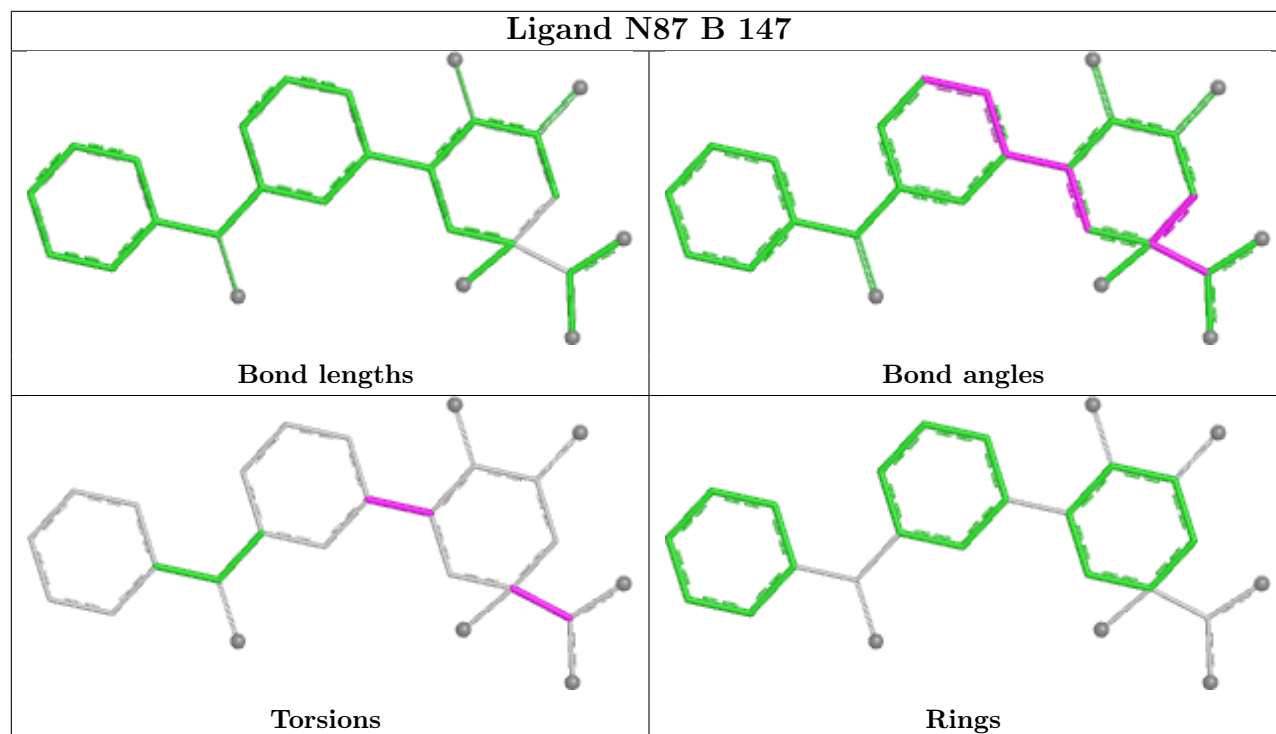
Ligand N87 R 147



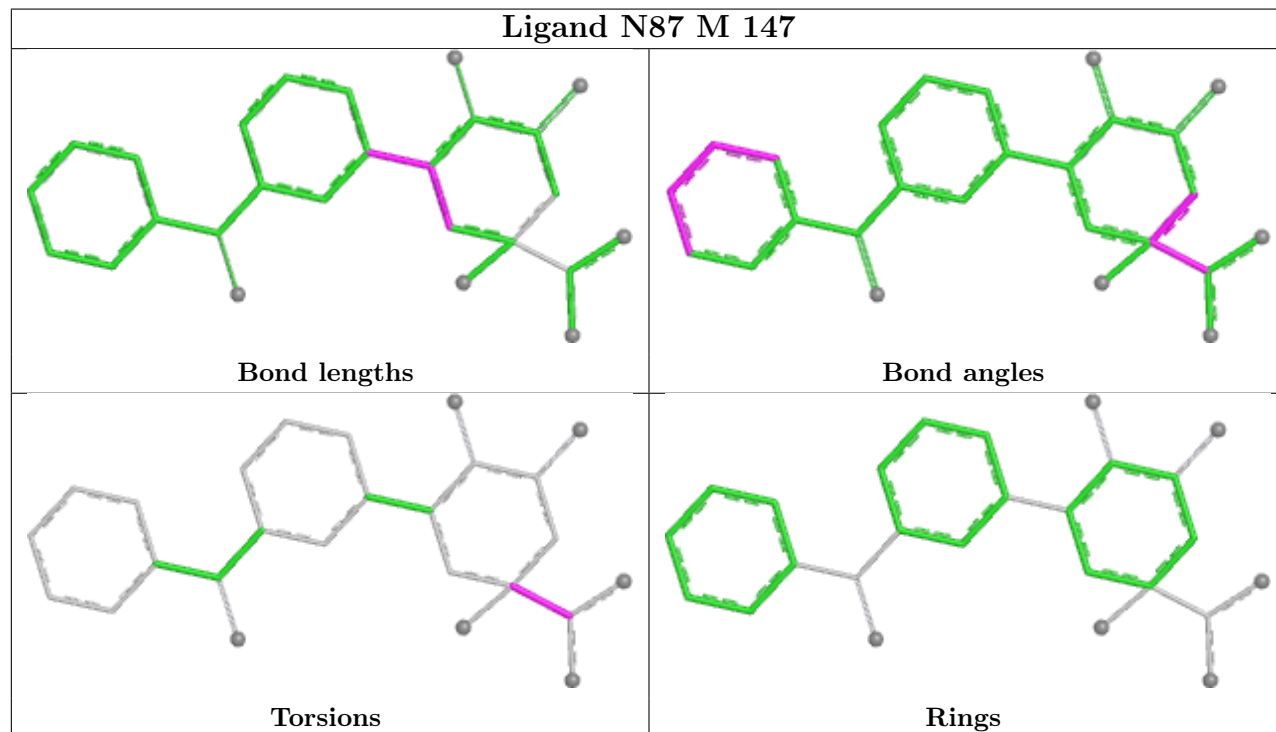
Ligand N87 X 147



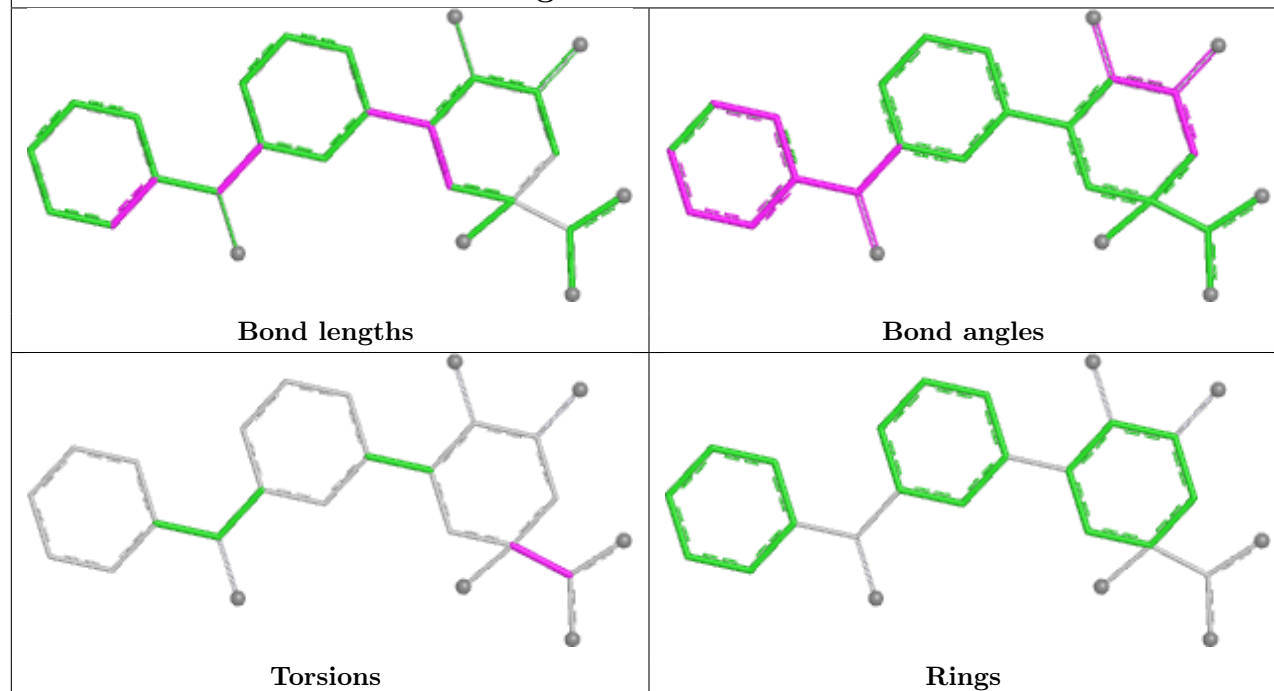
Ligand N87 B 147



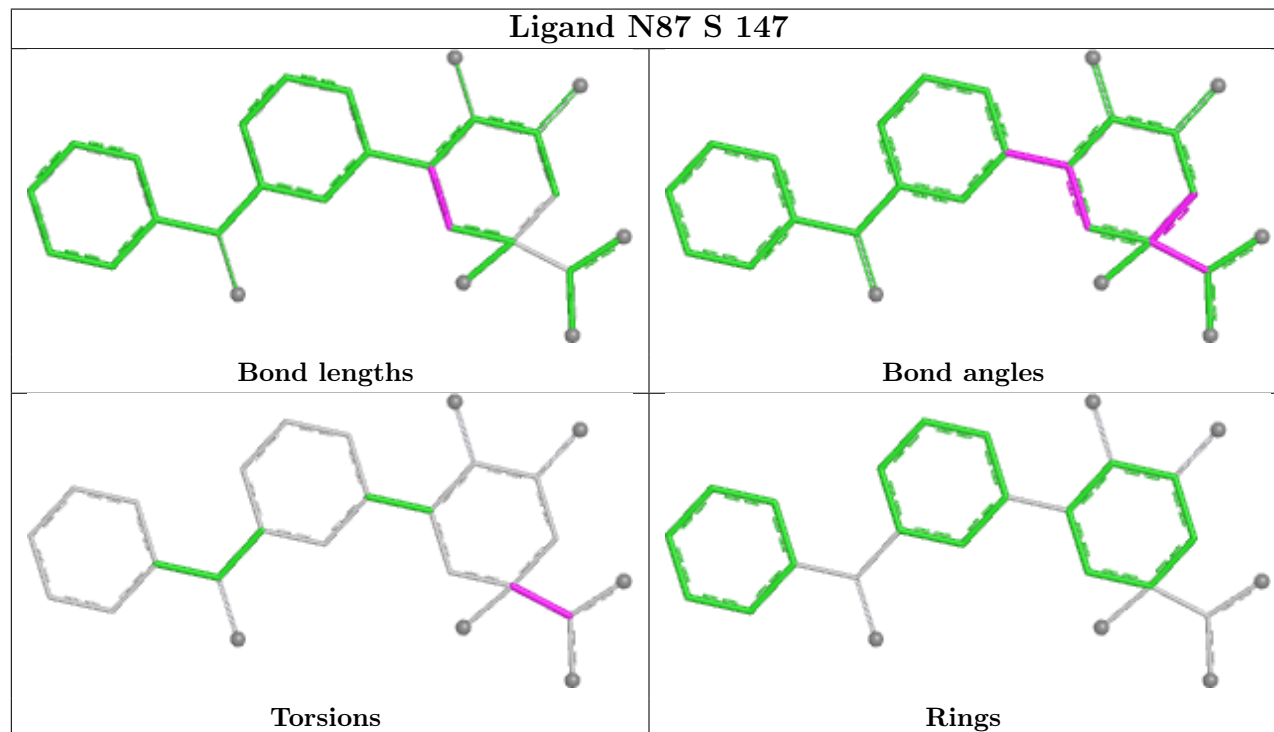
Ligand N87 M 147



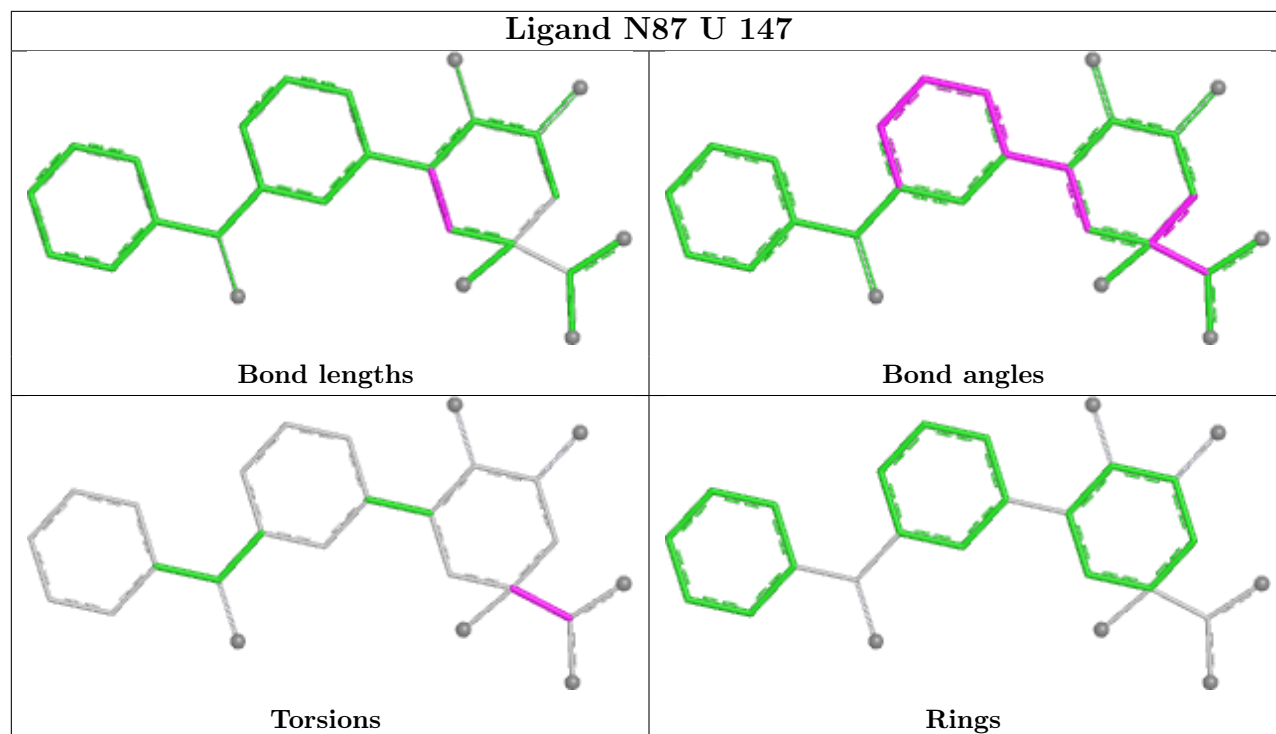
Ligand N87 D 147



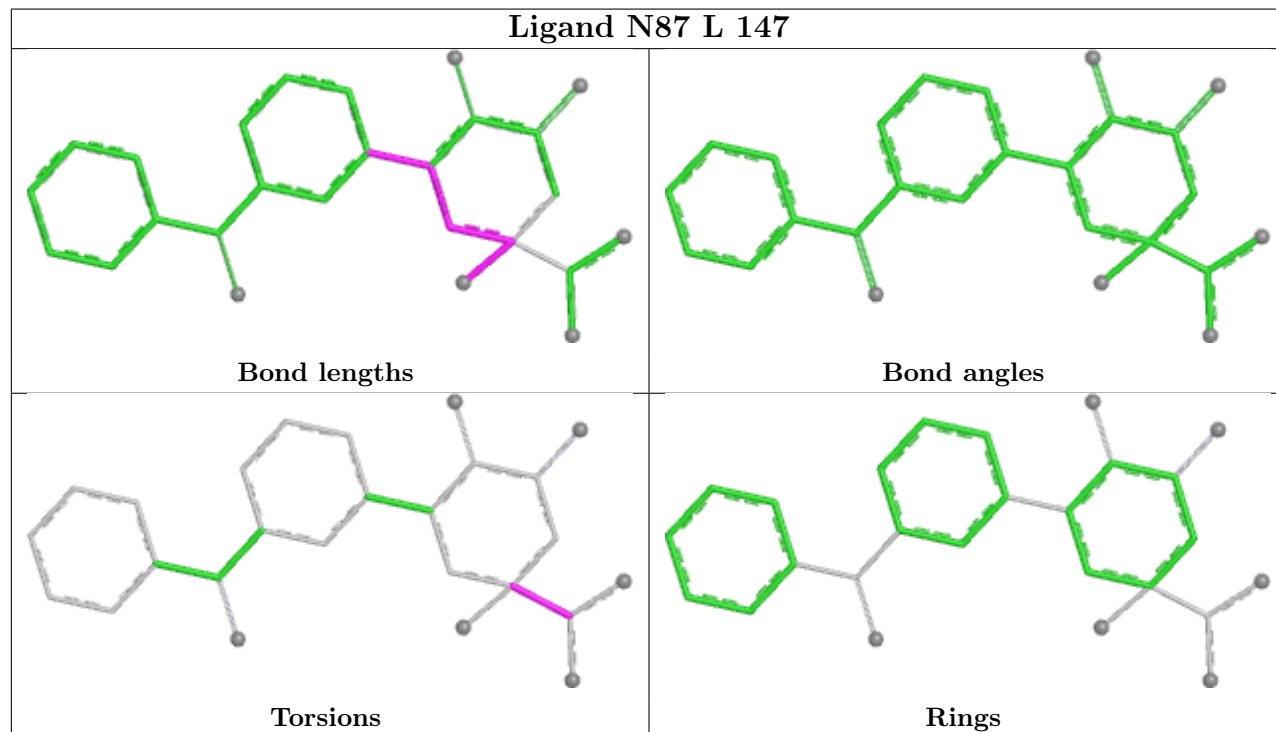
Ligand N87 S 147



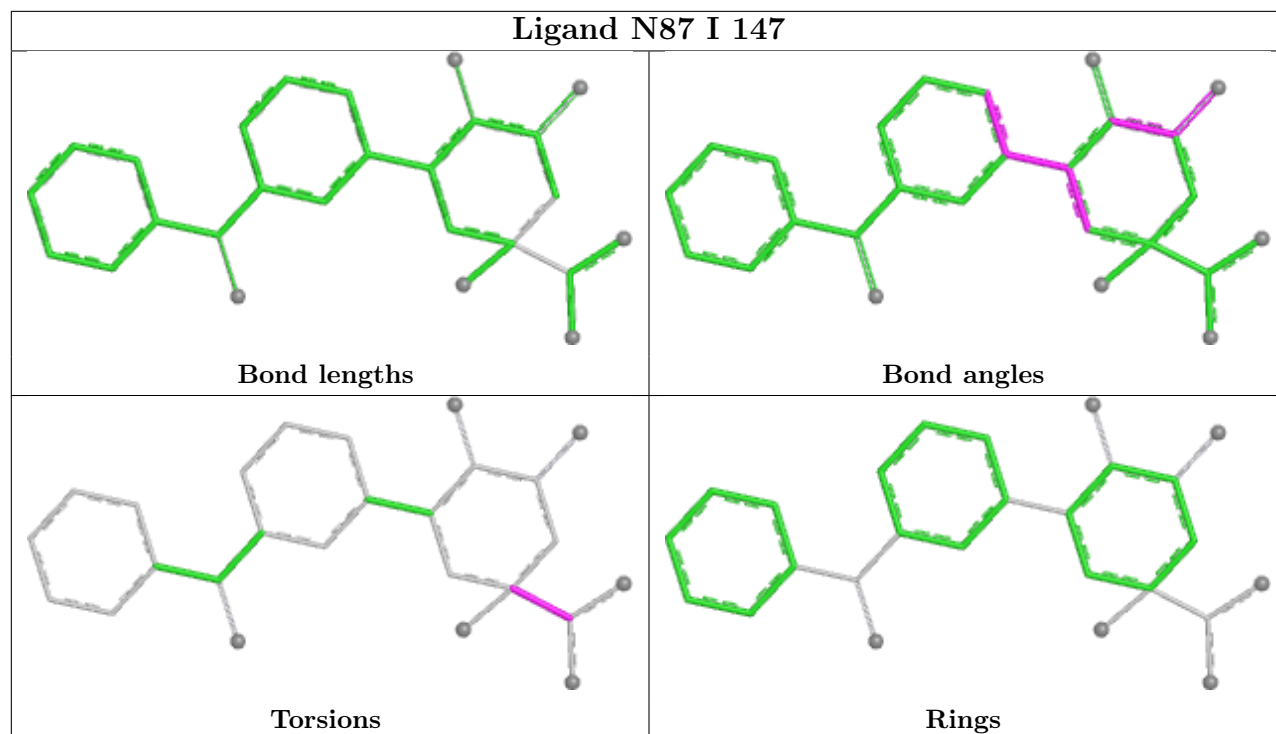
Ligand N87 U 147



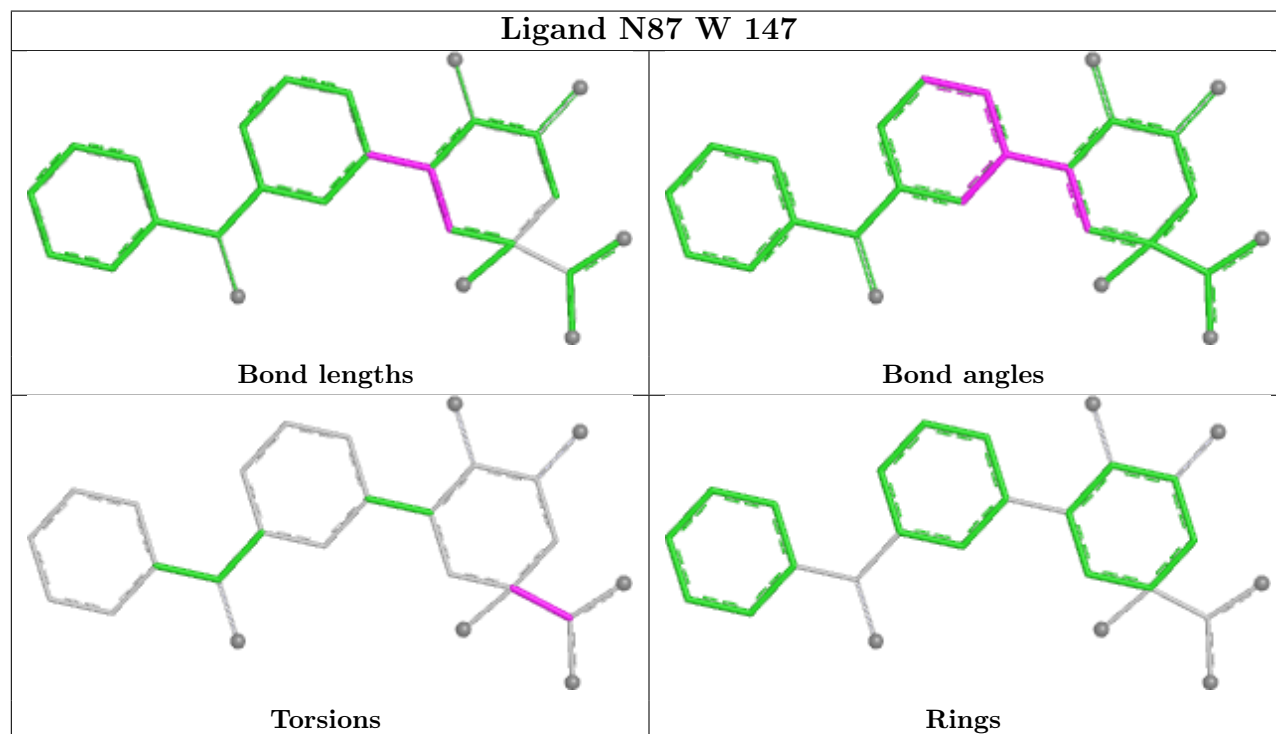
Ligand N87 L 147



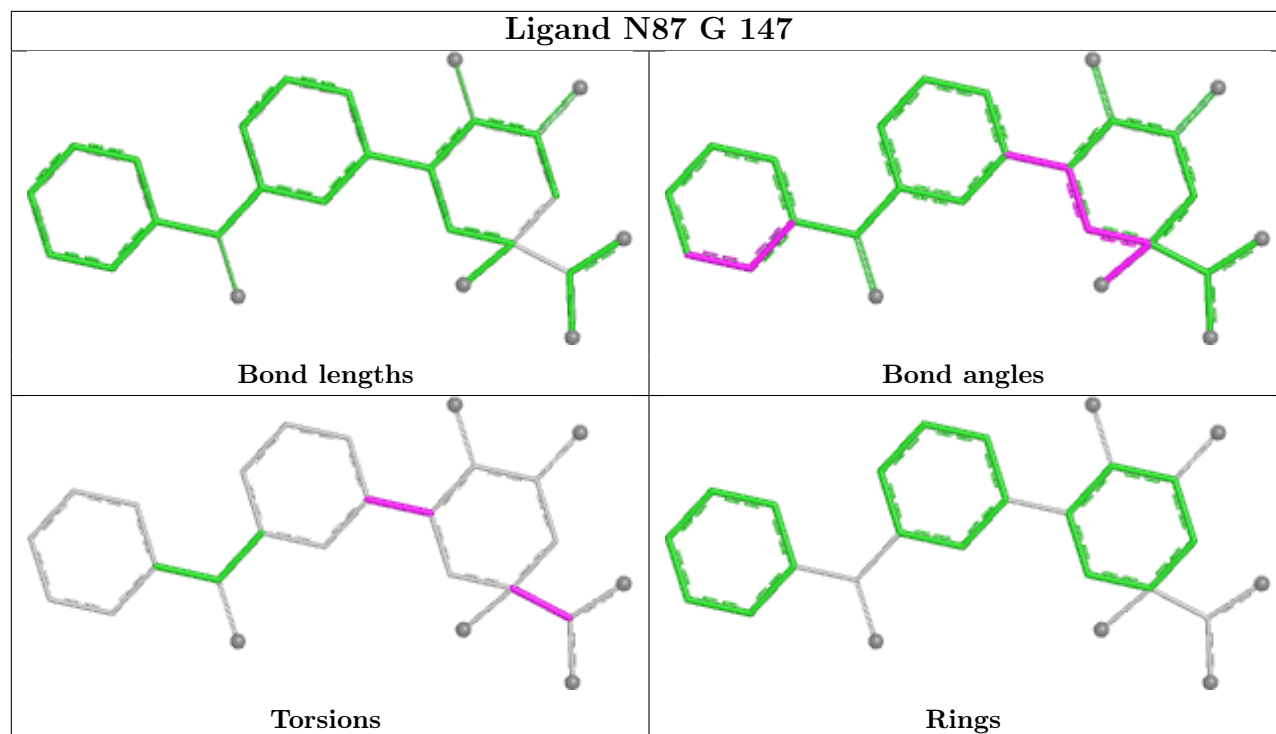
Ligand N87 I 147



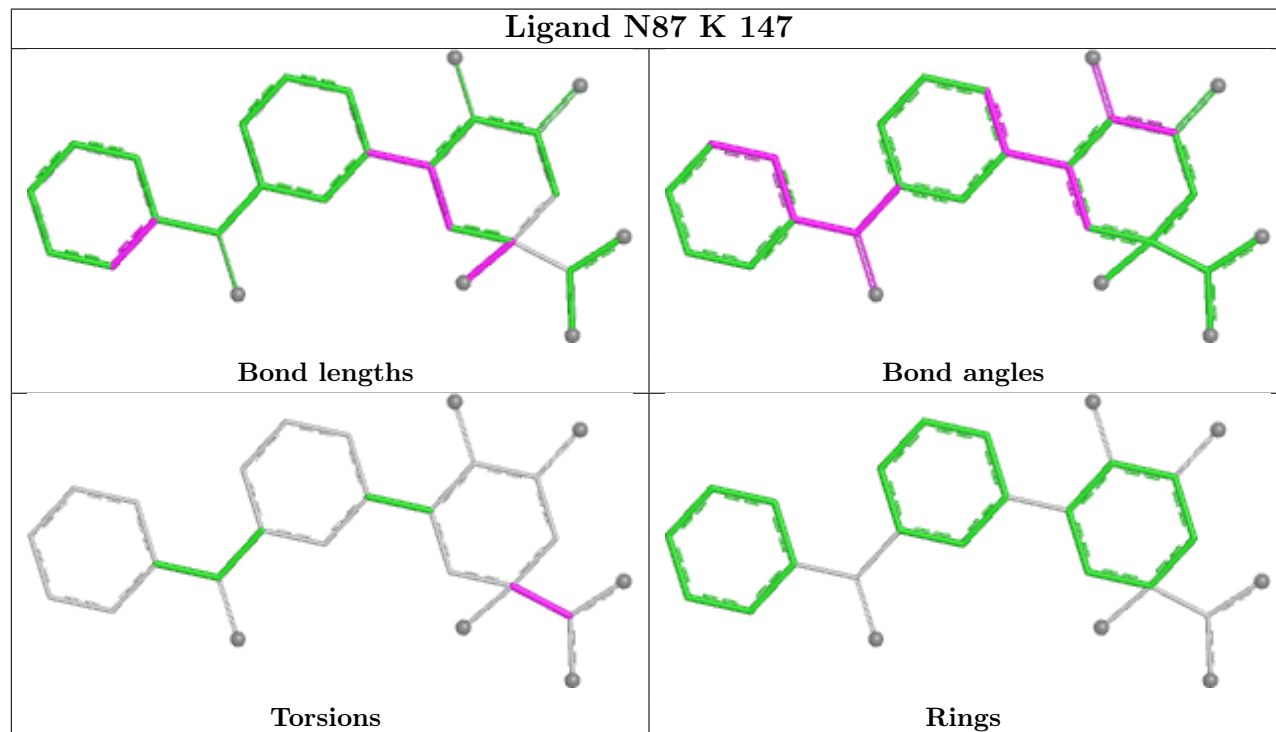
Ligand N87 W 147



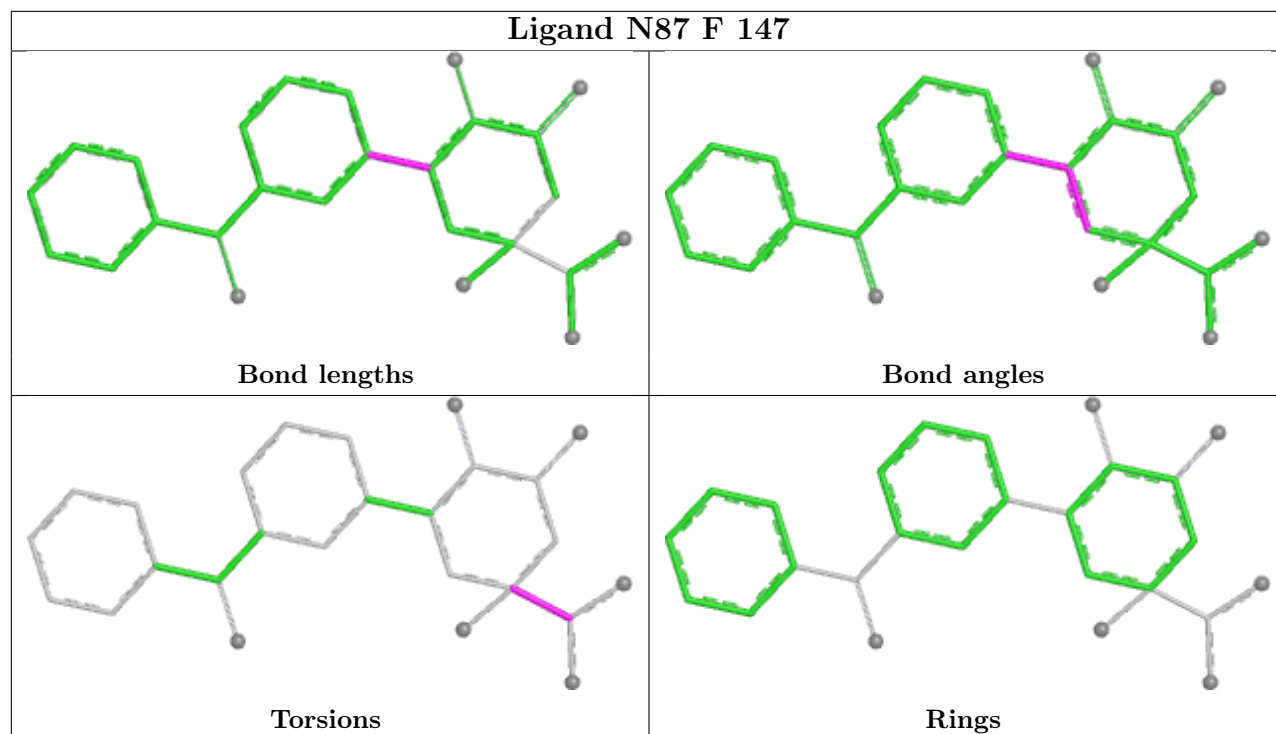
Ligand N87 G 147



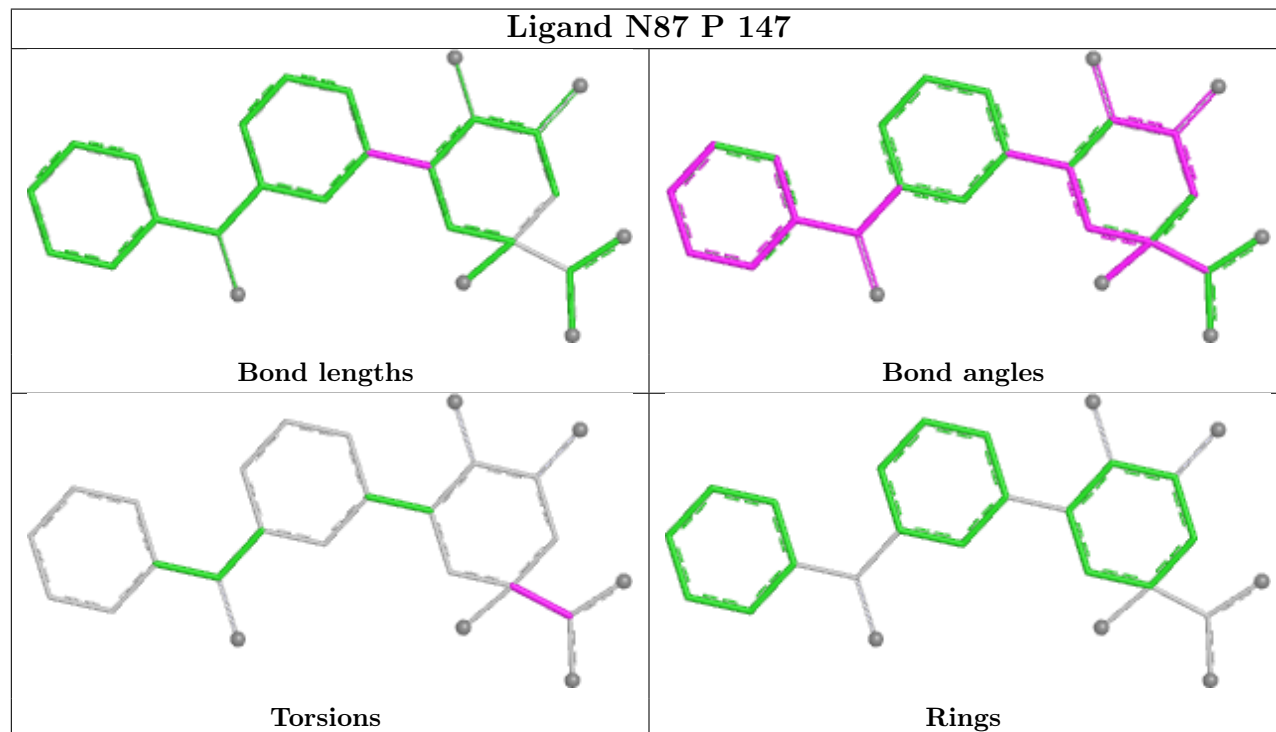
Ligand N87 K 147



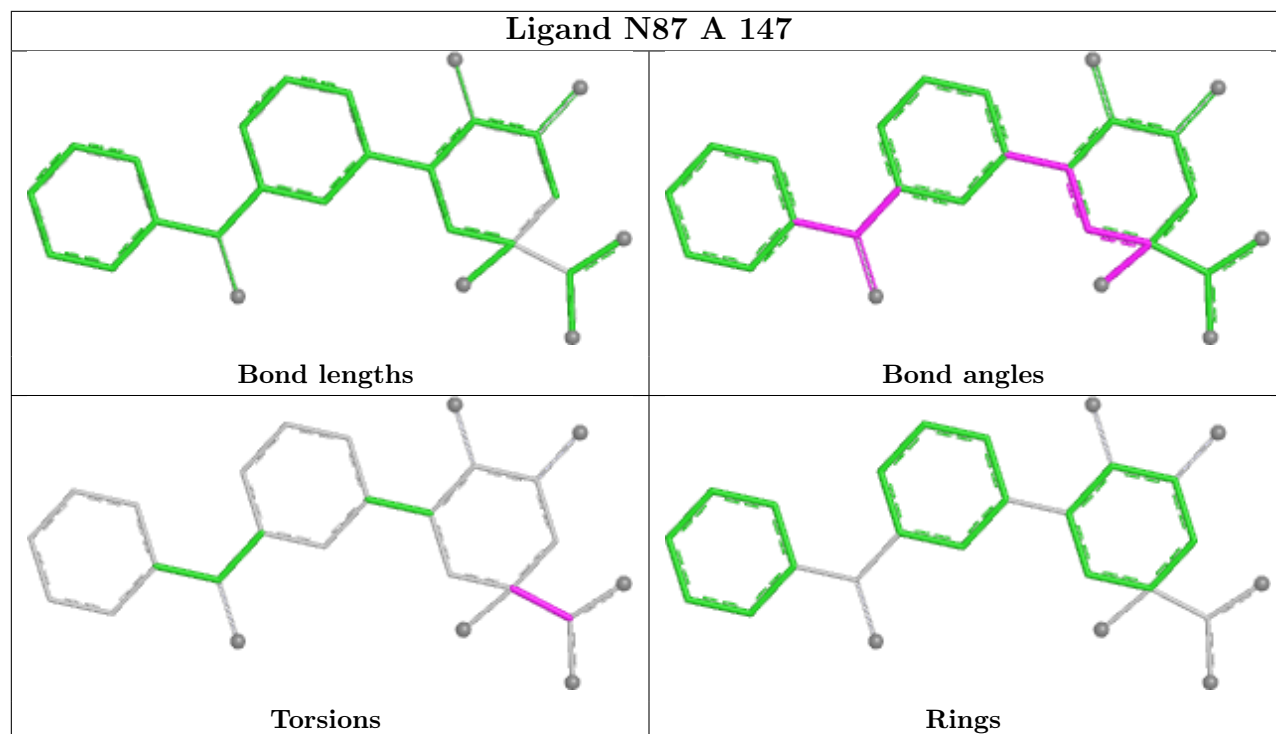
Ligand N87 F 147



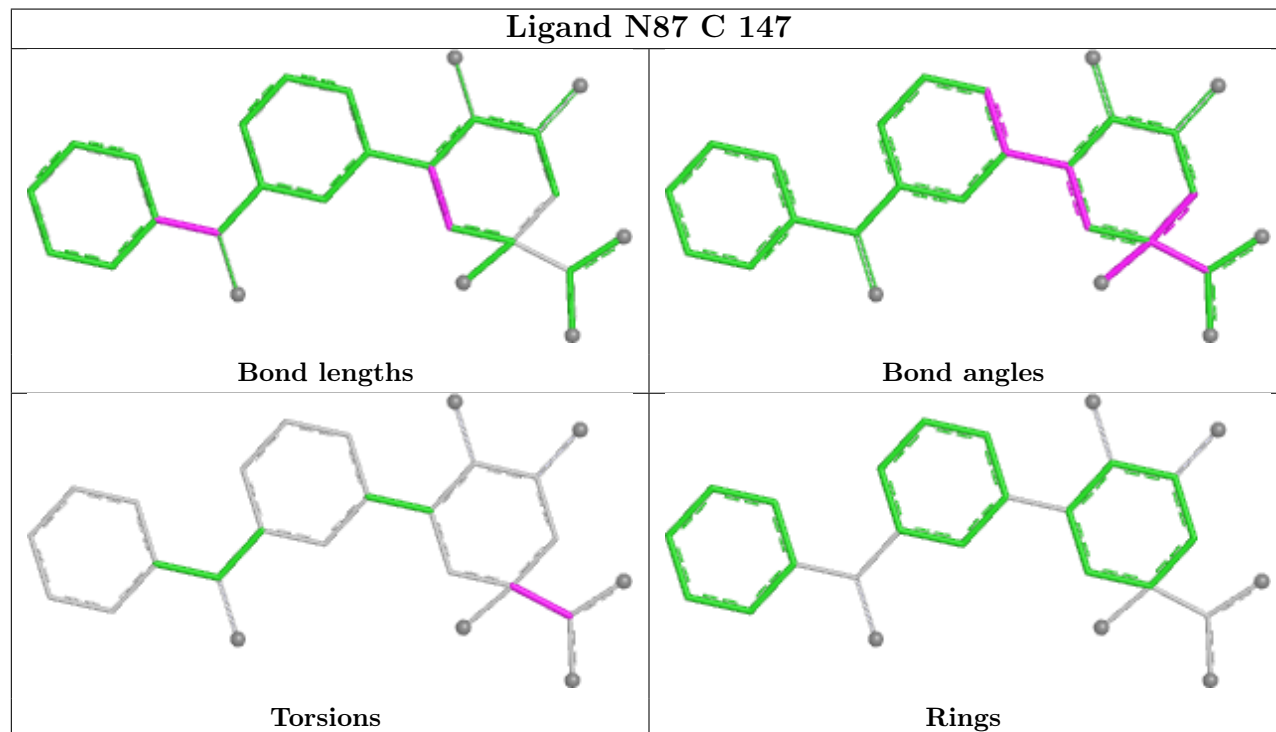
Ligand N87 P 147



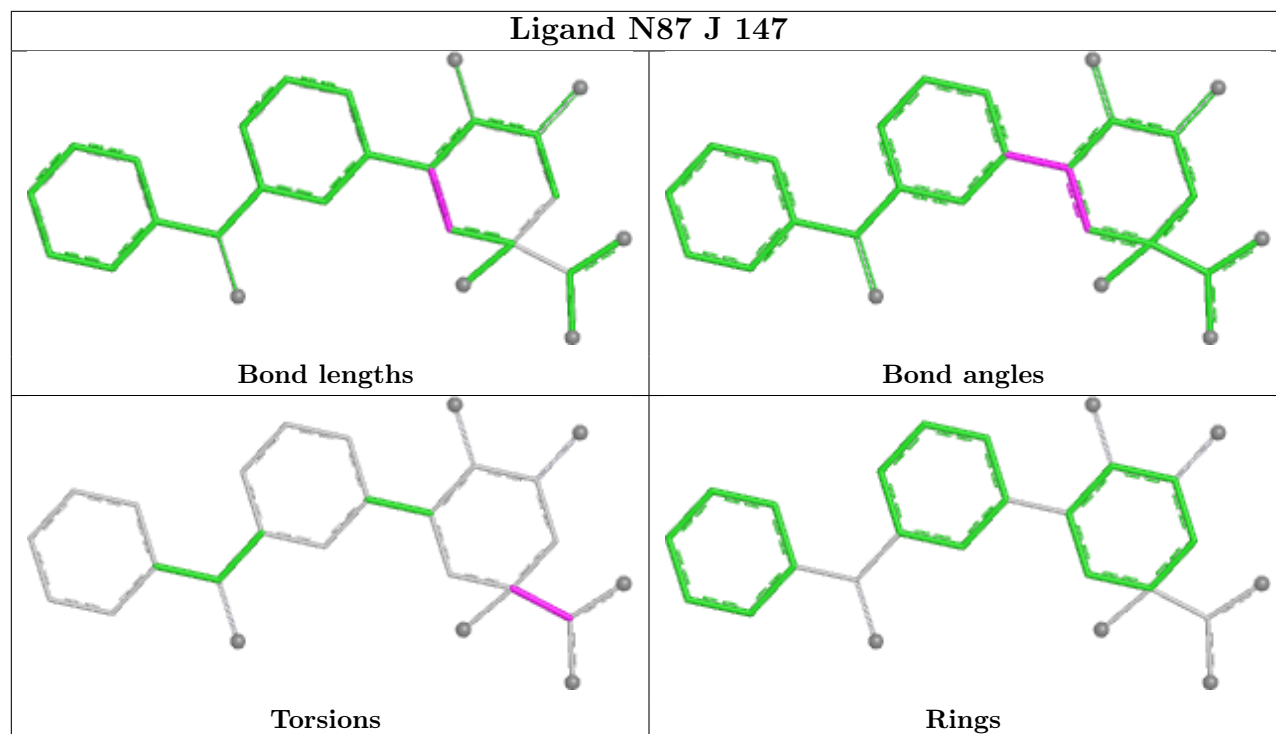
Ligand N87 A 147



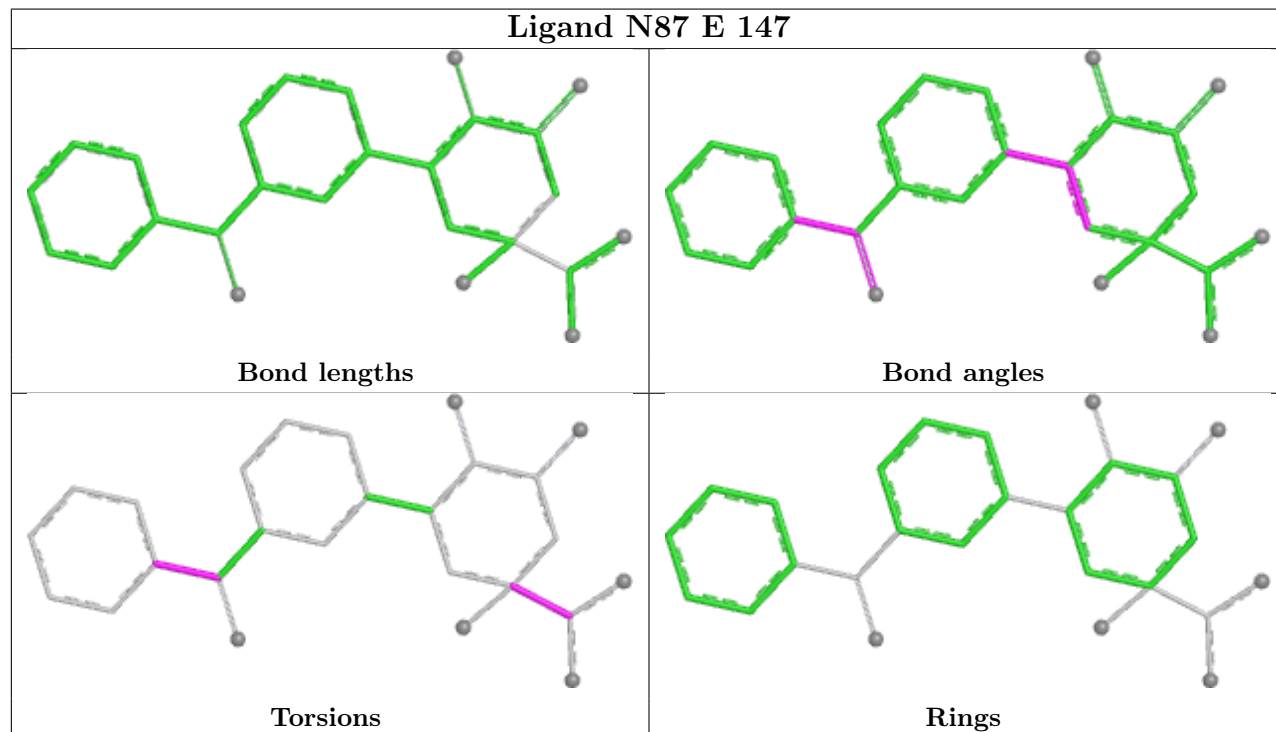
Ligand N87 C 147

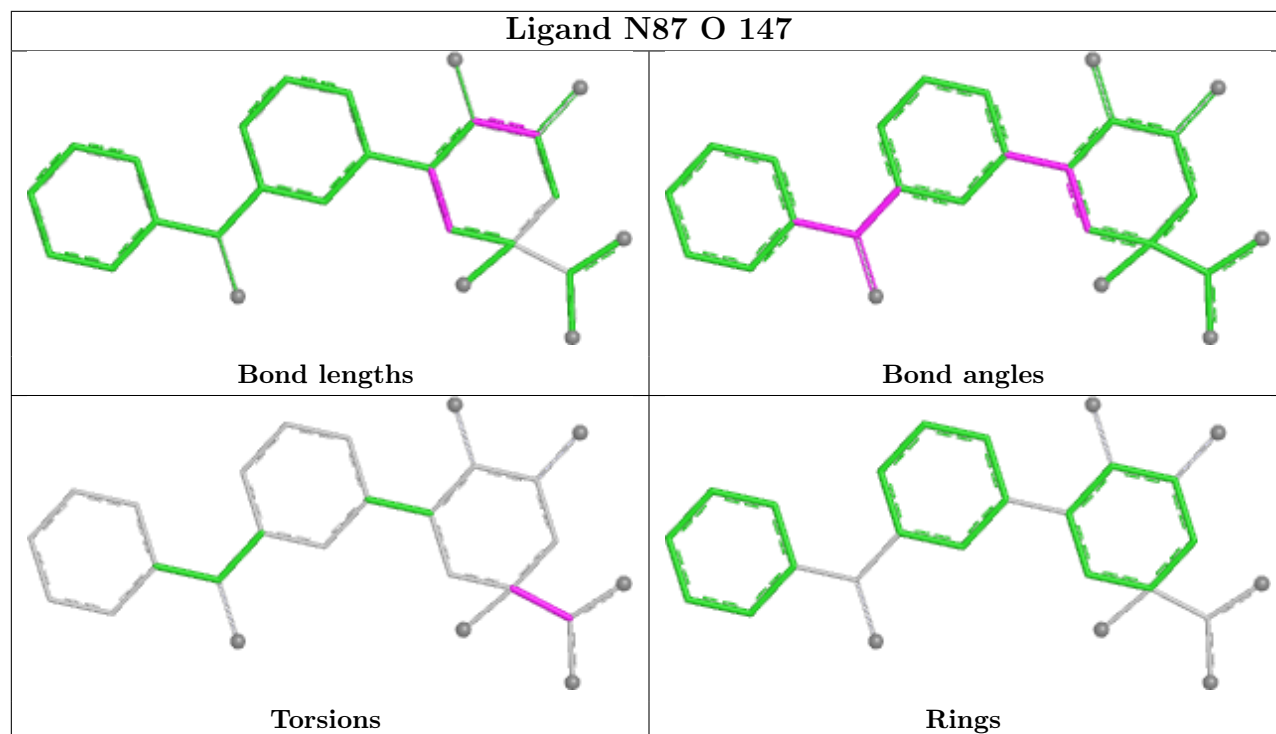


Ligand N87 J 147



Ligand N87 E 147





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	141/147 (95%)	-0.17	2 (1%) 73 69	24, 36, 56, 68	2 (1%)
1	B	141/147 (95%)	-0.57	0 100 100	13, 26, 41, 50	1 (0%)
1	C	141/147 (95%)	-0.36	4 (2%) 55 51	18, 30, 53, 62	0
1	D	141/147 (95%)	-0.16	3 (2%) 63 59	20, 35, 54, 65	0
1	E	141/147 (95%)	-0.26	3 (2%) 63 59	19, 31, 53, 64	0
1	F	141/147 (95%)	-0.34	1 (0%) 84 81	20, 30, 55, 63	1 (0%)
1	G	141/147 (95%)	-0.43	0 100 100	17, 28, 46, 62	1 (0%)
1	H	141/147 (95%)	-0.45	0 100 100	13, 30, 45, 53	0
1	I	141/147 (95%)	-0.22	1 (0%) 84 81	21, 33, 57, 68	0
1	J	141/147 (95%)	-0.45	1 (0%) 84 81	17, 27, 49, 63	0
1	K	141/147 (95%)	-0.26	2 (1%) 73 69	13, 34, 55, 61	0
1	L	141/147 (95%)	-0.34	1 (0%) 84 81	20, 35, 50, 58	0
1	M	141/147 (95%)	-0.36	1 (0%) 84 81	22, 32, 52, 58	0
1	N	141/147 (95%)	-0.20	2 (1%) 73 69	21, 35, 54, 63	1 (0%)
1	O	141/147 (95%)	-0.42	1 (0%) 84 81	20, 30, 54, 67	0
1	P	141/147 (95%)	-0.58	0 100 100	9, 27, 42, 56	0
1	Q	141/147 (95%)	-0.30	2 (1%) 73 69	20, 30, 49, 60	0
1	R	141/147 (95%)	-0.24	2 (1%) 73 69	21, 31, 54, 62	0
1	S	141/147 (95%)	-0.47	2 (1%) 73 69	13, 26, 45, 59	2 (1%)
1	T	141/147 (95%)	-0.53	0 100 100	17, 27, 42, 54	1 (0%)
1	U	141/147 (95%)	-0.42	2 (1%) 73 69	17, 29, 51, 59	1 (0%)
1	V	141/147 (95%)	-0.35	0 100 100	20, 29, 51, 63	1 (0%)
1	W	141/147 (95%)	-0.18	1 (0%) 84 81	20, 36, 56, 62	1 (0%)
1	X	141/147 (95%)	-0.32	2 (1%) 73 69	22, 33, 54, 64	1 (0%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	3384/3528 (95%)	-0.35	33 (0%) 79 76	9, 31, 54, 68	13 (0%)

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	W	23	VAL	5.7
1	E	22	ALA	4.8
1	R	22	ALA	4.0
1	C	21	PRO	4.0
1	U	23	VAL	3.6
1	Q	23	VAL	3.3
1	D	23	VAL	3.1
1	K	3	LEU	2.9
1	F	23	VAL	2.9
1	E	21	PRO	2.8
1	K	25	GLY	2.7
1	D	21	PRO	2.6
1	C	3	LEU	2.6
1	L	3	LEU	2.5
1	J	19	ARG	2.5
1	X	20	GLU	2.5
1	M	64	GLN	2.4
1	I	41	ALA	2.4
1	N	22	ALA	2.2
1	N	3	LEU	2.1
1	S	17	GLY	2.1
1	U	3	LEU	2.1
1	C	17	GLY	2.1
1	C	20	GLU	2.1
1	O	143	HIS	2.1
1	A	22	ALA	2.1
1	R	143	HIS	2.1
1	X	143	HIS	2.1
1	Q	22	ALA	2.0
1	A	25	GLY	2.0
1	D	4	ILE	2.0
1	E	23	VAL	2.0
1	S	22	ALA	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

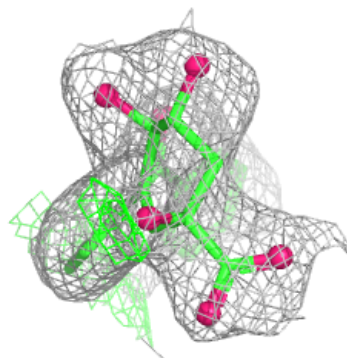
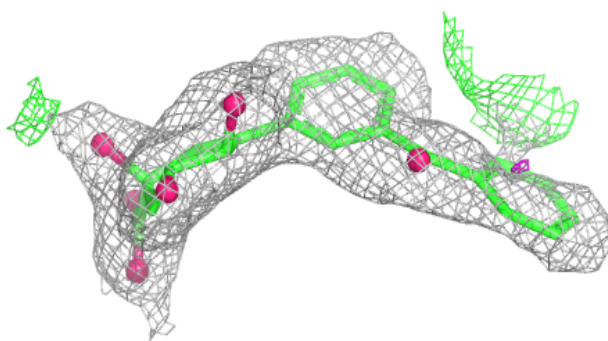
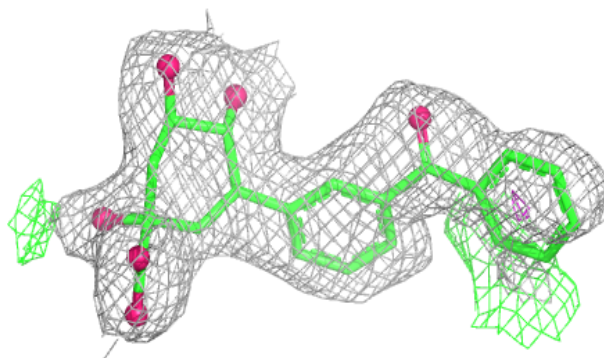
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	N87	K	147	26/26	0.90	0.10	29,42,56,57	0
2	N87	D	147	26/26	0.91	0.10	27,38,55,57	0
2	N87	I	147	26/26	0.91	0.11	35,46,66,68	0
2	N87	C	147	26/26	0.91	0.10	26,40,58,59	0
2	N87	O	147	26/26	0.91	0.10	40,46,54,55	0
2	N87	Q	147	26/26	0.91	0.10	34,40,49,51	0
2	N87	R	147	26/26	0.91	0.11	35,45,63,64	0
2	N87	X	147	26/26	0.91	0.11	39,51,58,59	0
2	N87	M	147	26/26	0.92	0.11	31,44,59,60	0
2	N87	N	147	26/26	0.92	0.10	26,38,55,57	0
2	N87	A	147	26/26	0.92	0.09	36,43,59,59	0
2	N87	W	147	26/26	0.93	0.10	31,42,59,60	0
2	N87	V	147	26/26	0.93	0.10	27,43,55,57	0
2	N87	U	147	26/26	0.94	0.08	24,38,57,59	0
2	N87	F	147	26/26	0.94	0.08	36,42,55,55	0
2	N87	E	147	26/26	0.94	0.10	33,41,60,61	0
2	N87	J	147	26/26	0.94	0.09	28,39,56,58	0
2	N87	L	147	26/26	0.95	0.07	27,36,47,49	0
2	N87	T	147	26/26	0.96	0.08	28,35,47,48	0
2	N87	B	147	26/26	0.96	0.07	23,28,37,38	0
2	N87	G	147	26/26	0.96	0.07	31,39,50,51	0
2	N87	H	147	26/26	0.96	0.07	18,29,30,32	0
2	N87	S	147	26/26	0.96	0.07	17,30,48,49	0
2	N87	P	147	26/26	0.97	0.06	15,24,28,29	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.

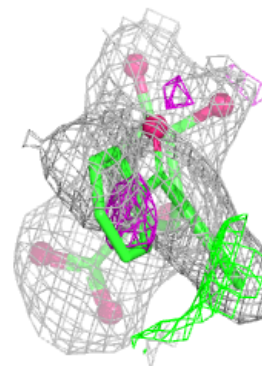
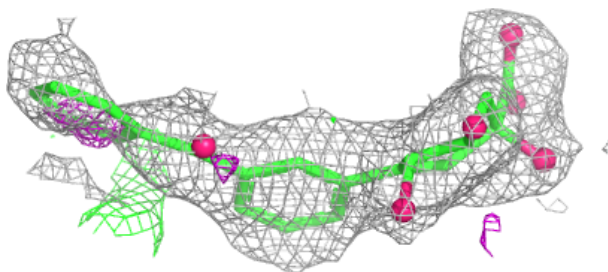
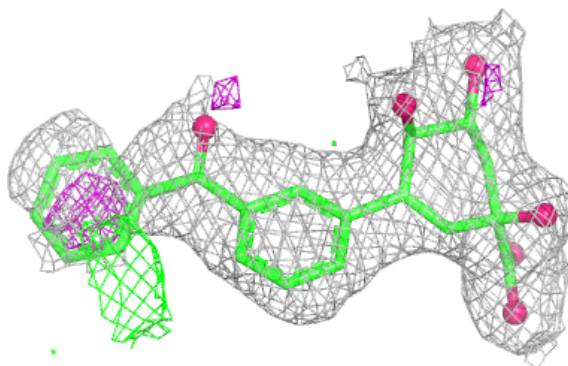
Electron density around N87 K 147:

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



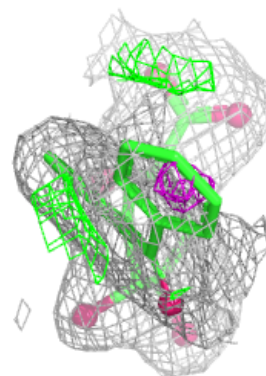
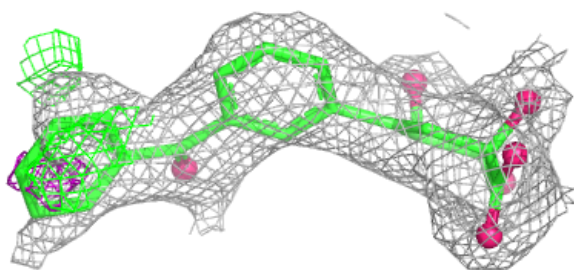
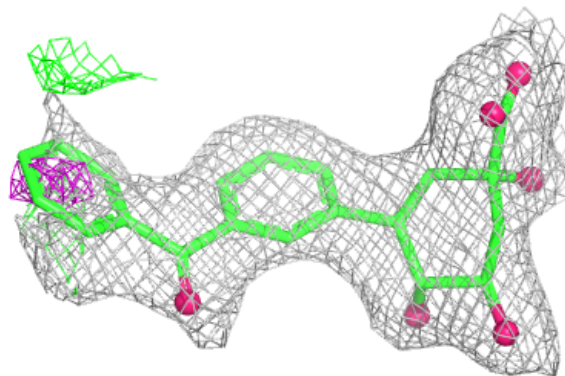
Electron density around N87 D 147:

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

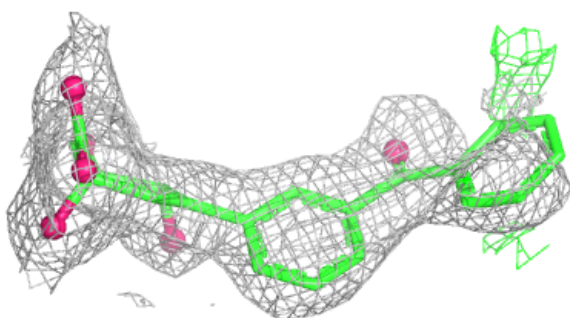
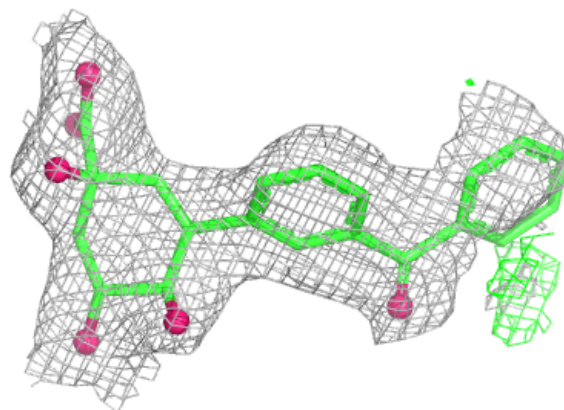


Electron density around N87 I 147:

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

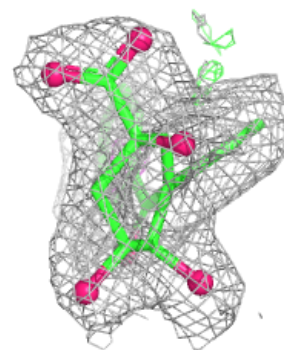
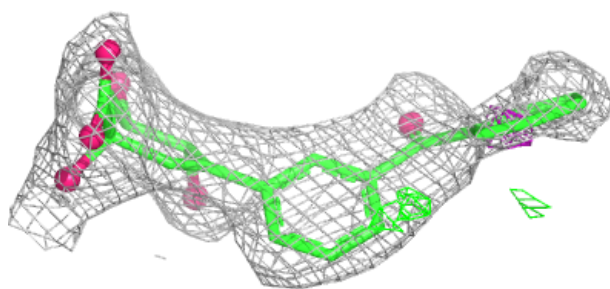
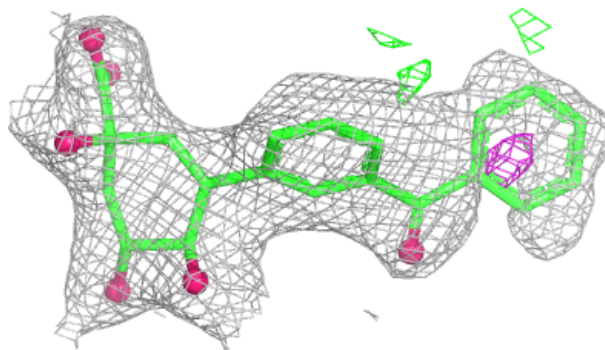
**Electron density around N87 C 147:**

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

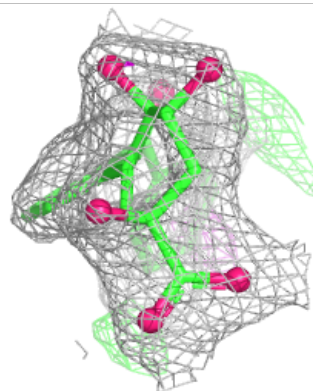
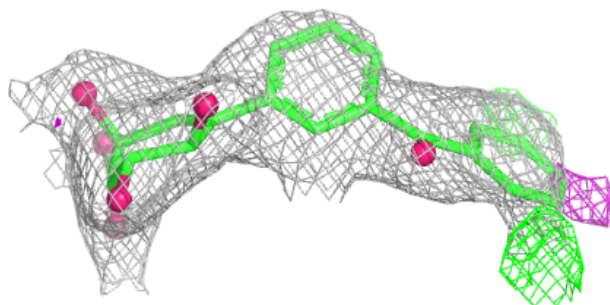
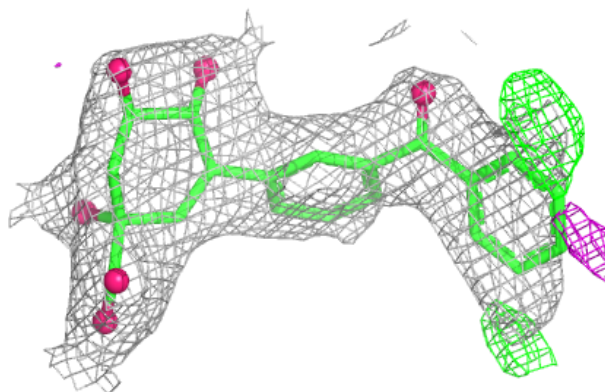


Electron density around N87 O 147:

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

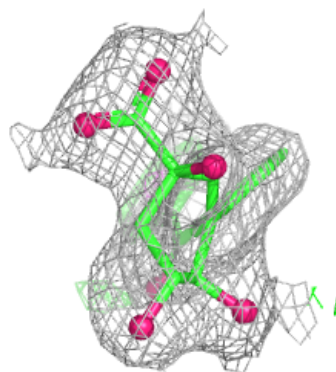
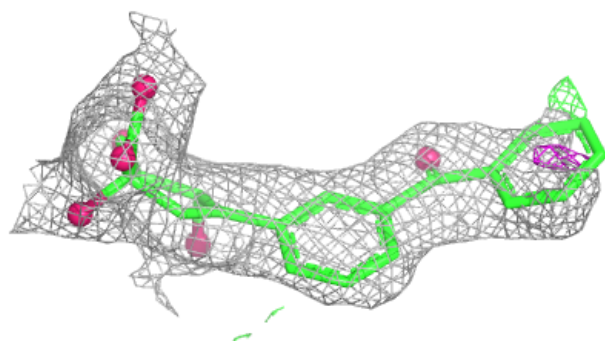
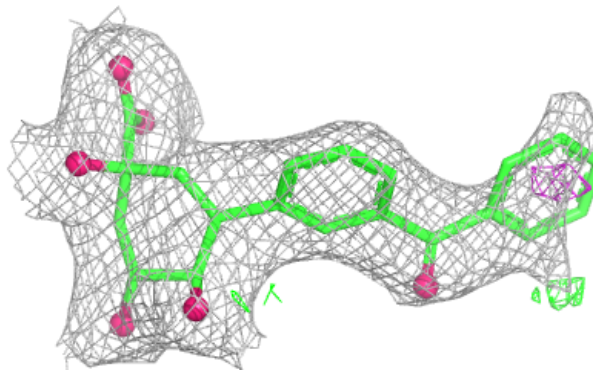
**Electron density around N87 Q 147:**

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

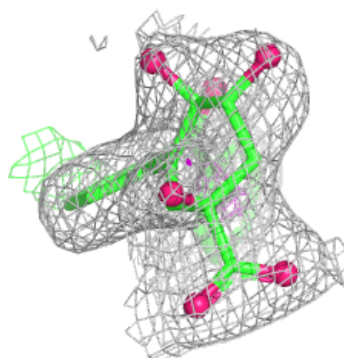
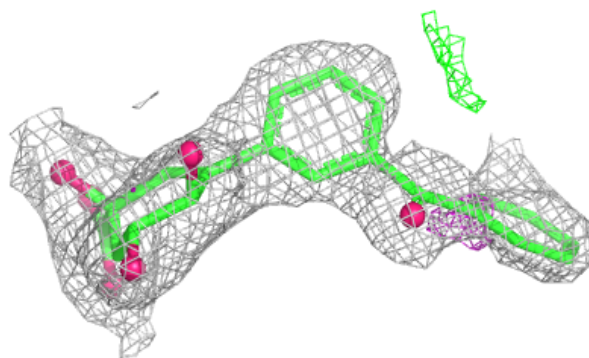
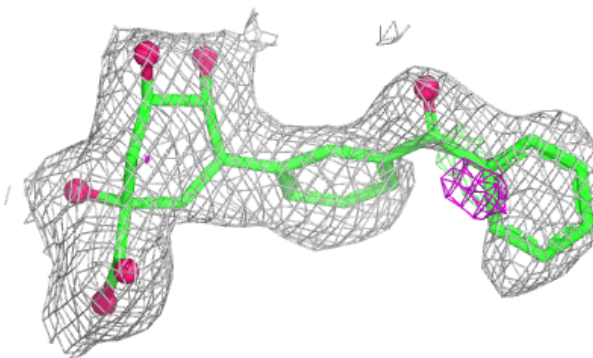


Electron density around N87 R 147:

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

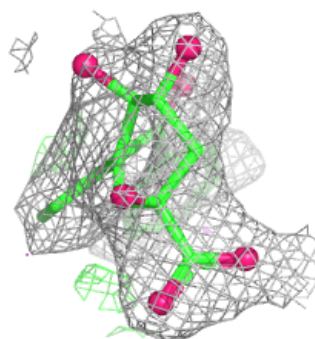
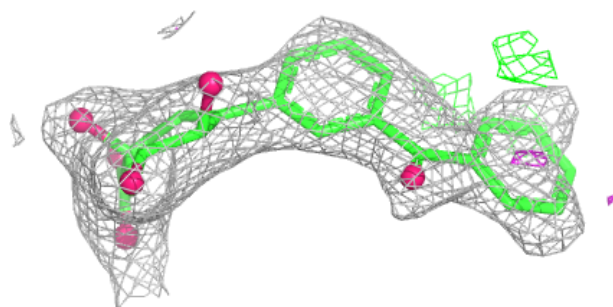
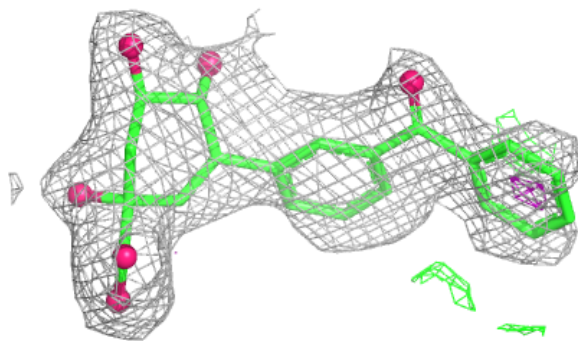
**Electron density around N87 X 147:**

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

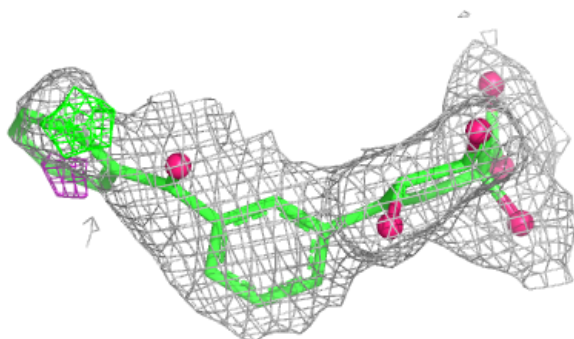
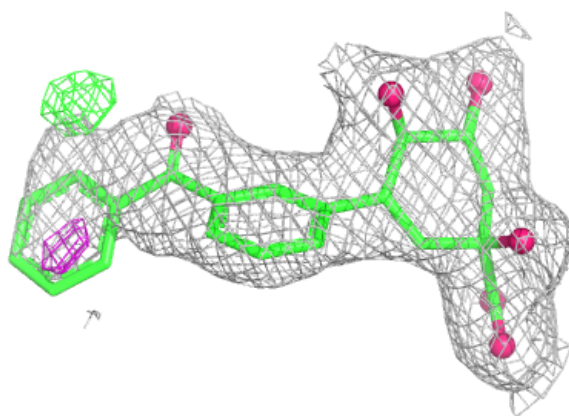


Electron density around N87 M 147:

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

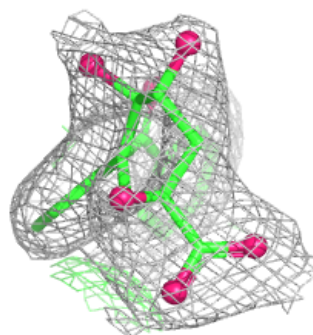
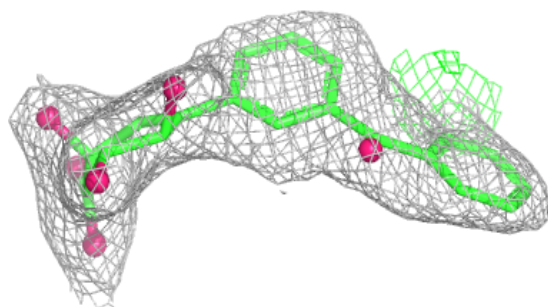
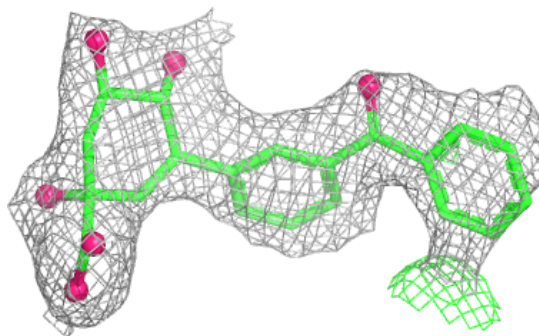
**Electron density around N87 N 147:**

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

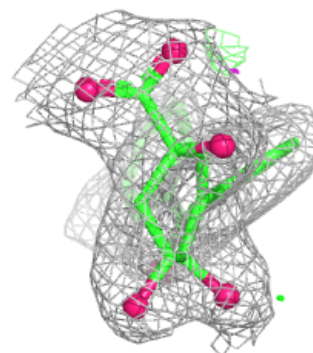
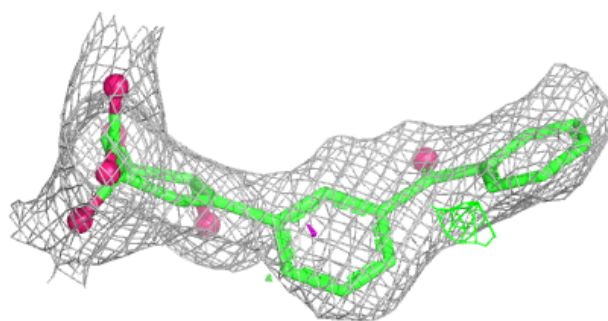
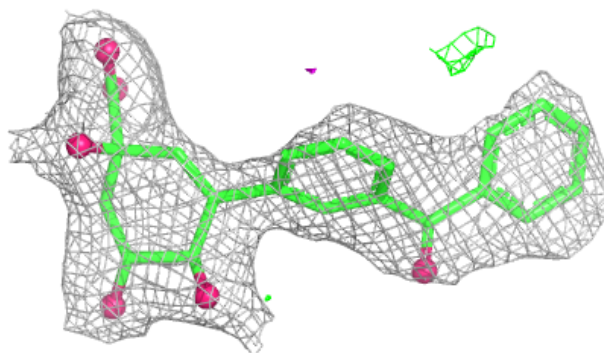


Electron density around N87 A 147:

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

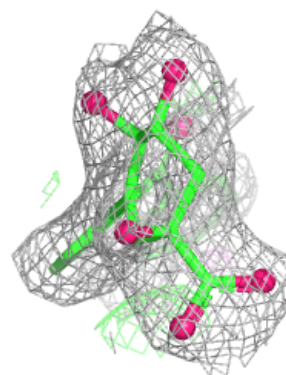
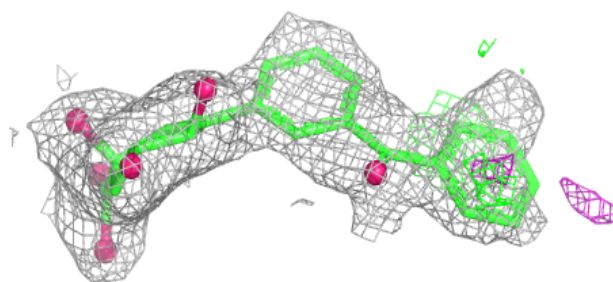
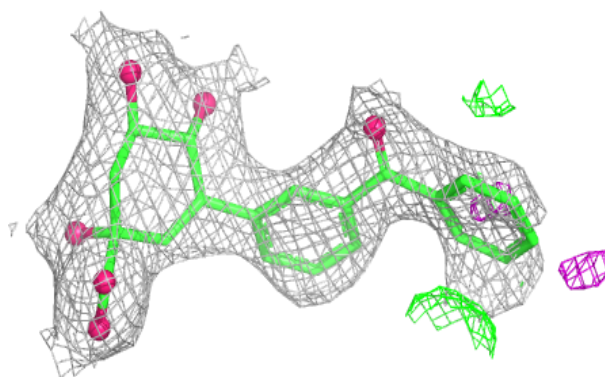
**Electron density around N87 W 147:**

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

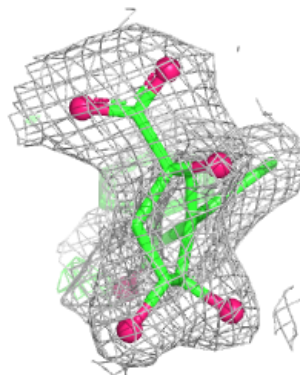
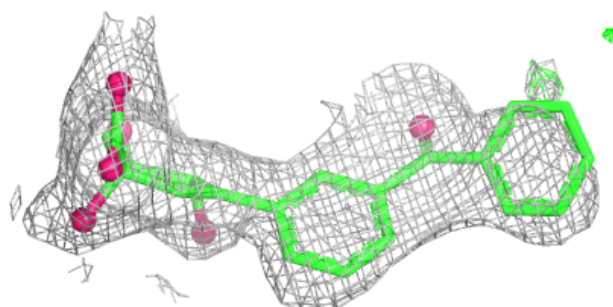
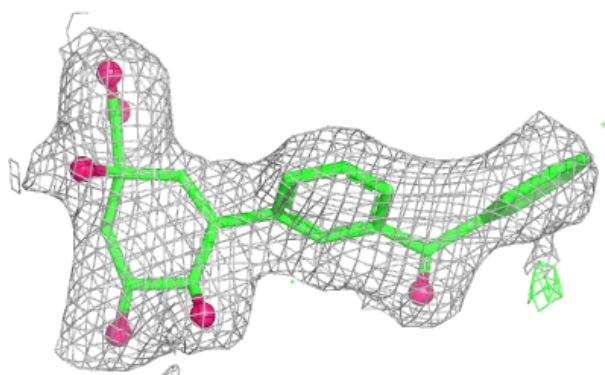


Electron density around N87 V 147:

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

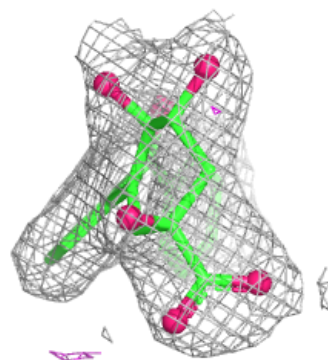
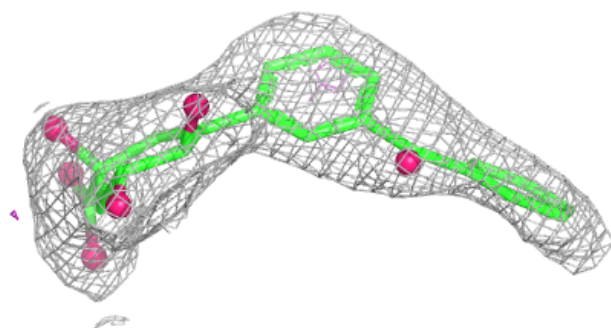
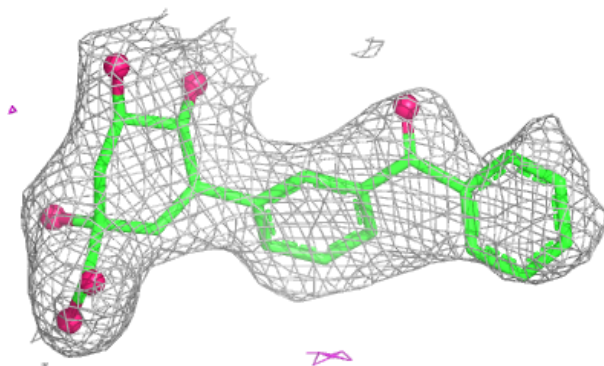
**Electron density around N87 U 147:**

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

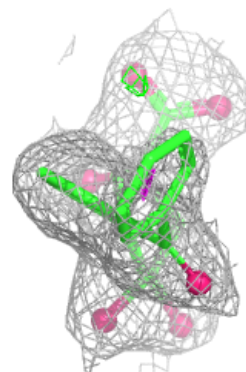
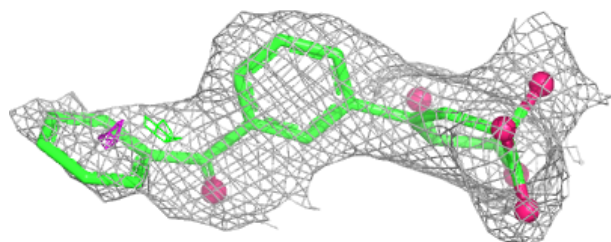
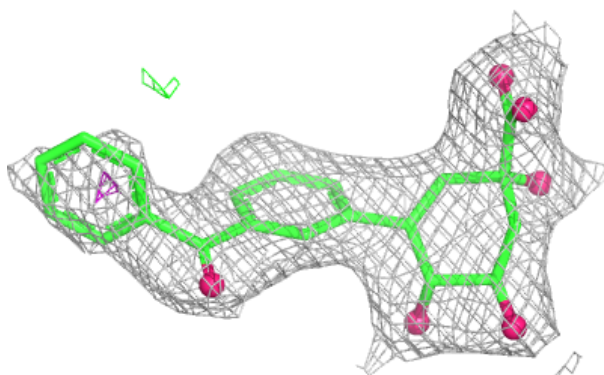


Electron density around N87 F 147:

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

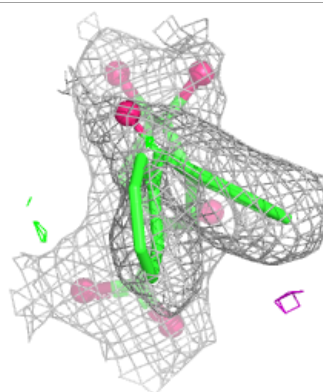
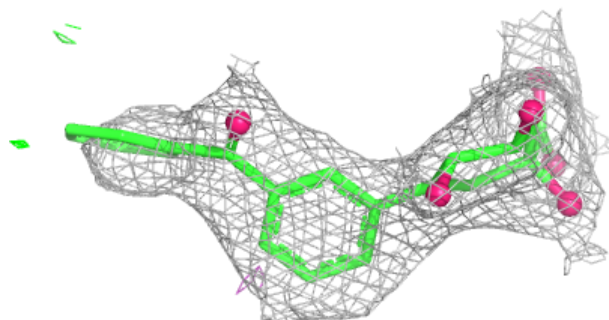
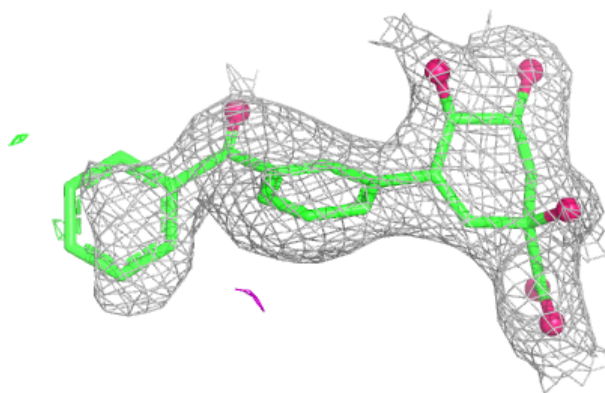
**Electron density around N87 E 147:**

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

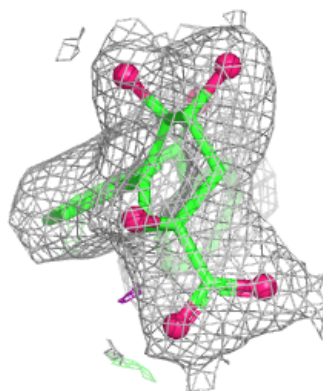
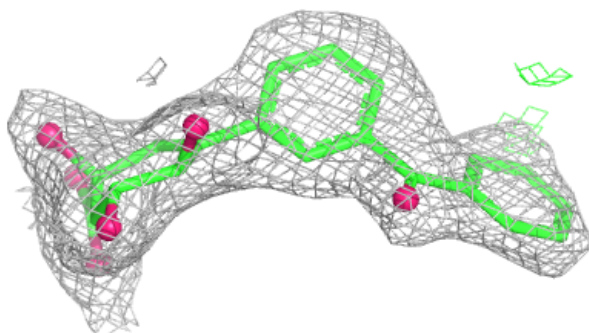
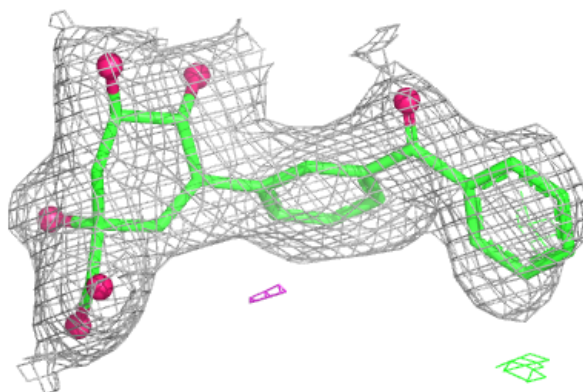


Electron density around N87 J 147:

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

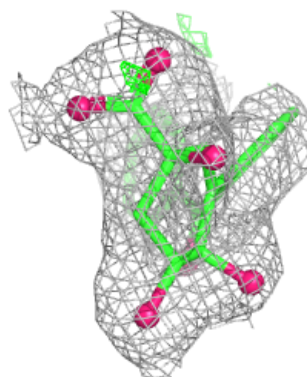
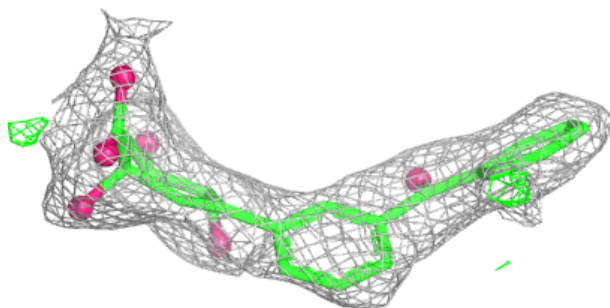
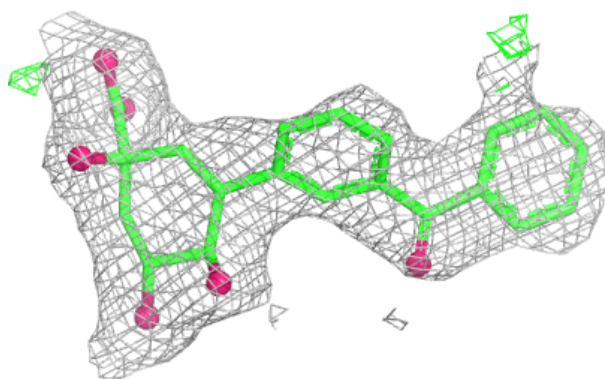
**Electron density around N87 L 147:**

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

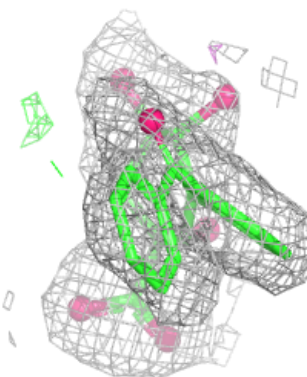
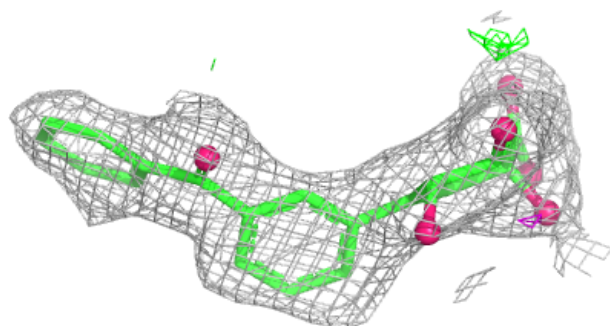
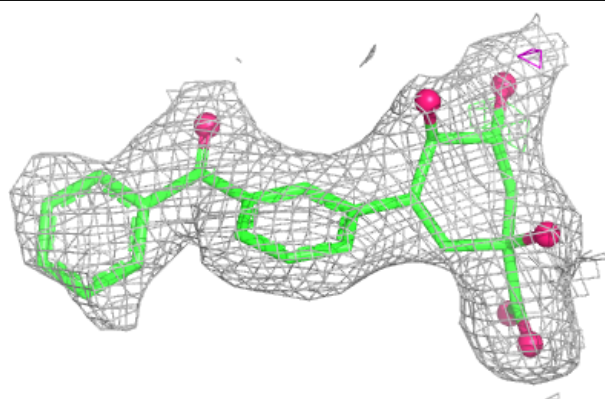


Electron density around N87 T 147:

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

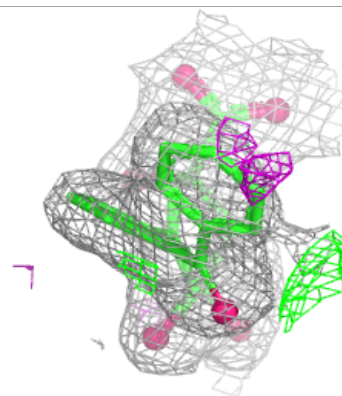
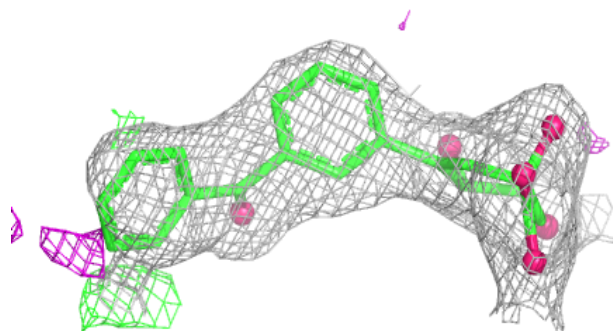
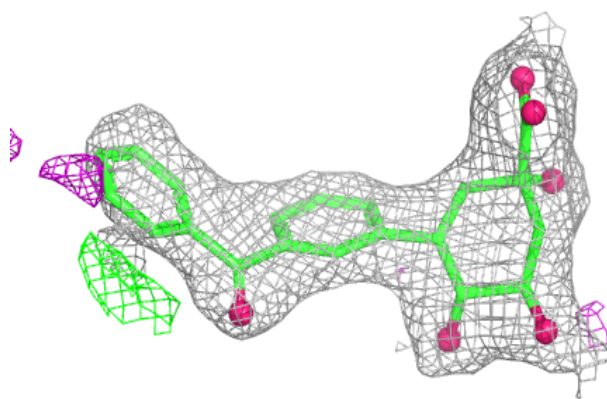
**Electron density around N87 B 147:**

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

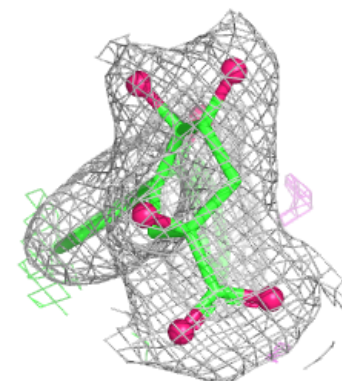
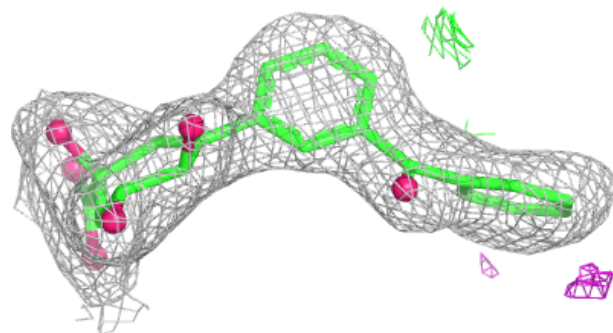
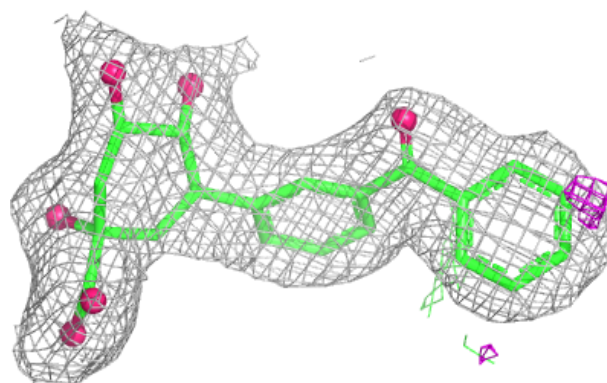


Electron density around N87 G 147:

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

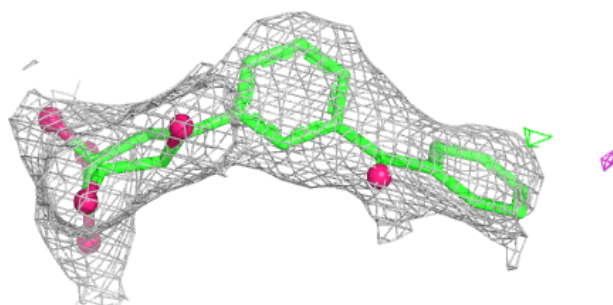
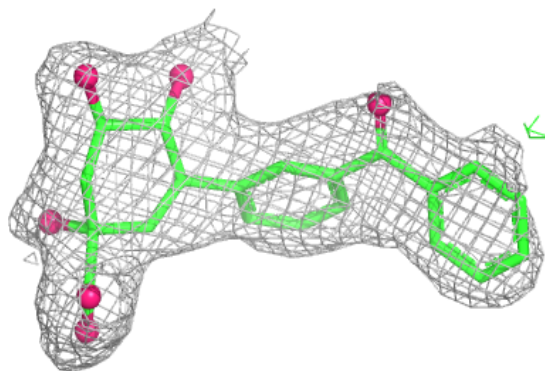
**Electron density around N87 H 147:**

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

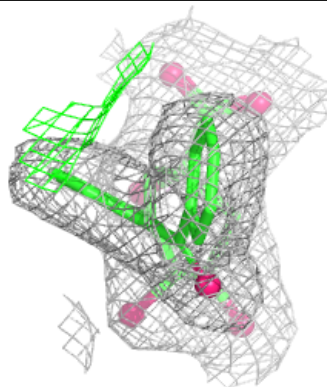
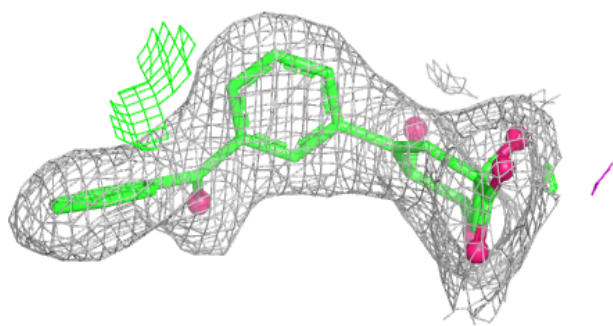
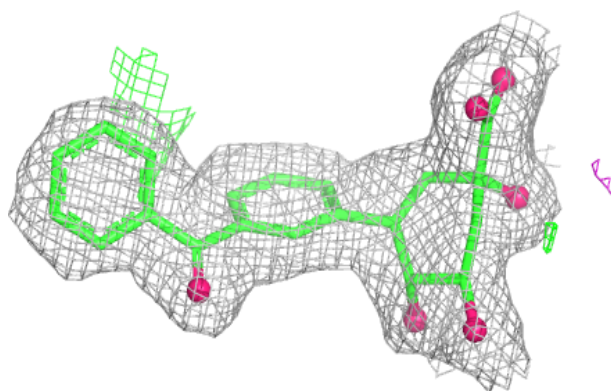


Electron density around N87 S 147:

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

**Electron density around N87 P 147:**

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



6.5 Other polymers ⓘ

There are no such residues in this entry.