



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 12, 2026 – 06:13 AM UTC

PDB ID : 1GQ2 / pdb_00001gq2
Title : Malic Enzyme from Pigeon Liver
Authors : Yang, Z.; Zhang, H.; Liang, T.
Deposited on : 2001-11-19
Resolution : 2.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

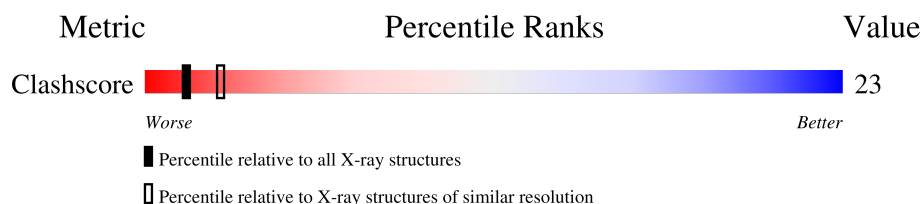
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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))
Clashscore	190562	6492 (2.50-2.50)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	555	 58% 41% .
1	B	555	 60% 39% .
1	C	555	 62% 37% .
1	D	555	 62% 37% .
1	E	555	 63% 36% .
1	F	555	 64% 35% .
1	G	555	 60% 39% .
1	H	555	 63% 36% .
1	I	555	 65% 34% .
1	J	555	 65% 33% .

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Mol	Chain	Length	Quality of chain
1	K	555	 59% 41%
1	L	555	 59% 40% .
1	M	555	 64% 35% .
1	N	555	 61% 38% .
1	O	555	 64% 35% .
1	P	555	 65% 35%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	OXL	C	1582	-	-	X	-
3	OXL	D	1582	-	-	X	-
3	OXL	O	1582	-	X	-	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 71519 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 MALIC ENZYME.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	555	Total	C	N	O	S	Se	0	0	0
			4345	2772	742	806	11	14			
1	B	555	Total	C	N	O	S	Se	0	0	0
			4345	2772	742	806	11	14			
1	C	555	Total	C	N	O	S	Se	0	0	0
			4345	2772	742	806	11	14			
1	D	555	Total	C	N	O	S	Se	0	0	0
			4345	2772	742	806	11	14			
1	E	555	Total	C	N	O	S	Se	0	0	0
			4345	2772	742	806	11	14			
1	F	555	Total	C	N	O	S	Se	0	0	0
			4345	2772	742	806	11	14			
1	G	555	Total	C	N	O	S	Se	0	0	0
			4345	2772	742	806	11	14			
1	H	555	Total	C	N	O	S	Se	0	0	0
			4345	2772	742	806	11	14			
1	I	555	Total	C	N	O	S	Se	0	0	0
			4345	2772	742	806	11	14			
1	J	555	Total	C	N	O	S	Se	0	0	0
			4345	2772	742	806	11	14			
1	K	555	Total	C	N	O	S	Se	0	0	0
			4345	2772	742	806	11	14			
1	L	555	Total	C	N	O	S	Se	0	0	0
			4345	2772	742	806	11	14			
1	M	555	Total	C	N	O	S	Se	0	0	0
			4345	2772	742	806	11	14			
1	N	555	Total	C	N	O	S	Se	0	0	0
			4345	2772	742	806	11	14			
1	O	555	Total	C	N	O	S	Se	0	0	0
			4345	2772	742	806	11	14			
1	P	555	Total	C	N	O	S	Se	0	0	0
			4346	2772	742	807	11	14			

There are 224 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	38	MSE	MET	modified residue	UNP P40927
A	86	MSE	MET	modified residue	UNP P40927
A	108	MSE	MET	modified residue	UNP P40927
A	146	MSE	MET	modified residue	UNP P40927
A	177	MSE	MET	modified residue	UNP P40927
A	202	MSE	MET	modified residue	UNP P40927
A	239	MSE	MET	modified residue	UNP P40927
A	248	MSE	MET	modified residue	UNP P40927
A	325	MSE	MET	modified residue	UNP P40927
A	327	MSE	MET	modified residue	UNP P40927
A	343	MSE	MET	modified residue	UNP P40927
A	374	MSE	MET	modified residue	UNP P40927
A	407	MSE	MET	modified residue	UNP P40927
A	577	MSE	MET	modified residue	UNP P40927
B	38	MSE	MET	modified residue	UNP P40927
B	86	MSE	MET	modified residue	UNP P40927
B	108	MSE	MET	modified residue	UNP P40927
B	146	MSE	MET	modified residue	UNP P40927
B	177	MSE	MET	modified residue	UNP P40927
B	202	MSE	MET	modified residue	UNP P40927
B	239	MSE	MET	modified residue	UNP P40927
B	248	MSE	MET	modified residue	UNP P40927
B	325	MSE	MET	modified residue	UNP P40927
B	327	MSE	MET	modified residue	UNP P40927
B	343	MSE	MET	modified residue	UNP P40927
B	374	MSE	MET	modified residue	UNP P40927
B	407	MSE	MET	modified residue	UNP P40927
B	577	MSE	MET	modified residue	UNP P40927
C	38	MSE	MET	modified residue	UNP P40927
C	86	MSE	MET	modified residue	UNP P40927
C	108	MSE	MET	modified residue	UNP P40927
C	146	MSE	MET	modified residue	UNP P40927
C	177	MSE	MET	modified residue	UNP P40927
C	202	MSE	MET	modified residue	UNP P40927
C	239	MSE	MET	modified residue	UNP P40927
C	248	MSE	MET	modified residue	UNP P40927
C	325	MSE	MET	modified residue	UNP P40927
C	327	MSE	MET	modified residue	UNP P40927
C	343	MSE	MET	modified residue	UNP P40927
C	374	MSE	MET	modified residue	UNP P40927
C	407	MSE	MET	modified residue	UNP P40927
C	577	MSE	MET	modified residue	UNP P40927

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Chain	Residue	Modelled	Actual	Comment	Reference
D	38	MSE	MET	modified residue	UNP P40927
D	86	MSE	MET	modified residue	UNP P40927
D	108	MSE	MET	modified residue	UNP P40927
D	146	MSE	MET	modified residue	UNP P40927
D	177	MSE	MET	modified residue	UNP P40927
D	202	MSE	MET	modified residue	UNP P40927
D	239	MSE	MET	modified residue	UNP P40927
D	248	MSE	MET	modified residue	UNP P40927
D	325	MSE	MET	modified residue	UNP P40927
D	327	MSE	MET	modified residue	UNP P40927
D	343	MSE	MET	modified residue	UNP P40927
D	374	MSE	MET	modified residue	UNP P40927
D	407	MSE	MET	modified residue	UNP P40927
D	577	MSE	MET	modified residue	UNP P40927
E	38	MSE	MET	modified residue	UNP P40927
E	86	MSE	MET	modified residue	UNP P40927
E	108	MSE	MET	modified residue	UNP P40927
E	146	MSE	MET	modified residue	UNP P40927
E	177	MSE	MET	modified residue	UNP P40927
E	202	MSE	MET	modified residue	UNP P40927
E	239	MSE	MET	modified residue	UNP P40927
E	248	MSE	MET	modified residue	UNP P40927
E	325	MSE	MET	modified residue	UNP P40927
E	327	MSE	MET	modified residue	UNP P40927
E	343	MSE	MET	modified residue	UNP P40927
E	374	MSE	MET	modified residue	UNP P40927
E	407	MSE	MET	modified residue	UNP P40927
E	577	MSE	MET	modified residue	UNP P40927
F	38	MSE	MET	modified residue	UNP P40927
F	86	MSE	MET	modified residue	UNP P40927
F	108	MSE	MET	modified residue	UNP P40927
F	146	MSE	MET	modified residue	UNP P40927
F	177	MSE	MET	modified residue	UNP P40927
F	202	MSE	MET	modified residue	UNP P40927
F	239	MSE	MET	modified residue	UNP P40927
F	248	MSE	MET	modified residue	UNP P40927
F	325	MSE	MET	modified residue	UNP P40927
F	327	MSE	MET	modified residue	UNP P40927
F	343	MSE	MET	modified residue	UNP P40927
F	374	MSE	MET	modified residue	UNP P40927
F	407	MSE	MET	modified residue	UNP P40927
F	577	MSE	MET	modified residue	UNP P40927

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Chain	Residue	Modelled	Actual	Comment	Reference
G	38	MSE	MET	modified residue	UNP P40927
G	86	MSE	MET	modified residue	UNP P40927
G	108	MSE	MET	modified residue	UNP P40927
G	146	MSE	MET	modified residue	UNP P40927
G	177	MSE	MET	modified residue	UNP P40927
G	202	MSE	MET	modified residue	UNP P40927
G	239	MSE	MET	modified residue	UNP P40927
G	248	MSE	MET	modified residue	UNP P40927
G	325	MSE	MET	modified residue	UNP P40927
G	327	MSE	MET	modified residue	UNP P40927
G	343	MSE	MET	modified residue	UNP P40927
G	374	MSE	MET	modified residue	UNP P40927
G	407	MSE	MET	modified residue	UNP P40927
G	577	MSE	MET	modified residue	UNP P40927
H	38	MSE	MET	modified residue	UNP P40927
H	86	MSE	MET	modified residue	UNP P40927
H	108	MSE	MET	modified residue	UNP P40927
H	146	MSE	MET	modified residue	UNP P40927
H	177	MSE	MET	modified residue	UNP P40927
H	202	MSE	MET	modified residue	UNP P40927
H	239	MSE	MET	modified residue	UNP P40927
H	248	MSE	MET	modified residue	UNP P40927
H	325	MSE	MET	modified residue	UNP P40927
H	327	MSE	MET	modified residue	UNP P40927
H	343	MSE	MET	modified residue	UNP P40927
H	374	MSE	MET	modified residue	UNP P40927
H	407	MSE	MET	modified residue	UNP P40927
H	577	MSE	MET	modified residue	UNP P40927
I	38	MSE	MET	modified residue	UNP P40927
I	86	MSE	MET	modified residue	UNP P40927
I	108	MSE	MET	modified residue	UNP P40927
I	146	MSE	MET	modified residue	UNP P40927
I	177	MSE	MET	modified residue	UNP P40927
I	202	MSE	MET	modified residue	UNP P40927
I	239	MSE	MET	modified residue	UNP P40927
I	248	MSE	MET	modified residue	UNP P40927
I	325	MSE	MET	modified residue	UNP P40927
I	327	MSE	MET	modified residue	UNP P40927
I	343	MSE	MET	modified residue	UNP P40927
I	374	MSE	MET	modified residue	UNP P40927
I	407	MSE	MET	modified residue	UNP P40927
I	577	MSE	MET	modified residue	UNP P40927

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Chain	Residue	Modelled	Actual	Comment	Reference
J	38	MSE	MET	modified residue	UNP P40927
J	86	MSE	MET	modified residue	UNP P40927
J	108	MSE	MET	modified residue	UNP P40927
J	146	MSE	MET	modified residue	UNP P40927
J	177	MSE	MET	modified residue	UNP P40927
J	202	MSE	MET	modified residue	UNP P40927
J	239	MSE	MET	modified residue	UNP P40927
J	248	MSE	MET	modified residue	UNP P40927
J	325	MSE	MET	modified residue	UNP P40927
J	327	MSE	MET	modified residue	UNP P40927
J	343	MSE	MET	modified residue	UNP P40927
J	374	MSE	MET	modified residue	UNP P40927
J	407	MSE	MET	modified residue	UNP P40927
J	577	MSE	MET	modified residue	UNP P40927
K	38	MSE	MET	modified residue	UNP P40927
K	86	MSE	MET	modified residue	UNP P40927
K	108	MSE	MET	modified residue	UNP P40927
K	146	MSE	MET	modified residue	UNP P40927
K	177	MSE	MET	modified residue	UNP P40927
K	202	MSE	MET	modified residue	UNP P40927
K	239	MSE	MET	modified residue	UNP P40927
K	248	MSE	MET	modified residue	UNP P40927
K	325	MSE	MET	modified residue	UNP P40927
K	327	MSE	MET	modified residue	UNP P40927
K	343	MSE	MET	modified residue	UNP P40927
K	374	MSE	MET	modified residue	UNP P40927
K	407	MSE	MET	modified residue	UNP P40927
K	577	MSE	MET	modified residue	UNP P40927
L	38	MSE	MET	modified residue	UNP P40927
L	86	MSE	MET	modified residue	UNP P40927
L	108	MSE	MET	modified residue	UNP P40927
L	146	MSE	MET	modified residue	UNP P40927
L	177	MSE	MET	modified residue	UNP P40927
L	202	MSE	MET	modified residue	UNP P40927
L	239	MSE	MET	modified residue	UNP P40927
L	248	MSE	MET	modified residue	UNP P40927
L	325	MSE	MET	modified residue	UNP P40927
L	327	MSE	MET	modified residue	UNP P40927
L	343	MSE	MET	modified residue	UNP P40927
L	374	MSE	MET	modified residue	UNP P40927
L	407	MSE	MET	modified residue	UNP P40927
L	577	MSE	MET	modified residue	UNP P40927

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Chain	Residue	Modelled	Actual	Comment	Reference
M	38	MSE	MET	modified residue	UNP P40927
M	86	MSE	MET	modified residue	UNP P40927
M	108	MSE	MET	modified residue	UNP P40927
M	146	MSE	MET	modified residue	UNP P40927
M	177	MSE	MET	modified residue	UNP P40927
M	202	MSE	MET	modified residue	UNP P40927
M	239	MSE	MET	modified residue	UNP P40927
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M	374	MSE	MET	modified residue	UNP P40927
M	407	MSE	MET	modified residue	UNP P40927
M	577	MSE	MET	modified residue	UNP P40927
N	38	MSE	MET	modified residue	UNP P40927
N	86	MSE	MET	modified residue	UNP P40927
N	108	MSE	MET	modified residue	UNP P40927
N	146	MSE	MET	modified residue	UNP P40927
N	177	MSE	MET	modified residue	UNP P40927
N	202	MSE	MET	modified residue	UNP P40927
N	239	MSE	MET	modified residue	UNP P40927
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N	327	MSE	MET	modified residue	UNP P40927
N	343	MSE	MET	modified residue	UNP P40927
N	374	MSE	MET	modified residue	UNP P40927
N	407	MSE	MET	modified residue	UNP P40927
N	577	MSE	MET	modified residue	UNP P40927
O	38	MSE	MET	modified residue	UNP P40927
O	86	MSE	MET	modified residue	UNP P40927
O	108	MSE	MET	modified residue	UNP P40927
O	146	MSE	MET	modified residue	UNP P40927
O	177	MSE	MET	modified residue	UNP P40927
O	202	MSE	MET	modified residue	UNP P40927
O	239	MSE	MET	modified residue	UNP P40927
O	248	MSE	MET	modified residue	UNP P40927
O	325	MSE	MET	modified residue	UNP P40927
O	327	MSE	MET	modified residue	UNP P40927
O	343	MSE	MET	modified residue	UNP P40927
O	374	MSE	MET	modified residue	UNP P40927
O	407	MSE	MET	modified residue	UNP P40927
O	577	MSE	MET	modified residue	UNP P40927

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Chain	Residue	Modelled	Actual	Comment	Reference
P	38	MSE	MET	modified residue	UNP P40927
P	86	MSE	MET	modified residue	UNP P40927
P	108	MSE	MET	modified residue	UNP P40927
P	146	MSE	MET	modified residue	UNP P40927
P	177	MSE	MET	modified residue	UNP P40927
P	202	MSE	MET	modified residue	UNP P40927
P	239	MSE	MET	modified residue	UNP P40927
P	248	MSE	MET	modified residue	UNP P40927
P	325	MSE	MET	modified residue	UNP P40927
P	327	MSE	MET	modified residue	UNP P40927
P	343	MSE	MET	modified residue	UNP P40927
P	374	MSE	MET	modified residue	UNP P40927
P	407	MSE	MET	modified residue	UNP P40927
P	577	MSE	MET	modified residue	UNP P40927

- # NAP

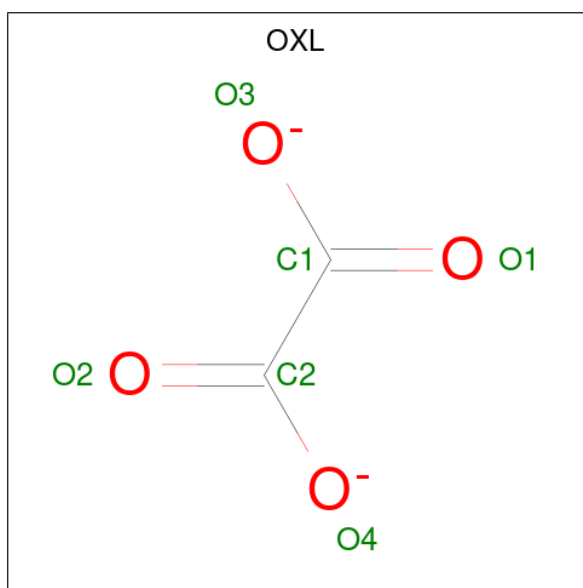
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 48	C 21	N 7	O 17	P 3	0	0
2	B	1	Total 48	C 21	N 7	O 17	P 3	0	0
2	C	1	Total 48	C 21	N 7	O 17	P 3	0	0
2	D	1	Total 48	C 21	N 7	O 17	P 3	0	0



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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	E	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	F	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	G	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	H	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	I	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	J	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	K	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	L	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	M	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	N	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	O	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	P	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is OXALATE ION (CCD ID: OXL) (formula: C_2O_4).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 2 4	0	0
3	B	1	Total C O 6 2 4	0	0
3	C	1	Total C O 6 2 4	0	0
3	D	1	Total C O 6 2 4	0	0
3	E	1	Total C O 6 2 4	0	0
3	F	1	Total C O 6 2 4	0	0
3	G	1	Total C O 6 2 4	0	0
3	H	1	Total C O 6 2 4	0	0
3	I	1	Total C O 6 2 4	0	0
3	J	1	Total C O 6 2 4	0	0
3	K	1	Total C O 6 2 4	0	0
3	L	1	Total C O 6 2 4	0	0
3	M	1	Total C O 6 2 4	0	0
3	N	1	Total C O 6 2 4	0	0
3	O	1	Total C O 6 2 4	0	0
3	P	1	Total C O 6 2 4	0	0

- Molecule 4 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Mn 1 1	0	0
4	B	1	Total Mn 1 1	0	0
4	C	1	Total Mn 1 1	0	0
4	D	1	Total Mn 1 1	0	0

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

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total 1	Cl 1	0	0
5	C	4	Total 4	Cl 4	0	0
5	E	3	Total 3	Cl 3	0	0
5	F	2	Total 2	Cl 2	0	0
5	G	1	Total 1	Cl 1	0	0
5	H	1	Total 1	Cl 1	0	0
5	I	5	Total 5	Cl 5	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	J	2	Total 2	Cl 2	0	0
5	K	1	Total 1	Cl 1	0	0
5	L	1	Total 1	Cl 1	0	0
5	M	3	Total 3	Cl 3	0	0
5	N	2	Total 2	Cl 2	0	0
5	O	4	Total 4	Cl 4	0	0
5	P	3	Total 3	Cl 3	0	0

- Molecule 6 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	4	Total 4	Na 4	0	0
6	D	2	Total 2	Na 2	0	0
6	F	2	Total 2	Na 2	0	0
6	G	1	Total 1	Na 1	0	0
6	H	5	Total 5	Na 5	0	0
6	I	2	Total 2	Na 2	0	0
6	J	2	Total 2	Na 2	0	0
6	K	1	Total 1	Na 1	0	0
6	L	1	Total 1	Na 1	0	0
6	M	6	Total 6	Na 6	0	0
6	N	1	Total 1	Na 1	0	0
6	O	4	Total 4	Na 4	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	P	5	Total	Na	0	0
			5	5		

- Molecule 7 is water.

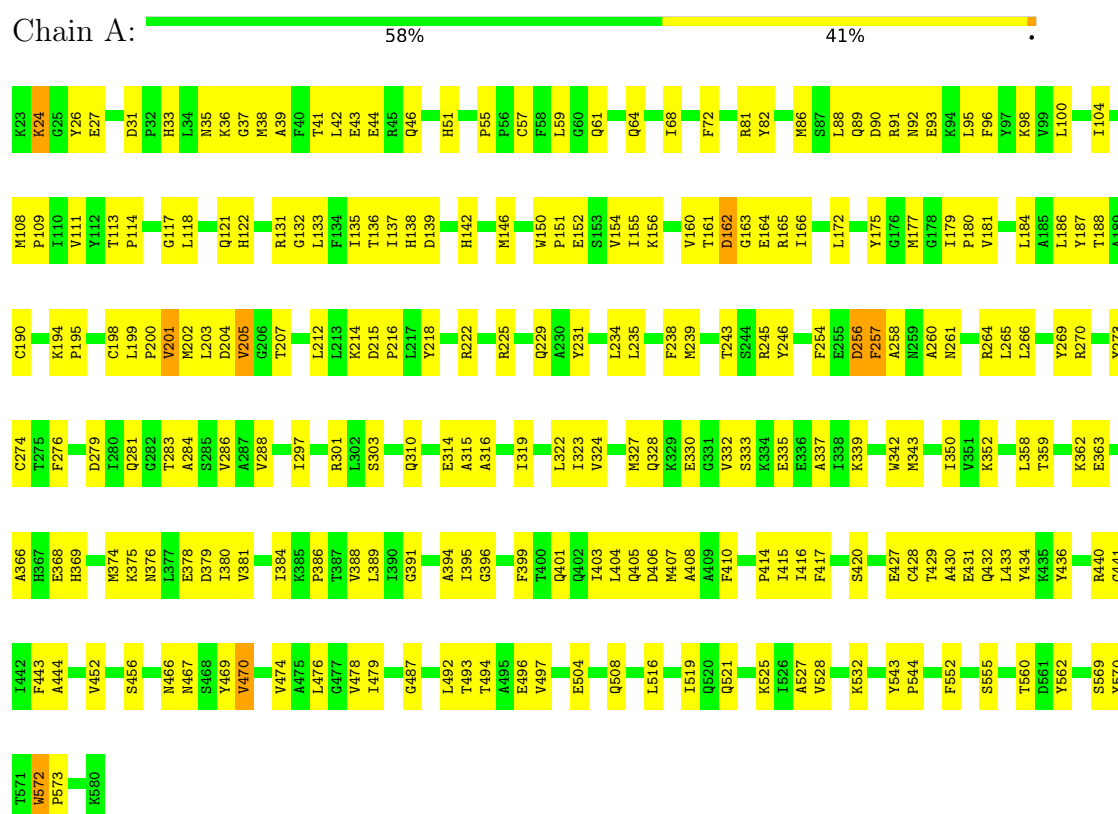
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	35	Total	O	0	0
			35	35		
7	B	42	Total	O	0	0
			42	42		
7	C	77	Total	O	0	0
			77	77		
7	D	49	Total	O	0	0
			49	49		
7	E	58	Total	O	0	0
			58	58		
7	F	78	Total	O	0	0
			78	78		
7	G	65	Total	O	0	0
			65	65		
7	H	77	Total	O	0	0
			77	77		
7	I	80	Total	O	0	0
			80	80		
7	J	63	Total	O	0	0
			63	63		
7	K	41	Total	O	0	0
			41	41		
7	L	75	Total	O	0	0
			75	75		
7	M	81	Total	O	0	0
			81	81		
7	N	71	Total	O	0	0
			71	71		
7	O	78	Total	O	0	0
			78	78		
7	P	79	Total	O	0	0
			79	79		

3 Residue-property plots

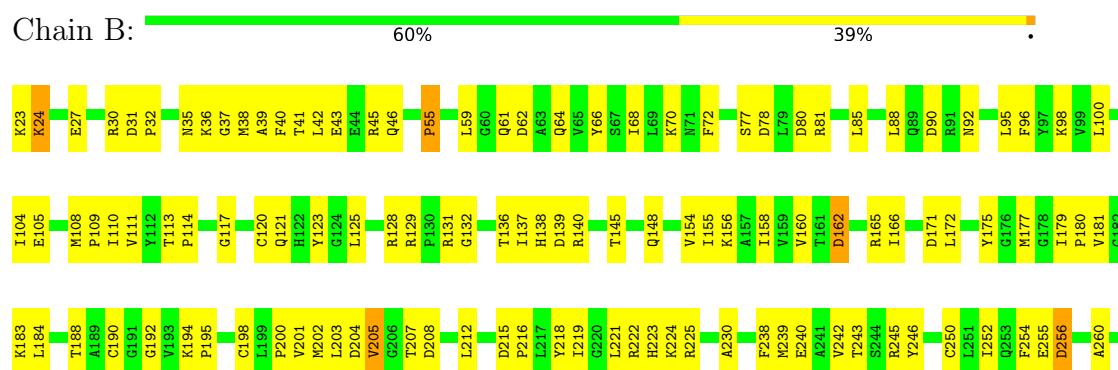
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

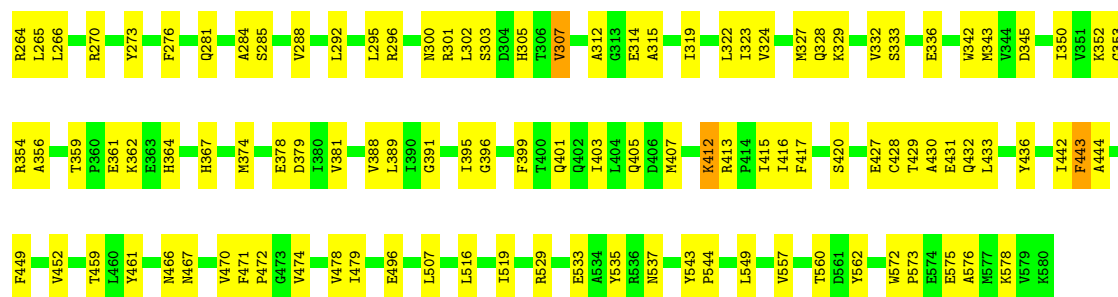
Note EDS was not executed.

• Molecule 1: MALIC ENZYME

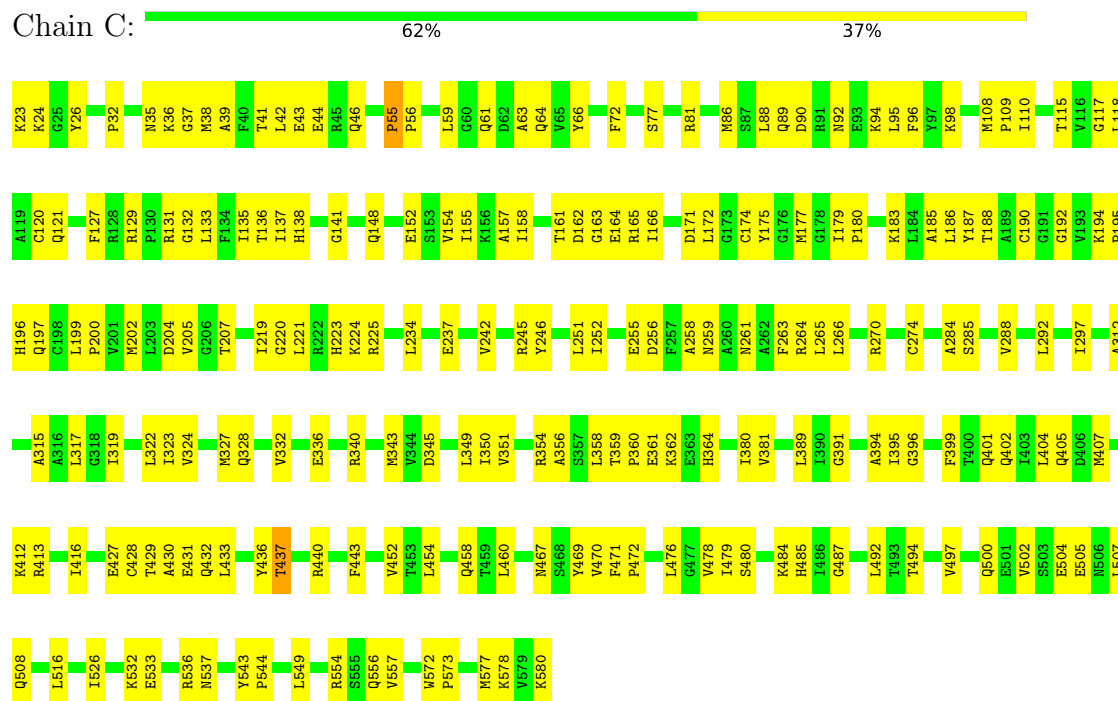


• Molecule 1: MALIC ENZYME

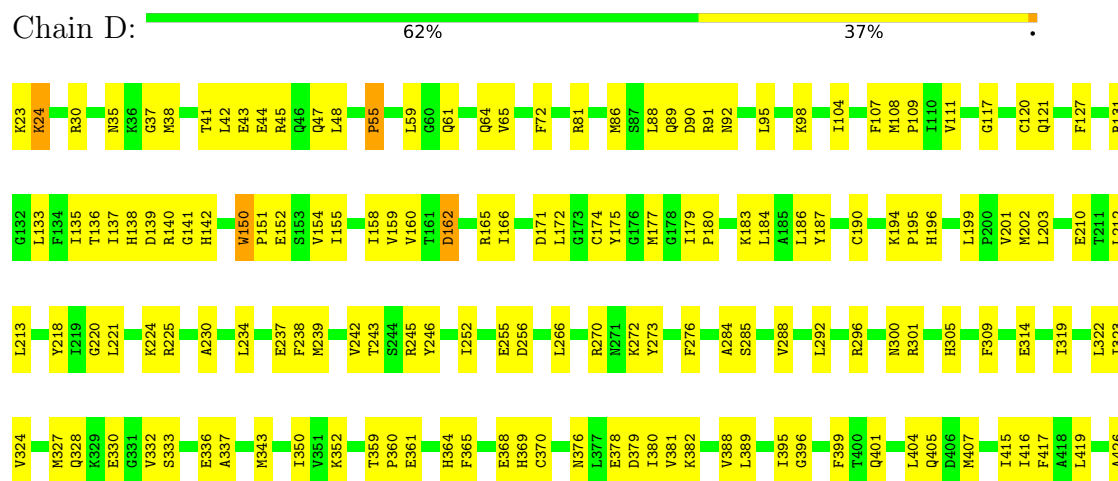


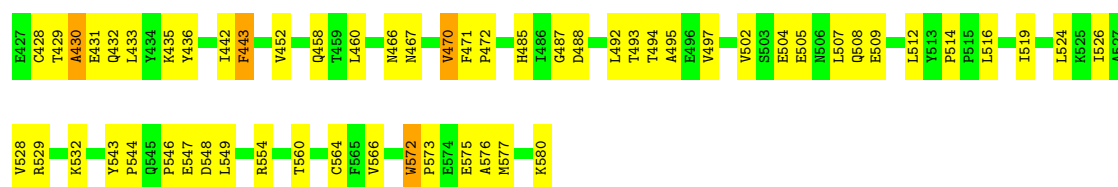


• Molecule 1: MALIC ENZYME



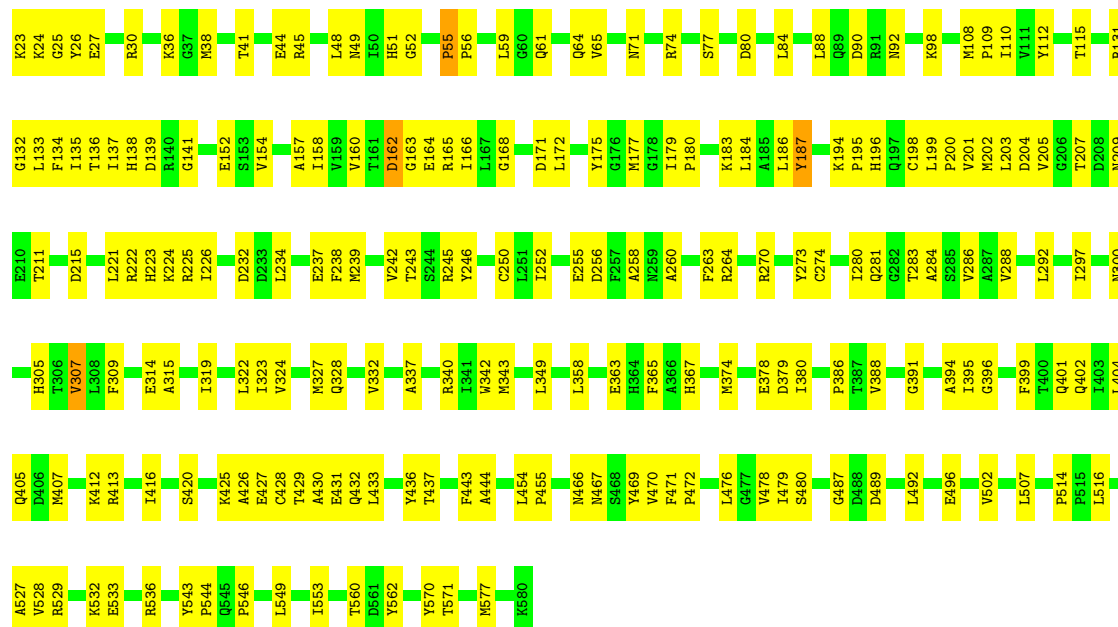
• Molecule 1: MALIC ENZYME





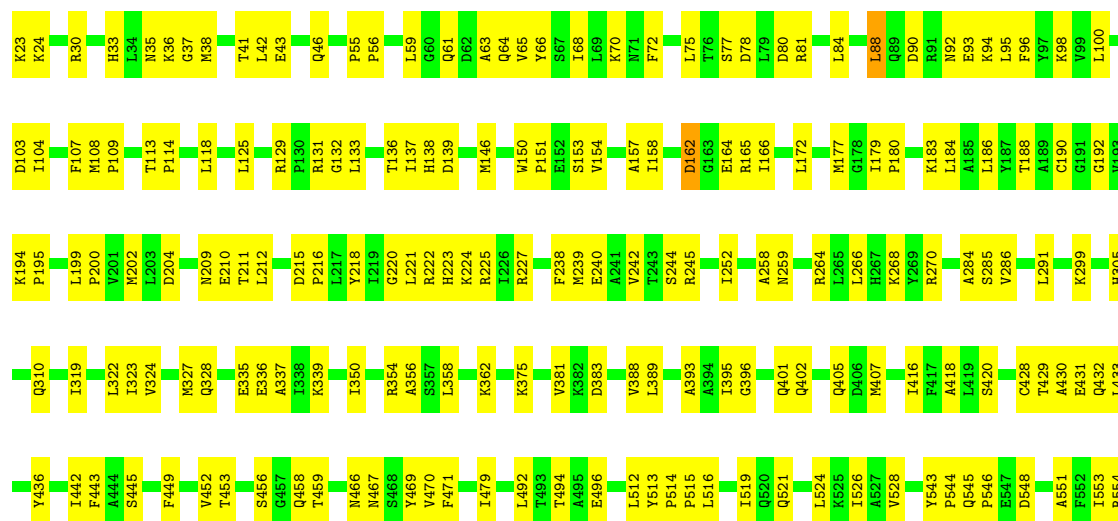
• Molecule 1: MALIC ENZYME

Chain E: 63% 36%



• Molecule 1: MALIC ENZYME

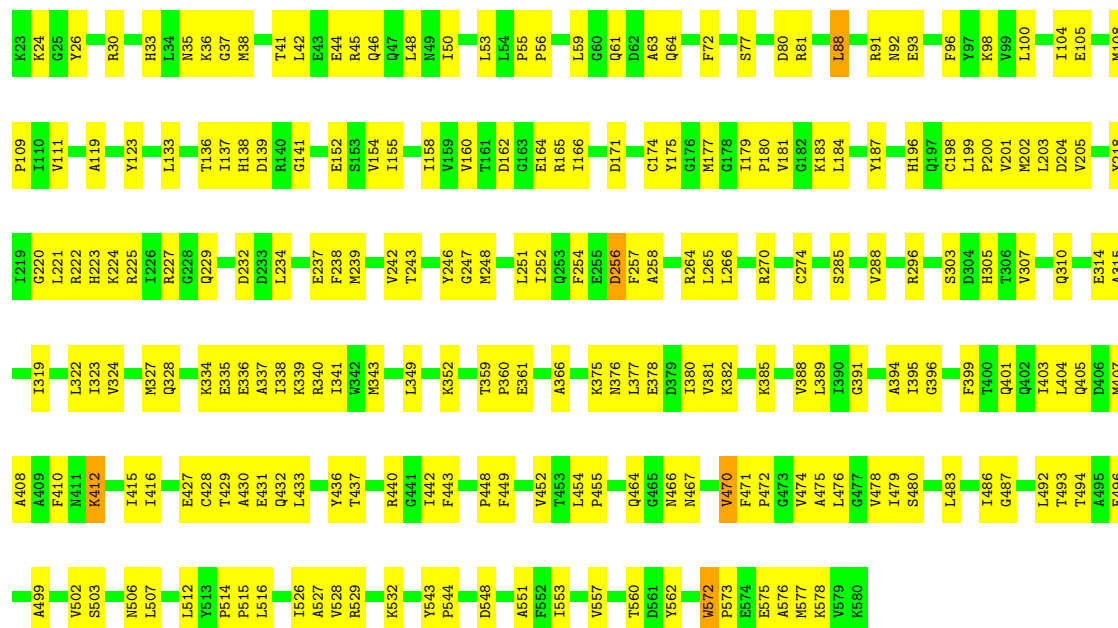
Chain F: 64% 35%





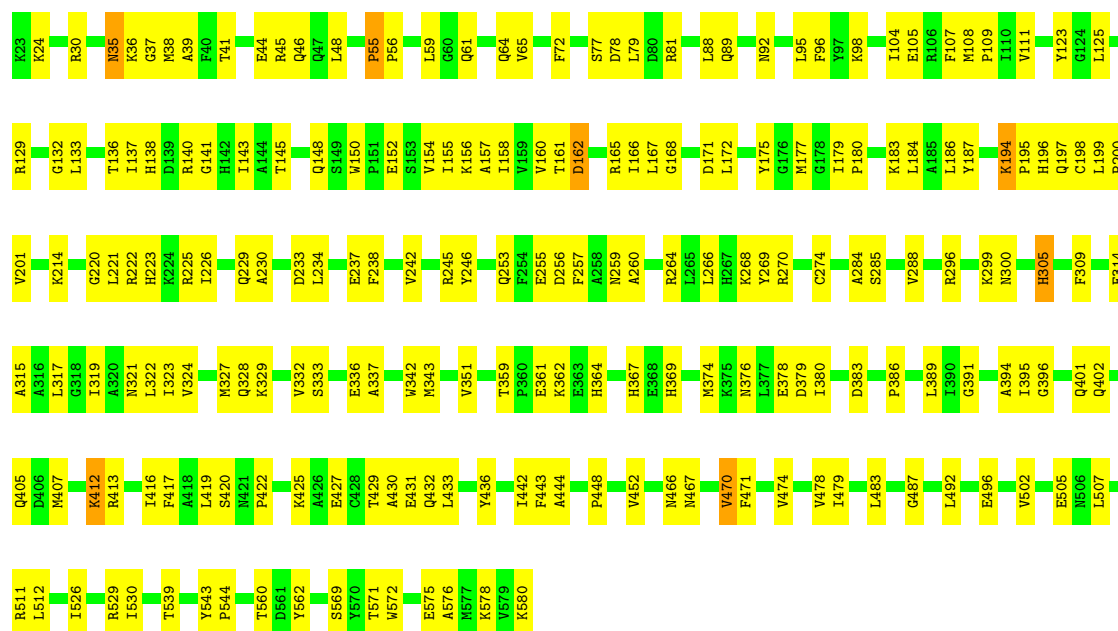
• Molecule 1: MALIC ENZYME

Chain G: 60% 39%



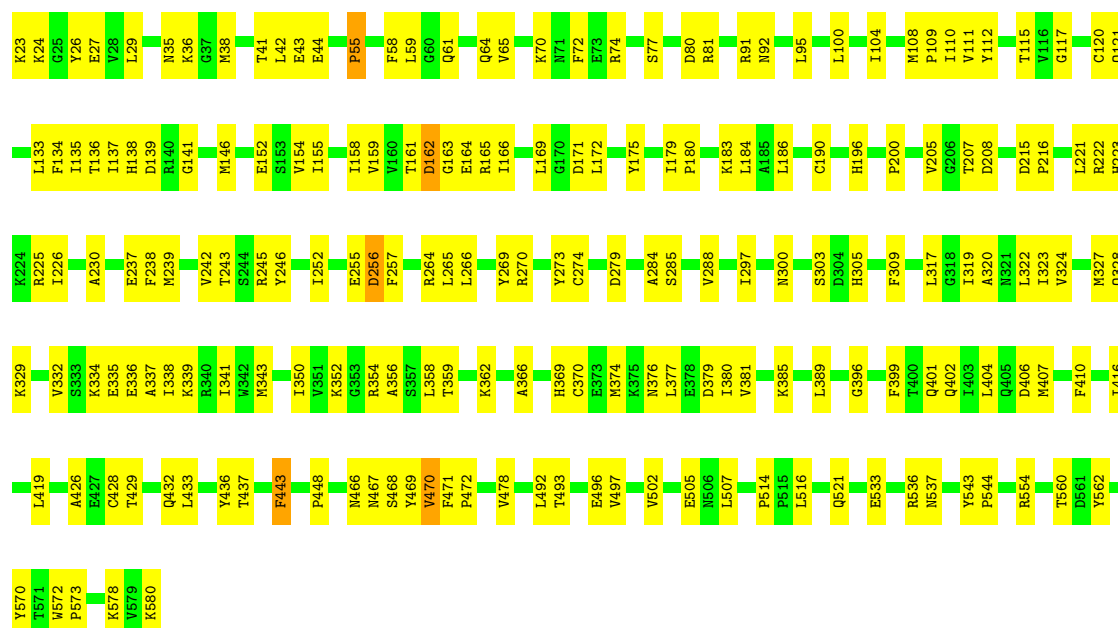
• Molecule 1: MALIC ENZYME

Chain H: 63% 36%



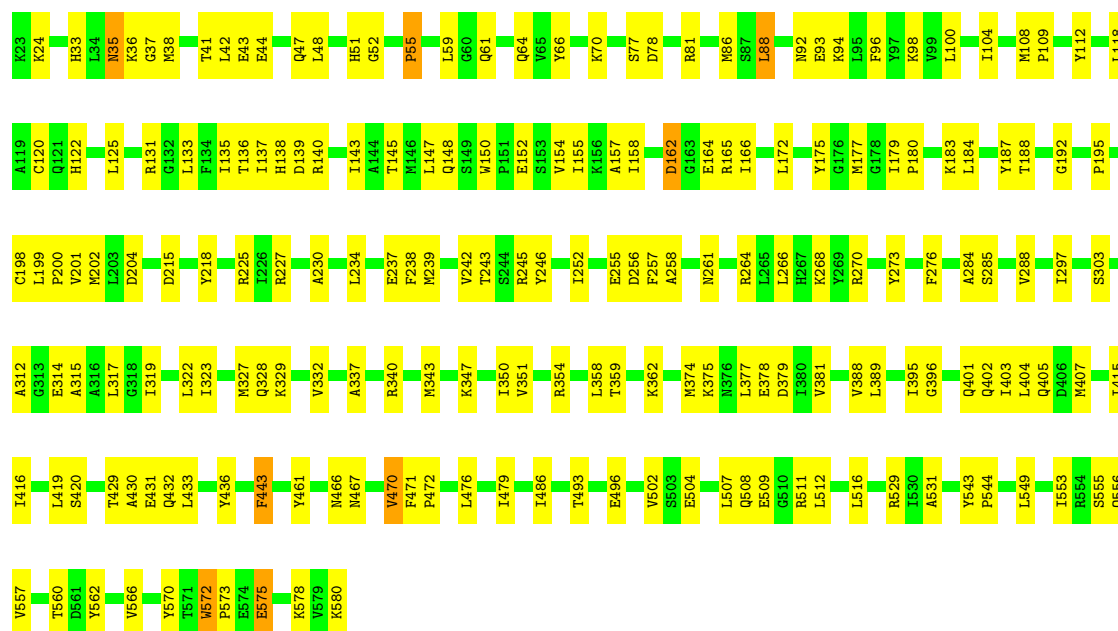
• Molecule 1: MALIC ENZYME

Chain I:  65% 34% .



• Molecule 1: MALIC ENZYME

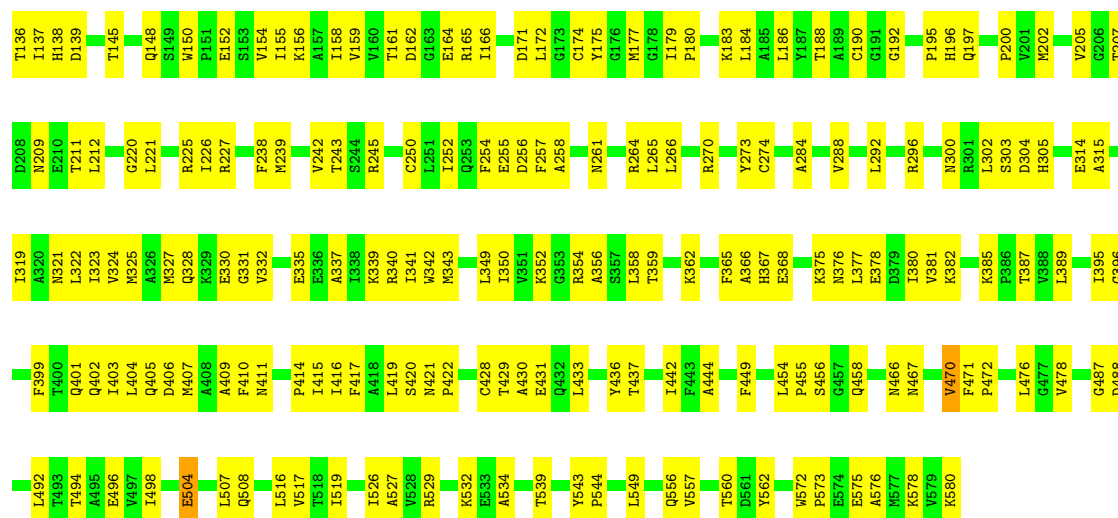
Chain J:  65% 33% .



• Molecule 1: MALIC ENZYME

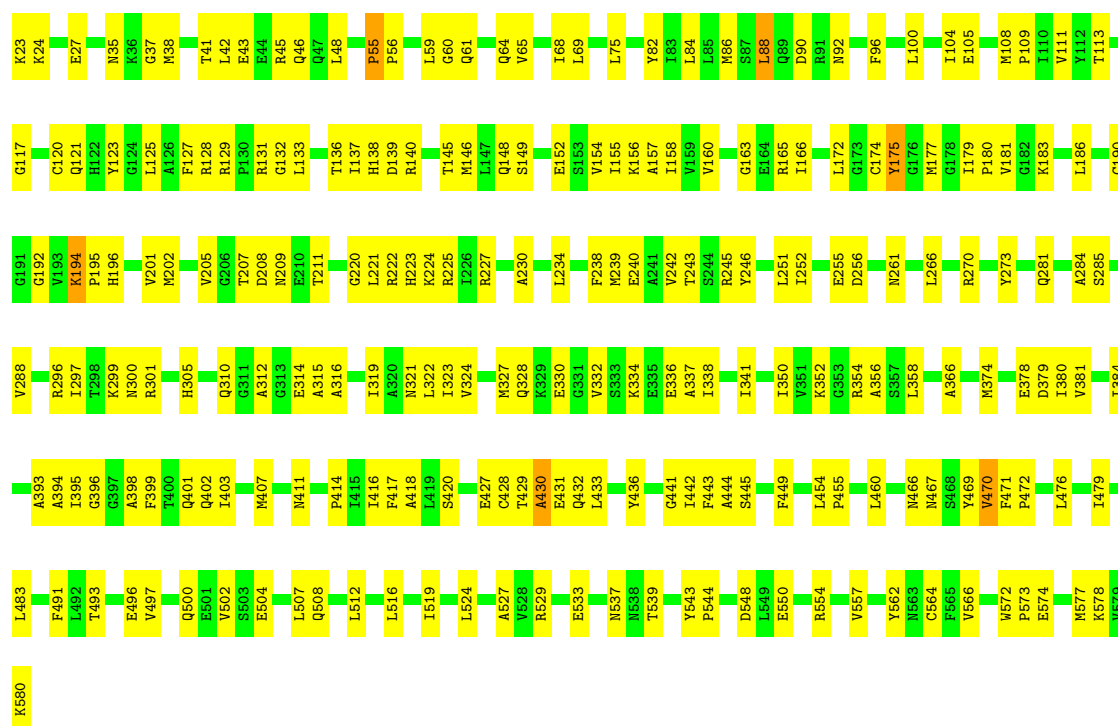
Chain K:  59% 41% .





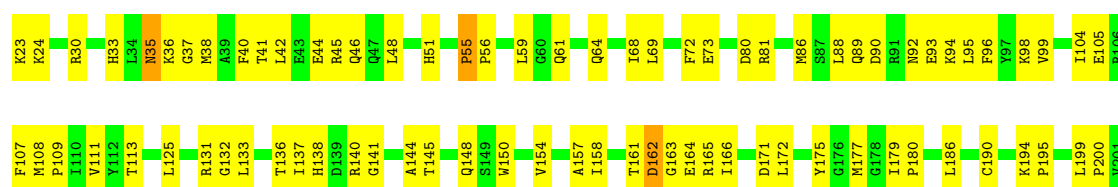
• Molecule 1: MALIC ENZYME

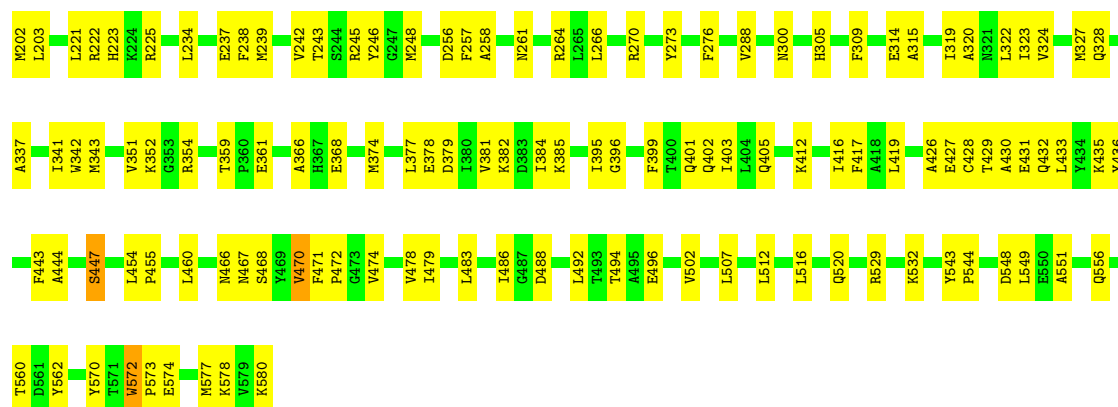
Chain L: 59% 40%



• Molecule 1: MALIC ENZYME

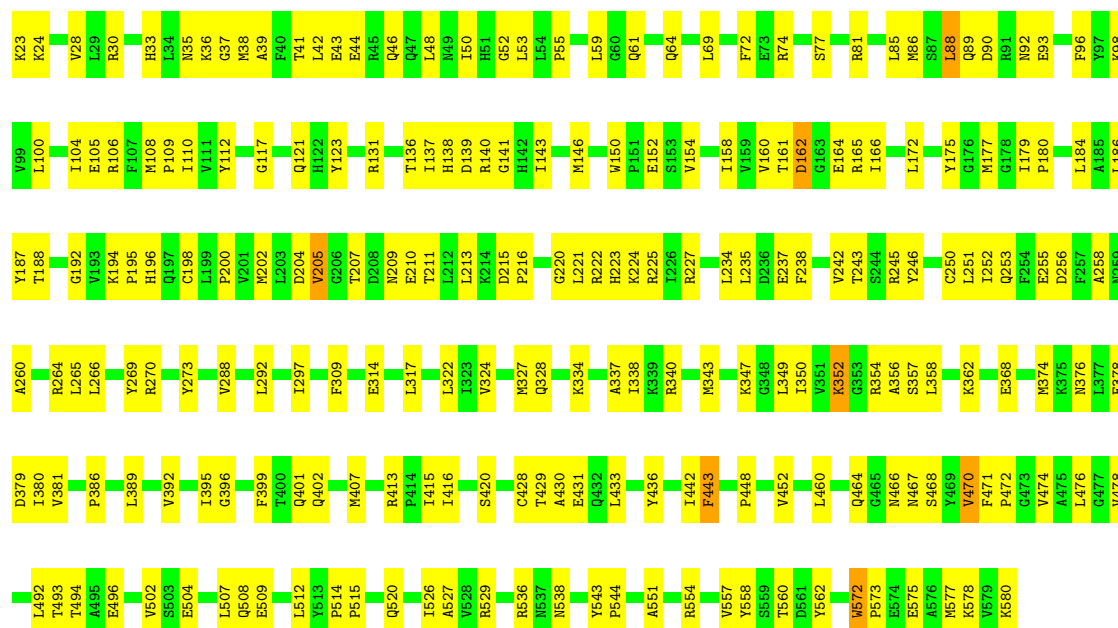
Chain M: 64% 35%





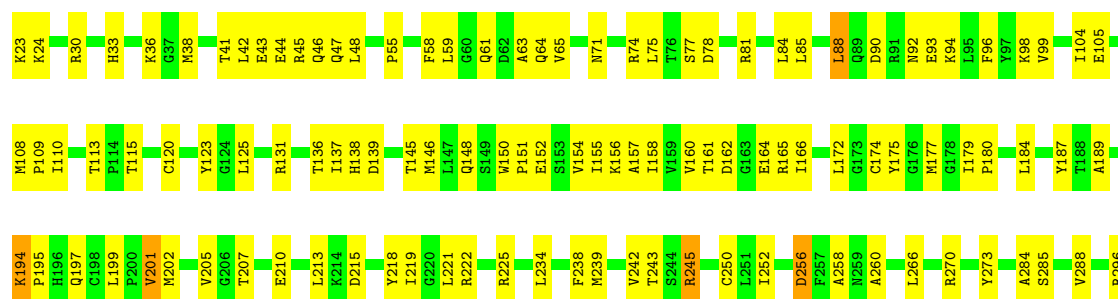
• Molecule 1: MALIC ENZYME

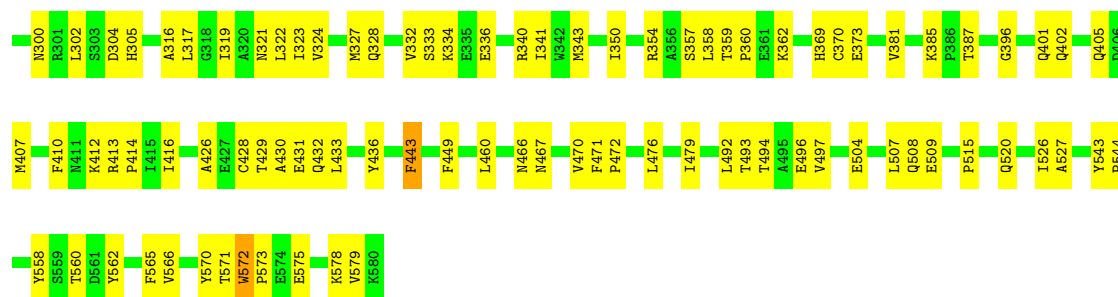
Chain N: 61% 38%



• Molecule 1: MALIC ENZYME

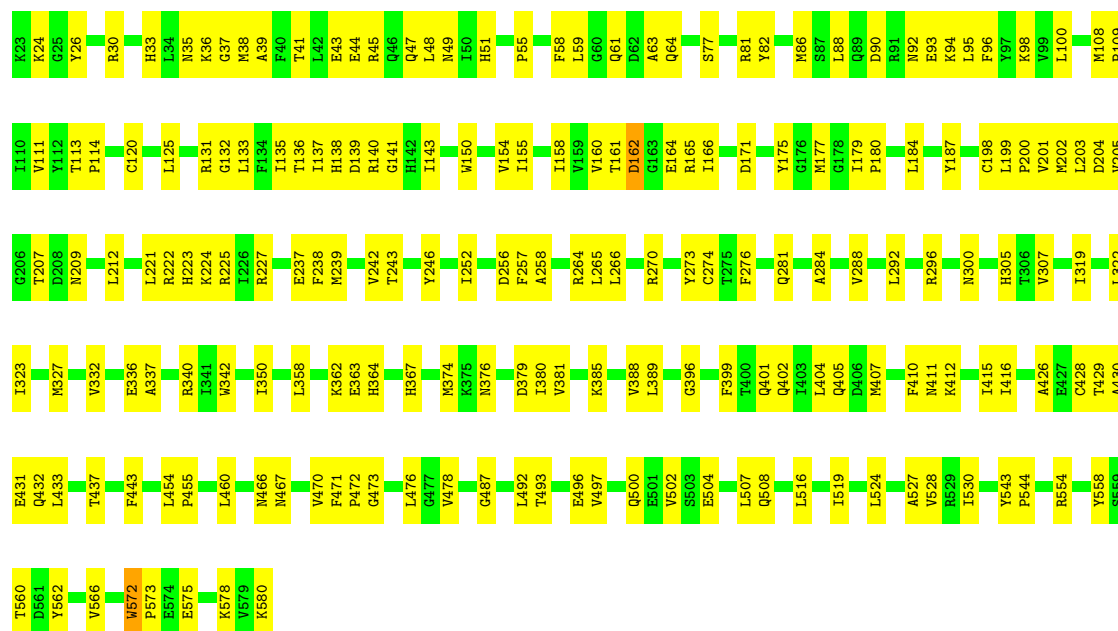
Chain O: 64% 35%





● Molecule 1: MALIC ENZYME

Chain P: 65% 35%



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	124.15Å 140.86Å 167.08Å 90.05° 87.16° 75.63°	Depositor
Resolution (Å)	10.00 – 2.50	Depositor
% Data completeness (in resolution range)	83.0 (10.00-2.50)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.210 , 0.256	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	71519	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAP, NA, OXL, CL, MN

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	0.45	0/4420	0.93	10/5962 (0.2%)
1	B	0.45	0/4420	0.94	11/5962 (0.2%)
1	C	0.48	0/4420	0.92	8/5962 (0.1%)
1	D	0.47	0/4420	0.95	15/5962 (0.3%)
1	E	0.46	0/4420	0.93	10/5962 (0.2%)
1	F	0.48	0/4420	0.95	7/5962 (0.1%)
1	G	0.47	0/4420	0.94	12/5962 (0.2%)
1	H	0.49	1/4420 (0.0%)	0.94	12/5962 (0.2%)
1	I	0.50	0/4420	0.95	12/5962 (0.2%)
1	J	0.48	0/4420	0.94	14/5962 (0.2%)
1	K	0.46	0/4420	0.92	11/5962 (0.2%)
1	L	0.47	0/4420	0.94	10/5962 (0.2%)
1	M	0.50	0/4420	0.94	14/5962 (0.2%)
1	N	0.48	0/4420	0.96	11/5962 (0.2%)
1	O	0.48	0/4420	0.93	12/5962 (0.2%)
1	P	0.48	0/4421	0.93	9/5962 (0.2%)
All	All	0.47	1/70721 (0.0%)	0.94	178/95392 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	55	PRO	CA-C	5.61	1.54	1.51

The worst 5 of 178 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	470	VAL	N-CA-C	9.43	119.67	111.56
1	N	470	VAL	N-CA-C	8.99	119.93	111.48
1	J	470	VAL	N-CA-C	8.94	119.24	111.56
1	E	470	VAL	N-CA-C	8.93	119.24	111.56
1	G	470	VAL	N-CA-C	8.83	119.78	111.48

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4345	0	4366	235	0
1	B	4345	0	4366	224	0
1	C	4345	0	4366	222	0
1	D	4345	0	4366	200	0
1	E	4345	0	4366	193	0
1	F	4345	0	4366	198	0
1	G	4345	0	4366	199	0
1	H	4345	0	4366	186	0
1	I	4345	0	4366	185	0
1	J	4345	0	4366	205	0
1	K	4345	0	4366	211	0
1	L	4345	0	4366	230	0
1	M	4345	0	4366	192	0
1	N	4345	0	4366	211	0
1	O	4345	0	4366	228	0
1	P	4346	0	4366	198	0
2	A	48	0	25	4	0
2	B	48	0	25	4	0
2	C	48	0	25	2	0
2	D	48	0	25	2	0
2	E	48	0	25	3	0
2	F	48	0	25	2	0
2	G	48	0	25	3	0
2	H	48	0	25	3	0
2	I	48	0	25	3	0
2	J	48	0	25	4	0
2	K	48	0	25	5	0
2	L	48	0	25	5	0
2	M	48	0	25	3	0
2	N	48	0	25	3	0
2	O	48	0	25	2	0
2	P	48	0	25	1	0
3	A	6	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	6	0	0	1	0
3	C	6	0	0	3	0
3	D	6	0	0	2	0
3	E	6	0	0	1	0
3	F	6	0	0	1	0
3	G	6	0	0	1	0
3	H	6	0	0	1	0
3	I	6	0	0	0	0
3	J	6	0	0	1	0
3	K	6	0	0	1	0
3	L	6	0	0	1	0
3	M	6	0	0	0	0
3	N	6	0	0	1	0
3	O	6	0	0	0	0
3	P	6	0	0	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
4	I	1	0	0	0	0
4	J	1	0	0	0	0
4	K	1	0	0	0	0
4	L	1	0	0	0	0
4	M	1	0	0	0	0
4	N	1	0	0	0	0
4	O	1	0	0	0	0
4	P	1	0	0	0	0
5	B	1	0	0	0	0
5	C	4	0	0	1	0
5	E	3	0	0	1	0
5	F	2	0	0	1	0
5	G	1	0	0	0	0
5	H	1	0	0	0	0
5	I	5	0	0	1	0
5	J	2	0	0	0	0
5	K	1	0	0	0	0
5	L	1	0	0	0	0
5	M	3	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	N	2	0	0	1	0
5	O	4	0	0	3	0
5	P	3	0	0	3	0
6	C	4	0	0	0	0
6	D	2	0	0	0	0
6	F	2	0	0	0	0
6	G	1	0	0	0	0
6	H	5	0	0	0	0
6	I	2	0	0	0	0
6	J	2	0	0	0	0
6	K	1	0	0	0	0
6	L	1	0	0	0	0
6	M	6	0	0	0	0
6	N	1	0	0	0	0
6	O	4	0	0	0	0
6	P	5	0	0	0	0
7	A	35	0	0	6	0
7	B	42	0	0	6	0
7	C	77	0	0	7	0
7	D	49	0	0	2	0
7	E	58	0	0	5	0
7	F	78	0	0	6	0
7	G	65	0	0	6	0
7	H	77	0	0	7	0
7	I	80	0	0	7	0
7	J	63	0	0	3	0
7	K	41	0	0	5	0
7	L	75	0	0	7	0
7	M	81	0	0	7	0
7	N	71	0	0	7	0
7	O	78	0	0	8	0
7	P	79	0	0	4	0
All	All	71519	0	70256	3218	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 23.

The worst 5 of 3218 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:H:136:THR:HG22	1:H:138:HIS:H	1.08	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:136:THR:HG22	1:N:138:HIS:H	1.04	1.17
1:K:98:LYS:HD3	1:K:560:THR:HG21	1.30	1.14
1:B:136:THR:HG22	1:B:138:HIS:H	1.06	1.13
1:F:136:THR:HG22	1:F:138:HIS:H	1.10	1.13

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 117 ligands modelled in this entry, 85 are monoatomic - leaving 32 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	OXL	D	1582	6,4	5,5,5	1.89	2 (40%)	6,6,6	2.40	2 (33%)
2	NAP	P	1581	-	50,52,52	1.94	10 (20%)	71,80,80	1.86	12 (16%)
3	OXL	K	1582	4	5,5,5	1.90	2 (40%)	6,6,6	2.47	3 (50%)
3	OXL	B	1582	4	5,5,5	1.63	2 (40%)	6,6,6	2.50	2 (33%)
3	OXL	J	1582	4	5,5,5	1.90	2 (40%)	6,6,6	2.47	2 (33%)
3	OXL	L	1582	4	5,5,5	2.01	2 (40%)	6,6,6	2.43	2 (33%)
2	NAP	O	1581	-	50,52,52	1.98	10 (20%)	71,80,80	1.88	12 (16%)
2	NAP	A	1581	-	50,52,52	1.90	12 (24%)	71,80,80	1.87	11 (15%)
3	OXL	G	1582	4	5,5,5	1.74	2 (40%)	6,6,6	2.49	2 (33%)
3	OXL	M	1582	4	5,5,5	1.95	2 (40%)	6,6,6	2.42	2 (33%)
3	OXL	P	1582	4	5,5,5	1.88	2 (40%)	6,6,6	2.44	2 (33%)
2	NAP	H	1581	-	50,52,52	1.99	13 (26%)	71,80,80	1.89	12 (16%)
2	NAP	J	1581	-	50,52,52	2.01	11 (22%)	71,80,80	1.90	13 (18%)
2	NAP	C	1581	-	50,52,52	1.92	9 (18%)	71,80,80	1.85	12 (16%)
2	NAP	B	1581	-	50,52,52	1.95	14 (28%)	71,80,80	1.85	12 (16%)
2	NAP	N	1581	-	50,52,52	1.99	11 (22%)	71,80,80	1.93	11 (15%)
2	NAP	I	1581	-	50,52,52	2.10	14 (28%)	71,80,80	1.85	12 (16%)
2	NAP	L	1581	-	50,52,52	2.02	13 (26%)	71,80,80	1.85	10 (14%)
3	OXL	O	1582	4	5,5,5	1.79	2 (40%)	6,6,6	2.56	4 (66%)
2	NAP	G	1581	-	50,52,52	1.87	11 (22%)	71,80,80	1.85	11 (15%)
3	OXL	N	1582	4	5,5,5	1.89	2 (40%)	6,6,6	2.37	2 (33%)
3	OXL	A	1583	4	5,5,5	1.90	2 (40%)	6,6,6	2.39	2 (33%)
2	NAP	F	1581	-	50,52,52	1.84	8 (16%)	71,80,80	1.87	11 (15%)
3	OXL	C	1582	4	5,5,5	1.75	2 (40%)	6,6,6	2.44	2 (33%)
2	NAP	M	1581	-	50,52,52	1.90	10 (20%)	71,80,80	1.85	12 (16%)
3	OXL	E	1582	4	5,5,5	1.70	2 (40%)	6,6,6	2.50	2 (33%)
2	NAP	E	1581	-	50,52,52	2.03	13 (26%)	71,80,80	1.86	12 (16%)
2	NAP	D	1581	-	50,52,52	1.92	9 (18%)	71,80,80	1.85	12 (16%)
3	OXL	H	1582	4	5,5,5	1.90	2 (40%)	6,6,6	2.41	2 (33%)
2	NAP	K	1581	-	50,52,52	2.00	9 (18%)	71,80,80	1.88	13 (18%)
3	OXL	I	1582	4	5,5,5	1.94	2 (40%)	6,6,6	2.45	2 (33%)
3	OXL	F	1582	4	5,5,5	1.89	2 (40%)	6,6,6	2.38	2 (33%)

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
3	OXL	D	1582	6,4	-	0/4/4/4	-
2	NAP	P	1581	-	-	5/35/67/67	0/5/5/5
3	OXL	K	1582	4	-	0/4/4/4	-
3	OXL	B	1582	4	-	0/4/4/4	-
3	OXL	J	1582	4	-	0/4/4/4	-
3	OXL	L	1582	4	-	0/4/4/4	-
2	NAP	O	1581	-	-	4/35/67/67	0/5/5/5
2	NAP	A	1581	-	-	3/35/67/67	0/5/5/5
3	OXL	G	1582	4	-	0/4/4/4	-
3	OXL	M	1582	4	-	0/4/4/4	-
3	OXL	P	1582	4	-	0/4/4/4	-
2	NAP	H	1581	-	-	7/35/67/67	0/5/5/5
2	NAP	J	1581	-	-	6/35/67/67	0/5/5/5
2	NAP	C	1581	-	-	6/35/67/67	0/5/5/5
2	NAP	B	1581	-	-	4/35/67/67	0/5/5/5
2	NAP	N	1581	-	-	5/35/67/67	0/5/5/5
2	NAP	I	1581	-	-	4/35/67/67	0/5/5/5
2	NAP	L	1581	-	-	4/35/67/67	0/5/5/5
3	OXL	O	1582	4	-	0/4/4/4	-
2	NAP	G	1581	-	-	4/35/67/67	0/5/5/5
3	OXL	N	1582	4	-	0/4/4/4	-
3	OXL	A	1583	4	-	0/4/4/4	-
2	NAP	F	1581	-	-	4/35/67/67	0/5/5/5
3	OXL	C	1582	4	-	0/4/4/4	-
2	NAP	M	1581	-	-	6/35/67/67	0/5/5/5
3	OXL	E	1582	4	-	0/4/4/4	-
2	NAP	E	1581	-	-	4/35/67/67	0/5/5/5
2	NAP	D	1581	-	-	7/35/67/67	0/5/5/5
3	OXL	H	1582	4	-	0/4/4/4	-
2	NAP	K	1581	-	-	5/35/67/67	0/5/5/5
3	OXL	I	1582	4	-	0/4/4/4	-
3	OXL	F	1582	4	-	0/4/4/4	-

The worst 5 of 209 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	1581	NAP	C2N-N1N	8.01	1.43	1.35
2	J	1581	NAP	C2N-N1N	7.92	1.43	1.35
2	E	1581	NAP	C2N-N1N	7.72	1.43	1.35
2	P	1581	NAP	C2N-N1N	7.72	1.43	1.35
2	D	1581	NAP	C2N-N1N	7.53	1.43	1.35

The worst 5 of 223 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	1581	NAP	C5A-C4A-N3A	-6.20	118.18	126.72
2	K	1581	NAP	C5A-C4A-N3A	-6.06	118.37	126.72
2	B	1581	NAP	C5A-C4A-N3A	-5.99	118.47	126.72
2	O	1581	NAP	C5A-C4A-N3A	-5.96	118.51	126.72
2	A	1581	NAP	C5A-C4A-N3A	-5.93	118.55	126.72

There are no chirality outliers.

5 of 78 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1581	NAP	O4D-C1D-N1N-C6N
2	C	1581	NAP	O4D-C1D-N1N-C6N
2	D	1581	NAP	O4D-C1D-N1N-C6N
2	F	1581	NAP	O4D-C1D-N1N-C6N
2	H	1581	NAP	C5B-O5B-PA-O1A

There are no ring outliers.

29 monomers are involved in 65 short contacts:

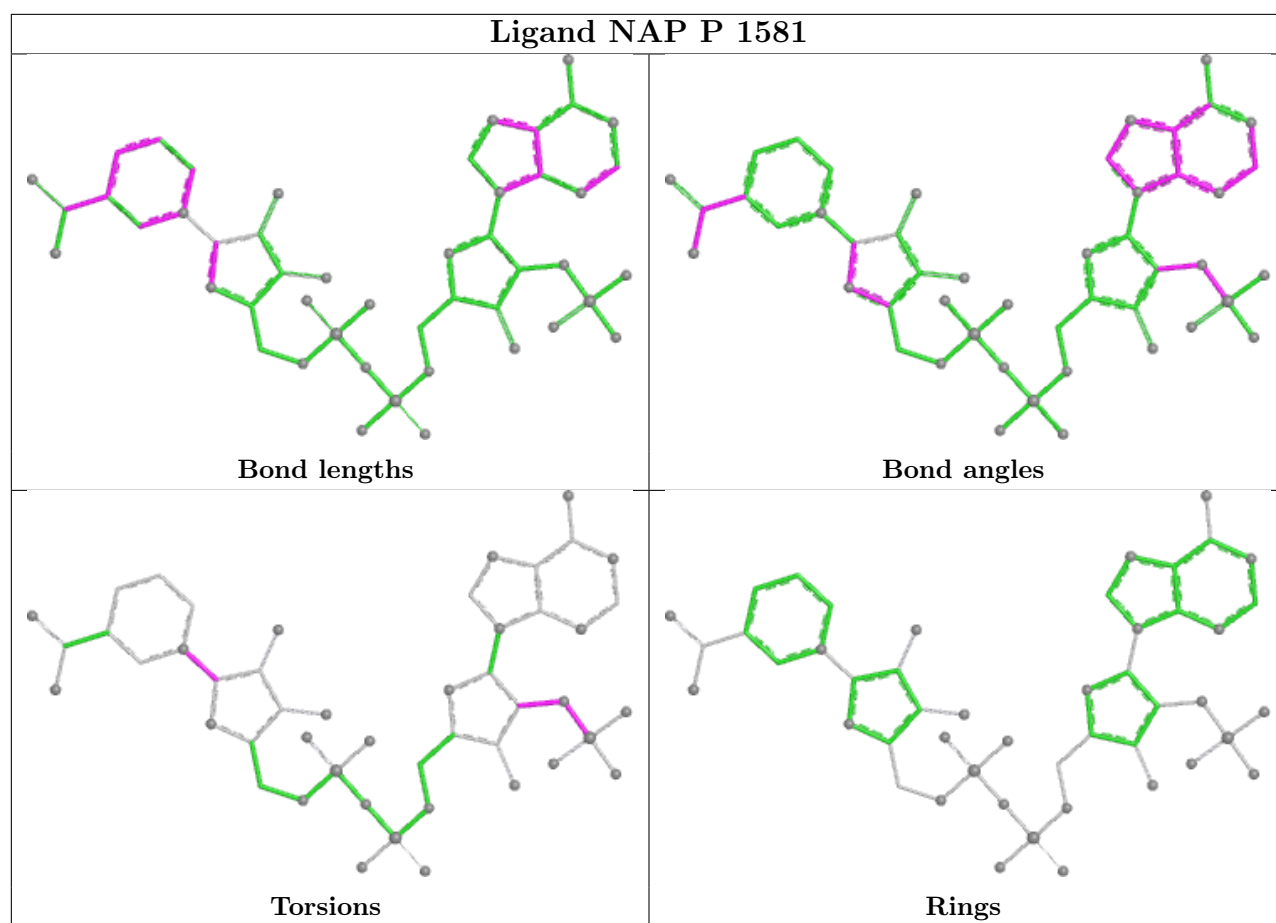
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1582	OXL	2	0
2	P	1581	NAP	1	0
3	K	1582	OXL	1	0
3	B	1582	OXL	1	0
3	J	1582	OXL	1	0
3	L	1582	OXL	1	0
2	O	1581	NAP	2	0
2	A	1581	NAP	4	0
3	G	1582	OXL	1	0
3	P	1582	OXL	1	0
2	H	1581	NAP	3	0
2	J	1581	NAP	4	0
2	C	1581	NAP	2	0

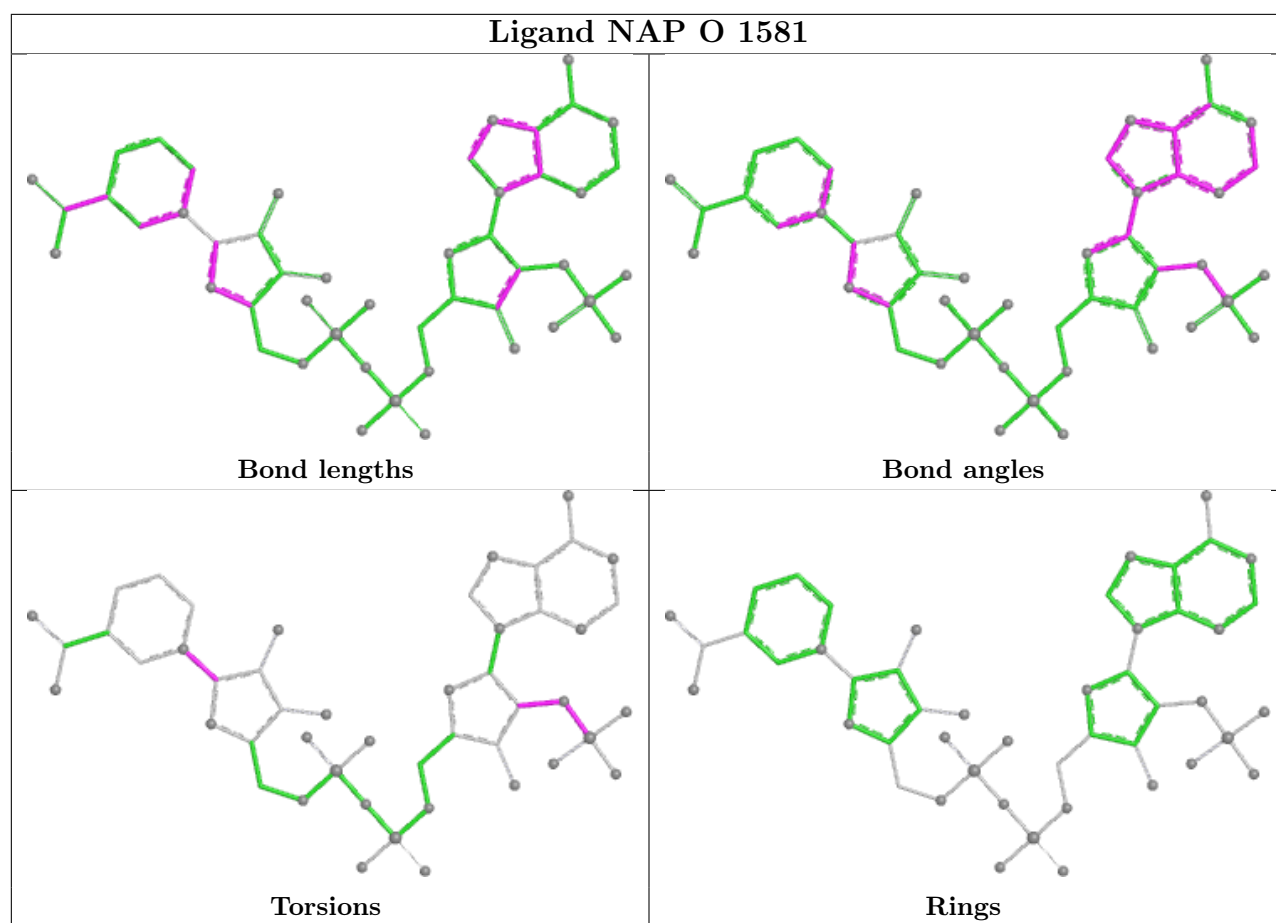
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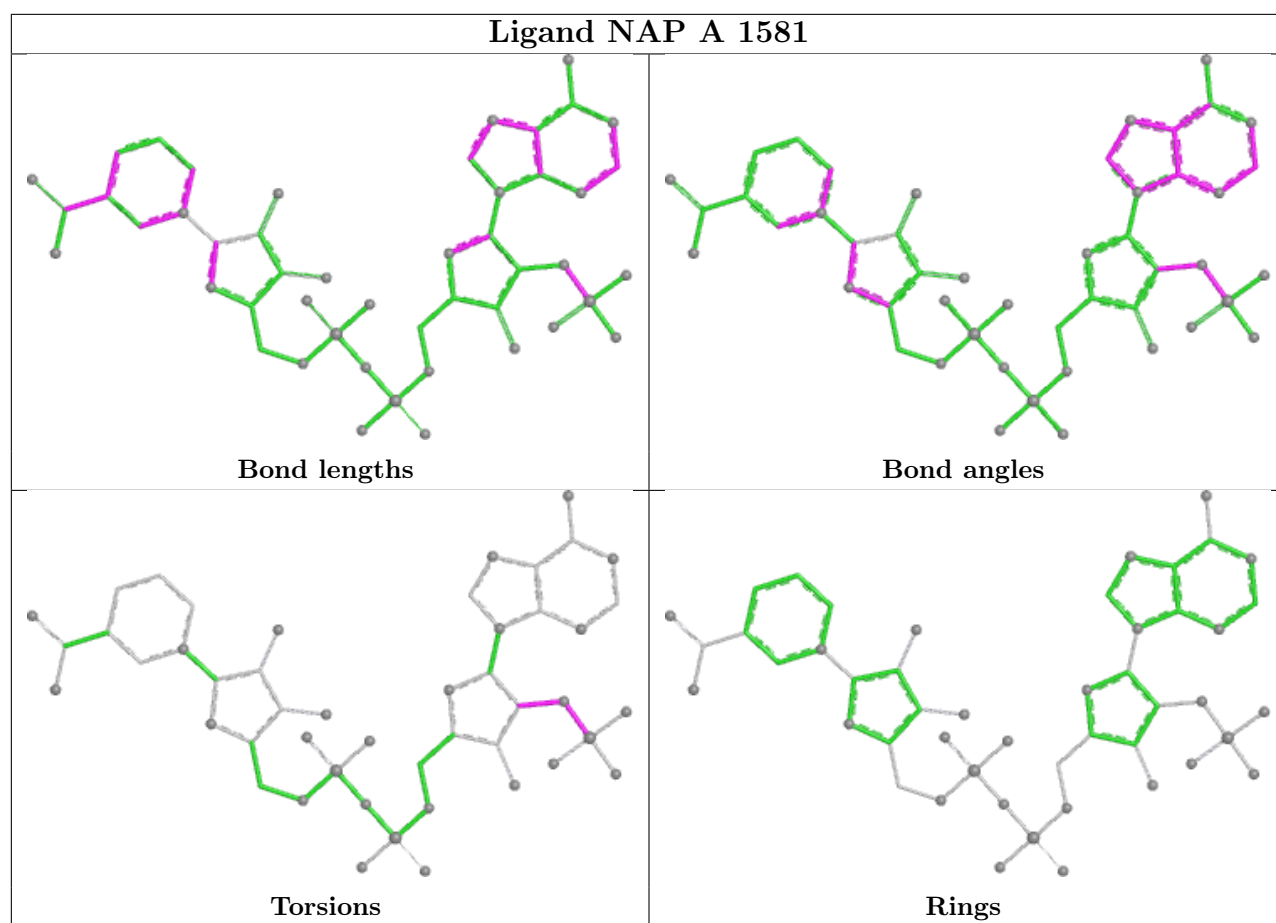
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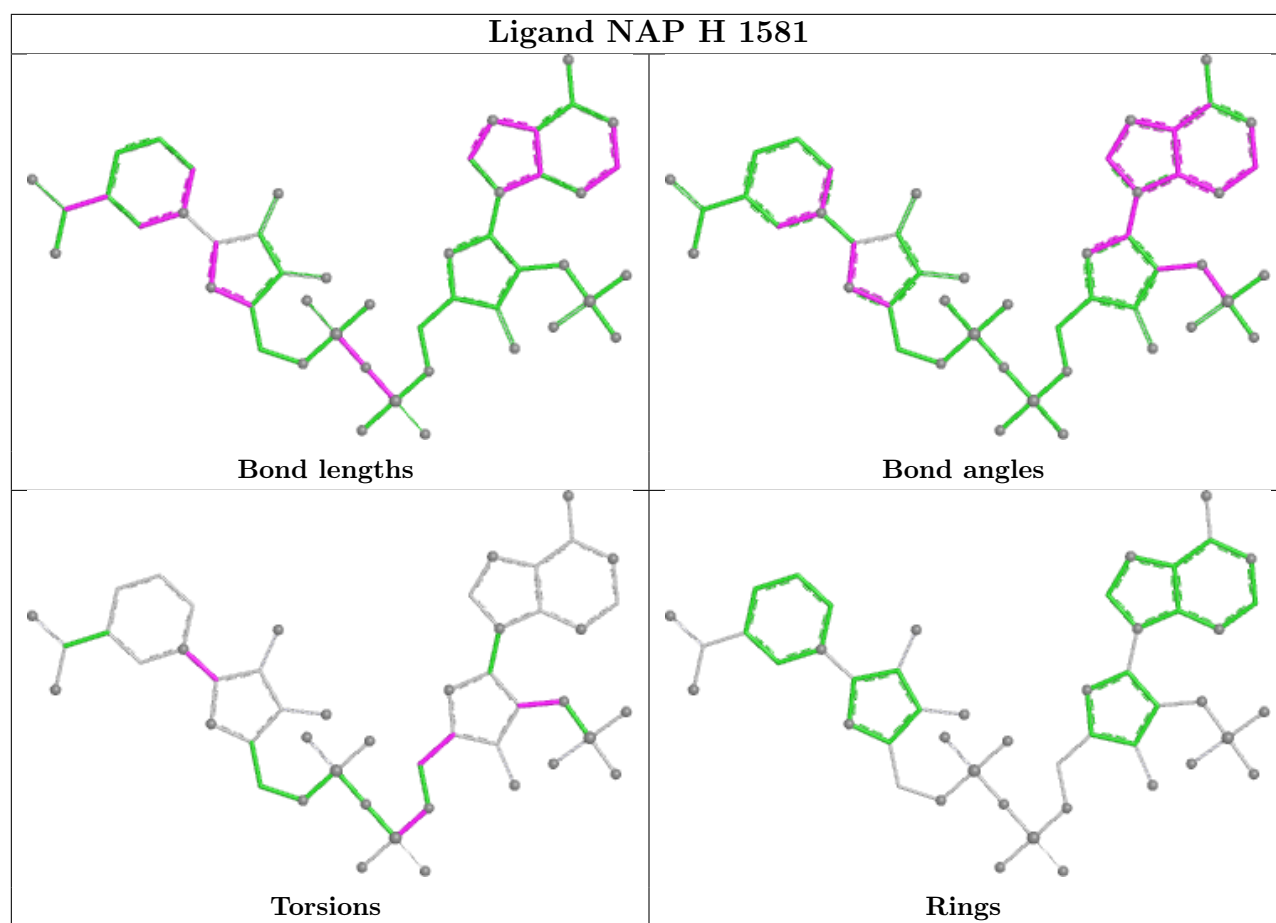
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1581	NAP	4	0
2	N	1581	NAP	3	0
2	I	1581	NAP	3	0
2	L	1581	NAP	5	0
2	G	1581	NAP	3	0
3	N	1582	OXL	1	0
3	A	1583	OXL	1	0
2	F	1581	NAP	2	0
3	C	1582	OXL	3	0
2	M	1581	NAP	3	0
3	E	1582	OXL	1	0
2	E	1581	NAP	3	0
2	D	1581	NAP	2	0
3	H	1582	OXL	1	0
2	K	1581	NAP	5	0
3	F	1582	OXL	1	0

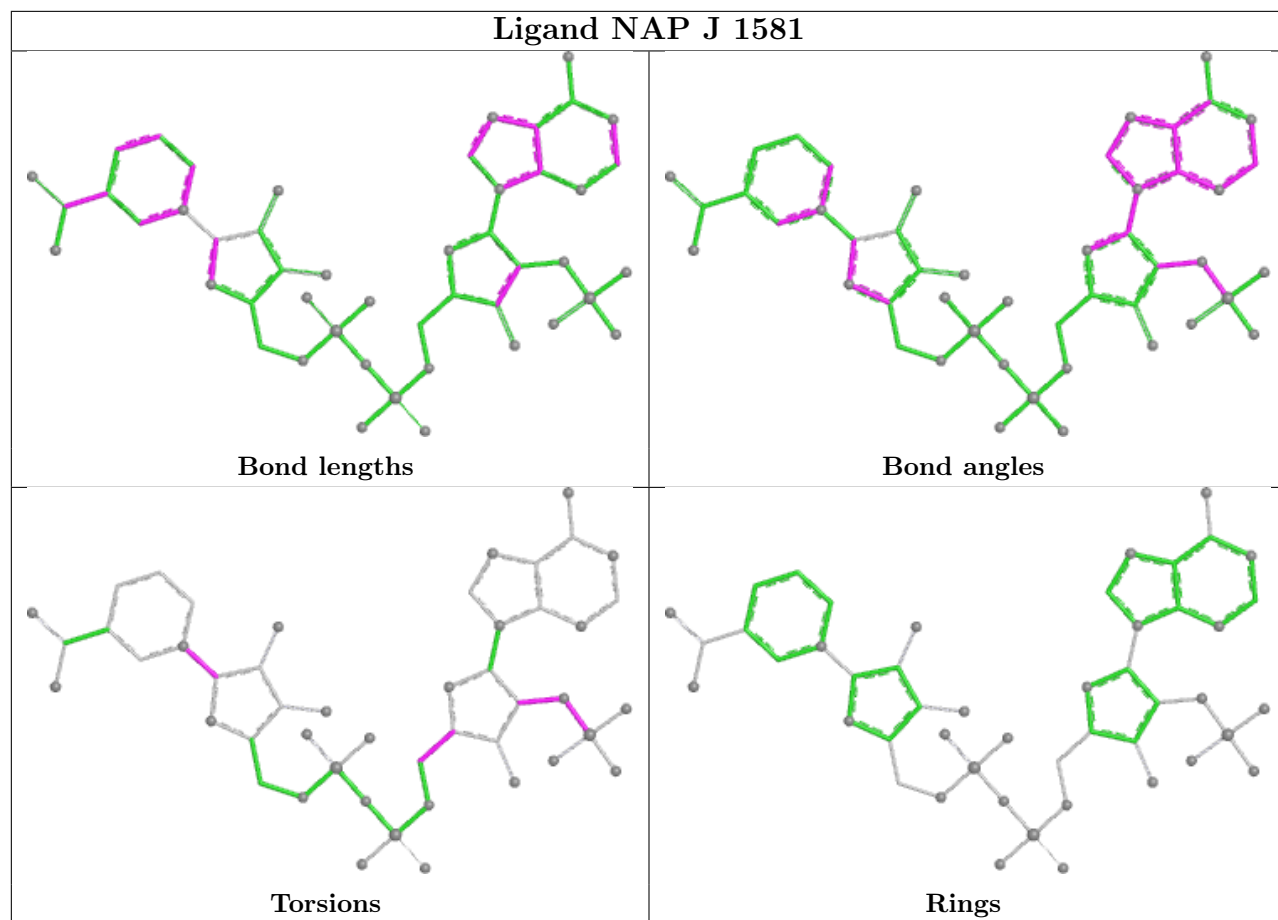
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

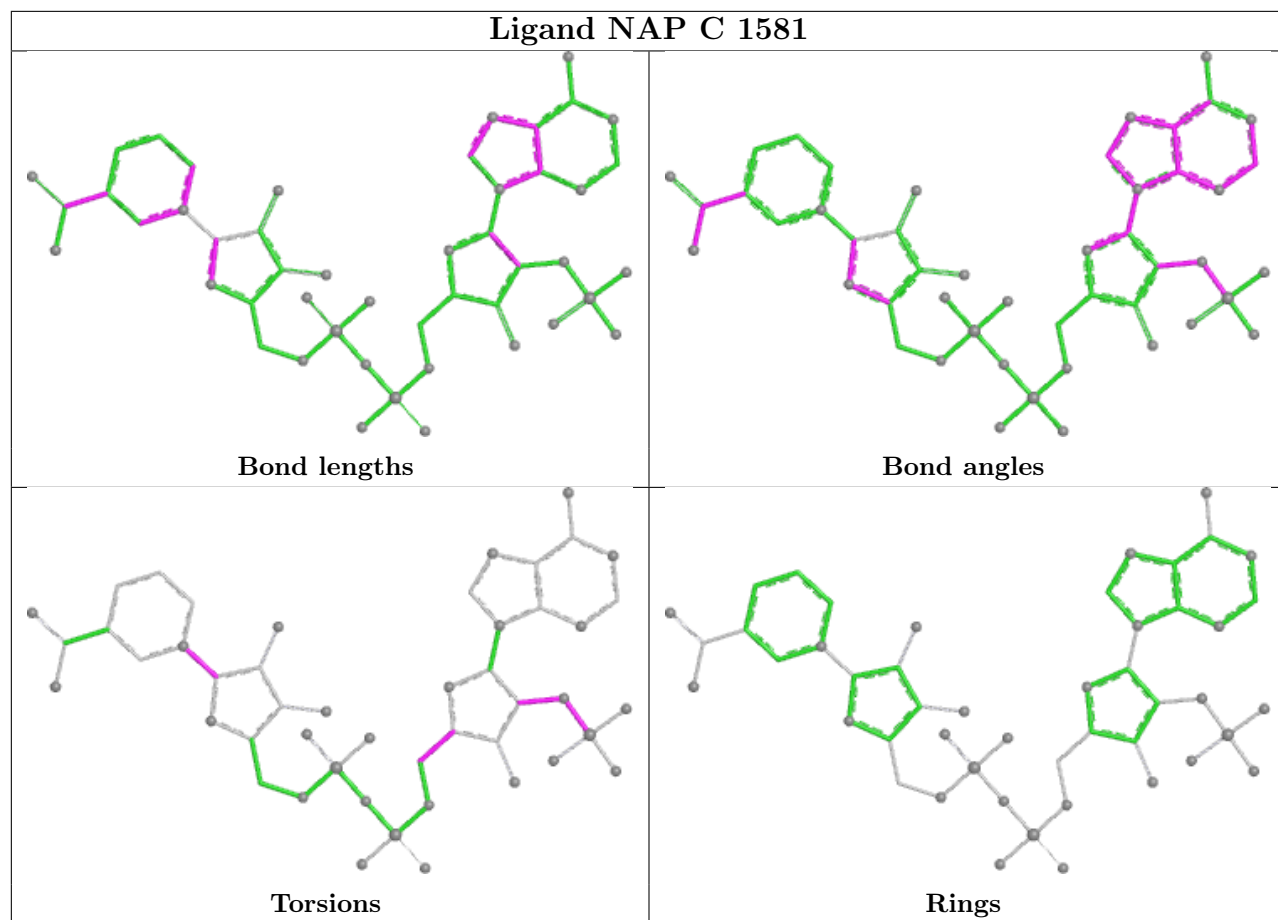


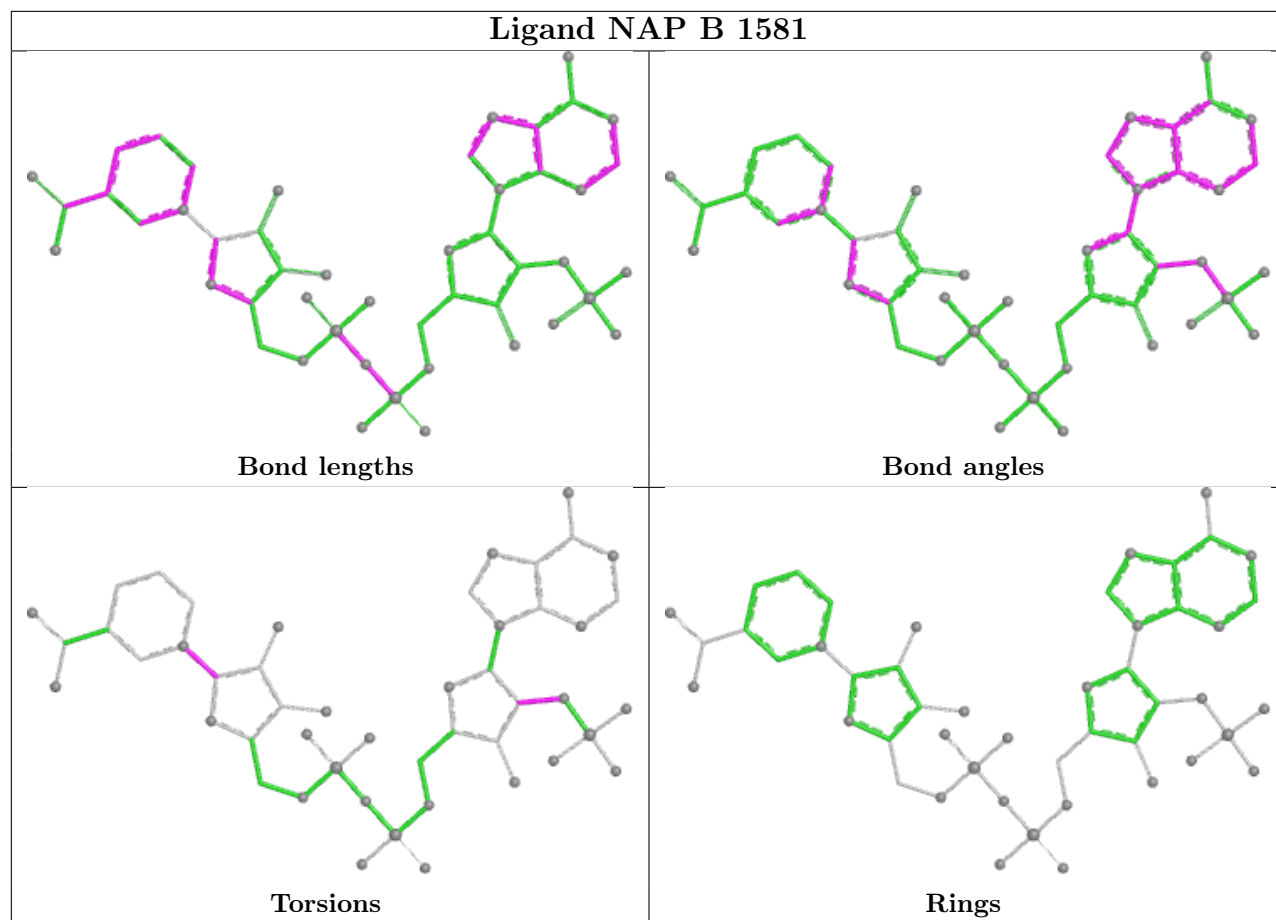


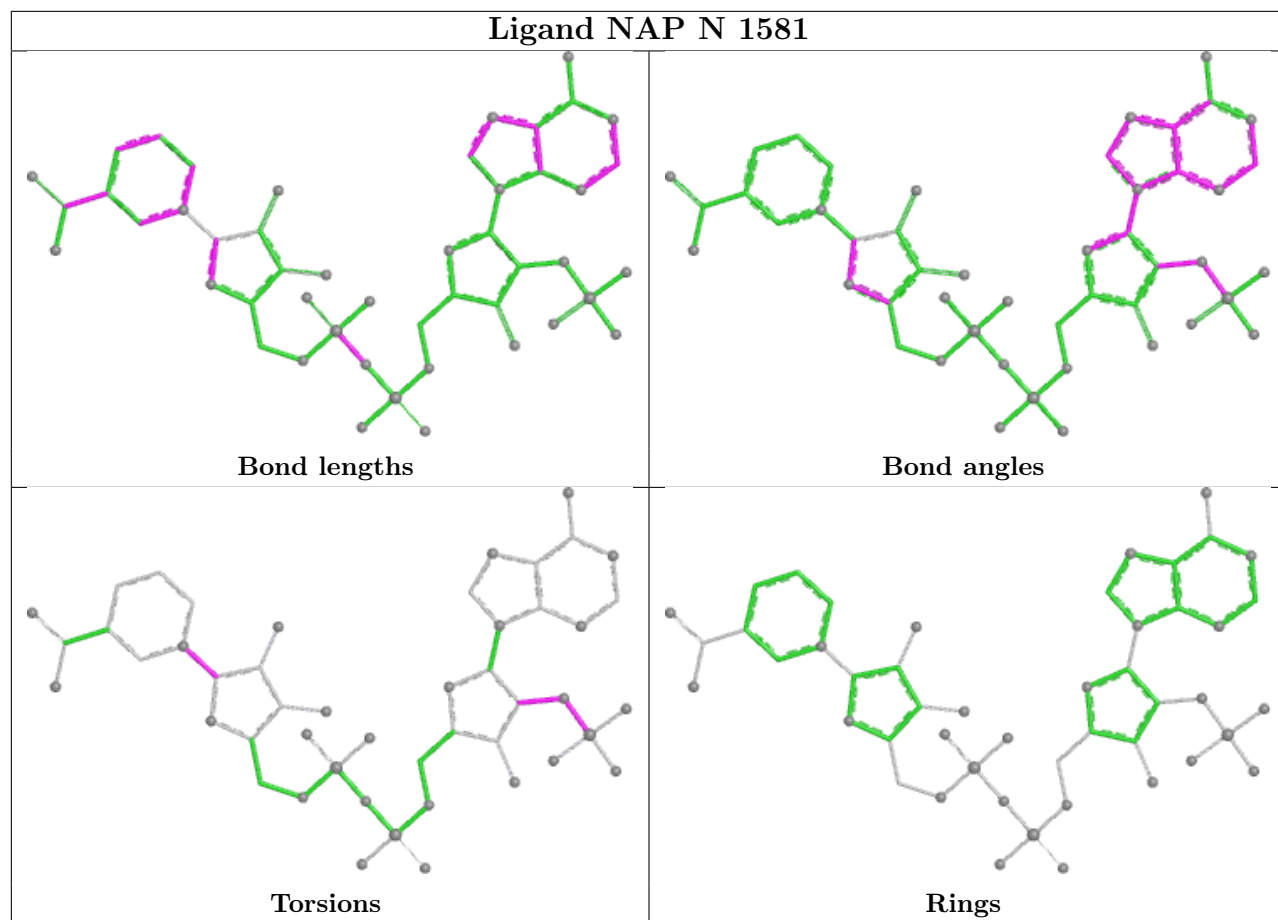


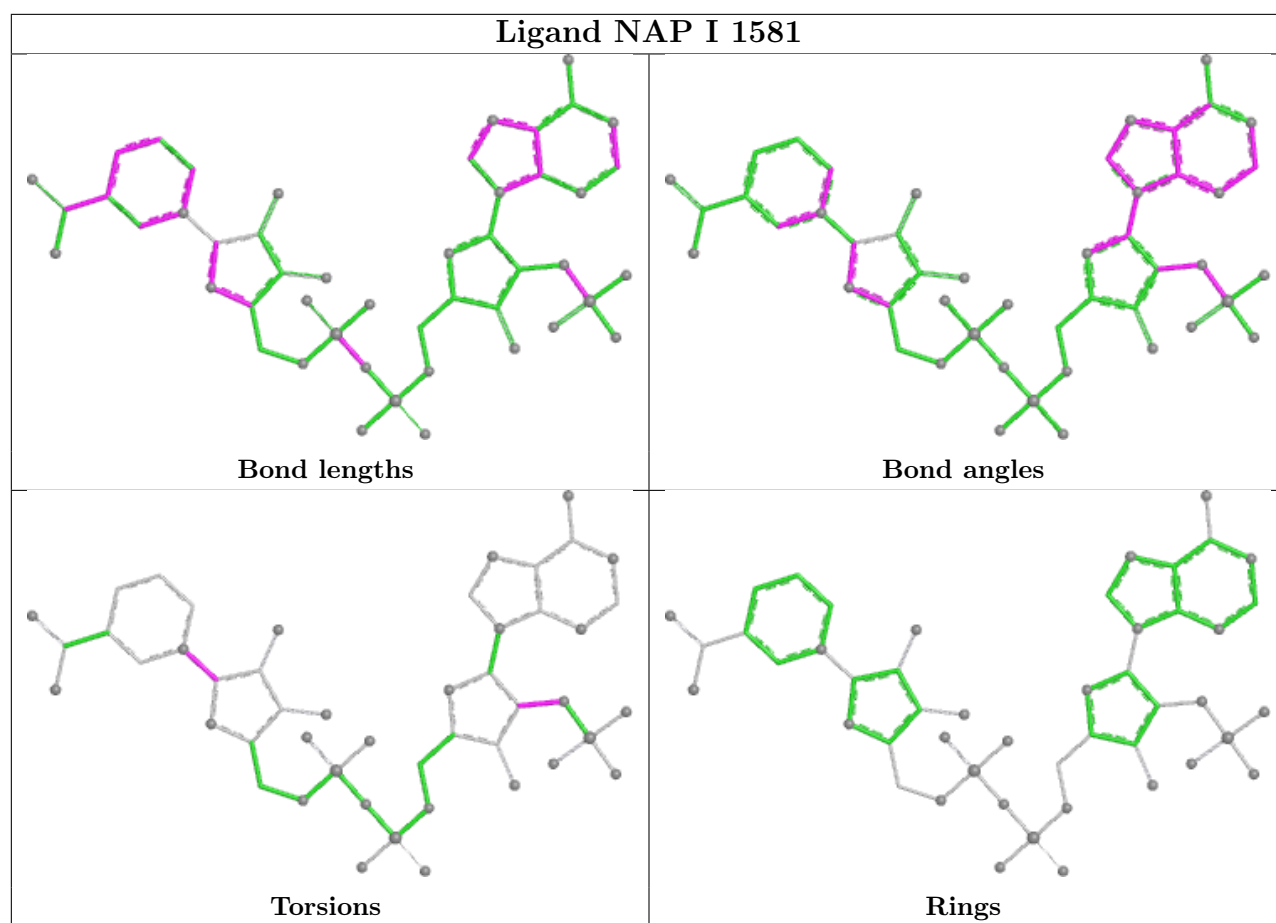


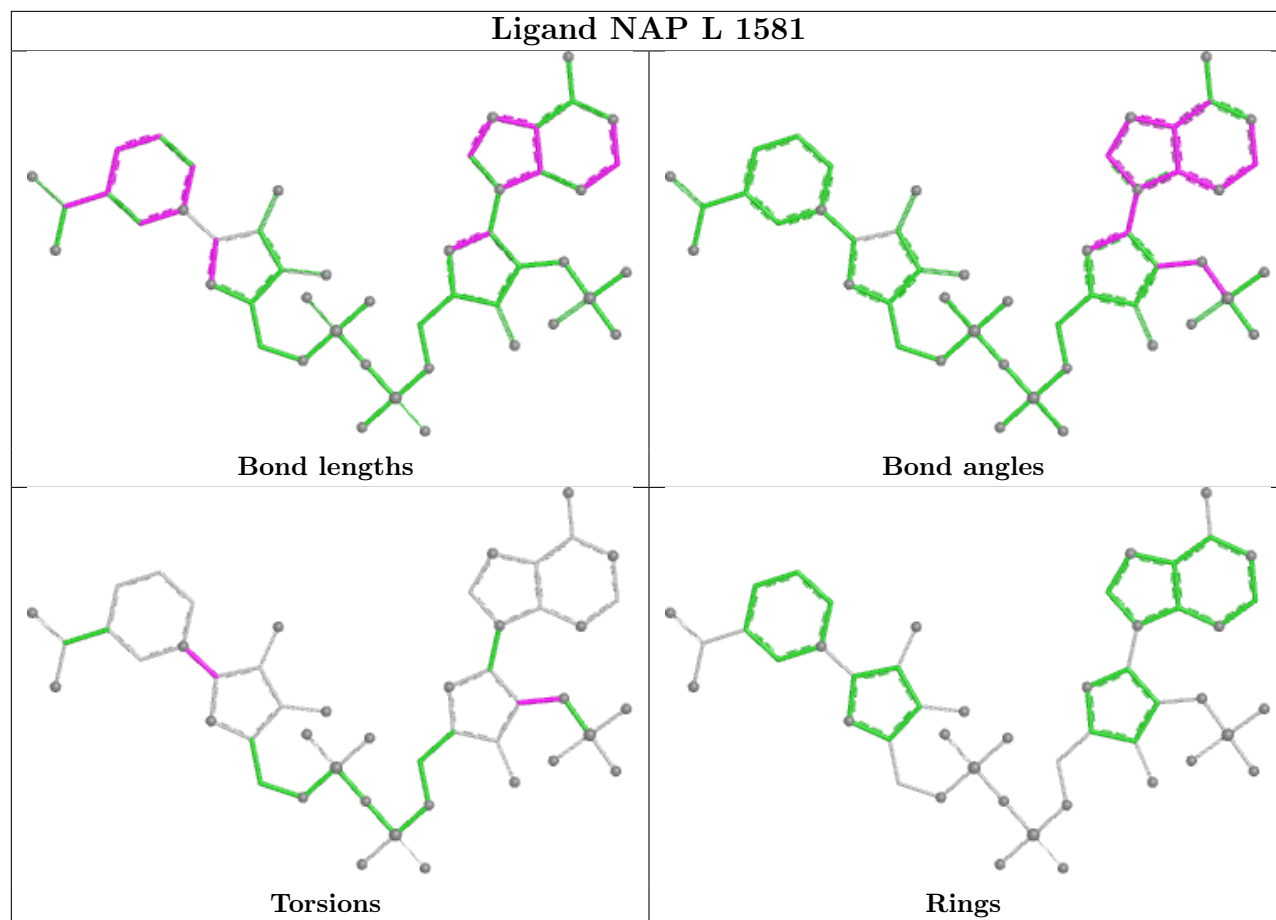


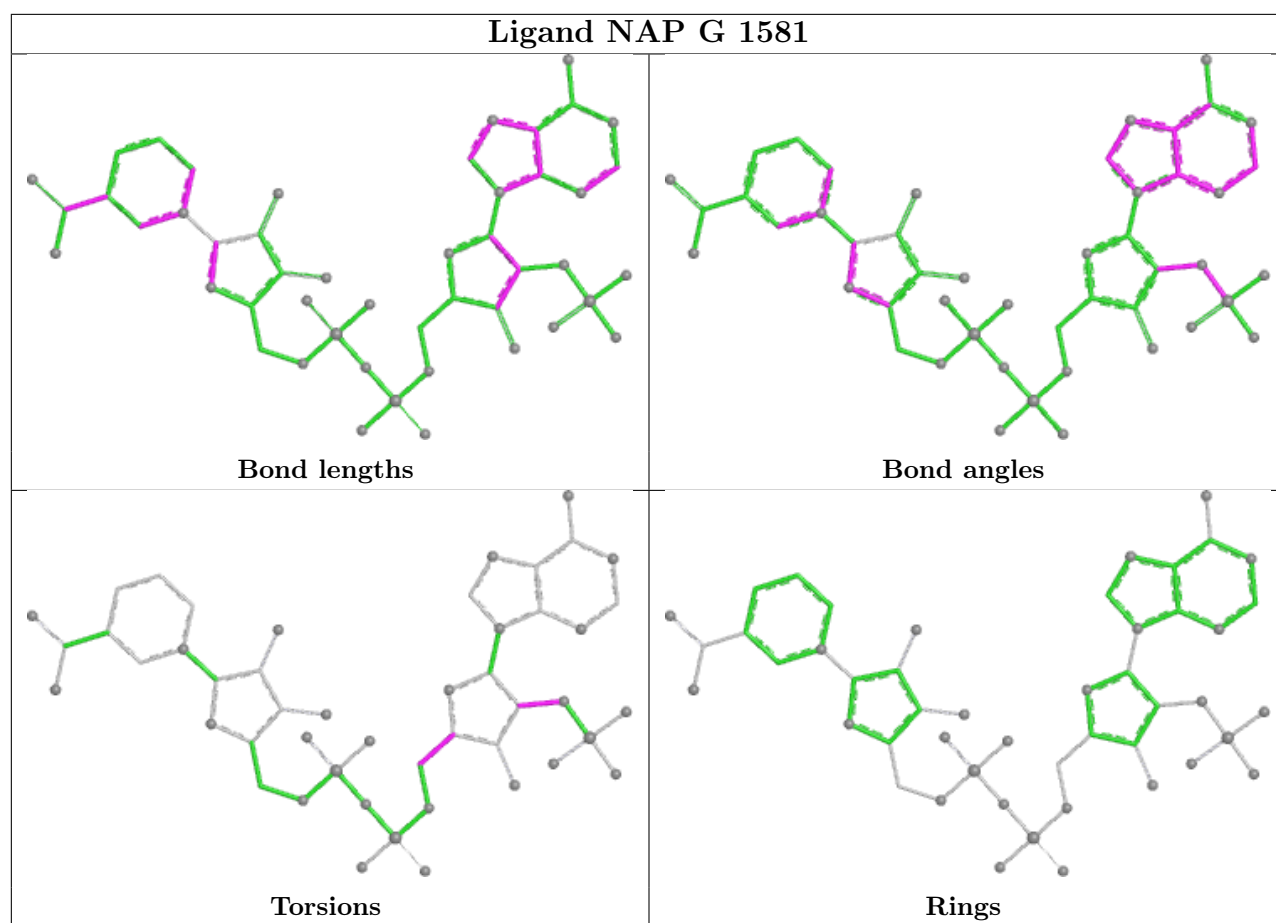


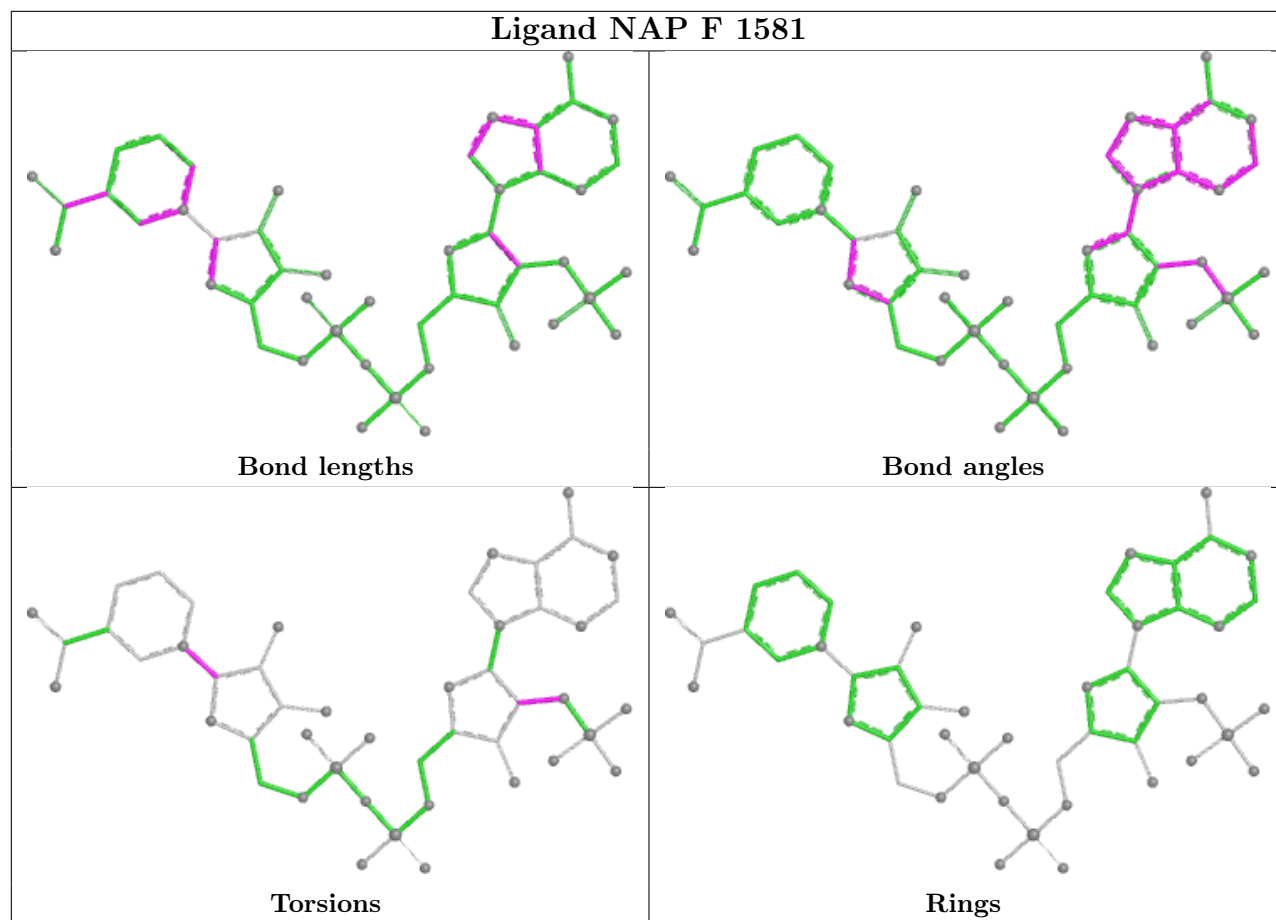




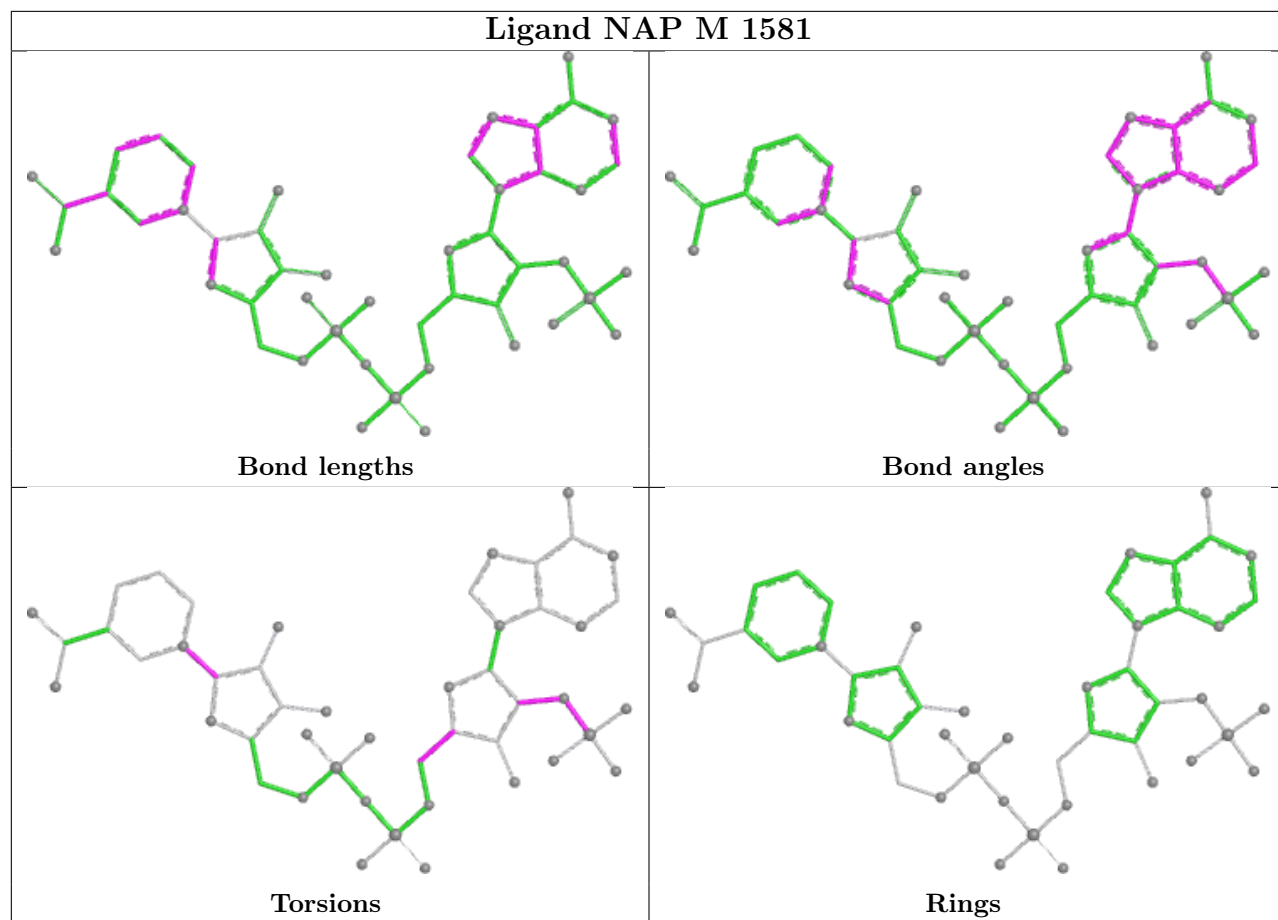


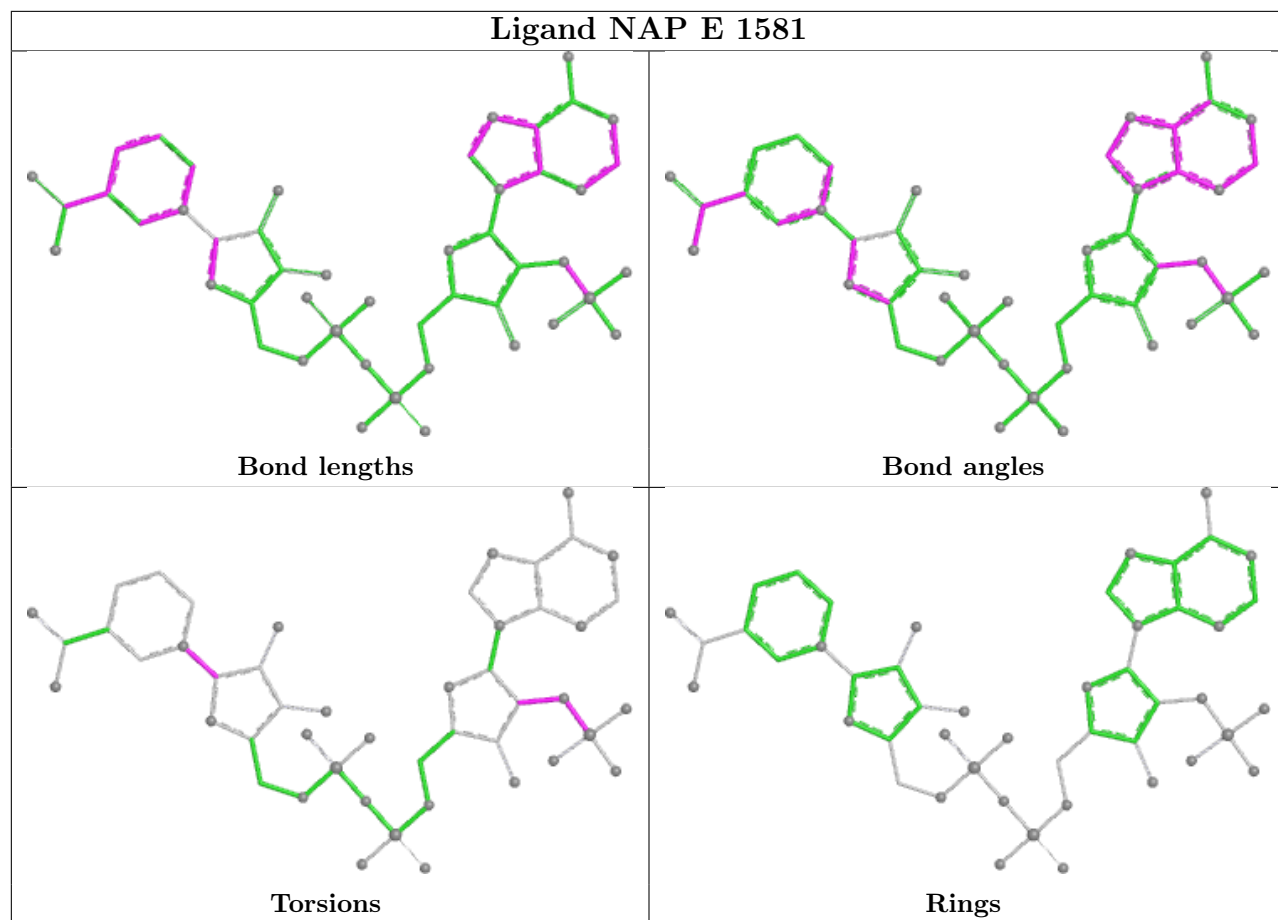


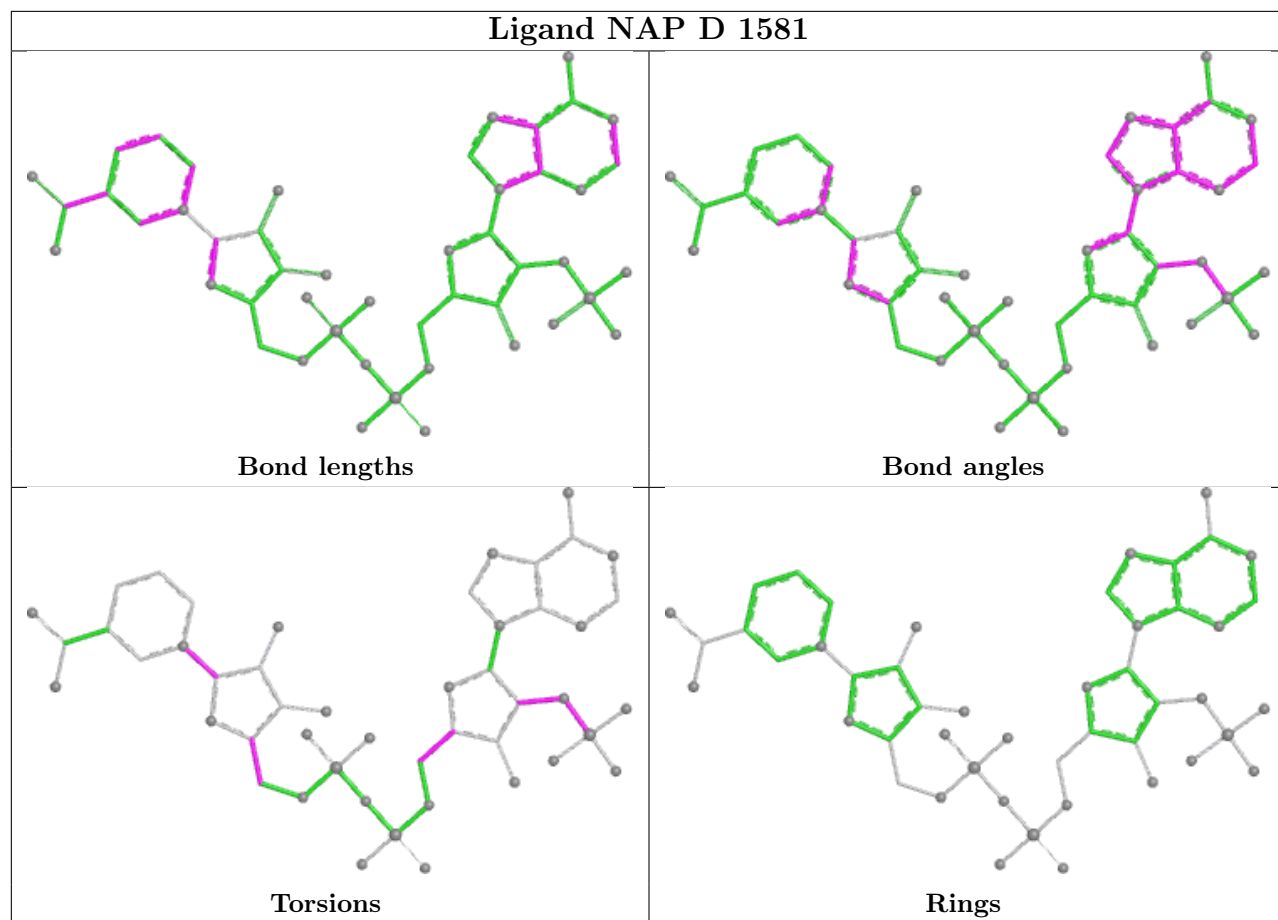


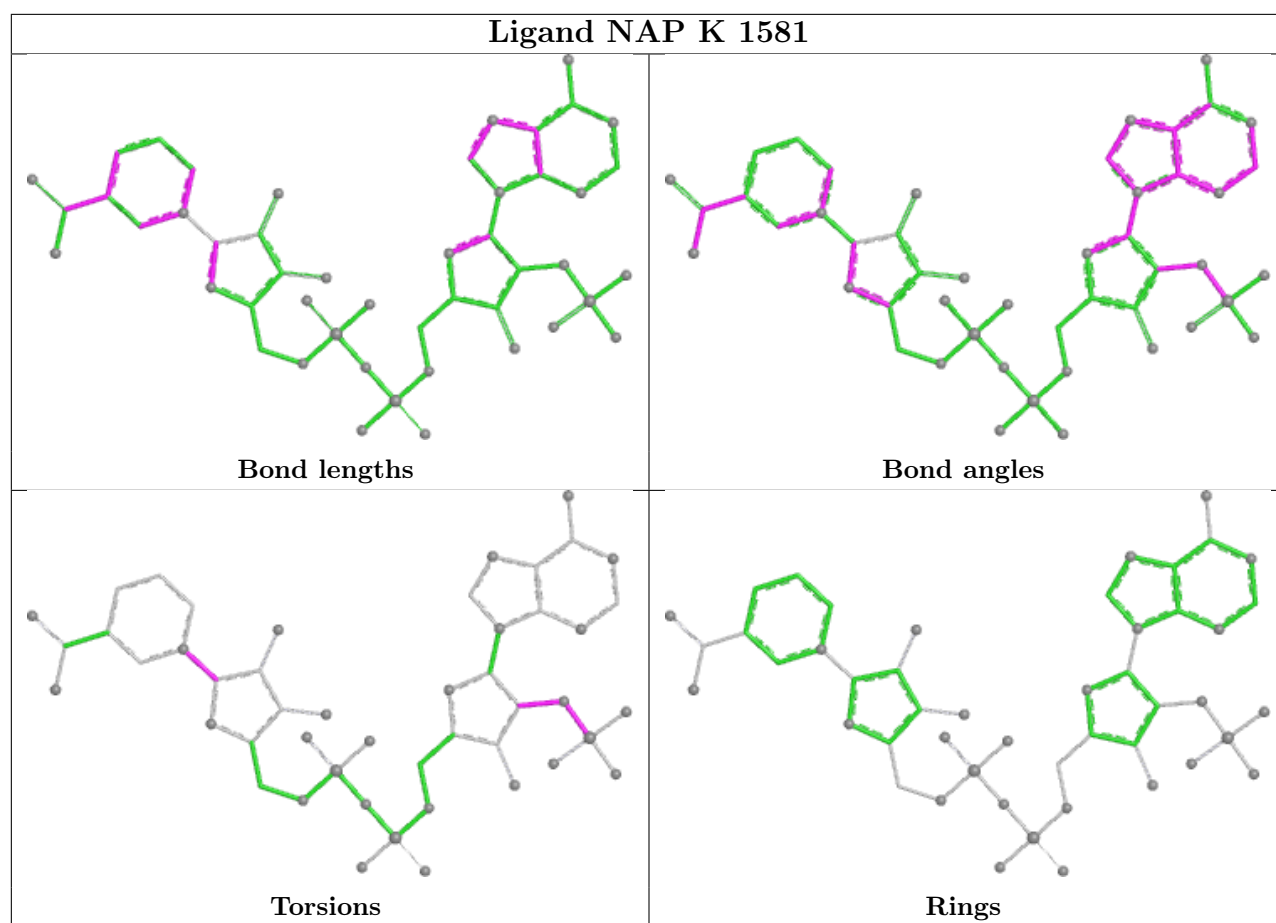


Ligand NAP M 1581









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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.