



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:05 AM UTC

PDB ID : 9HAQ / pdb\_00009haq  
Title : Crystal structure of methionine gamma-lyase from *Brevibacterium sandarakinum* in complex with PLP and norleucine at pH 8.5  
Authors : Kopecny, D.; Ferchaud, N.; Briozzo, P.  
Deposited on : 2024-11-04  
Resolution : 2.69 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](mailto: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>.

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

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

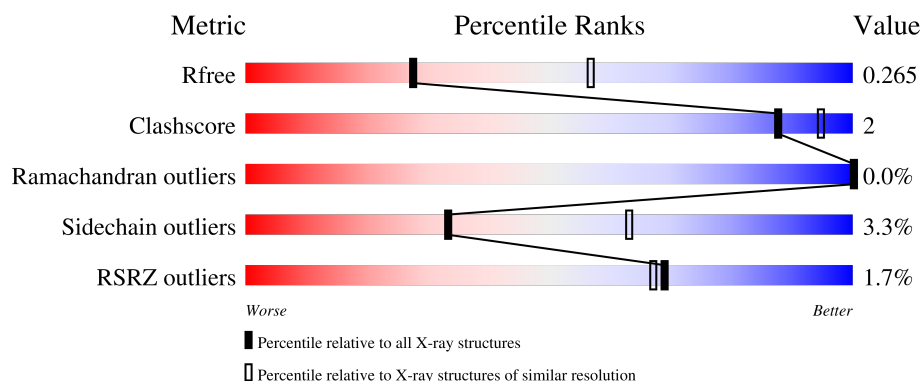
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.69 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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  $\geq 3$ , 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	414	<div> <div>86%</div> <div>7% • 7%</div> </div>
1	B	414	<div> <div>87%</div> <div>6% • 6%</div> </div>
1	D	414	<div> <div>86%</div> <div>7% 7%</div> </div>
1	F	414	<div> <div>88%</div> <div>5% • 6%</div> </div>
1	H	414	<div> <div>4%</div> <div>83%</div> <div>6% • 10%</div> </div>

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Mol	Chain	Length	Quality of chain
1	I	414	 88% 5% 6%
1	J	414	 86% 6% 7%
1	L	414	 85% 6% 9%
1	P	414	 86% 7% 7%
2	C	413	 86% 8% 6%
2	E	413	 90% 6%
2	G	413	 87% 7% 6%
2	K	413	 87% 6% 7%
2	M	413	 87% 5% 8%
2	N	413	 88% 5% 6%
2	O	413	 86% 6% 8%

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 89962 atoms, of which 44658 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 Cystathionine gamma-synthase.

Mol	Chain	Residues	Atoms								ZeroOcc	AltConf	Trace
1	A	386	Total	C	H	N	O	P	S		0	0	0
			5597	1761	2780	497	545	1	13				
1	B	388	Total	C	H	N	O	P	S		0	0	0
			5638	1773	2800	504	547	1	13				
1	D	383	Total	C	H	N	O	P	S		0	0	0
			5556	1748	2758	494	542	1	13				
1	F	387	Total	C	H	N	O	P	S		0	0	0
			5624	1769	2794	502	545	1	13				
1	H	372	Total	C	H	N	O	P	S		0	1	0
			5425	1709	2693	482	527	1	13				
1	I	387	Total	C	H	N	O	P	S		0	1	0
			5648	1776	2807	505	546	1	13				
1	J	384	Total	C	H	N	O	P	S		0	0	0
			5585	1758	2776	497	540	1	13				
1	L	374	Total	C	H	N	O	P	S		0	0	0
			5427	1710	2690	483	530	1	13				
1	P	385	Total	C	H	N	O	P	S		0	1	0
			5626	1769	2797	502	544	1	13				

There are 180 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP A0A1H1YBL2
A	-18	GLY	-	expression tag	UNP A0A1H1YBL2
A	-17	SER	-	expression tag	UNP A0A1H1YBL2
A	-16	SER	-	expression tag	UNP A0A1H1YBL2
A	-15	HIS	-	expression tag	UNP A0A1H1YBL2
A	-14	HIS	-	expression tag	UNP A0A1H1YBL2
A	-13	HIS	-	expression tag	UNP A0A1H1YBL2
A	-12	HIS	-	expression tag	UNP A0A1H1YBL2
A	-11	HIS	-	expression tag	UNP A0A1H1YBL2
A	-10	HIS	-	expression tag	UNP A0A1H1YBL2
A	-9	SER	-	expression tag	UNP A0A1H1YBL2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	SER	-	expression tag	UNP A0A1H1YBL2
A	-7	GLY	-	expression tag	UNP A0A1H1YBL2
A	-6	LEU	-	expression tag	UNP A0A1H1YBL2
A	-5	VAL	-	expression tag	UNP A0A1H1YBL2
A	-4	PRO	-	expression tag	UNP A0A1H1YBL2
A	-3	ARG	-	expression tag	UNP A0A1H1YBL2
A	-2	GLY	-	expression tag	UNP A0A1H1YBL2
A	-1	SER	-	expression tag	UNP A0A1H1YBL2
A	0	HIS	-	expression tag	UNP A0A1H1YBL2
B	-19	MET	-	initiating methionine	UNP A0A1H1YBL2
B	-18	GLY	-	expression tag	UNP A0A1H1YBL2
B	-17	SER	-	expression tag	UNP A0A1H1YBL2
B	-16	SER	-	expression tag	UNP A0A1H1YBL2
B	-15	HIS	-	expression tag	UNP A0A1H1YBL2
B	-14	HIS	-	expression tag	UNP A0A1H1YBL2
B	-13	HIS	-	expression tag	UNP A0A1H1YBL2
B	-12	HIS	-	expression tag	UNP A0A1H1YBL2
B	-11	HIS	-	expression tag	UNP A0A1H1YBL2
B	-10	HIS	-	expression tag	UNP A0A1H1YBL2
B	-9	SER	-	expression tag	UNP A0A1H1YBL2
B	-8	SER	-	expression tag	UNP A0A1H1YBL2
B	-7	GLY	-	expression tag	UNP A0A1H1YBL2
B	-6	LEU	-	expression tag	UNP A0A1H1YBL2
B	-5	VAL	-	expression tag	UNP A0A1H1YBL2
B	-4	PRO	-	expression tag	UNP A0A1H1YBL2
B	-3	ARG	-	expression tag	UNP A0A1H1YBL2
B	-2	GLY	-	expression tag	UNP A0A1H1YBL2
B	-1	SER	-	expression tag	UNP A0A1H1YBL2
B	0	HIS	-	expression tag	UNP A0A1H1YBL2
D	-19	MET	-	initiating methionine	UNP A0A1H1YBL2
D	-18	GLY	-	expression tag	UNP A0A1H1YBL2
D	-17	SER	-	expression tag	UNP A0A1H1YBL2
D	-16	SER	-	expression tag	UNP A0A1H1YBL2
D	-15	HIS	-	expression tag	UNP A0A1H1YBL2
D	-14	HIS	-	expression tag	UNP A0A1H1YBL2
D	-13	HIS	-	expression tag	UNP A0A1H1YBL2
D	-12	HIS	-	expression tag	UNP A0A1H1YBL2
D	-11	HIS	-	expression tag	UNP A0A1H1YBL2
D	-10	HIS	-	expression tag	UNP A0A1H1YBL2
D	-9	SER	-	expression tag	UNP A0A1H1YBL2
D	-8	SER	-	expression tag	UNP A0A1H1YBL2
D	-7	GLY	-	expression tag	UNP A0A1H1YBL2

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-6	LEU	-	expression tag	UNP A0A1H1YBL2
D	-5	VAL	-	expression tag	UNP A0A1H1YBL2
D	-4	PRO	-	expression tag	UNP A0A1H1YBL2
D	-3	ARG	-	expression tag	UNP A0A1H1YBL2
D	-2	GLY	-	expression tag	UNP A0A1H1YBL2
D	-1	SER	-	expression tag	UNP A0A1H1YBL2
D	0	HIS	-	expression tag	UNP A0A1H1YBL2
F	-19	MET	-	initiating methionine	UNP A0A1H1YBL2
F	-18	GLY	-	expression tag	UNP A0A1H1YBL2
F	-17	SER	-	expression tag	UNP A0A1H1YBL2
F	-16	SER	-	expression tag	UNP A0A1H1YBL2
F	-15	HIS	-	expression tag	UNP A0A1H1YBL2
F	-14	HIS	-	expression tag	UNP A0A1H1YBL2
F	-13	HIS	-	expression tag	UNP A0A1H1YBL2
F	-12	HIS	-	expression tag	UNP A0A1H1YBL2
F	-11	HIS	-	expression tag	UNP A0A1H1YBL2
F	-10	HIS	-	expression tag	UNP A0A1H1YBL2
F	-9	SER	-	expression tag	UNP A0A1H1YBL2
F	-8	SER	-	expression tag	UNP A0A1H1YBL2
F	-7	GLY	-	expression tag	UNP A0A1H1YBL2
F	-6	LEU	-	expression tag	UNP A0A1H1YBL2
F	-5	VAL	-	expression tag	UNP A0A1H1YBL2
F	-4	PRO	-	expression tag	UNP A0A1H1YBL2
F	-3	ARG	-	expression tag	UNP A0A1H1YBL2
F	-2	GLY	-	expression tag	UNP A0A1H1YBL2
F	-1	SER	-	expression tag	UNP A0A1H1YBL2
F	0	HIS	-	expression tag	UNP A0A1H1YBL2
H	-19	MET	-	initiating methionine	UNP A0A1H1YBL2
H	-18	GLY	-	expression tag	UNP A0A1H1YBL2
H	-17	SER	-	expression tag	UNP A0A1H1YBL2
H	-16	SER	-	expression tag	UNP A0A1H1YBL2
H	-15	HIS	-	expression tag	UNP A0A1H1YBL2
H	-14	HIS	-	expression tag	UNP A0A1H1YBL2
H	-13	HIS	-	expression tag	UNP A0A1H1YBL2
H	-12	HIS	-	expression tag	UNP A0A1H1YBL2
H	-11	HIS	-	expression tag	UNP A0A1H1YBL2
H	-10	HIS	-	expression tag	UNP A0A1H1YBL2
H	-9	SER	-	expression tag	UNP A0A1H1YBL2
H	-8	SER	-	expression tag	UNP A0A1H1YBL2
H	-7	GLY	-	expression tag	UNP A0A1H1YBL2
H	-6	LEU	-	expression tag	UNP A0A1H1YBL2
H	-5	VAL	-	expression tag	UNP A0A1H1YBL2

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-4	PRO	-	expression tag	UNP A0A1H1YBL2
H	-3	ARG	-	expression tag	UNP A0A1H1YBL2
H	-2	GLY	-	expression tag	UNP A0A1H1YBL2
H	-1	SER	-	expression tag	UNP A0A1H1YBL2
H	0	HIS	-	expression tag	UNP A0A1H1YBL2
I	-19	MET	-	initiating methionine	UNP A0A1H1YBL2
I	-18	GLY	-	expression tag	UNP A0A1H1YBL2
I	-17	SER	-	expression tag	UNP A0A1H1YBL2
I	-16	SER	-	expression tag	UNP A0A1H1YBL2
I	-15	HIS	-	expression tag	UNP A0A1H1YBL2
I	-14	HIS	-	expression tag	UNP A0A1H1YBL2
I	-13	HIS	-	expression tag	UNP A0A1H1YBL2
I	-12	HIS	-	expression tag	UNP A0A1H1YBL2
I	-11	HIS	-	expression tag	UNP A0A1H1YBL2
I	-10	HIS	-	expression tag	UNP A0A1H1YBL2
I	-9	SER	-	expression tag	UNP A0A1H1YBL2
I	-8	SER	-	expression tag	UNP A0A1H1YBL2
I	-7	GLY	-	expression tag	UNP A0A1H1YBL2
I	-6	LEU	-	expression tag	UNP A0A1H1YBL2
I	-5	VAL	-	expression tag	UNP A0A1H1YBL2
I	-4	PRO	-	expression tag	UNP A0A1H1YBL2
I	-3	ARG	-	expression tag	UNP A0A1H1YBL2
I	-2	GLY	-	expression tag	UNP A0A1H1YBL2
I	-1	SER	-	expression tag	UNP A0A1H1YBL2
I	0	HIS	-	expression tag	UNP A0A1H1YBL2
J	-19	MET	-	initiating methionine	UNP A0A1H1YBL2
J	-18	GLY	-	expression tag	UNP A0A1H1YBL2
J	-17	SER	-	expression tag	UNP A0A1H1YBL2
J	-16	SER	-	expression tag	UNP A0A1H1YBL2
J	-15	HIS	-	expression tag	UNP A0A1H1YBL2
J	-14	HIS	-	expression tag	UNP A0A1H1YBL2
J	-13	HIS	-	expression tag	UNP A0A1H1YBL2
J	-12	HIS	-	expression tag	UNP A0A1H1YBL2
J	-11	HIS	-	expression tag	UNP A0A1H1YBL2
J	-10	HIS	-	expression tag	UNP A0A1H1YBL2
J	-9	SER	-	expression tag	UNP A0A1H1YBL2
J	-8	SER	-	expression tag	UNP A0A1H1YBL2
J	-7	GLY	-	expression tag	UNP A0A1H1YBL2
J	-6	LEU	-	expression tag	UNP A0A1H1YBL2
J	-5	VAL	-	expression tag	UNP A0A1H1YBL2
J	-4	PRO	-	expression tag	UNP A0A1H1YBL2
J	-3	ARG	-	expression tag	UNP A0A1H1YBL2

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Chain	Residue	Modelled	Actual	Comment	Reference
J	-2	GLY	-	expression tag	UNP A0A1H1YBL2
J	-1	SER	-	expression tag	UNP A0A1H1YBL2
J	0	HIS	-	expression tag	UNP A0A1H1YBL2
L	-19	MET	-	initiating methionine	UNP A0A1H1YBL2
L	-18	GLY	-	expression tag	UNP A0A1H1YBL2
L	-17	SER	-	expression tag	UNP A0A1H1YBL2
L	-16	SER	-	expression tag	UNP A0A1H1YBL2
L	-15	HIS	-	expression tag	UNP A0A1H1YBL2
L	-14	HIS	-	expression tag	UNP A0A1H1YBL2
L	-13	HIS	-	expression tag	UNP A0A1H1YBL2
L	-12	HIS	-	expression tag	UNP A0A1H1YBL2
L	-11	HIS	-	expression tag	UNP A0A1H1YBL2
L	-10	HIS	-	expression tag	UNP A0A1H1YBL2
L	-9	SER	-	expression tag	UNP A0A1H1YBL2
L	-8	SER	-	expression tag	UNP A0A1H1YBL2
L	-7	GLY	-	expression tag	UNP A0A1H1YBL2
L	-6	LEU	-	expression tag	UNP A0A1H1YBL2
L	-5	VAL	-	expression tag	UNP A0A1H1YBL2
L	-4	PRO	-	expression tag	UNP A0A1H1YBL2
L	-3	ARG	-	expression tag	UNP A0A1H1YBL2
L	-2	GLY	-	expression tag	UNP A0A1H1YBL2
L	-1	SER	-	expression tag	UNP A0A1H1YBL2
L	0	HIS	-	expression tag	UNP A0A1H1YBL2
P	-19	MET	-	initiating methionine	UNP A0A1H1YBL2
P	-18	GLY	-	expression tag	UNP A0A1H1YBL2
P	-17	SER	-	expression tag	UNP A0A1H1YBL2
P	-16	SER	-	expression tag	UNP A0A1H1YBL2
P	-15	HIS	-	expression tag	UNP A0A1H1YBL2
P	-14	HIS	-	expression tag	UNP A0A1H1YBL2
P	-13	HIS	-	expression tag	UNP A0A1H1YBL2
P	-12	HIS	-	expression tag	UNP A0A1H1YBL2
P	-11	HIS	-	expression tag	UNP A0A1H1YBL2
P	-10	HIS	-	expression tag	UNP A0A1H1YBL2
P	-9	SER	-	expression tag	UNP A0A1H1YBL2
P	-8	SER	-	expression tag	UNP A0A1H1YBL2
P	-7	GLY	-	expression tag	UNP A0A1H1YBL2
P	-6	LEU	-	expression tag	UNP A0A1H1YBL2
P	-5	VAL	-	expression tag	UNP A0A1H1YBL2
P	-4	PRO	-	expression tag	UNP A0A1H1YBL2
P	-3	ARG	-	expression tag	UNP A0A1H1YBL2
P	-2	GLY	-	expression tag	UNP A0A1H1YBL2
P	-1	SER	-	expression tag	UNP A0A1H1YBL2

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Chain	Residue	Modelled	Actual	Comment	Reference
P	0	HIS	-	expression tag	UNP A0A1H1YBL2

- Molecule 2 is a protein called Cystathionine gamma-synthase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	C	388	Total	C	H	N	O	S	0	0	0
			5618	1765	2795	503	542	13			
2	E	389	Total	C	H	N	O	S	0	0	0
			5638	1770	2807	506	542	13			
2	G	387	Total	C	H	N	O	S	0	0	0
			5607	1762	2790	502	540	13			
2	K	386	Total	C	H	N	O	S	0	0	0
			5594	1759	2783	500	539	13			
2	M	382	Total	C	H	N	O	S	0	0	0
			5543	1743	2757	496	534	13			
2	N	387	Total	C	H	N	O	S	0	0	0
			5604	1761	2789	501	540	13			
2	O	380	Total	C	H	N	O	S	0	0	0
			5517	1735	2745	493	531	13			

There are 140 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-19	MET	-	initiating methionine	UNP A0A1H1YBL2
C	-18	GLY	-	expression tag	UNP A0A1H1YBL2
C	-17	SER	-	expression tag	UNP A0A1H1YBL2
C	-16	SER	-	expression tag	UNP A0A1H1YBL2
C	-15	HIS	-	expression tag	UNP A0A1H1YBL2
C	-14	HIS	-	expression tag	UNP A0A1H1YBL2
C	-13	HIS	-	expression tag	UNP A0A1H1YBL2
C	-12	HIS	-	expression tag	UNP A0A1H1YBL2
C	-11	HIS	-	expression tag	UNP A0A1H1YBL2
C	-10	HIS	-	expression tag	UNP A0A1H1YBL2
C	-9	SER	-	expression tag	UNP A0A1H1YBL2
C	-8	SER	-	expression tag	UNP A0A1H1YBL2
C	-7	GLY	-	expression tag	UNP A0A1H1YBL2
C	-6	LEU	-	expression tag	UNP A0A1H1YBL2
C	-5	VAL	-	expression tag	UNP A0A1H1YBL2
C	-4	PRO	-	expression tag	UNP A0A1H1YBL2
C	-3	ARG	-	expression tag	UNP A0A1H1YBL2
C	-2	GLY	-	expression tag	UNP A0A1H1YBL2
C	-1	SER	-	expression tag	UNP A0A1H1YBL2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	0	HIS	-	expression tag	UNP A0A1H1YBL2
E	-19	MET	-	initiating methionine	UNP A0A1H1YBL2
E	-18	GLY	-	expression tag	UNP A0A1H1YBL2
E	-17	SER	-	expression tag	UNP A0A1H1YBL2
E	-16	SER	-	expression tag	UNP A0A1H1YBL2
E	-15	HIS	-	expression tag	UNP A0A1H1YBL2
E	-14	HIS	-	expression tag	UNP A0A1H1YBL2
E	-13	HIS	-	expression tag	UNP A0A1H1YBL2
E	-12	HIS	-	expression tag	UNP A0A1H1YBL2
E	-11	HIS	-	expression tag	UNP A0A1H1YBL2
E	-10	HIS	-	expression tag	UNP A0A1H1YBL2
E	-9	SER	-	expression tag	UNP A0A1H1YBL2
E	-8	SER	-	expression tag	UNP A0A1H1YBL2
E	-7	GLY	-	expression tag	UNP A0A1H1YBL2
E	-6	LEU	-	expression tag	UNP A0A1H1YBL2
E	-5	VAL	-	expression tag	UNP A0A1H1YBL2
E	-4	PRO	-	expression tag	UNP A0A1H1YBL2
E	-3	ARG	-	expression tag	UNP A0A1H1YBL2
E	-2	GLY	-	expression tag	UNP A0A1H1YBL2
E	-1	SER	-	expression tag	UNP A0A1H1YBL2
E	0	HIS	-	expression tag	UNP A0A1H1YBL2
G	-19	MET	-	initiating methionine	UNP A0A1H1YBL2
G	-18	GLY	-	expression tag	UNP A0A1H1YBL2
G	-17	SER	-	expression tag	UNP A0A1H1YBL2
G	-16	SER	-	expression tag	UNP A0A1H1YBL2
G	-15	HIS	-	expression tag	UNP A0A1H1YBL2
G	-14	HIS	-	expression tag	UNP A0A1H1YBL2
G	-13	HIS	-	expression tag	UNP A0A1H1YBL2
G	-12	HIS	-	expression tag	UNP A0A1H1YBL2
G	-11	HIS	-	expression tag	UNP A0A1H1YBL2
G	-10	HIS	-	expression tag	UNP A0A1H1YBL2
G	-9	SER	-	expression tag	UNP A0A1H1YBL2
G	-8	SER	-	expression tag	UNP A0A1H1YBL2
G	-7	GLY	-	expression tag	UNP A0A1H1YBL2
G	-6	LEU	-	expression tag	UNP A0A1H1YBL2
G	-5	VAL	-	expression tag	UNP A0A1H1YBL2
G	-4	PRO	-	expression tag	UNP A0A1H1YBL2
G	-3	ARG	-	expression tag	UNP A0A1H1YBL2
G	-2	GLY	-	expression tag	UNP A0A1H1YBL2
G	-1	SER	-	expression tag	UNP A0A1H1YBL2
G	0	HIS	-	expression tag	UNP A0A1H1YBL2
K	-19	MET	-	initiating methionine	UNP A0A1H1YBL2

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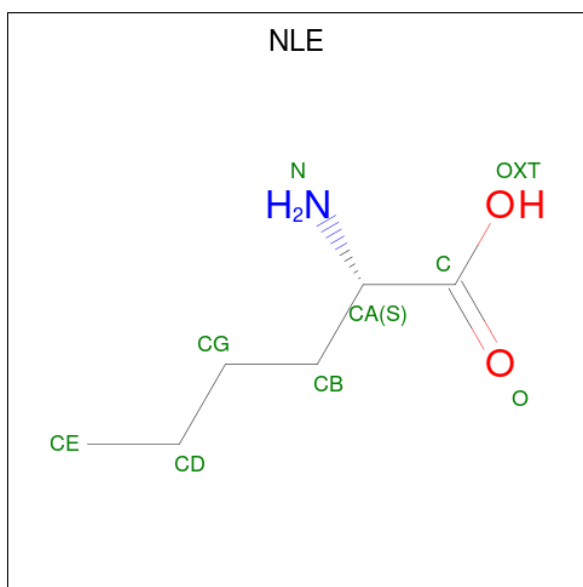
Chain	Residue	Modelled	Actual	Comment	Reference
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K	-17	SER	-	expression tag	UNP A0A1H1YBL2
K	-16	SER	-	expression tag	UNP A0A1H1YBL2
K	-15	HIS	-	expression tag	UNP A0A1H1YBL2
K	-14	HIS	-	expression tag	UNP A0A1H1YBL2
K	-13	HIS	-	expression tag	UNP A0A1H1YBL2
K	-12	HIS	-	expression tag	UNP A0A1H1YBL2
K	-11	HIS	-	expression tag	UNP A0A1H1YBL2
K	-10	HIS	-	expression tag	UNP A0A1H1YBL2
K	-9	SER	-	expression tag	UNP A0A1H1YBL2
K	-8	SER	-	expression tag	UNP A0A1H1YBL2
K	-7	GLY	-	expression tag	UNP A0A1H1YBL2
K	-6	LEU	-	expression tag	UNP A0A1H1YBL2
K	-5	VAL	-	expression tag	UNP A0A1H1YBL2
K	-4	PRO	-	expression tag	UNP A0A1H1YBL2
K	-3	ARG	-	expression tag	UNP A0A1H1YBL2
K	-2	GLY	-	expression tag	UNP A0A1H1YBL2
K	-1	SER	-	expression tag	UNP A0A1H1YBL2
K	0	HIS	-	expression tag	UNP A0A1H1YBL2
M	-19	MET	-	initiating methionine	UNP A0A1H1YBL2
M	-18	GLY	-	expression tag	UNP A0A1H1YBL2
M	-17	SER	-	expression tag	UNP A0A1H1YBL2
M	-16	SER	-	expression tag	UNP A0A1H1YBL2
M	-15	HIS	-	expression tag	UNP A0A1H1YBL2
M	-14	HIS	-	expression tag	UNP A0A1H1YBL2
M	-13	HIS	-	expression tag	UNP A0A1H1YBL2
M	-12	HIS	-	expression tag	UNP A0A1H1YBL2
M	-11	HIS	-	expression tag	UNP A0A1H1YBL2
M	-10	HIS	-	expression tag	UNP A0A1H1YBL2
M	-9	SER	-	expression tag	UNP A0A1H1YBL2
M	-8	SER	-	expression tag	UNP A0A1H1YBL2
M	-7	GLY	-	expression tag	UNP A0A1H1YBL2
M	-6	LEU	-	expression tag	UNP A0A1H1YBL2
M	-5	VAL	-	expression tag	UNP A0A1H1YBL2
M	-4	PRO	-	expression tag	UNP A0A1H1YBL2
M	-3	ARG	-	expression tag	UNP A0A1H1YBL2
M	-2	GLY	-	expression tag	UNP A0A1H1YBL2
M	-1	SER	-	expression tag	UNP A0A1H1YBL2
M	0	HIS	-	expression tag	UNP A0A1H1YBL2
N	-19	MET	-	initiating methionine	UNP A0A1H1YBL2
N	-18	GLY	-	expression tag	UNP A0A1H1YBL2
N	-17	SER	-	expression tag	UNP A0A1H1YBL2

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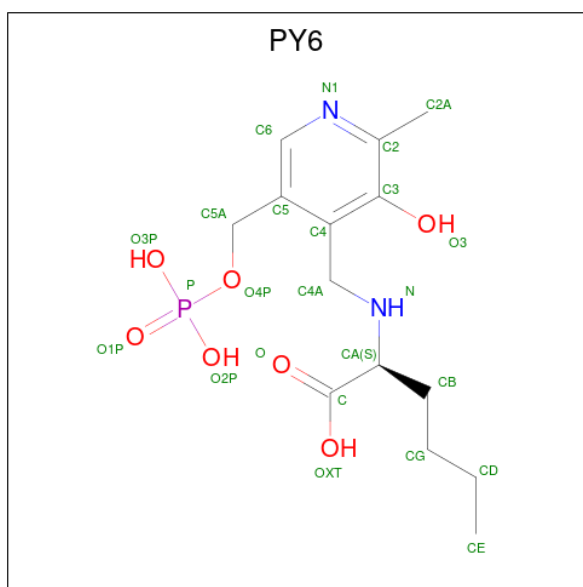
Chain	Residue	Modelled	Actual	Comment	Reference
N	-16	SER	-	expression tag	UNP A0A1H1YBL2
N	-15	HIS	-	expression tag	UNP A0A1H1YBL2
N	-14	HIS	-	expression tag	UNP A0A1H1YBL2
N	-13	HIS	-	expression tag	UNP A0A1H1YBL2
N	-12	HIS	-	expression tag	UNP A0A1H1YBL2
N	-11	HIS	-	expression tag	UNP A0A1H1YBL2
N	-10	HIS	-	expression tag	UNP A0A1H1YBL2
N	-9	SER	-	expression tag	UNP A0A1H1YBL2
N	-8	SER	-	expression tag	UNP A0A1H1YBL2
N	-7	GLY	-	expression tag	UNP A0A1H1YBL2
N	-6	LEU	-	expression tag	UNP A0A1H1YBL2
N	-5	VAL	-	expression tag	UNP A0A1H1YBL2
N	-4	PRO	-	expression tag	UNP A0A1H1YBL2
N	-3	ARG	-	expression tag	UNP A0A1H1YBL2
N	-2	GLY	-	expression tag	UNP A0A1H1YBL2
N	-1	SER	-	expression tag	UNP A0A1H1YBL2
N	0	HIS	-	expression tag	UNP A0A1H1YBL2
O	-19	MET	-	initiating methionine	UNP A0A1H1YBL2
O	-18	GLY	-	expression tag	UNP A0A1H1YBL2
O	-17	SER	-	expression tag	UNP A0A1H1YBL2
O	-16	SER	-	expression tag	UNP A0A1H1YBL2
O	-15	HIS	-	expression tag	UNP A0A1H1YBL2
O	-14	HIS	-	expression tag	UNP A0A1H1YBL2
O	-13	HIS	-	expression tag	UNP A0A1H1YBL2
O	-12	HIS	-	expression tag	UNP A0A1H1YBL2
O	-11	HIS	-	expression tag	UNP A0A1H1YBL2
O	-10	HIS	-	expression tag	UNP A0A1H1YBL2
O	-9	SER	-	expression tag	UNP A0A1H1YBL2
O	-8	SER	-	expression tag	UNP A0A1H1YBL2
O	-7	GLY	-	expression tag	UNP A0A1H1YBL2
O	-6	LEU	-	expression tag	UNP A0A1H1YBL2
O	-5	VAL	-	expression tag	UNP A0A1H1YBL2
O	-4	PRO	-	expression tag	UNP A0A1H1YBL2
O	-3	ARG	-	expression tag	UNP A0A1H1YBL2
O	-2	GLY	-	expression tag	UNP A0A1H1YBL2
O	-1	SER	-	expression tag	UNP A0A1H1YBL2
O	0	HIS	-	expression tag	UNP A0A1H1YBL2

- Molecule 3 is NORLEUCINE (CCD ID: NLE) (formula:  $C_6H_{13}NO_2$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	0	0
			21	6	12	1	2		
3	B	1	Total	C	H	N	O	0	0
			21	6	12	1	2		
3	D	1	Total	C	H	N	O	0	0
			22	6	13	1	2		
3	F	1	Total	C	H	N	O	0	0
			21	6	12	1	2		
3	J	1	Total	C	H	N	O	0	0
			21	6	12	1	2		

- Molecule 4 is 2-[O-PHOSPHONOPYRIDOXYL]-AMINO-HEXANOIC ACID (CCD ID: PY6) (formula: C<sub>14</sub>H<sub>23</sub>N<sub>2</sub>O<sub>7</sub>P) (labeled as "Ligand of Interest" by depositor).



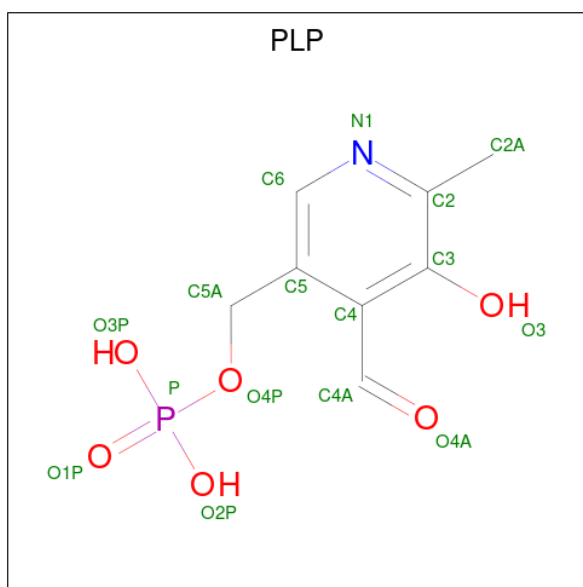
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	C	1	Total	C	H	N	O	P	0	0
			44	14	20	2	7	1		
4	E	1	Total	C	H	N	O	P	0	0
			44	14	20	2	7	1		
4	G	1	Total	C	H	N	O	P	0	0
			44	14	20	2	7	1		
4	H	1	Total	C	H	N	O	P	0	1
			44	14	20	2	7	1		
4	I	1	Total	C	H	N	O	P	0	1
			44	14	20	2	7	1		
4	K	1	Total	C	H	N	O	P	0	0
			43	14	19	2	7	1		
4	M	1	Total	C	H	N	O	P	0	0
			44	14	20	2	7	1		
4	N	1	Total	C	H	N	O	P	0	0
			44	14	20	2	7	1		
4	O	1	Total	C	H	N	O	P	0	0
			44	14	20	2	7	1		
4	P	1	Total	C	H	N	O	P	0	1
			44	14	20	2	7	1		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula:  $C_4H_{10}O_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	D	1	Total	C	H	O	0	0
			17	4	10	3		
5	F	1	Total	C	H	O	0	0
			17	4	10	3		
5	J	1	Total	C	H	O	0	0
			17	4	10	3		

- Molecule 6 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula:  $C_8H_{10}NO_6P$ ).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	P	1	Total	C	H	N	O	P	0	1
			22	8	7	1	5	1		

- Molecule 7 is water.

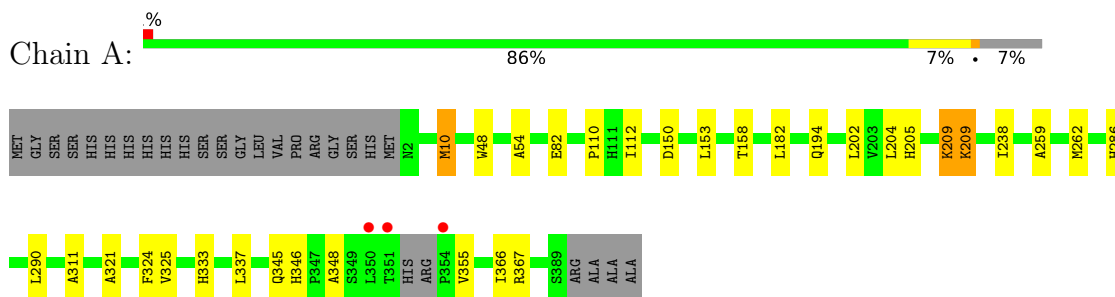
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	19	Total O 19 19	0	0
7	B	11	Total O 11 11	0	0
7	C	10	Total O 10 10	0	0
7	D	10	Total O 10 10	0	0
7	E	2	Total O 2 2	0	0
7	F	6	Total O 6 6	0	0
7	G	5	Total O 5 5	0	0
7	H	2	Total O 2 2	0	0
7	I	2	Total O 2 2	0	0
7	J	10	Total O 10 10	0	0
7	K	3	Total O 3 3	0	0
7	L	2	Total O 2 2	0	0
7	M	9	Total O 9 9	0	0
7	O	2	Total O 2 2	0	0
7	P	4	Total O 4 4	0	0



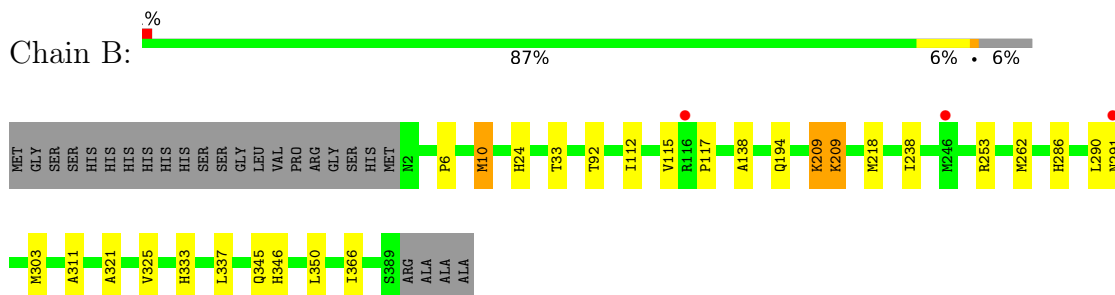
### 3 Residue-property plots [i](#)

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.

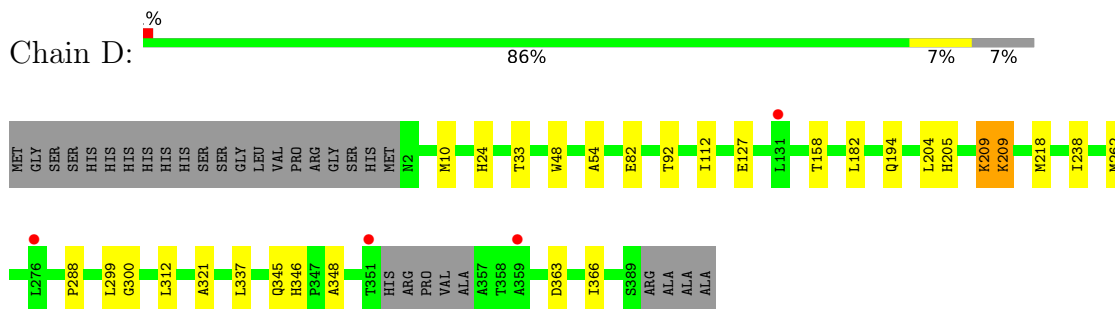
- Molecule 1: Cystathionine gamma-synthase



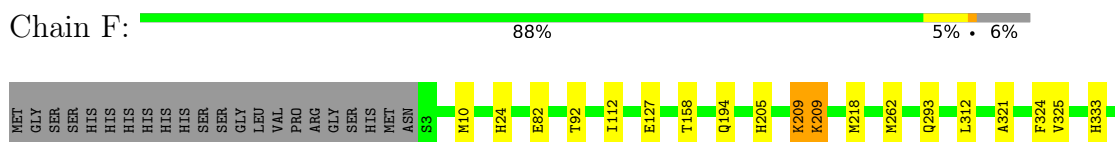
- Molecule 1: Cystathionine gamma-synthase



- Molecule 1: Cystathionine gamma-synthase

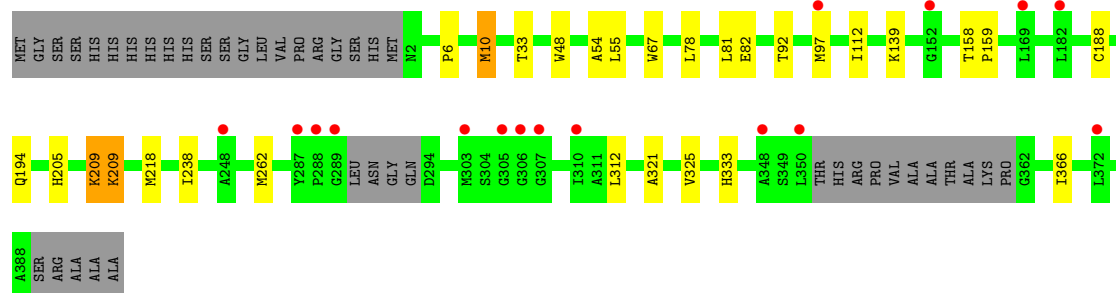
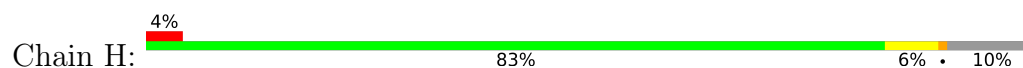


- Molecule 1: Cystathionine gamma-synthase

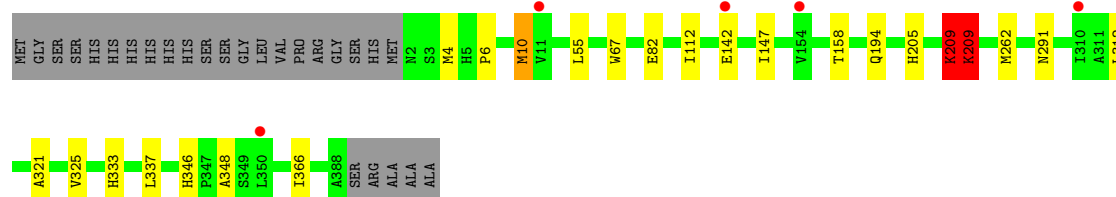
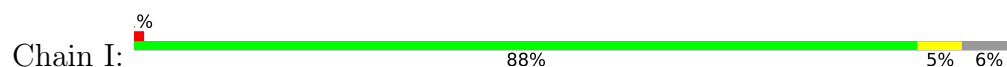




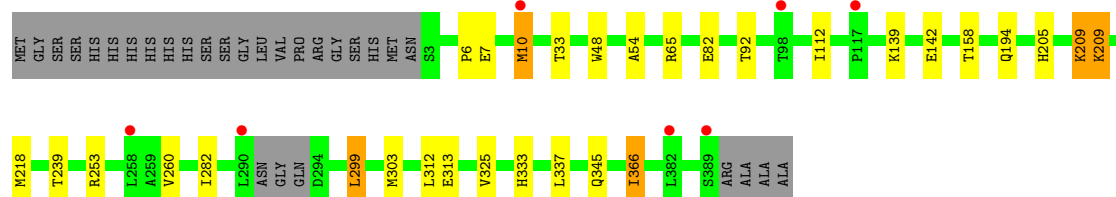
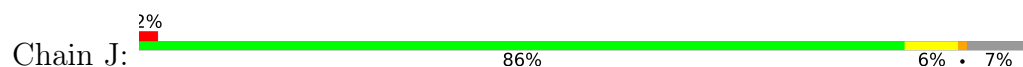
• Molecule 1: Cystathionine gamma-synthase



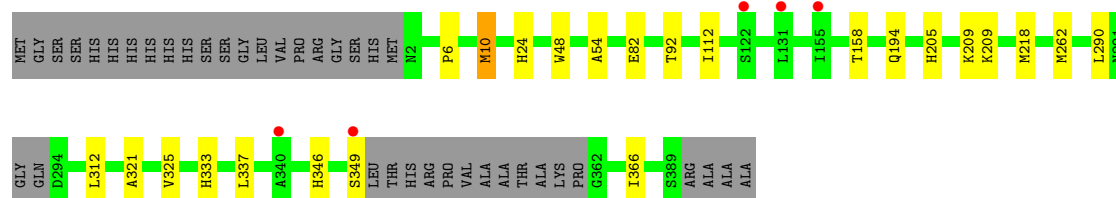
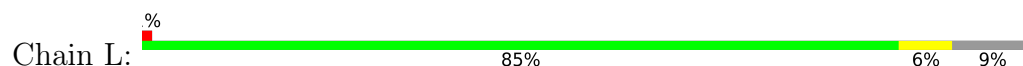
• Molecule 1: Cystathionine gamma-synthase



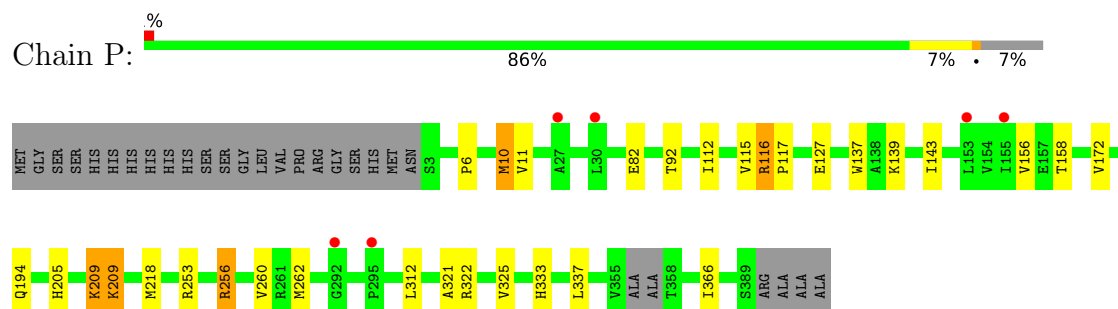
• Molecule 1: Cystathionine gamma-synthase



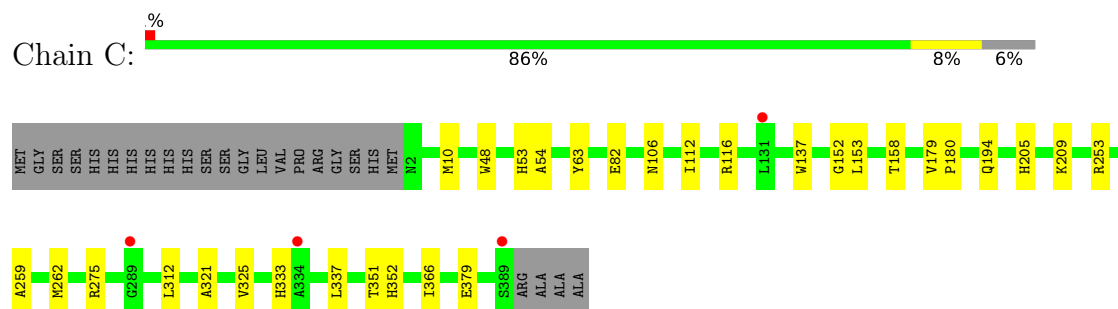
• Molecule 1: Cystathionine gamma-synthase



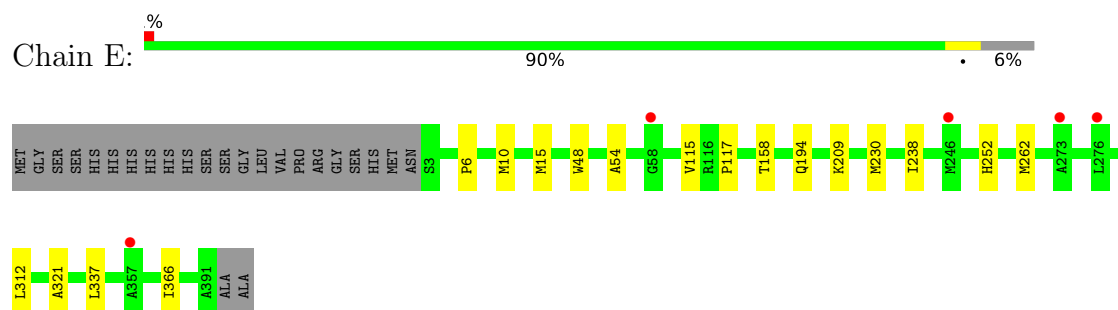
- Molecule 1: Cystathionine gamma-synthase



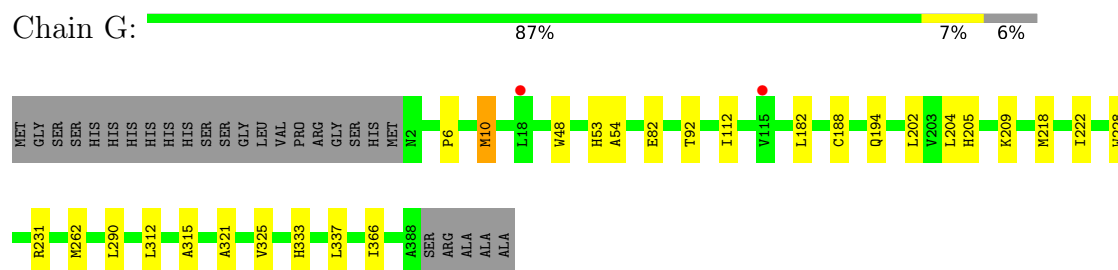
- Molecule 2: Cystathionine gamma-synthase



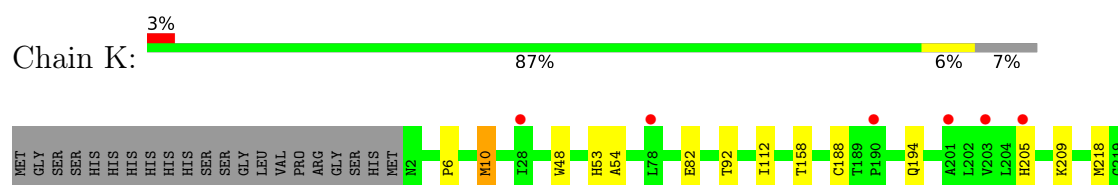
- Molecule 2: Cystathionine gamma-synthase

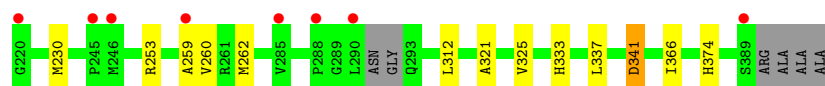


- Molecule 2: Cystathionine gamma-synthase

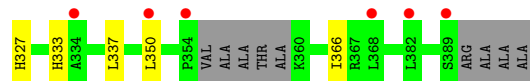
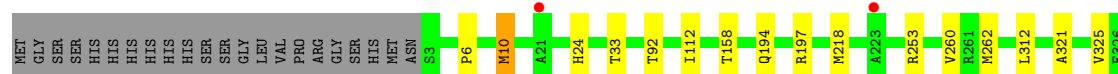
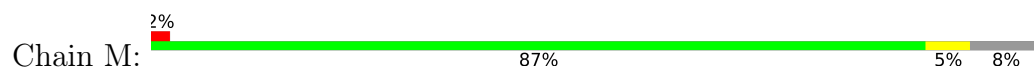


- Molecule 2: Cystathionine gamma-synthase

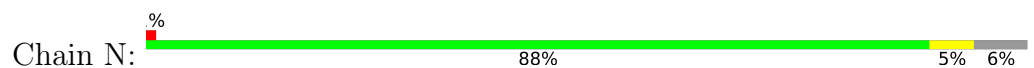




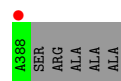
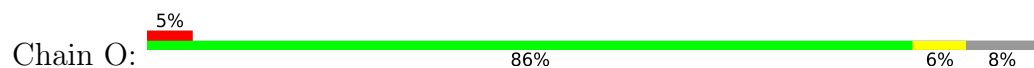
• Molecule 2: Cystathionine gamma-synthase



• Molecule 2: Cystathionine gamma-synthase



• Molecule 2: Cystathionine gamma-synthase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	113.83Å 151.94Å 316.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	136.98 – 2.69 136.98 – 2.69	Depositor EDS
% Data completeness (in resolution range)	79.0 (136.98-2.69) 79.0 (136.98-2.69)	Depositor EDS
$R_{merge}$	0.23	Depositor
$R_{sym}$	0.22	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.55 (at 2.69Å)	Xtriage
Refinement program	BUSTER 2.10.4	Depositor
R, $R_{free}$	0.258 , 0.278 0.247 , 0.265	Depositor DCC
$R_{free}$ test set	6037 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	70.5	Xtriage
Anisotropy	0.054	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 49.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	89962	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.33% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: PY6, PEG, PLP, NLE, LLP

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	0.73	0/2845	1.01	2/3886 (0.1%)
1	B	0.72	0/2868	0.98	0/3919
1	D	0.72	0/2825	0.98	0/3858
1	F	0.72	0/2860	0.98	1/3908 (0.0%)
1	H	0.72	0/2757	0.97	0/3762
1	I	0.73	0/2871	0.99	0/3922
1	J	0.75	0/2838	0.98	0/3877
1	L	0.72	0/2762	0.97	0/3770
1	P	0.73	0/2858	0.99	0/3902
2	C	0.73	0/2878	0.99	1/3933 (0.0%)
2	E	0.74	0/2886	0.99	0/3943
2	G	0.73	0/2872	1.00	0/3925
2	K	0.74	0/2865	0.99	1/3914 (0.0%)
2	M	0.73	1/2840 (0.0%)	0.98	0/3878
2	N	0.72	0/2870	0.98	0/3922
2	O	0.74	0/2824	0.99	1/3855 (0.0%)
All	All	0.73	1/45519 (0.0%)	0.98	6/62174 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	350	LEU	CA-C	5.84	1.57	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	341	ASP	CA-CB-CG	9.18	121.78	112.60
2	C	179	VAL	N-CA-CB	5.78	116.42	110.23
1	A	324	PHE	CA-CB-CG	5.42	119.22	113.80
2	O	38	ASP	CA-CB-CG	5.37	117.97	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	324	PHE	CA-CB-CG	5.26	119.06	113.80
1	A	290	LEU	N-CA-C	-5.00	101.49	108.54

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	2817	2780	2779	17	0
1	B	2838	2800	2799	13	0
1	D	2798	2758	2757	14	0
1	F	2830	2794	2793	17	0
1	H	2732	2693	2690	10	0
1	I	2841	2807	2805	7	2
1	J	2809	2776	2775	15	0
1	L	2737	2690	2690	8	0
1	P	2829	2797	2793	15	0
2	C	2823	2795	2795	14	0
2	E	2831	2807	2807	9	0
2	G	2817	2790	2790	12	2
2	K	2811	2783	2785	17	0
2	M	2786	2757	2757	10	0
2	N	2815	2789	2789	7	0
2	O	2772	2745	2745	11	0
3	A	9	12	12	3	0
3	B	9	12	12	2	0
3	D	9	13	12	0	0
3	F	9	12	12	3	0
3	J	9	12	12	3	0
4	C	24	20	20	0	0
4	E	24	20	20	3	0
4	G	24	20	20	0	0
4	H	24	20	19	0	0
4	I	24	20	19	0	0
4	K	24	19	19	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	M	24	20	20	0	0
4	N	24	20	20	0	0
4	O	24	20	20	2	0
4	P	24	20	19	0	0
5	D	7	10	10	1	0
5	F	7	10	10	0	0
5	J	7	10	10	0	0
6	P	15	7	6	0	0
7	A	19	0	0	0	0
7	B	11	0	0	0	0
7	C	10	0	0	0	0
7	D	10	0	0	0	0
7	E	2	0	0	0	0
7	F	6	0	0	0	0
7	G	5	0	0	0	0
7	H	2	0	0	0	0
7	I	2	0	0	0	0
7	J	10	0	0	0	0
7	K	3	0	0	0	0
7	L	2	0	0	0	0
7	M	9	0	0	0	0
7	O	2	0	0	0	0
7	P	4	0	0	0	0
All	All	45304	44658	44641	175	2

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 2.

All (175) 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)
2:E:209:LYS:HE3	4:E:401:PY6:H4A2	1.48	0.95
2:O:209:LYS:HE3	4:O:401:PY6:H4A2	1.49	0.93
2:K:209:LYS:HZ2	4:K:401:PY6:H4A2	1.34	0.92
2:K:209:LYS:HZ1	4:K:401:PY6:HA	1.39	0.86
1:F:209:LLP:H4'1	3:F:401:NLE:H	1.42	0.85
1:J:209:LLP:H4'1	3:J:401:NLE:H	1.42	0.83
1:A:209:LLP:H4'1	3:A:401:NLE:H	1.46	0.79
1:F:209:LLP:C4'	3:F:401:NLE:H	1.97	0.78
1:J:209:LLP:C4'	3:J:401:NLE:H	1.96	0.78
2:K:209:LYS:NZ	4:K:401:PY6:HA	1.98	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:LLP:C4'	3:A:401:NLE:H	1.97	0.76
1:F:209:LLP:H4'1	3:F:401:NLE:N	2.03	0.74
1:J:209:LLP:H4'1	3:J:401:NLE:N	2.02	0.73
2:O:209:LYS:CE	4:O:401:PY6:H4A2	2.20	0.72
2:E:209:LYS:CE	4:E:401:PY6:H4A2	2.19	0.71
1:A:209:LLP:H4'1	3:A:401:NLE:N	2.05	0.71
2:K:209:LYS:NZ	4:K:401:PY6:H4A2	2.07	0.69
2:E:115:VAL:HG12	2:E:117:PRO:HD2	1.77	0.67
2:G:53:HIS:NE2	2:M:327:HIS:NE2	2.42	0.67
4:K:401:PY6:O2P	4:K:401:PY6:H4A1	1.96	0.67
1:I:82:GLU:OE2	1:I:205:HIS:NE2	2.29	0.66
1:D:127:GLU:HB3	1:F:127:GLU:OE1	1.97	0.65
2:K:53:HIS:CD2	2:K:230:MET:HE2	2.32	0.64
2:C:53:HIS:NE2	1:F:363:ASP:OD2	2.31	0.62
1:B:209:LLP:H4'1	3:B:401:NLE:N	2.14	0.62
2:G:53:HIS:CE1	2:M:327:HIS:NE2	2.70	0.59
1:A:286:HIS:HB2	1:A:311:ALA:HB3	1.85	0.59
2:G:82:GLU:OE2	2:G:205:HIS:NE2	2.35	0.59
2:E:6:PRO:O	2:E:10:MET:HG2	2.02	0.58
1:L:82:GLU:OE2	1:L:205:HIS:HE1	1.86	0.57
1:D:321:ALA:HB1	1:D:366:ILE:HD11	1.87	0.56
1:D:363:ASP:OD2	2:E:230:MET:SD	2.64	0.56
2:G:182:LEU:HD11	2:G:204:LEU:HB2	1.88	0.56
1:J:299:LEU:O	1:J:303:MET:O	2.25	0.55
1:A:182:LEU:HD11	1:A:204:LEU:HB2	1.89	0.55
1:J:7:GLU:OE2	2:K:374:HIS:HD2	1.89	0.54
1:J:260:VAL:HG12	2:K:260:VAL:HG12	1.90	0.54
1:D:127:GLU:OE1	1:F:127:GLU:O	2.25	0.54
1:I:325:VAL:HG13	1:I:333:HIS:CG	2.44	0.53
1:L:321:ALA:HB1	1:L:366:ILE:HD11	1.91	0.53
1:B:115:VAL:HG12	1:B:117:PRO:HD2	1.91	0.52
2:M:325:VAL:HG13	2:M:333:HIS:CG	2.44	0.52
2:K:325:VAL:HG13	2:K:333:HIS:CG	2.45	0.52
1:H:10:MET:HE3	1:H:81:LEU:HD22	1.92	0.51
2:M:260:VAL:HG12	1:P:260:VAL:HG12	1.93	0.51
1:L:48:TRP:NE1	1:L:54:ALA:O	2.41	0.51
1:P:127:GLU:OE2	1:P:137:TRP:NE1	2.43	0.50
1:B:321:ALA:HB3	1:B:346:HIS:CE1	2.47	0.50
2:C:325:VAL:HG13	2:C:333:HIS:CG	2.47	0.50
1:D:182:LEU:HD11	1:D:204:LEU:HB2	1.92	0.50
2:E:48:TRP:NE1	2:E:54:ALA:O	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:325:VAL:HG13	1:J:333:HIS:CG	2.47	0.50
1:A:48:TRP:NE1	1:A:54:ALA:O	2.41	0.50
2:M:33:THR:O	2:O:24:HIS:HB2	2.11	0.50
2:K:48:TRP:NE1	2:K:54:ALA:O	2.41	0.50
2:O:48:TRP:NE1	2:O:54:ALA:O	2.42	0.50
1:B:325:VAL:HG13	1:B:333:HIS:CG	2.47	0.49
1:D:300:GLY:O	5:D:402:PEG:H41	2.12	0.49
1:L:325:VAL:HG13	1:L:333:HIS:CG	2.47	0.49
2:G:228:TRP:CE2	2:G:231:ARG:NH2	2.81	0.49
2:C:48:TRP:NE1	2:C:54:ALA:O	2.41	0.49
2:K:209:LYS:HZ1	4:K:401:PY6:CA	2.17	0.49
2:G:325:VAL:HG13	2:G:333:HIS:CG	2.47	0.49
2:G:202:LEU:HD23	2:G:222:ILE:HG21	1.95	0.49
1:H:325:VAL:HG13	1:H:333:HIS:CG	2.47	0.48
2:N:325:VAL:HG13	2:N:333:HIS:CG	2.48	0.48
1:A:82:GLU:OE2	1:A:205:HIS:NE2	2.39	0.48
1:P:116:ARG:NH2	1:P:137:TRP:CE2	2.81	0.48
1:A:153:LEU:HD21	1:A:202:LEU:HD13	1.94	0.48
1:J:82:GLU:OE2	1:J:205:HIS:NE2	2.44	0.48
1:F:325:VAL:HG13	1:F:333:HIS:CG	2.48	0.48
1:I:209[B]:LLP:OP2	1:J:65:ARG:NH1	2.46	0.48
2:C:116:ARG:NH1	2:C:137:TRP:CD1	2.82	0.48
1:P:11:VAL:O	1:P:256:ARG:HD3	2.14	0.47
1:H:48:TRP:NE1	1:H:54:ALA:O	2.42	0.47
1:P:115:VAL:HG12	1:P:117:PRO:HD2	1.97	0.47
2:G:321:ALA:HB1	2:G:366:ILE:HD11	1.96	0.47
1:P:82:GLU:OE2	1:P:205:HIS:NE2	2.48	0.47
1:A:325:VAL:CG1	1:A:333:HIS:CG	2.97	0.47
1:A:325:VAL:CG1	1:A:333:HIS:CD2	2.97	0.47
1:A:325:VAL:HG13	1:A:333:HIS:CG	2.50	0.47
1:D:288:PRO:O	1:D:299:LEU:HD11	2.13	0.47
1:H:82:GLU:OE2	1:H:205:HIS:NE2	2.47	0.47
1:H:321:ALA:HB1	1:H:366:ILE:HD11	1.97	0.47
1:A:321:ALA:HB1	1:A:366:ILE:HD11	1.96	0.46
2:O:15:MET:HE2	2:O:252:HIS:NE2	2.30	0.46
1:B:33:THR:O	1:D:24:HIS:HB2	2.16	0.46
1:J:48:TRP:NE1	1:J:54:ALA:O	2.41	0.46
1:A:346:HIS:CE1	1:A:348:ALA:HB3	2.51	0.46
1:B:321:ALA:HB1	1:B:366:ILE:HD11	1.97	0.46
2:N:82:GLU:OE2	2:N:205:HIS:NE2	2.47	0.46
1:F:325:VAL:CG1	1:F:333:HIS:CG	2.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:106:ASN:OD1	1:F:358:THR:OG1	2.30	0.46
2:C:321:ALA:HB1	2:C:366:ILE:HD11	1.97	0.46
1:D:82:GLU:OE2	1:D:205:HIS:NE2	2.47	0.46
2:K:321:ALA:HB1	2:K:366:ILE:HD11	1.97	0.46
2:M:24:HIS:HB2	2:O:33:THR:O	2.16	0.46
1:F:82:GLU:OE2	1:F:205:HIS:NE2	2.47	0.46
2:N:48:TRP:NE1	2:N:54:ALA:O	2.41	0.46
2:N:321:ALA:HB1	2:N:366:ILE:HD11	1.98	0.46
2:K:209:LYS:NZ	4:K:401:PY6:CA	2.74	0.46
2:E:321:ALA:HB1	2:E:366:ILE:HD11	1.98	0.45
2:K:6:PRO:O	2:K:10:MET:SD	2.74	0.45
1:P:325:VAL:CG1	1:P:333:HIS:CG	3.00	0.45
1:P:321:ALA:HB1	1:P:366:ILE:HD11	1.98	0.45
2:C:152:GLY:O	2:C:180:PRO:HD2	2.17	0.45
2:M:92:THR:HG22	2:M:218:MET:HE3	1.98	0.45
1:I:321:ALA:HB1	1:I:366:ILE:HD11	1.98	0.45
1:B:286:HIS:HB2	1:B:311:ALA:HB3	1.98	0.44
2:E:209:LYS:HZ2	4:E:401:PY6:HA	1.82	0.44
2:K:82:GLU:OE2	2:K:205:HIS:NE2	2.47	0.44
2:M:321:ALA:HB1	2:M:366:ILE:HD11	1.98	0.44
1:B:209:LLP:C4'	3:B:401:NLE:N	2.79	0.44
2:G:48:TRP:NE1	2:G:54:ALA:O	2.41	0.44
1:F:325:VAL:CG1	1:F:333:HIS:CD2	3.01	0.44
2:C:275:ARG:NH1	2:C:379:GLU:OE1	2.50	0.44
1:P:156:VAL:HG21	1:P:172:VAL:HG11	1.99	0.44
1:P:325:VAL:HG13	1:P:333:HIS:CG	2.52	0.44
1:F:24:HIS:HB2	1:H:33:THR:O	2.18	0.43
1:H:159:PRO:HD3	1:H:188:CYS:SG	2.58	0.43
2:O:124:HIS:CE1	2:O:128:THR:HG23	2.52	0.43
1:F:321:ALA:HB1	1:F:366:ILE:HD11	1.99	0.43
1:J:33:THR:O	1:L:24:HIS:HB2	2.19	0.43
1:F:325:VAL:HG13	1:F:333:HIS:CD2	2.54	0.43
1:H:6:PRO:O	1:H:10:MET:SD	2.76	0.43
1:D:48:TRP:NE1	1:D:54:ALA:O	2.41	0.43
2:C:63:TYR:OH	1:D:209:LLP:OP2	2.33	0.43
1:H:55:LEU:HD22	1:H:67:TRP:CD1	2.54	0.43
2:N:182:LEU:HD11	2:N:204:LEU:HB2	2.00	0.43
1:A:110:PRO:HD2	1:A:150:ASP:OD1	2.18	0.42
1:J:345:GLN:O	1:J:366:ILE:HG13	2.18	0.42
2:O:124:HIS:CE1	2:O:128:THR:CG2	3.02	0.42
1:B:253:ARG:NH1	2:C:253:ARG:NH1	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:10:MET:SD	2:C:259:ALA:HB2	2.59	0.42
2:C:53:HIS:CD2	1:F:363:ASP:OD2	2.72	0.42
2:M:253:ARG:NH1	1:P:253:ARG:NH1	2.68	0.42
1:L:321:ALA:HB3	1:L:346:HIS:CE1	2.54	0.42
1:D:92:THR:HG22	1:D:218:MET:HE3	2.02	0.42
1:L:92:THR:HG22	1:L:218:MET:HE3	2.02	0.42
2:M:6:PRO:O	2:M:10:MET:SD	2.78	0.42
1:B:92:THR:HG22	1:B:218:MET:HE3	2.02	0.42
1:F:345:GLN:HE21	1:F:367:ARG:CZ	2.33	0.42
1:J:92:THR:HG22	1:J:218:MET:HE3	2.02	0.42
2:O:6:PRO:O	2:O:10:MET:SD	2.78	0.42
2:G:202:LEU:HD11	2:G:228:TRP:CD2	2.55	0.41
2:N:6:PRO:O	2:N:10:MET:SD	2.78	0.41
1:P:325:VAL:CG1	1:P:333:HIS:CD2	3.02	0.41
1:D:346:HIS:CE1	1:D:348:ALA:HB3	2.55	0.41
1:P:139:LYS:O	1:P:143:ILE:HG13	2.20	0.41
1:I:346:HIS:CE1	1:I:348:ALA:HB3	2.56	0.41
1:A:325:VAL:HG13	1:A:333:HIS:CD2	2.56	0.41
1:I:6:PRO:O	1:I:10:MET:SD	2.79	0.41
1:P:92:THR:HG22	1:P:218:MET:HE3	2.02	0.41
1:A:345:GLN:HE21	1:A:367:ARG:CZ	2.34	0.41
1:B:24:HIS:HB2	1:D:33:THR:O	2.20	0.41
1:F:92:THR:HG22	1:F:218:MET:HE3	2.03	0.41
2:K:92:THR:HG22	2:K:218:MET:HE3	2.02	0.41
1:L:6:PRO:O	1:L:10:MET:SD	2.79	0.41
1:B:115:VAL:HA	1:B:138:ALA:O	2.20	0.41
2:C:82:GLU:OE2	2:C:205:HIS:NE2	2.51	0.41
2:C:351:THR:HG22	2:C:352:HIS:CE1	2.55	0.41
2:E:15:MET:HE2	2:E:252:HIS:CE1	2.56	0.41
2:G:6:PRO:O	2:G:10:MET:SD	2.78	0.41
2:G:92:THR:HG22	2:G:218:MET:HE3	2.03	0.41
1:H:92:THR:HG22	1:H:218:MET:HE3	2.03	0.41
1:J:6:PRO:O	1:J:10:MET:SD	2.79	0.41
1:P:6:PRO:O	1:P:10:MET:SD	2.78	0.41
2:N:92:THR:HG22	2:N:218:MET:HE3	2.03	0.41
2:O:82:GLU:OE2	2:O:205:HIS:NE2	2.54	0.40
1:A:10:MET:SD	1:A:259:ALA:HB2	2.62	0.40
2:K:10:MET:SD	2:K:259:ALA:HB2	2.61	0.40
2:O:92:THR:HG22	2:O:218:MET:HE3	2.03	0.40
1:B:6:PRO:O	1:B:10:MET:SD	2.79	0.40
1:I:55:LEU:HD22	1:I:67:TRP:CD1	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:253:ARG:NH1	2:K:253:ARG:NH1	2.70	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:315:ALA:HB3	1:I:147:ILE:O[3_745]	1.47	0.13
2:G:315:ALA:CB	1:I:147:ILE:O[3_745]	2.10	0.10

## 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	381/414 (92%)	366 (96%)	14 (4%)	1 (0%)	36	60
1	B	385/414 (93%)	371 (96%)	14 (4%)	0	100	100
1	D	378/414 (91%)	365 (97%)	13 (3%)	0	100	100
1	F	384/414 (93%)	368 (96%)	16 (4%)	0	100	100
1	H	365/414 (88%)	354 (97%)	11 (3%)	0	100	100
1	I	384/414 (93%)	367 (96%)	16 (4%)	1 (0%)	36	60
1	J	379/414 (92%)	368 (97%)	11 (3%)	0	100	100
1	L	367/414 (89%)	353 (96%)	14 (4%)	0	100	100
1	P	380/414 (92%)	358 (94%)	22 (6%)	0	100	100
2	C	386/413 (94%)	371 (96%)	15 (4%)	0	100	100
2	E	387/413 (94%)	373 (96%)	14 (4%)	0	100	100
2	G	385/413 (93%)	367 (95%)	18 (5%)	0	100	100
2	K	382/413 (92%)	367 (96%)	15 (4%)	0	100	100
2	M	378/413 (92%)	363 (96%)	15 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	N	385/413 (93%)	370 (96%)	15 (4%)	0	100	100
2	O	374/413 (91%)	359 (96%)	15 (4%)	0	100	100
All	All	6080/6617 (92%)	5840 (96%)	238 (4%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	291	ASN
1	A	355	VAL

### 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	283/305 (93%)	276 (98%)	7 (2%)	42	71
1	B	285/305 (93%)	274 (96%)	11 (4%)	28	57
1	D	281/305 (92%)	272 (97%)	9 (3%)	34	64
1	F	284/305 (93%)	275 (97%)	9 (3%)	34	64
1	H	274/305 (90%)	263 (96%)	11 (4%)	28	56
1	I	285/305 (93%)	275 (96%)	10 (4%)	32	61
1	J	282/305 (92%)	269 (95%)	13 (5%)	24	51
1	L	275/305 (90%)	266 (97%)	9 (3%)	33	63
1	P	285/305 (93%)	274 (96%)	11 (4%)	28	57
2	C	286/305 (94%)	278 (97%)	8 (3%)	38	68
2	E	286/305 (94%)	280 (98%)	6 (2%)	47	75
2	G	285/305 (93%)	276 (97%)	9 (3%)	34	64
2	K	285/305 (93%)	276 (97%)	9 (3%)	34	64
2	M	283/305 (93%)	275 (97%)	8 (3%)	38	68
2	N	285/305 (93%)	276 (97%)	9 (3%)	34	64
2	O	281/305 (92%)	270 (96%)	11 (4%)	28	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	4525/4880 (93%)	4375 (97%)	150 (3%)	33 63

All (150) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	MET
1	A	112	ILE
1	A	158	THR
1	A	194	GLN
1	A	238	ILE
1	A	262	MET
1	A	337	LEU
1	B	10	MET
1	B	112	ILE
1	B	194	GLN
1	B	238	ILE
1	B	262	MET
1	B	290	LEU
1	B	291	ASN
1	B	303	MET
1	B	337	LEU
1	B	345	GLN
1	B	350	LEU
2	C	112	ILE
2	C	153	LEU
2	C	158	THR
2	C	194	GLN
2	C	209	LYS
2	C	262	MET
2	C	312	LEU
2	C	337	LEU
1	D	10	MET
1	D	112	ILE
1	D	158	THR
1	D	194	GLN
1	D	238	ILE
1	D	262	MET
1	D	312	LEU
1	D	337	LEU
1	D	345	GLN
2	E	158	THR
2	E	194	GLN

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Mol	Chain	Res	Type
2	E	238	ILE
2	E	262	MET
2	E	312	LEU
2	E	337	LEU
1	F	10	MET
1	F	112	ILE
1	F	158	THR
1	F	194	GLN
1	F	262	MET
1	F	293	GLN
1	F	312	LEU
1	F	337	LEU
1	F	358	THR
2	G	10	MET
2	G	112	ILE
2	G	188	CYS
2	G	194	GLN
2	G	209	LYS
2	G	262	MET
2	G	290	LEU
2	G	312	LEU
2	G	337	LEU
1	H	10	MET
1	H	78	LEU
1	H	97	MET
1	H	112	ILE
1	H	139	LYS
1	H	158	THR
1	H	194	GLN
1	H	209[A]	LYS
1	H	238	ILE
1	H	262	MET
1	H	312	LEU
1	I	4	MET
1	I	10	MET
1	I	112	ILE
1	I	142	GLU
1	I	158	THR
1	I	194	GLN
1	I	209[A]	LYS
1	I	262	MET
1	I	312	LEU

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Mol	Chain	Res	Type
1	I	337	LEU
1	J	10	MET
1	J	112	ILE
1	J	139	LYS
1	J	142	GLU
1	J	158	THR
1	J	194	GLN
1	J	239	THR
1	J	282	ILE
1	J	299	LEU
1	J	312	LEU
1	J	313	GLU
1	J	337	LEU
1	J	366	ILE
2	K	10	MET
2	K	112	ILE
2	K	158	THR
2	K	188	CYS
2	K	194	GLN
2	K	262	MET
2	K	312	LEU
2	K	337	LEU
2	K	341	ASP
1	L	10	MET
1	L	112	ILE
1	L	158	THR
1	L	194	GLN
1	L	262	MET
1	L	290	LEU
1	L	312	LEU
1	L	337	LEU
1	L	349	SER
2	M	10	MET
2	M	112	ILE
2	M	158	THR
2	M	194	GLN
2	M	197	ARG
2	M	262	MET
2	M	312	LEU
2	M	337	LEU
2	N	10	MET
2	N	112	ILE

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Mol	Chain	Res	Type
2	N	158	THR
2	N	194	GLN
2	N	209	LYS
2	N	262	MET
2	N	293	GLN
2	N	312	LEU
2	N	337	LEU
2	O	10	MET
2	O	112	ILE
2	O	139	LYS
2	O	142	GLU
2	O	158	THR
2	O	262	MET
2	O	290	LEU
2	O	301	ARG
2	O	312	LEU
2	O	326	GLU
2	O	337	LEU
1	P	10	MET
1	P	112	ILE
1	P	116	ARG
1	P	158	THR
1	P	194	GLN
1	P	209[A]	LYS
1	P	256	ARG
1	P	262	MET
1	P	312	LEU
1	P	322	ARG
1	P	337	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (63) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	GLN
1	A	148	GLN
1	A	194	GLN
1	A	345	GLN
1	B	2	ASN
1	B	34	ASN
1	B	194	GLN
1	B	352	HIS
2	C	34	ASN

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Mol	Chain	Res	Type
2	C	124	HIS
2	C	148	GLN
2	C	194	GLN
1	D	34	ASN
1	D	64	GLN
1	D	148	GLN
2	E	24	HIS
2	E	124	HIS
2	E	193	GLN
2	E	194	GLN
1	F	34	ASN
1	F	124	HIS
1	F	148	GLN
1	F	345	GLN
2	G	34	ASN
2	G	124	HIS
2	G	148	GLN
2	G	193	GLN
2	G	194	GLN
1	H	53	HIS
1	H	124	HIS
1	H	148	GLN
1	H	194	GLN
1	I	34	ASN
1	I	124	HIS
1	I	148	GLN
1	I	345	GLN
1	J	124	HIS
1	J	148	GLN
1	J	194	GLN
2	K	34	ASN
2	K	124	HIS
2	K	148	GLN
2	K	194	GLN
1	L	34	ASN
1	L	124	HIS
1	L	148	GLN
1	L	194	GLN
1	L	205	HIS
2	M	53	HIS
2	M	124	HIS
2	M	148	GLN

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Mol	Chain	Res	Type
2	M	194	GLN
2	M	293	GLN
2	N	34	ASN
2	N	124	HIS
2	N	148	GLN
2	N	194	GLN
2	O	124	HIS
2	O	148	GLN
1	P	34	ASN
1	P	124	HIS
1	P	148	GLN
1	P	194	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

9 non-standard protein/DNA/RNA residues 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$
1	LLP	B	209	1	23,24,25	1.64	2 (8%)	25,32,34	0.82	0
1	LLP	J	209	1	23,24,25	1.67	2 (8%)	25,32,34	0.83	0
1	LLP	P	209[B]	1	23,24,25	1.39	1 (4%)	25,32,34	0.78	0
1	LLP	I	209[B]	1	23,24,25	1.38	1 (4%)	25,32,34	0.74	0
1	LLP	F	209	1	23,24,25	1.67	2 (8%)	25,32,34	0.80	0
1	LLP	A	209	1	23,24,25	1.61	2 (8%)	25,32,34	0.81	0
1	LLP	L	209	1	23,24,25	1.44	1 (4%)	25,32,34	0.88	0
1	LLP	H	209[B]	1	23,24,25	1.39	1 (4%)	25,32,34	0.72	0
1	LLP	D	209	1	23,24,25	1.62	2 (8%)	25,32,34	0.84	0

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
1	LLP	B	209	1	-	6/16/17/19	0/1/1/1
1	LLP	J	209	1	-	6/16/17/19	0/1/1/1
1	LLP	P	209[B]	1	-	4/16/17/19	0/1/1/1
1	LLP	I	209[B]	1	-	4/16/17/19	0/1/1/1
1	LLP	F	209	1	-	6/16/17/19	0/1/1/1
1	LLP	A	209	1	-	6/16/17/19	0/1/1/1
1	LLP	L	209	1	-	5/16/17/19	0/1/1/1
1	LLP	H	209[B]	1	-	4/16/17/19	0/1/1/1
1	LLP	D	209	1	-	6/16/17/19	0/1/1/1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	209	LLP	C4'-NZ	7.11	1.51	1.27
1	F	209	LLP	C4'-NZ	7.04	1.50	1.27
1	B	209	LLP	C4'-NZ	6.99	1.50	1.27
1	D	209	LLP	C4'-NZ	6.90	1.50	1.27
1	A	209	LLP	C4'-NZ	6.83	1.50	1.27
1	L	209	LLP	C4'-NZ	6.26	1.48	1.27
1	H	209[B]	LLP	C4'-NZ	6.19	1.47	1.27
1	P	209[B]	LLP	C4'-NZ	6.15	1.47	1.27
1	I	209[B]	LLP	C4'-NZ	6.14	1.47	1.27
1	F	209	LLP	CE-NZ	2.72	1.52	1.46
1	J	209	LLP	CE-NZ	2.66	1.52	1.46
1	A	209	LLP	CE-NZ	2.50	1.52	1.46
1	D	209	LLP	CE-NZ	2.45	1.52	1.46
1	B	209	LLP	CE-NZ	2.45	1.52	1.46

There are no bond angle outliers.

There are no chirality outliers.

All (47) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	209	LLP	N-CA-CB-CG
1	A	209	LLP	C-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
1	B	209	LLP	N-CA-CB-CG
1	B	209	LLP	C-CA-CB-CG
1	D	209	LLP	N-CA-CB-CG
1	D	209	LLP	C-CA-CB-CG
1	F	209	LLP	N-CA-CB-CG
1	F	209	LLP	C-CA-CB-CG
1	H	209[B]	LLP	C4-C4'-NZ-CE
1	I	209[B]	LLP	C4-C4'-NZ-CE
1	J	209	LLP	N-CA-CB-CG
1	J	209	LLP	C-CA-CB-CG
1	L	209	LLP	C4-C4'-NZ-CE
1	L	209	LLP	N-CA-CB-CG
1	L	209	LLP	C-CA-CB-CG
1	P	209[B]	LLP	C4-C4'-NZ-CE
1	A	209	LLP	C4-C4'-NZ-CE
1	B	209	LLP	C4-C4'-NZ-CE
1	D	209	LLP	C4-C4'-NZ-CE
1	F	209	LLP	C4-C4'-NZ-CE
1	J	209	LLP	C4-C4'-NZ-CE
1	A	209	LLP	CG-CD-CE-NZ
1	B	209	LLP	CG-CD-CE-NZ
1	D	209	LLP	CG-CD-CE-NZ
1	F	209	LLP	CG-CD-CE-NZ
1	J	209	LLP	CG-CD-CE-NZ
1	A	209	LLP	CD-CE-NZ-C4'
1	D	209	LLP	CD-CE-NZ-C4'
1	H	209[B]	LLP	CG-CD-CE-NZ
1	I	209[B]	LLP	CG-CD-CE-NZ
1	P	209[B]	LLP	CG-CD-CE-NZ
1	B	209	LLP	CD-CE-NZ-C4'
1	F	209	LLP	CD-CE-NZ-C4'
1	J	209	LLP	CD-CE-NZ-C4'
1	L	209	LLP	CD-CE-NZ-C4'
1	B	209	LLP	C3-C4-C4'-NZ
1	D	209	LLP	C3-C4-C4'-NZ
1	L	209	LLP	C3-C4-C4'-NZ
1	A	209	LLP	C3-C4-C4'-NZ
1	F	209	LLP	C3-C4-C4'-NZ
1	J	209	LLP	C3-C4-C4'-NZ
1	H	209[B]	LLP	CA-CB-CG-CD
1	I	209[B]	LLP	CA-CB-CG-CD
1	P	209[B]	LLP	CA-CB-CG-CD

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Mol	Chain	Res	Type	Atoms
1	H	209[B]	LLP	C3-C4-C4'-NZ
1	I	209[B]	LLP	C3-C4-C4'-NZ
1	P	209[B]	LLP	C3-C4-C4'-NZ

There are no ring outliers.

6 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	209	LLP	2	0
1	J	209	LLP	3	0
1	I	209[B]	LLP	1	0
1	F	209	LLP	3	0
1	A	209	LLP	3	0
1	D	209	LLP	1	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

19 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	$\# Z  > 2$
3	NLE	F	401	-	7,8,8	0.89	0	6,9,9	0.47	0
5	PEG	D	402	-	6,6,6	0.23	0	5,5,5	0.38	0
4	PY6	M	401	-	24,24,24	1.92	5 (20%)	29,33,33	2.07	14 (48%)
4	PY6	K	401	-	24,24,24	1.91	4 (16%)	29,33,33	2.02	13 (44%)
4	PY6	N	401	-	24,24,24	1.72	5 (20%)	29,33,33	1.77	10 (34%)
4	PY6	H	401[A]	-	24,24,24	2.16	6 (25%)	29,33,33	2.41	12 (41%)
3	NLE	D	401	-	7,8,8	0.93	0	6,9,9	0.42	0
5	PEG	J	402	-	6,6,6	0.25	0	5,5,5	0.24	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NLE	J	401	-	7,8,8	0.85	0	6,9,9	0.44	0
4	PY6	C	401	-	24,24,24	2.02	5 (20%)	29,33,33	2.27	14 (48%)
5	PEG	F	402	-	6,6,6	0.25	0	5,5,5	0.44	0
6	PLP	P	401[A]	4	15,15,16	0.73	1 (6%)	21,22,23	0.73	0
3	NLE	A	401	-	7,8,8	0.84	0	6,9,9	0.66	0
4	PY6	P	402[A]	6	24,24,24	2.16	6 (25%)	29,33,33	2.41	13 (44%)
4	PY6	E	401	-	24,24,24	1.80	6 (25%)	29,33,33	1.77	10 (34%)
3	NLE	B	401	-	7,8,8	1.10	0	6,9,9	0.45	0
4	PY6	G	401	-	24,24,24	1.70	5 (20%)	29,33,33	1.83	11 (37%)
4	PY6	O	401	-	24,24,24	1.79	6 (25%)	29,33,33	1.89	9 (31%)
4	PY6	I	401[A]	-	24,24,24	2.07	5 (20%)	29,33,33	2.44	14 (48%)

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	NLE	F	401	-	-	1/8/8/8	-
5	PEG	D	402	-	-	2/4/4/4	-
4	PY6	M	401	-	-	0/19/19/19	0/1/1/1
4	PY6	K	401	-	-	4/19/19/19	0/1/1/1
4	PY6	N	401	-	-	5/19/19/19	0/1/1/1
4	PY6	H	401[A]	-	-	5/19/19/19	0/1/1/1
3	NLE	D	401	-	-	3/8/8/8	-
5	PEG	J	402	-	-	2/4/4/4	-
3	NLE	J	401	-	-	2/8/8/8	-
4	PY6	C	401	-	-	5/19/19/19	0/1/1/1
5	PEG	F	402	-	-	2/4/4/4	-
6	PLP	P	401[A]	4	-	0/6/6/8	0/1/1/1
3	NLE	A	401	-	-	1/8/8/8	-
4	PY6	P	402[A]	6	-	5/19/19/19	0/1/1/1
4	PY6	E	401	-	-	5/19/19/19	0/1/1/1
3	NLE	B	401	-	-	3/8/8/8	-
4	PY6	G	401	-	-	5/19/19/19	0/1/1/1
4	PY6	O	401	-	-	5/19/19/19	0/1/1/1
4	PY6	I	401[A]	-	-	4/19/19/19	0/1/1/1



All (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	P	402[A]	PY6	P-O4P	7.17	1.82	1.60
4	M	401	PY6	P-O4P	7.09	1.82	1.60
4	C	401	PY6	P-O4P	7.07	1.82	1.60
4	K	401	PY6	P-O4P	7.04	1.82	1.60
4	H	401[A]	PY6	P-O4P	7.01	1.82	1.60
4	I	401[A]	PY6	P-O4P	6.57	1.81	1.60
4	G	401	PY6	P-O4P	5.77	1.78	1.60
4	N	401	PY6	P-O4P	5.76	1.78	1.60
4	E	401	PY6	P-O4P	5.60	1.78	1.60
4	O	401	PY6	P-O4P	5.47	1.77	1.60
4	H	401[A]	PY6	CA-N	4.39	1.56	1.46
4	P	402[A]	PY6	CA-N	4.31	1.56	1.46
4	I	401[A]	PY6	CA-N	4.14	1.56	1.46
4	C	401	PY6	CA-N	3.42	1.54	1.46
4	K	401	PY6	CA-C	3.40	1.61	1.52
4	E	401	PY6	C4A-C4	-3.16	1.47	1.52
4	O	401	PY6	C4A-C4	-3.15	1.47	1.52
4	H	401[A]	PY6	CA-C	3.09	1.60	1.52
4	I	401[A]	PY6	O4P-C5A	-2.90	1.34	1.44
4	E	401	PY6	CA-N	2.89	1.53	1.46
4	H	401[A]	PY6	O4P-C5A	-2.87	1.34	1.44
4	P	402[A]	PY6	O4P-C5A	-2.87	1.34	1.44
4	M	401	PY6	O4P-C5A	-2.85	1.34	1.44
4	I	401[A]	PY6	CA-C	2.84	1.59	1.52
4	G	401	PY6	O4P-C5A	-2.74	1.34	1.44
4	O	401	PY6	CA-N	2.74	1.52	1.46
4	C	401	PY6	O4P-C5A	-2.71	1.34	1.44
4	K	401	PY6	O4P-C5A	-2.68	1.35	1.44
4	O	401	PY6	O4P-C5A	-2.67	1.35	1.44
4	N	401	PY6	O4P-C5A	-2.66	1.35	1.44
4	O	401	PY6	CA-C	2.64	1.59	1.52
4	C	401	PY6	CA-C	2.62	1.59	1.52
4	G	401	PY6	CA-C	2.53	1.59	1.52
4	E	401	PY6	O4P-C5A	-2.49	1.35	1.44
4	E	401	PY6	CA-C	2.48	1.59	1.52
4	N	401	PY6	CA-C	2.47	1.58	1.52
4	P	402[A]	PY6	CA-C	2.45	1.58	1.52
4	M	401	PY6	C6-C5	2.44	1.42	1.37
4	G	401	PY6	CA-N	2.39	1.52	1.46
4	P	402[A]	PY6	C6-C5	2.35	1.42	1.37
4	N	401	PY6	CA-N	2.33	1.52	1.46
4	K	401	PY6	C6-C5	2.33	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	401	PY6	CA-N	2.32	1.51	1.46
4	H	401[A]	PY6	C6-C5	2.31	1.42	1.37
4	C	401	PY6	C6-C5	2.28	1.42	1.37
4	I	401[A]	PY6	C6-C5	2.27	1.42	1.37
4	G	401	PY6	C6-C5	2.27	1.42	1.37
4	H	401[A]	PY6	C4A-N	2.26	1.53	1.46
4	N	401	PY6	C6-C5	2.24	1.42	1.37
4	O	401	PY6	C6-C5	2.19	1.42	1.37
4	E	401	PY6	C6-C5	2.17	1.42	1.37
4	M	401	PY6	CA-C	2.17	1.58	1.52
4	P	402[A]	PY6	C4A-N	2.05	1.52	1.46
6	P	401[A]	PLP	C4A-C4	-2.02	1.47	1.51

All (120) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	401[A]	PY6	C4A-N-CA	5.78	124.70	113.84
4	I	401[A]	PY6	C4A-N-CA	5.77	124.67	113.84
4	P	402[A]	PY6	C4A-N-CA	5.73	124.59	113.84
4	C	401	PY6	C4A-N-CA	5.48	124.13	113.84
4	O	401	PY6	O2P-P-O4P	-4.51	94.90	106.67
4	I	401[A]	PY6	C5A-C5-C6	-4.19	112.53	119.36
4	H	401[A]	PY6	C5A-C5-C6	-4.15	112.59	119.36
4	P	402[A]	PY6	C5A-C5-C6	-4.15	112.59	119.36
4	H	401[A]	PY6	C3-C4-C5	-4.12	115.00	118.73
4	M	401	PY6	C5A-C5-C6	-4.11	112.66	119.36
4	P	402[A]	PY6	C3-C4-C5	-3.98	115.12	118.73
4	I	401[A]	PY6	C3-C4-C5	-3.95	115.15	118.73
4	C	401	PY6	C5A-C5-C6	-3.66	113.39	119.36
4	I	401[A]	PY6	O2P-P-O4P	-3.52	97.49	106.67
4	K	401	PY6	C5A-C5-C6	-3.44	113.75	119.36
4	C	401	PY6	C3-C4-C5	-3.41	115.64	118.73
4	M	401	PY6	C3-C4-C5	-3.40	115.65	118.73
4	P	402[A]	PY6	C4A-C4-C3	3.21	124.25	119.98
4	I	401[A]	PY6	C4A-C4-C3	3.20	124.23	119.98
4	K	401	PY6	C3-C4-C5	-3.17	115.85	118.73
4	E	401	PY6	C4A-N-CA	3.16	119.77	113.84
4	H	401[A]	PY6	C4A-C4-C3	3.15	124.17	119.98
4	C	401	PY6	C4A-C4-C3	3.13	124.14	119.98
4	O	401	PY6	C4A-N-CA	3.09	119.63	113.84
4	M	401	PY6	O2P-P-O4P	-3.08	98.63	106.67
4	I	401[A]	PY6	O3-C3-C4	3.05	127.03	118.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	401	PY6	O2P-P-O4P	-3.01	98.82	106.67
4	P	402[A]	PY6	O3-C3-C4	3.01	126.92	118.18
4	H	401[A]	PY6	O3-C3-C4	3.00	126.89	118.18
4	C	401	PY6	O3-C3-C4	3.00	126.88	118.18
4	K	401	PY6	O2P-P-O4P	-2.99	98.87	106.67
4	M	401	PY6	C5A-C5-C4	2.97	128.93	122.67
4	H	401[A]	PY6	C2A-C2-C3	2.90	124.20	120.80
4	N	401	PY6	C4A-N-CA	2.90	119.28	113.84
4	I	401[A]	PY6	O3-C3-C2	-2.89	111.59	117.58
4	H	401[A]	PY6	O3-C3-C2	-2.87	111.62	117.58
4	M	401	PY6	O3-C3-C4	2.87	126.51	118.18
4	P	402[A]	PY6	C2A-C2-C3	2.87	124.16	120.80
4	I	401[A]	PY6	O3P-P-O2P	2.86	118.53	107.80
4	H	401[A]	PY6	O4P-P-O1P	-2.85	98.73	106.44
4	M	401	PY6	C4A-C4-C5	2.85	122.85	119.75
4	M	401	PY6	O3-C3-C2	-2.84	111.70	117.58
4	I	401[A]	PY6	C2A-C2-C3	2.84	124.12	120.80
4	E	401	PY6	O3-C3-C4	2.83	126.38	118.18
4	O	401	PY6	O3-C3-C4	2.81	126.33	118.18
4	P	402[A]	PY6	O3-C3-C2	-2.81	111.76	117.58
4	P	402[A]	PY6	O3P-P-O2P	2.80	118.31	107.80
4	G	401	PY6	O3-C3-C4	2.80	126.29	118.18
4	H	401[A]	PY6	O3P-P-O2P	2.79	118.26	107.80
4	C	401	PY6	O3P-P-O2P	2.79	118.25	107.80
4	C	401	PY6	C2A-C2-C3	2.78	124.05	120.80
4	N	401	PY6	O3-C3-C4	2.77	126.22	118.18
4	K	401	PY6	O3P-P-O2P	2.76	118.16	107.80
4	K	401	PY6	O3-C3-C4	2.76	126.19	118.18
4	P	402[A]	PY6	O4P-P-O1P	-2.76	98.99	106.44
4	C	401	PY6	O3-C3-C2	-2.76	111.87	117.58
4	G	401	PY6	C4A-N-CA	2.74	118.98	113.84
4	M	401	PY6	O3P-P-O2P	2.72	117.98	107.80
4	I	401[A]	PY6	C5A-C5-C4	2.71	128.38	122.67
4	P	402[A]	PY6	O2P-P-O4P	-2.70	99.64	106.67
4	G	401	PY6	C2A-C2-C3	2.69	123.95	120.80
4	O	401	PY6	O3P-P-O2P	2.69	117.89	107.80
4	H	401[A]	PY6	C5A-C5-C4	2.67	128.29	122.67
4	H	401[A]	PY6	O2P-P-O4P	-2.67	99.71	106.67
4	P	402[A]	PY6	C5A-C5-C4	2.65	128.25	122.67
4	K	401	PY6	C2A-C2-C3	2.65	123.89	120.80
4	N	401	PY6	C5A-C5-C6	-2.64	115.06	119.36
4	E	401	PY6	C2A-C2-C3	2.62	123.87	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	K	401	PY6	O4P-P-O1P	-2.62	99.36	106.44
4	E	401	PY6	O3P-P-O2P	2.62	117.62	107.80
4	G	401	PY6	O3P-P-O2P	2.58	117.49	107.80
4	N	401	PY6	C2A-C2-C3	2.58	123.81	120.80
4	O	401	PY6	C2A-C2-C3	2.57	123.81	120.80
4	G	401	PY6	C5A-C5-C6	-2.57	115.18	119.36
4	K	401	PY6	O3-C3-C2	-2.53	112.34	117.58
4	H	401[A]	PY6	C2A-C2-N1	-2.52	112.89	117.64
4	E	401	PY6	C5A-C5-C6	-2.52	115.25	119.36
4	K	401	PY6	CB-CA-C	2.52	116.34	110.35
4	P	402[A]	PY6	C2A-C2-N1	-2.50	112.92	117.64
4	N	401	PY6	O3P-P-O2P	2.50	117.17	107.80
4	O	401	PY6	C5A-C5-C6	-2.49	115.31	119.36
4	I	401[A]	PY6	C2A-C2-N1	-2.46	113.00	117.64
4	G	401	PY6	O3P-P-O4P	-2.46	100.26	106.67
4	G	401	PY6	O3-C3-C2	-2.38	112.66	117.58
4	C	401	PY6	C2A-C2-N1	-2.36	113.19	117.64
4	E	401	PY6	O3P-P-O4P	-2.35	100.54	106.67
4	O	401	PY6	O3-C3-C2	-2.35	112.72	117.58
4	K	401	PY6	C5A-C5-C4	2.33	127.58	122.67
4	C	401	PY6	C5A-C5-C4	2.33	127.57	122.67
4	N	401	PY6	O3-C3-C2	-2.33	112.76	117.58
4	E	401	PY6	O3-C3-C2	-2.32	112.78	117.58
4	N	401	PY6	O4P-P-O1P	-2.28	100.28	106.44
4	O	401	PY6	CB-CA-C	2.28	115.77	110.35
4	G	401	PY6	O2P-P-O4P	-2.27	100.75	106.67
4	I	401[A]	PY6	O4P-P-O1P	-2.26	100.34	106.44
4	K	401	PY6	C2A-C2-N1	-2.25	113.40	117.64
4	G	401	PY6	C3-C4-C5	-2.25	116.69	118.73
4	M	401	PY6	C2A-C2-C3	2.23	123.41	120.80
4	E	401	PY6	O2P-P-O4P	-2.23	100.86	106.67
4	E	401	PY6	CB-CA-C	2.23	115.64	110.35
4	G	401	PY6	C2A-C2-N1	-2.22	113.47	117.64
4	G	401	PY6	CB-CA-C	2.19	115.56	110.35
4	N	401	PY6	O2P-P-O4P	-2.19	100.96	106.67
4	M	401	PY6	O4P-C5A-C5	2.19	113.46	109.36
4	M	401	PY6	O4P-P-O1P	-2.17	100.56	106.44
4	P	402[A]	PY6	CB-CA-C	2.17	115.50	110.35
4	C	401	PY6	O3P-P-O4P	-2.16	101.03	106.67
4	I	401[A]	PY6	O3P-P-O4P	-2.16	101.03	106.67
4	I	401[A]	PY6	CB-CA-C	2.16	115.48	110.35
4	K	401	PY6	O3P-P-O4P	-2.13	101.11	106.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	401	PY6	C4A-N-CA	2.12	117.82	113.84
4	N	401	PY6	CB-CA-C	2.11	115.36	110.35
4	C	401	PY6	O4P-P-O1P	-2.08	100.82	106.44
4	N	401	PY6	C2A-C2-N1	-2.07	113.74	117.64
4	K	401	PY6	C4A-C4-C5	2.05	121.98	119.75
4	M	401	PY6	O3P-P-O4P	-2.03	101.38	106.67
4	E	401	PY6	C2A-C2-N1	-2.03	113.82	117.64
4	O	401	PY6	C2A-C2-N1	-2.02	113.83	117.64
4	M	401	PY6	C2A-C2-N1	-2.02	113.84	117.64
4	C	401	PY6	CB-CA-C	2.01	115.12	110.35

There are no chirality outliers.

All (59) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	401	PY6	C3-C4-C4A-N
4	C	401	PY6	C5-C4-C4A-N
4	C	401	PY6	CB-CA-N-C4A
4	E	401	PY6	C-CA-N-C4A
4	H	401[A]	PY6	C5-C4-C4A-N
4	H	401[A]	PY6	CB-CA-N-C4A
4	I	401[A]	PY6	C5-C4-C4A-N
4	I	401[A]	PY6	CB-CA-N-C4A
4	N	401	PY6	C-CA-N-C4A
4	O	401	PY6	C-CA-N-C4A
4	P	402[A]	PY6	C5-C4-C4A-N
4	P	402[A]	PY6	CB-CA-N-C4A
4	K	401	PY6	C-CA-CB-CG
4	K	401	PY6	C4-C4A-N-CA
5	D	402	PEG	O2-C3-C4-O4
5	J	402	PEG	O2-C3-C4-O4
5	J	402	PEG	O1-C1-C2-O2
4	K	401	PY6	N-CA-CB-CG
4	E	401	PY6	C-CA-CB-CG
4	G	401	PY6	C-CA-CB-CG
4	N	401	PY6	C-CA-CB-CG
4	O	401	PY6	C-CA-CB-CG
4	P	402[A]	PY6	CE-CD-CG-CB
4	H	401[A]	PY6	CE-CD-CG-CB
4	C	401	PY6	CE-CD-CG-CB
3	D	401	NLE	OXT-C-CA-CB
4	H	401[A]	PY6	C3-C4-C4A-N

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Mol	Chain	Res	Type	Atoms
4	I	401[A]	PY6	C3-C4-C4A-N
4	P	402[A]	PY6	C3-C4-C4A-N
4	E	401	PY6	CB-CA-N-C4A
4	G	401	PY6	CB-CA-N-C4A
4	N	401	PY6	CB-CA-N-C4A
4	O	401	PY6	CB-CA-N-C4A
4	C	401	PY6	C-CA-N-C4A
4	G	401	PY6	C-CA-N-C4A
4	H	401[A]	PY6	C-CA-N-C4A
4	I	401[A]	PY6	C-CA-N-C4A
4	P	402[A]	PY6	C-CA-N-C4A
3	B	401	NLE	N-CA-CB-CG
3	D	401	NLE	CE-CD-CG-CB
3	B	401	NLE	O-C-CA-CB
3	B	401	NLE	OXT-C-CA-CB
3	D	401	NLE	O-C-CA-CB
5	D	402	PEG	C4-C3-O2-C2
5	F	402	PEG	C1-C2-O2-C3
5	F	402	PEG	C4-C3-O2-C2
4	E	401	PY6	C4-C4A-N-CA
4	N	401	PY6	C4-C4A-N-CA
4	O	401	PY6	C4-C4A-N-CA
4	E	401	PY6	N-CA-CB-CG
4	N	401	PY6	N-CA-CB-CG
4	O	401	PY6	N-CA-CB-CG
4	G	401	PY6	C4-C4A-N-CA
4	G	401	PY6	N-CA-CB-CG
4	K	401	PY6	CB-CA-N-C4A
3	A	401	NLE	CE-CD-CG-CB
3	F	401	NLE	CE-CD-CG-CB
3	J	401	NLE	CE-CD-CG-CB
3	J	401	NLE	OXT-C-CA-N

There are no ring outliers.

8 monomers are involved in 24 short contacts:

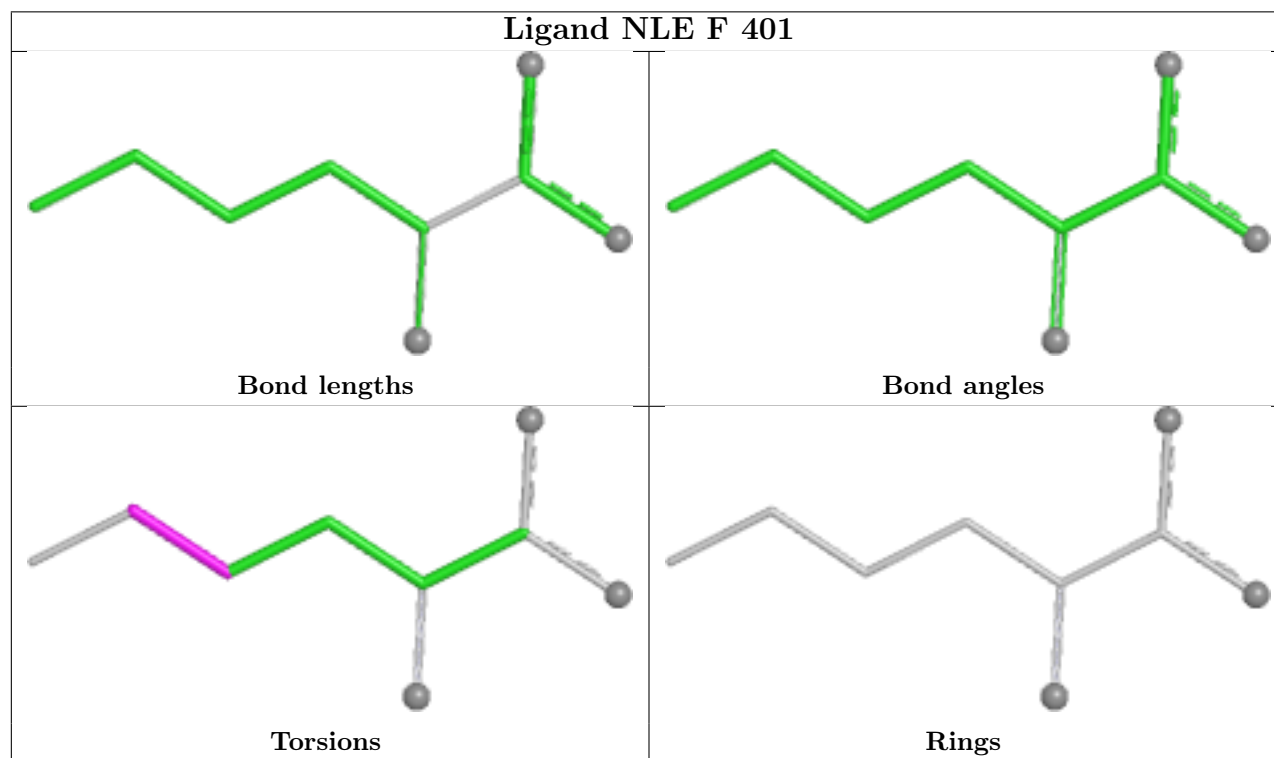
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	401	NLE	3	0
5	D	402	PEG	1	0
4	K	401	PY6	7	0
3	J	401	NLE	3	0
3	A	401	NLE	3	0

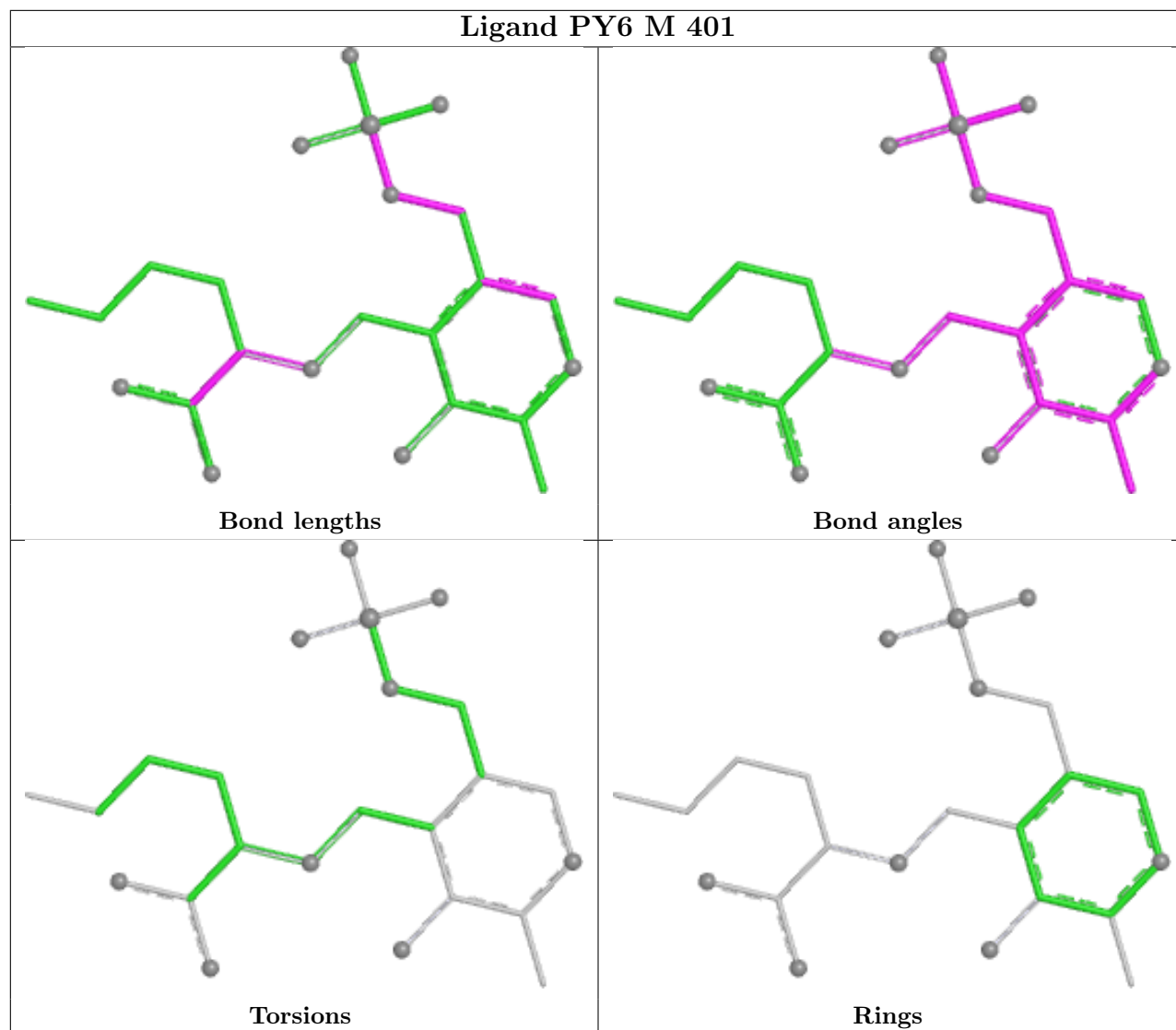
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	401	PY6	3	0
3	B	401	NLE	2	0
4	O	401	PY6	2	0

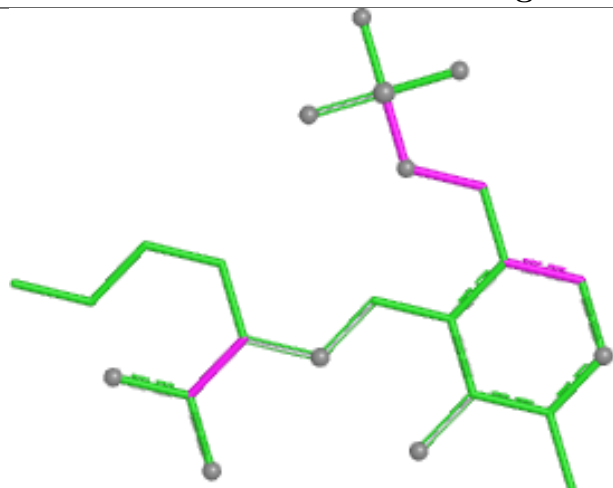
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



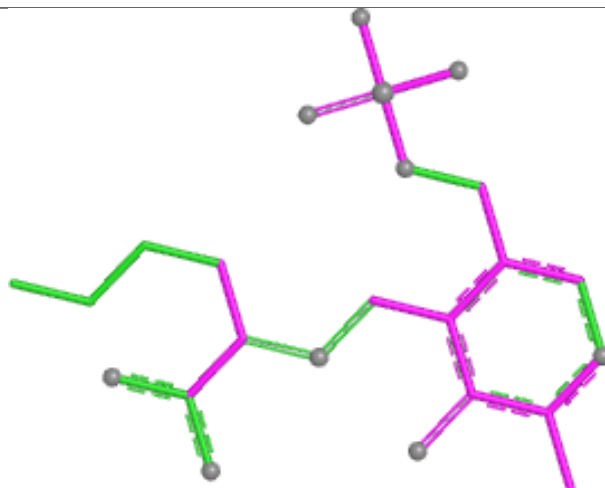




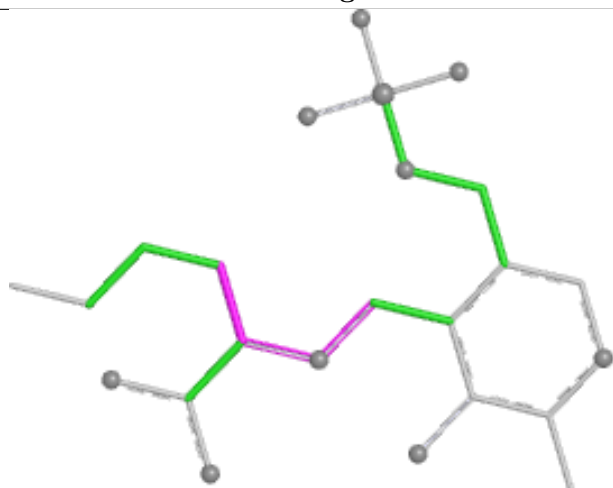
## Ligand PY6 K 401



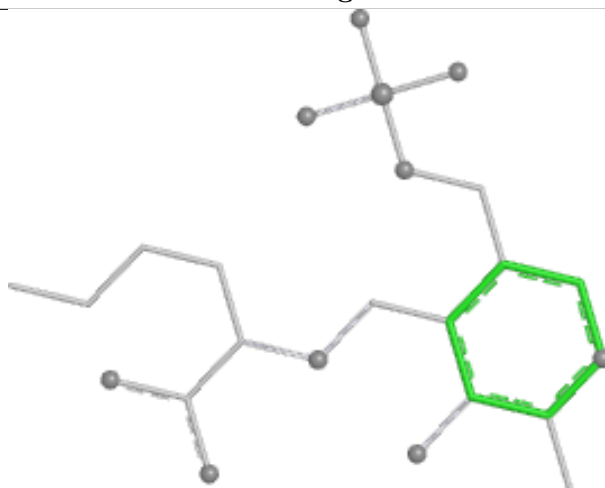
Bond lengths



Bond angles

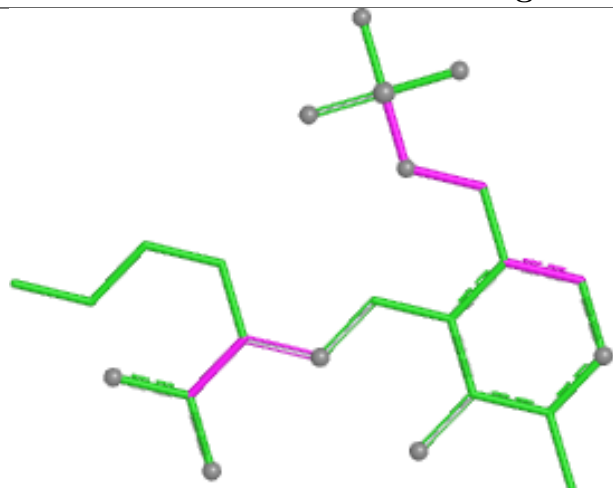


Torsions

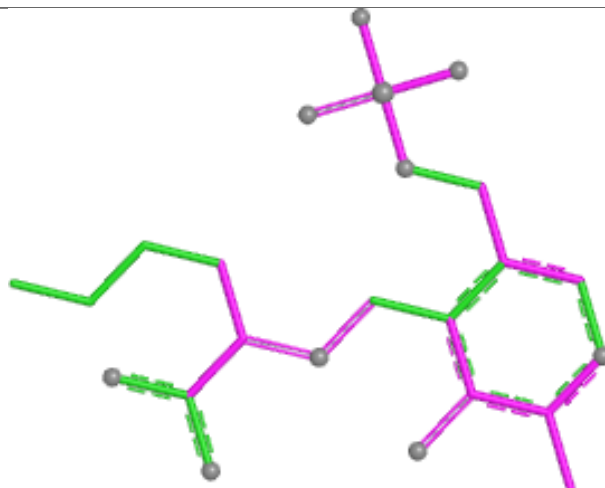


Rings

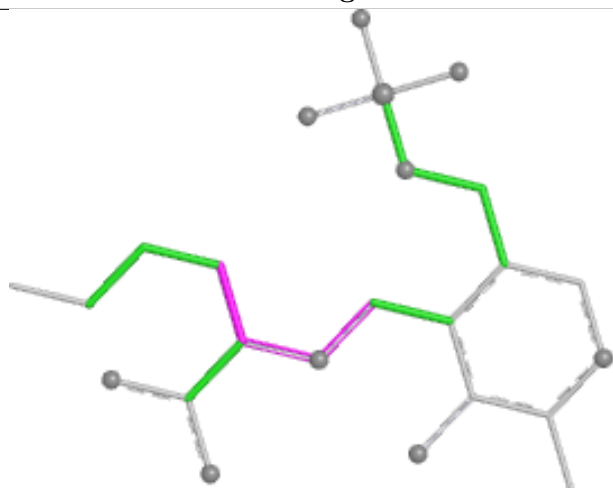
## Ligand PY6 N 401



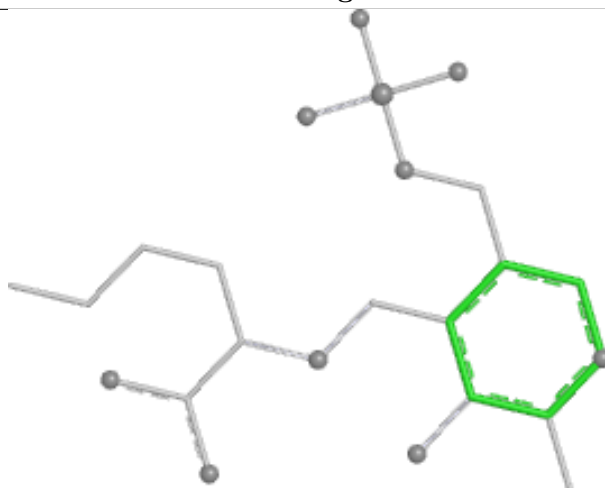
Bond lengths



Bond angles

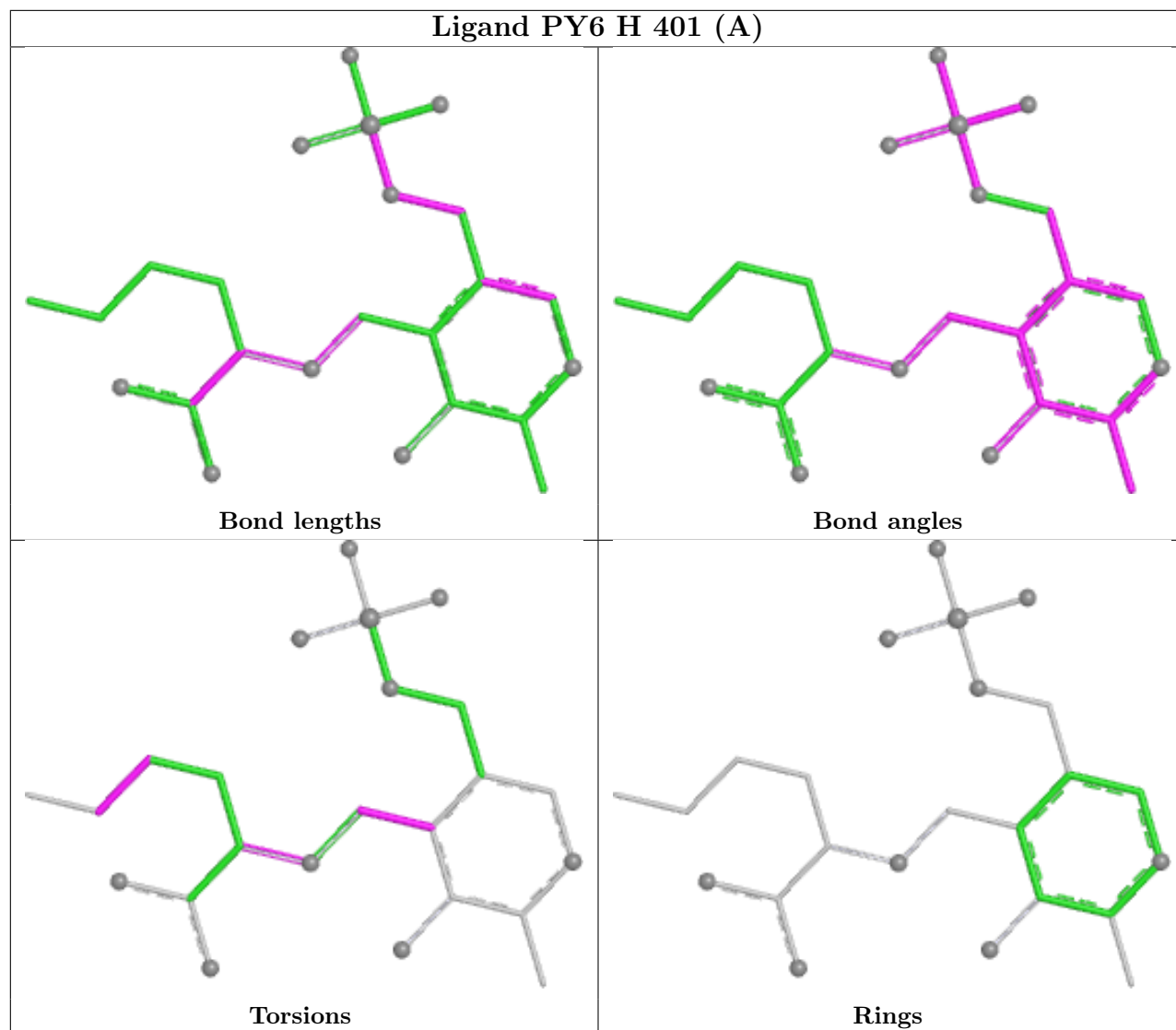


Torsions

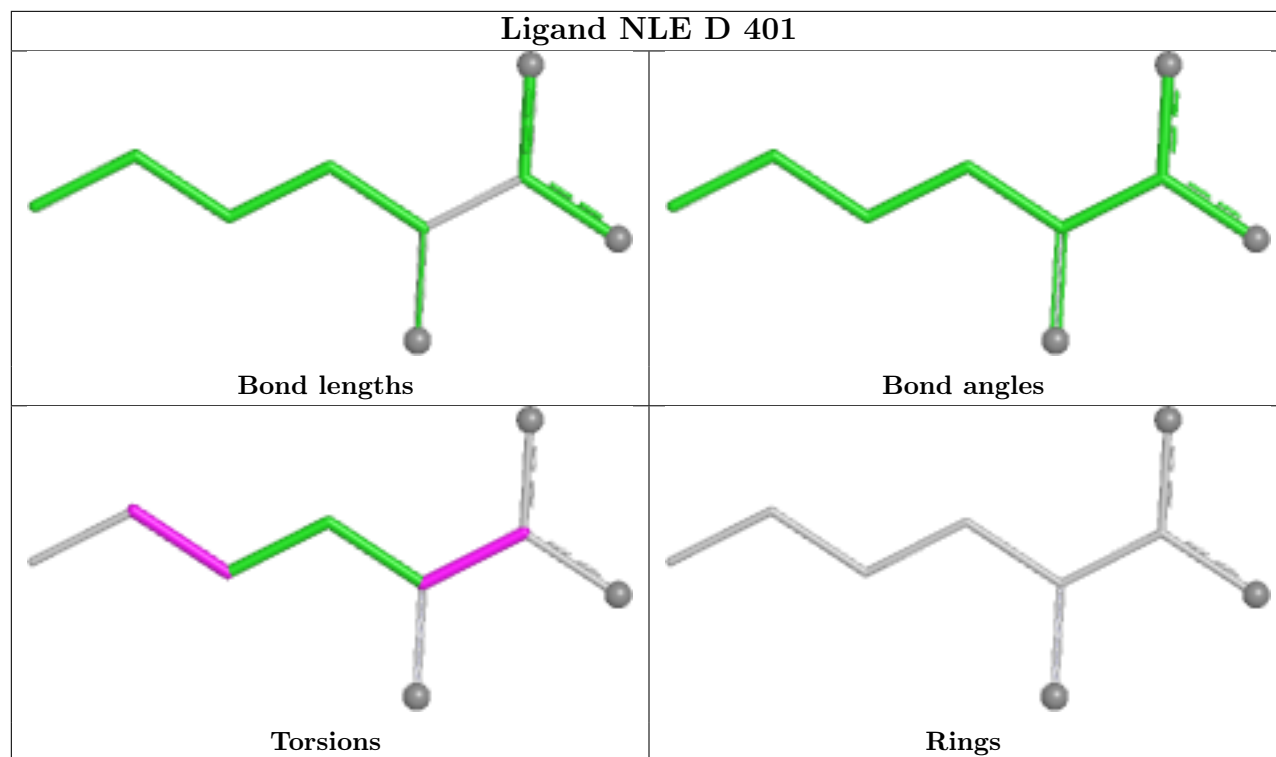


Rings

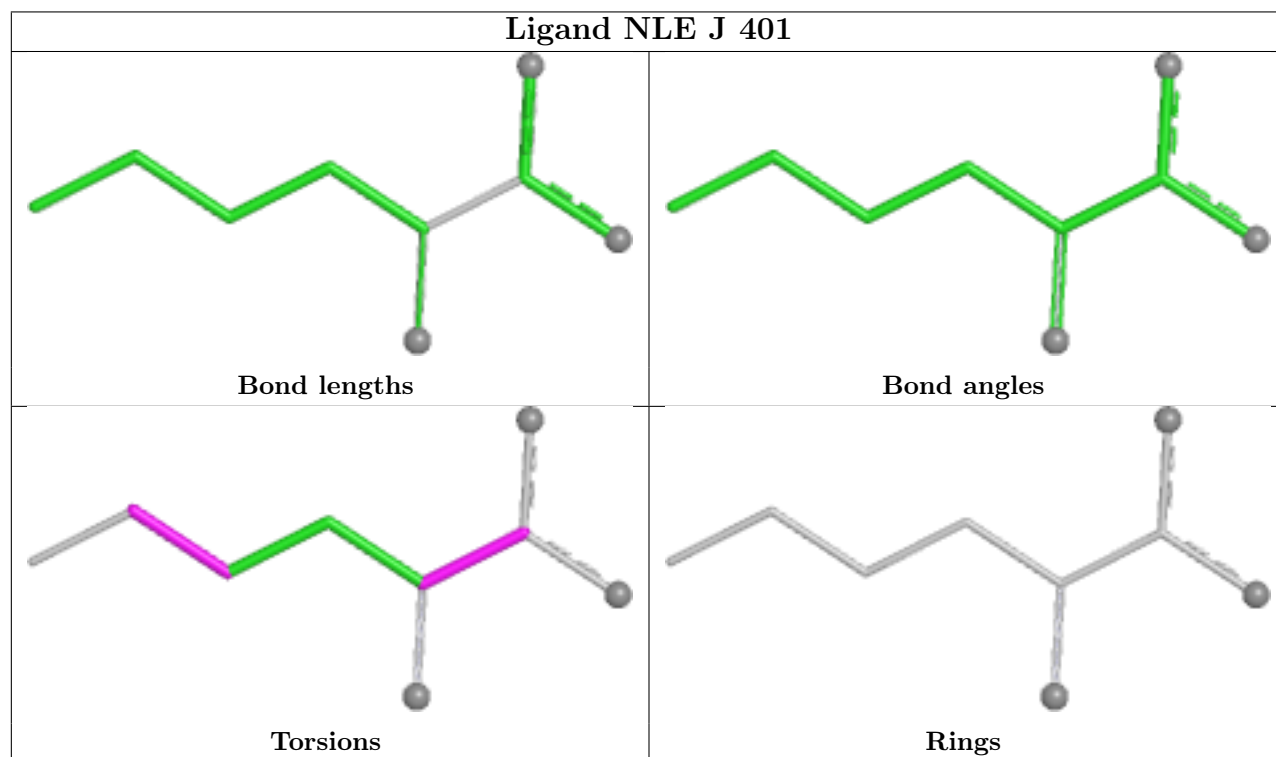
## Ligand PY6 H 401 (A)



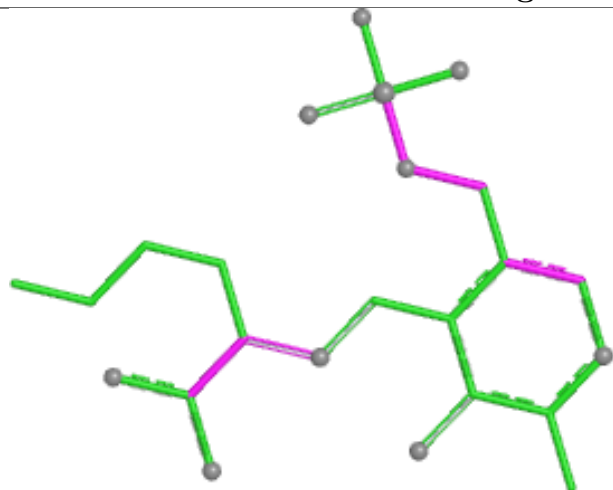
## Ligand NLE D 401



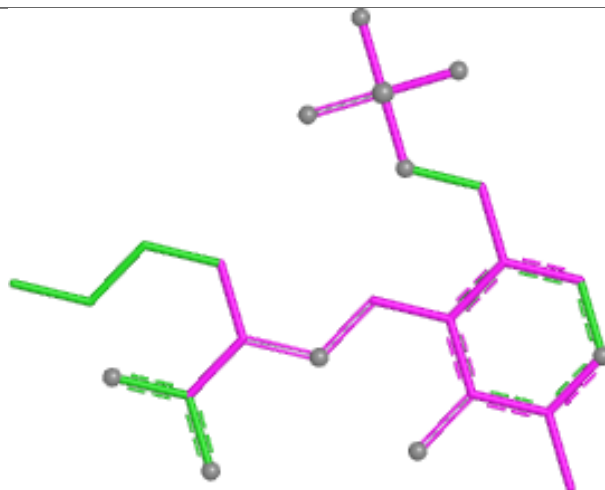
## Ligand NLE J 401



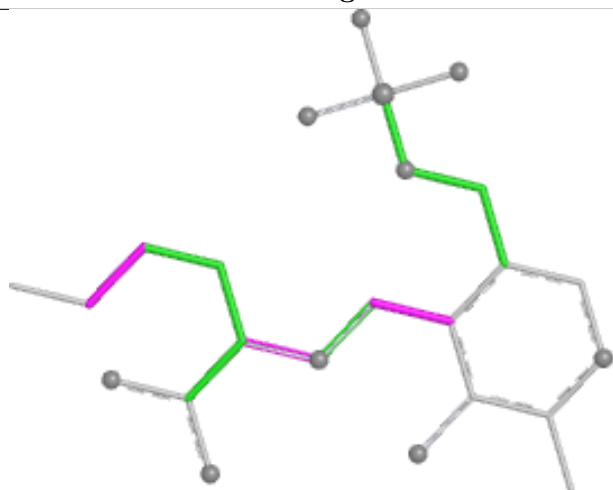
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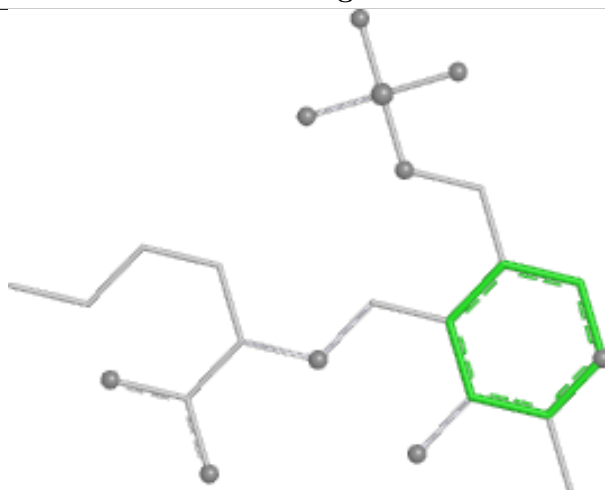
Bond lengths



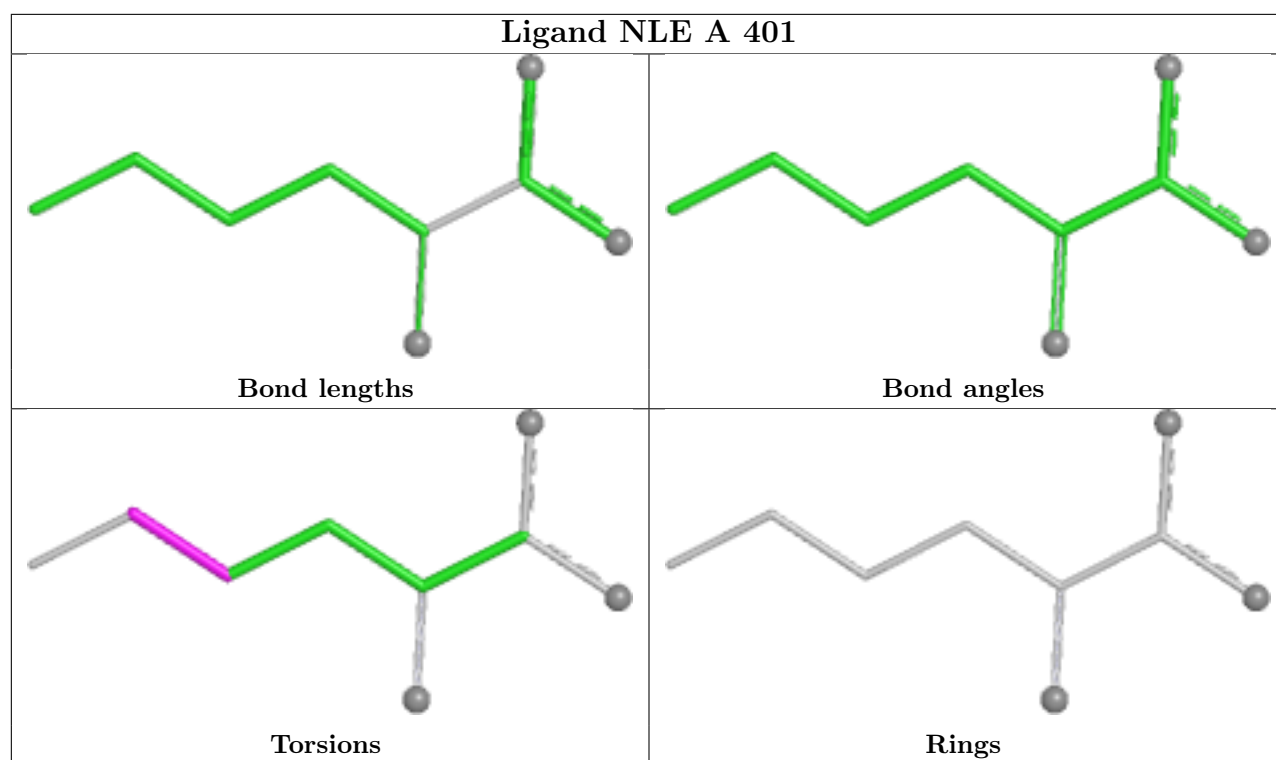
Bond angles



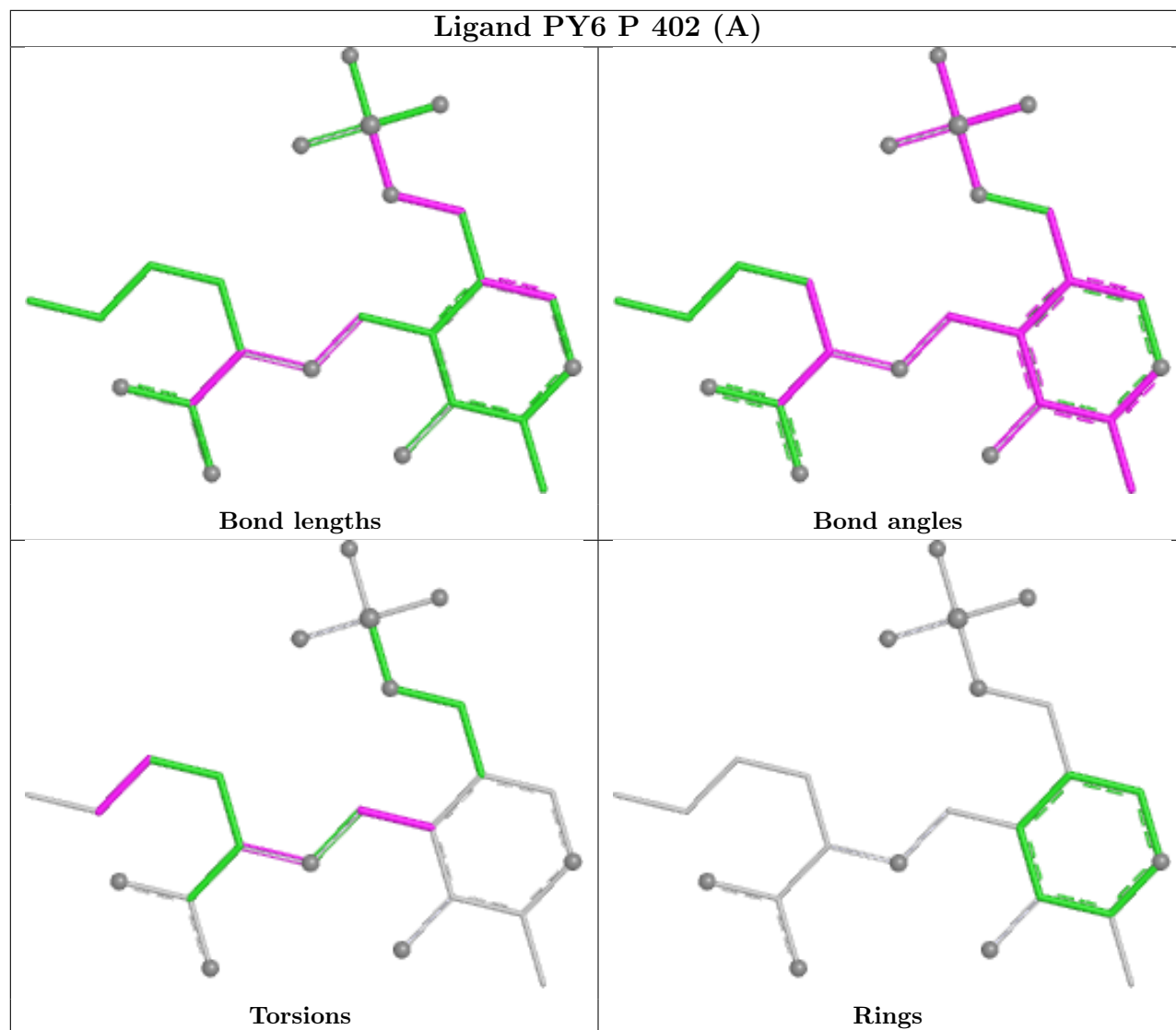
Torsions



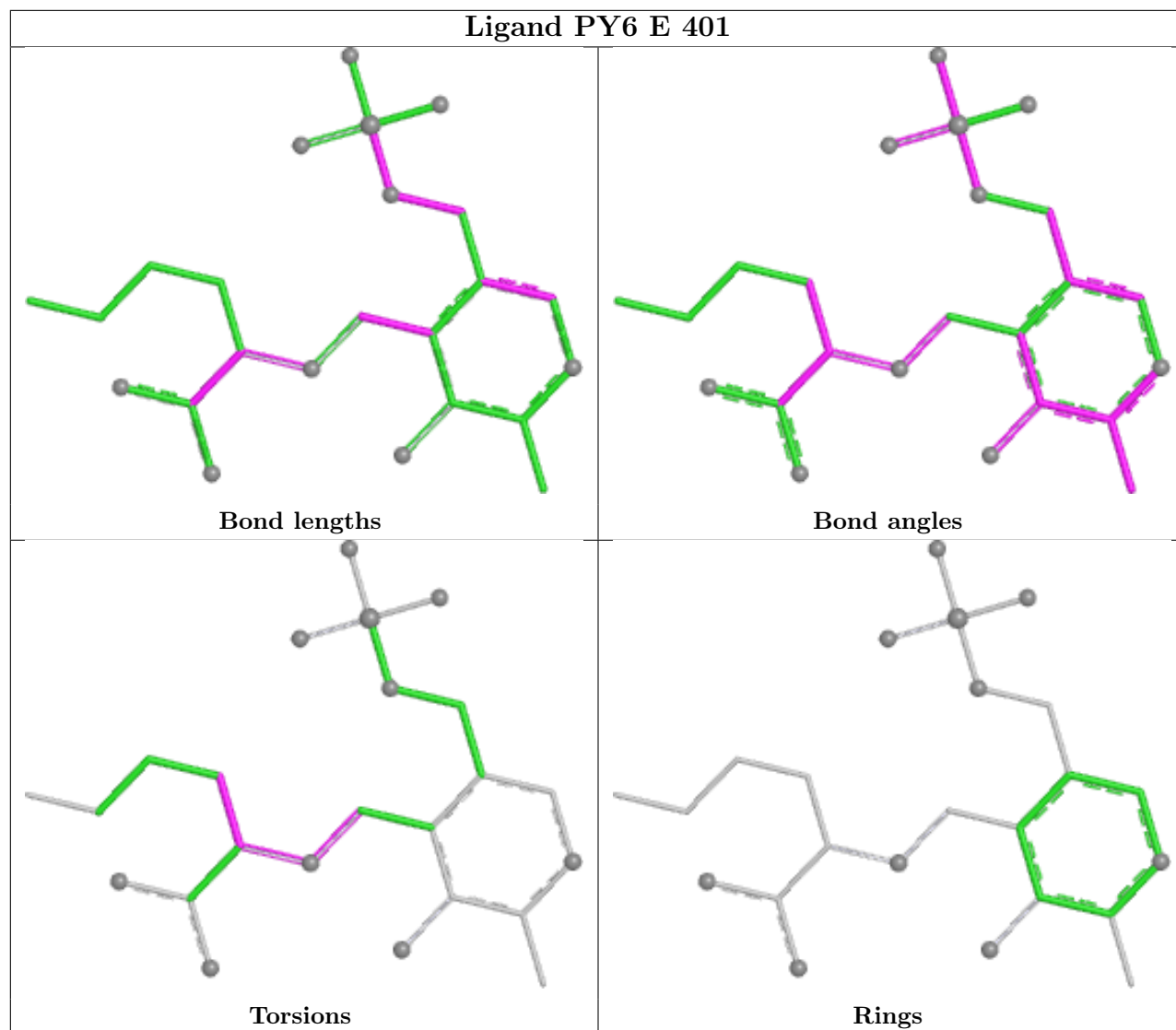
Rings



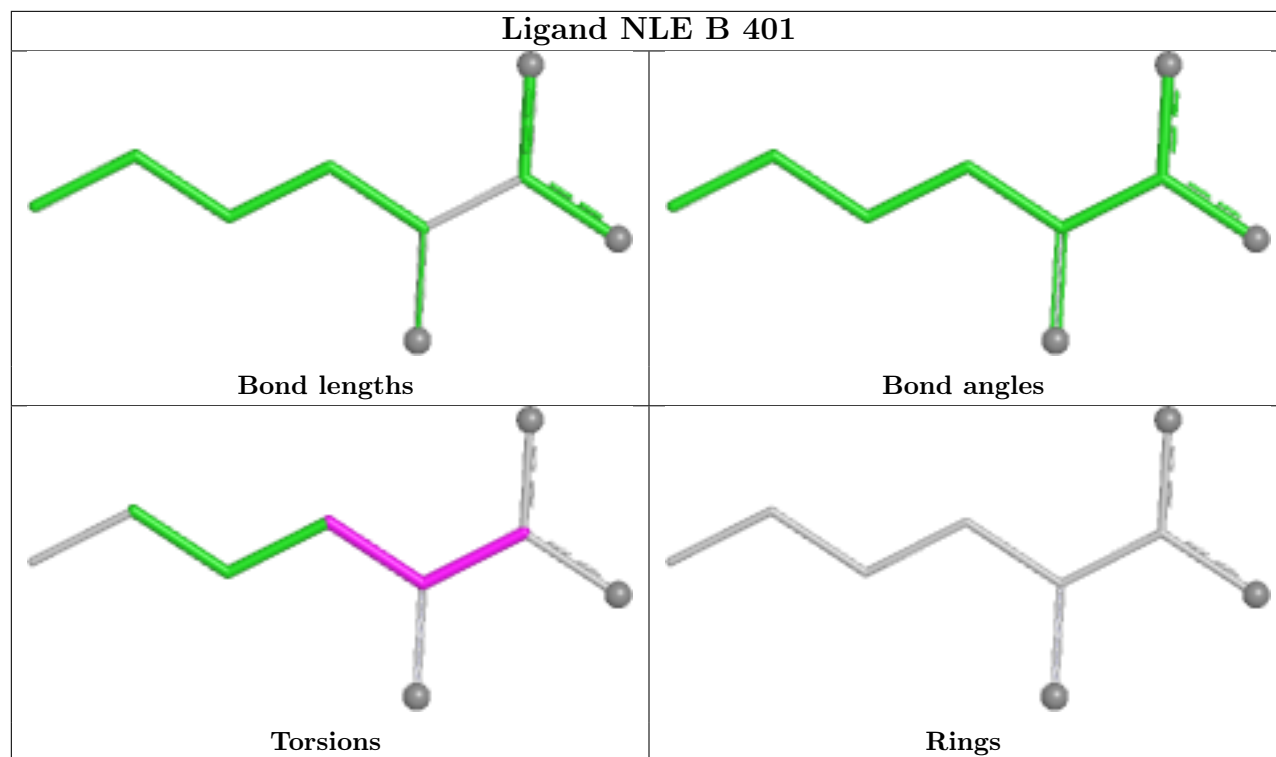
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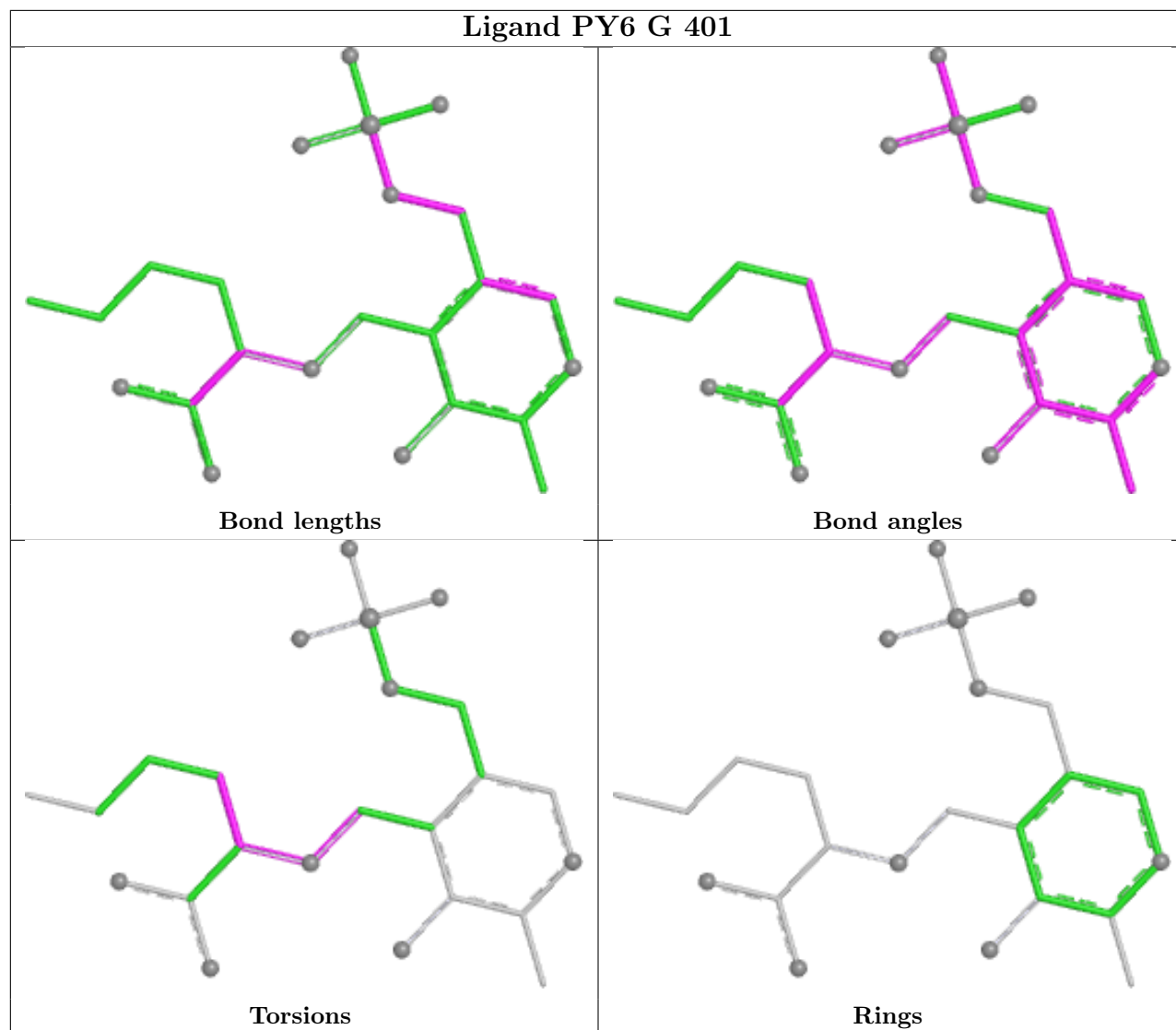
## Ligand PY6 E 401



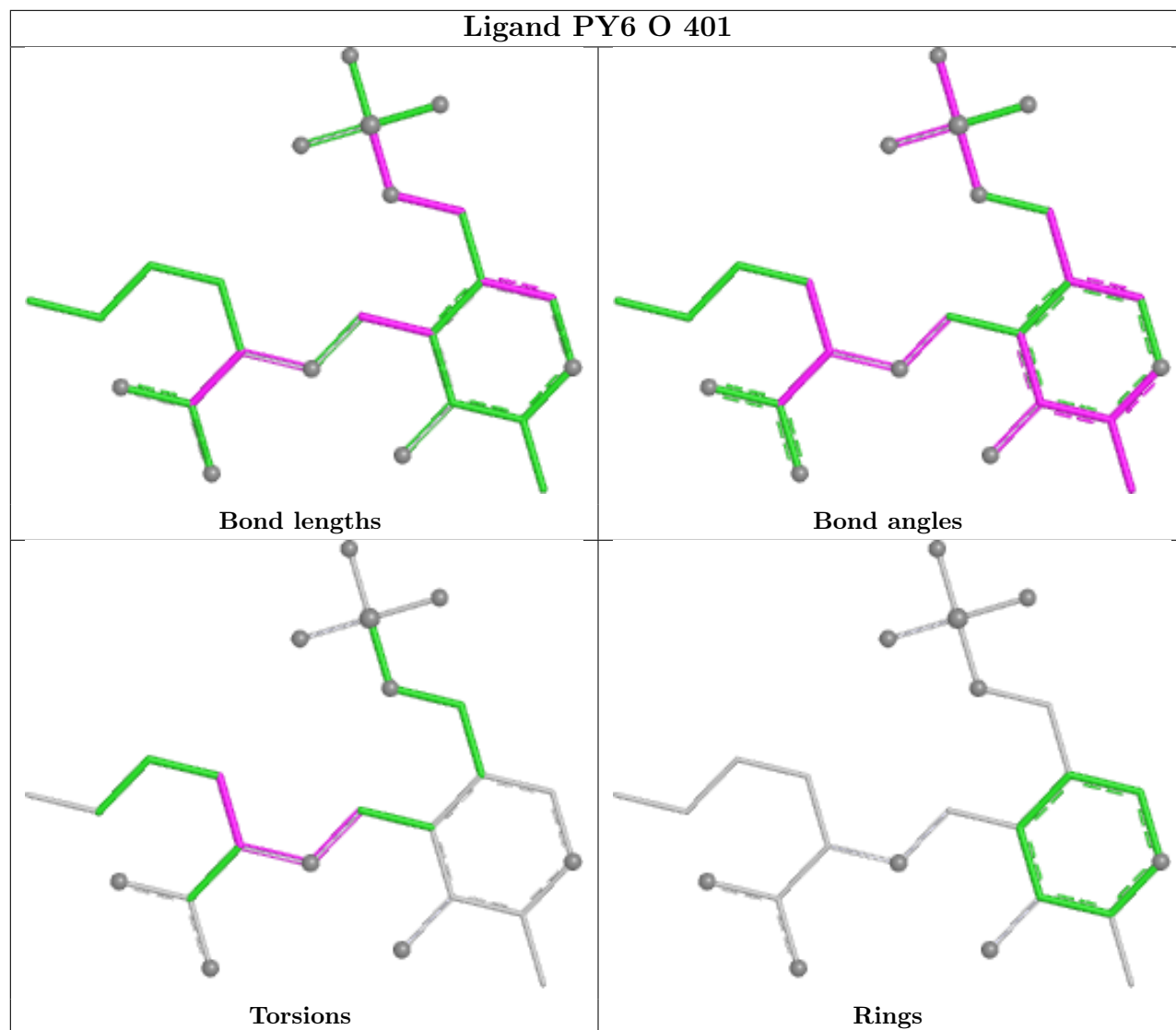


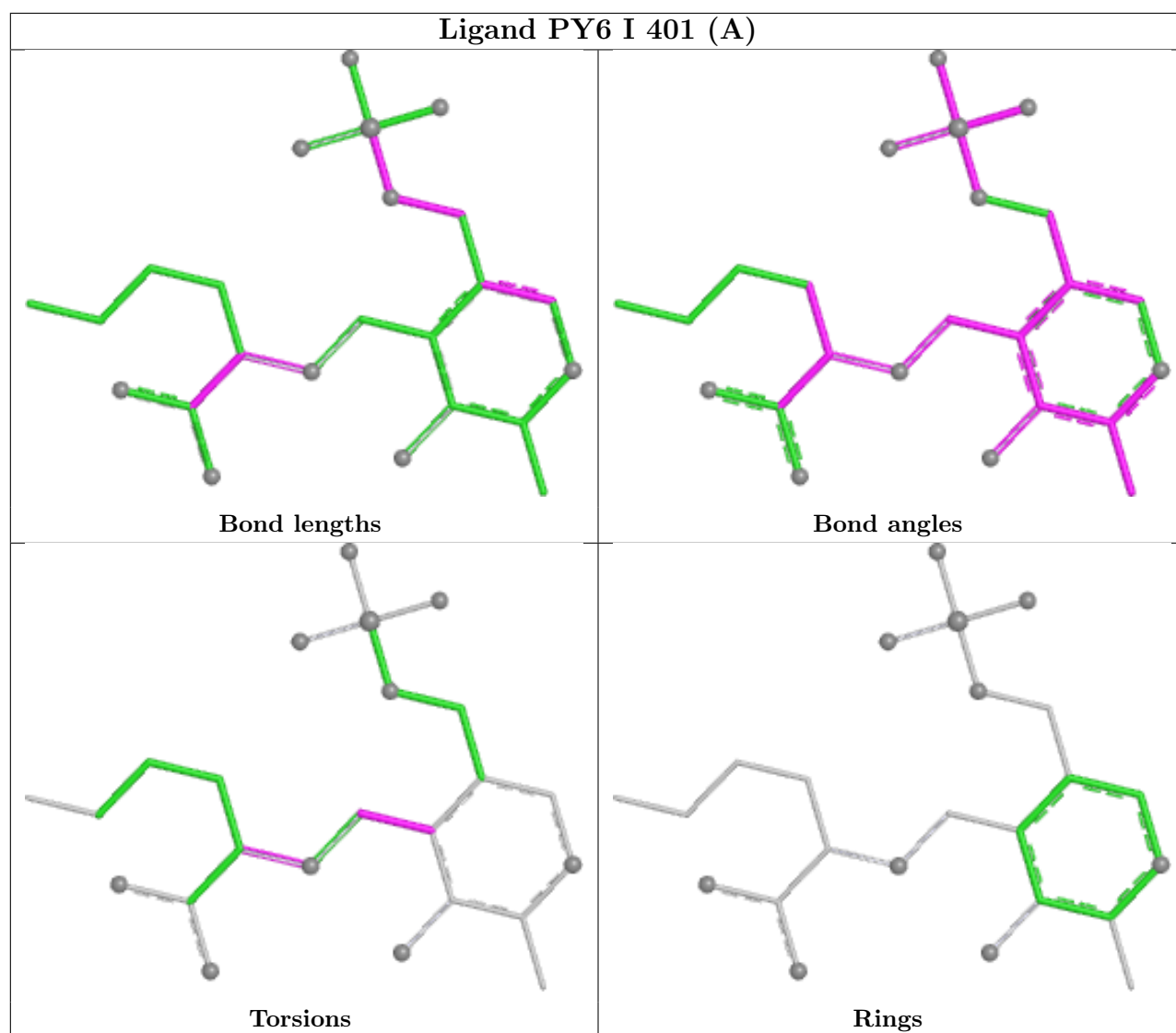


## Ligand PY6 G 401



## Ligand PY6 O 401





## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	385/414 (92%)	0.03	3 (0%) 82 81	45, 67, 89, 102	0
1	B	387/414 (93%)	0.03	3 (0%) 82 81	44, 62, 81, 93	0
1	D	382/414 (92%)	0.10	4 (1%) 79 78	48, 71, 91, 105	0
1	F	386/414 (93%)	0.08	1 (0%) 90 89	46, 70, 104, 114	0
1	H	371/414 (89%)	0.49	16 (4%) 40 36	59, 113, 197, 213	0
1	I	386/414 (93%)	0.26	5 (1%) 75 73	61, 87, 108, 115	0
1	J	383/414 (92%)	0.43	7 (1%) 67 65	62, 90, 124, 136	0
1	L	373/414 (90%)	0.29	5 (1%) 75 73	61, 90, 118, 124	0
1	P	384/414 (92%)	0.42	6 (1%) 70 68	67, 101, 141, 160	0
2	C	388/413 (93%)	0.10	4 (1%) 79 78	49, 75, 102, 111	0
2	E	389/413 (94%)	0.25	5 (1%) 75 73	61, 95, 135, 143	0
2	G	387/413 (93%)	0.22	2 (0%) 87 86	59, 88, 120, 142	0
2	K	386/413 (93%)	0.45	14 (3%) 46 42	67, 95, 116, 122	0
2	M	382/413 (92%)	0.30	8 (2%) 63 61	55, 89, 124, 139	0
2	N	387/413 (93%)	0.36	4 (1%) 79 78	74, 108, 138, 147	0
2	O	380/413 (92%)	0.60	20 (5%) 32 28	71, 129, 181, 189	0
All	All	6136/6617 (92%)	0.28	107 (1%) 69 67	44, 87, 139, 213	0

All (107) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	357	ALA	4.3
1	H	306	GLY	3.9
2	E	273	ALA	3.7
2	C	289	GLY	3.7
2	N	389	SER	3.5

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Mol	Chain	Res	Type	RSRZ
1	H	248	ALA	3.4
2	M	21	ALA	3.4
1	A	350	LEU	3.4
2	O	388	ALA	3.3
1	H	288	PRO	3.3
2	M	389	SER	3.2
2	K	190	PRO	3.2
2	K	203	VAL	3.2
1	J	389	SER	3.2
1	L	349	SER	3.2
1	A	351	THR	3.2
2	O	130	LEU	3.1
2	O	96	ALA	3.1
2	O	288	PRO	3.0
1	H	169	LEU	3.0
1	I	350	LEU	3.0
1	H	305	GLY	3.0
1	J	10	MET	2.9
1	H	289	GLY	2.9
1	J	290	LEU	2.8
1	J	98	THR	2.8
1	D	359	ALA	2.8
1	L	155	ILE	2.7
2	K	78	LEU	2.7
1	H	307	GLY	2.7
2	K	389	SER	2.7
1	I	11	VAL	2.7
1	H	97	MET	2.7
2	K	259	ALA	2.7
2	K	246	MET	2.7
2	O	246	MET	2.7
1	L	340	ALA	2.7
2	M	334	ALA	2.7
2	K	201	ALA	2.6
2	K	28	ILE	2.6
1	J	382	LEU	2.6
2	O	240	GLY	2.6
2	O	156	VAL	2.5
2	N	117	PRO	2.5
1	H	372	LEU	2.5
2	C	389	SER	2.5
2	K	245	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
2	M	354	PRO	2.5
1	I	310	ILE	2.4
2	O	169	LEU	2.4
1	A	354	PRO	2.4
2	O	90	PHE	2.4
2	M	368	LEU	2.4
2	O	122	SER	2.4
2	C	334	ALA	2.4
1	H	350	LEU	2.4
2	E	276	LEU	2.4
2	E	58	GLY	2.3
2	M	223	ALA	2.3
2	O	155	ILE	2.3
1	H	152	GLY	2.3
2	K	220	GLY	2.3
1	H	348	ALA	2.3
2	O	352	HIS	2.3
1	J	117	PRO	2.3
1	F	355	VAL	2.3
1	D	131	LEU	2.3
1	P	30	LEU	2.3
2	M	350	LEU	2.3
1	H	303	MET	2.2
2	E	246	MET	2.2
1	L	131	LEU	2.2
2	O	276	LEU	2.2
2	O	372	LEU	2.2
2	O	237	ALA	2.2
2	M	382	LEU	2.2
2	N	182	LEU	2.2
1	B	246	MET	2.2
2	K	285	VAL	2.2
1	P	27	ALA	2.2
2	O	223	ALA	2.2
1	P	295	PRO	2.2
1	D	276	LEU	2.2
2	O	241	ALA	2.1
1	B	291	ASN	2.1
2	C	131	LEU	2.1
2	G	18	LEU	2.1
1	P	292	GLY	2.1
1	I	154	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	P	155	ILE	2.1
2	O	291	ASN	2.1
1	L	122	SER	2.1
1	P	153	LEU	2.1
1	H	287	TYR	2.1
1	B	116	ARG	2.1
2	K	288	PRO	2.1
1	H	182	LEU	2.1
1	I	142	GLU	2.0
1	J	258	LEU	2.0
2	O	305	GLY	2.0
2	N	278	ALA	2.0
1	D	351	THR	2.0
2	K	290	LEU	2.0
2	K	205	HIS	2.0
1	H	310	ILE	2.0
2	G	115	VAL	2.0
2	O	62	VAL	2.0

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

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	LLP	P	209[B]	24/25	0.78	0.24	73,98,100,100	20
1	LLP	J	209	24/25	0.89	0.10	74,88,89,89	0
1	LLP	D	209	24/25	0.90	0.09	52,64,65,65	0
1	LLP	L	209	24/25	0.91	0.10	72,82,82,83	0
1	LLP	H	209[B]	24/25	0.92	0.10	92,110,110,110	42
1	LLP	F	209	24/25	0.93	0.08	53,66,68,68	0
1	LLP	A	209	24/25	0.93	0.09	51,55,57,57	0
1	LLP	I	209[B]	24/25	0.93	0.10	66,82,82,82	41
1	LLP	B	209	24/25	0.94	0.08	46,52,54,54	0

## 6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.



## 6.4 Ligands ⓘ

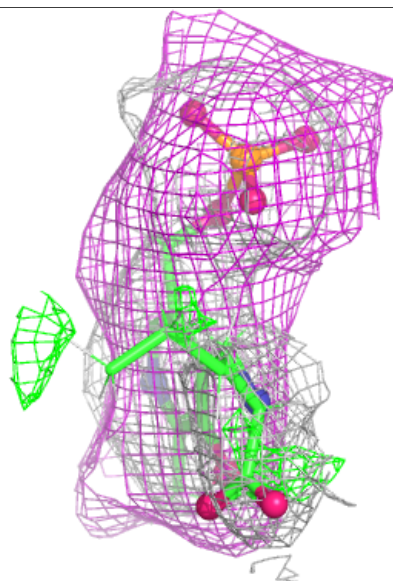
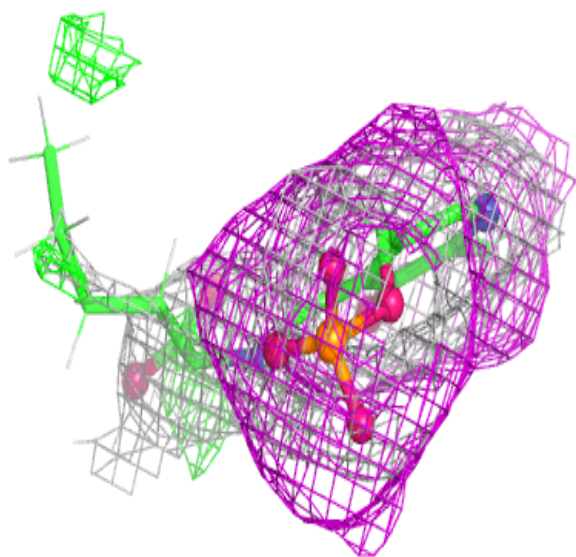
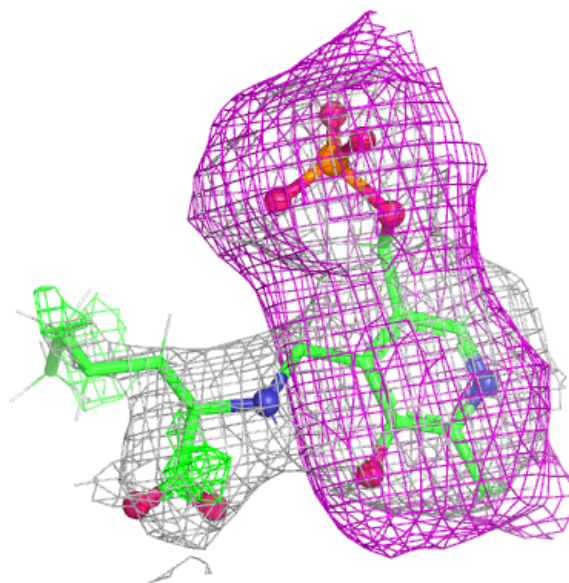
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	PY6	P	402[A]	24/24	0.07	0.31	71,72,72,72	44
5	PEG	J	402	7/7	0.58	0.14	96,96,97,97	0
5	PEG	D	402	7/7	0.77	0.10	73,73,73,73	0
6	PLP	P	401[A]	15/16	0.78	0.10	98,99,100,100	22
3	NLE	F	401	9/9	0.84	0.14	88,89,90,90	0
3	NLE	A	401	9/9	0.85	0.17	96,96,98,98	0
3	NLE	J	401	9/9	0.85	0.17	119,120,121,121	0
5	PEG	F	402	7/7	0.86	0.08	78,78,79,79	0
4	PY6	M	401	24/24	0.87	0.13	79,81,81,81	0
4	PY6	E	401	24/24	0.87	0.11	76,78,78,79	0
4	PY6	I	401[A]	24/24	0.89	0.12	46,47,47,47	44
4	PY6	O	401	24/24	0.91	0.09	108,109,109,109	0
4	PY6	K	401	24/24	0.91	0.09	66,67,69,69	0
3	NLE	B	401	9/9	0.91	0.10	64,65,67,67	0
4	PY6	G	401	24/24	0.93	0.10	68,69,69,69	0
3	NLE	D	401	9/9	0.93	0.13	97,98,100,100	0
4	PY6	N	401	24/24	0.93	0.08	79,80,81,81	0
4	PY6	H	401[A]	24/24	0.94	0.12	93,94,94,94	44
4	PY6	C	401	24/24	0.95	0.08	69,71,71,71	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.

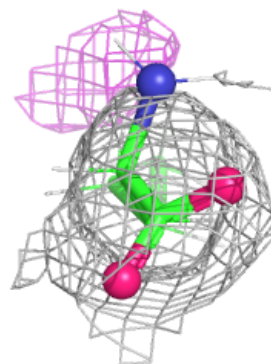
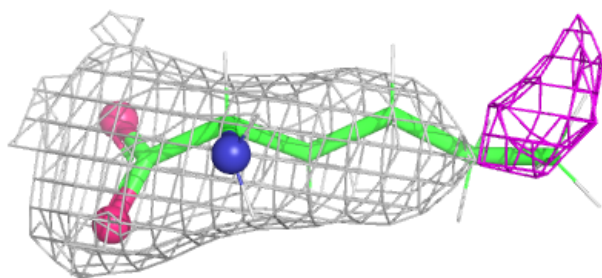
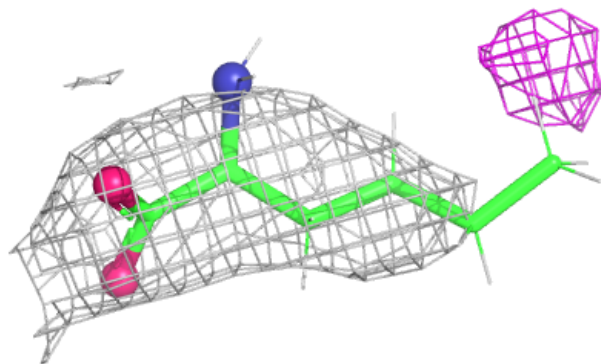
**Electron density around PY6 P 402 (A):**

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

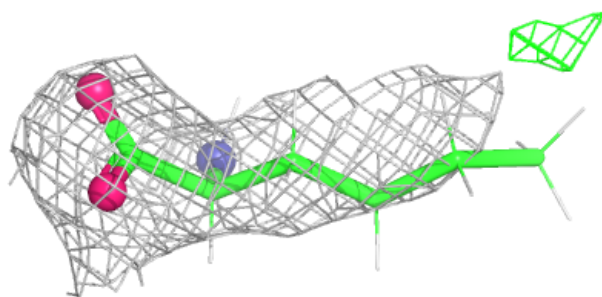
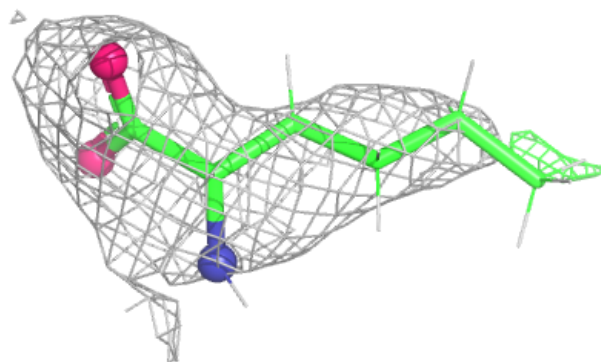


**Electron density around NLE F 401:**

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and green (positive)

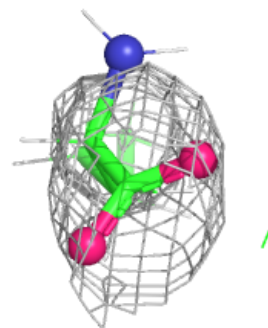
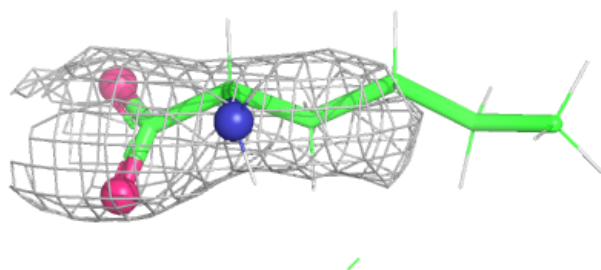
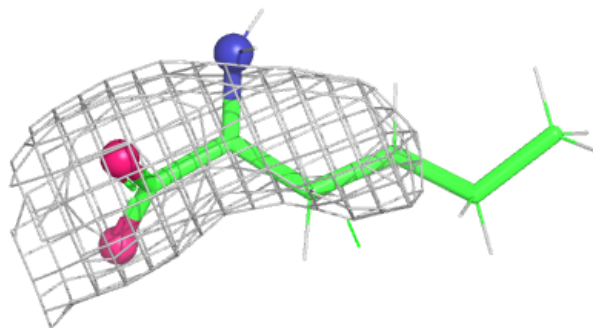
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and green (positive)



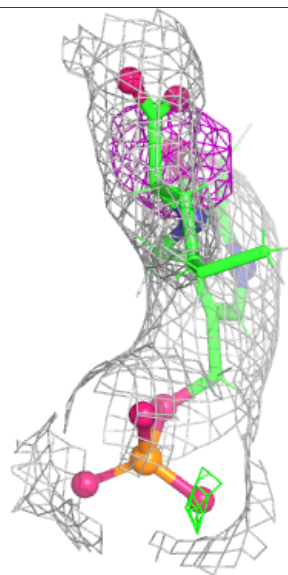
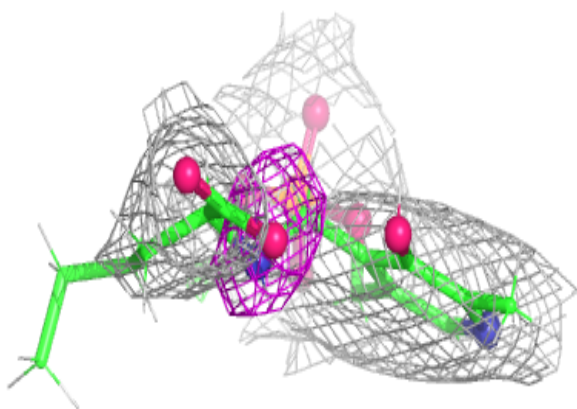
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and green (positive)



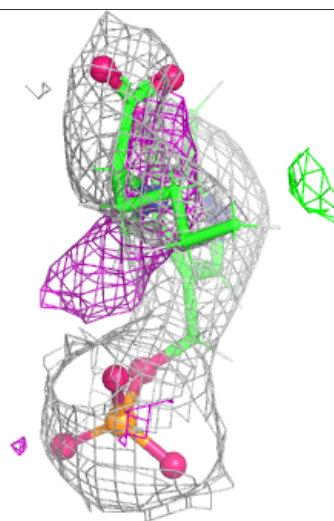
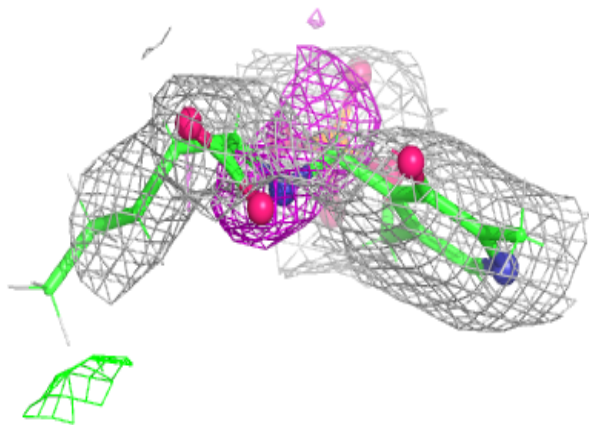
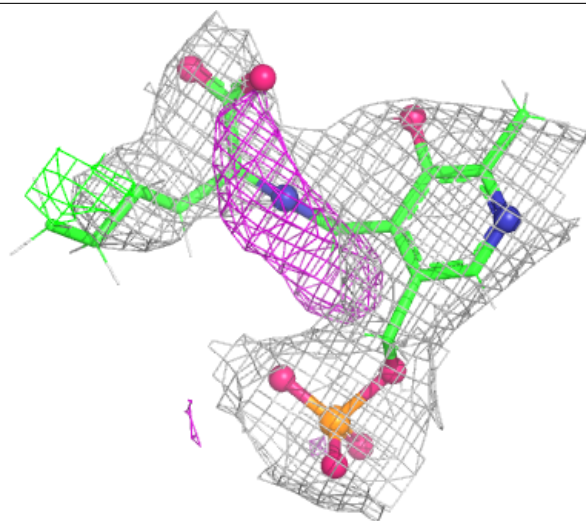
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and green (positive)



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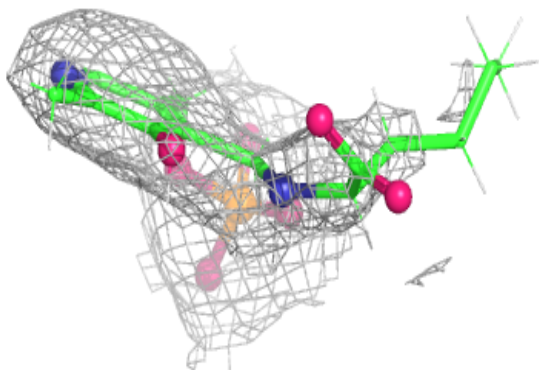
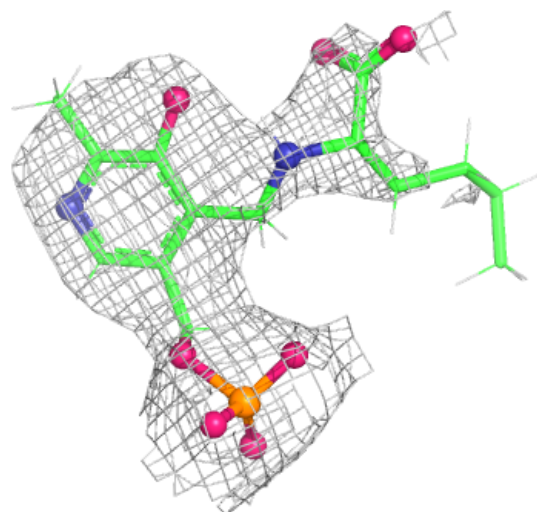
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and green (positive)





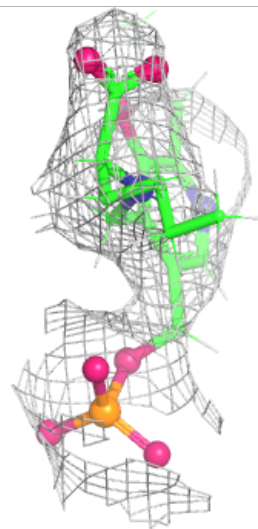
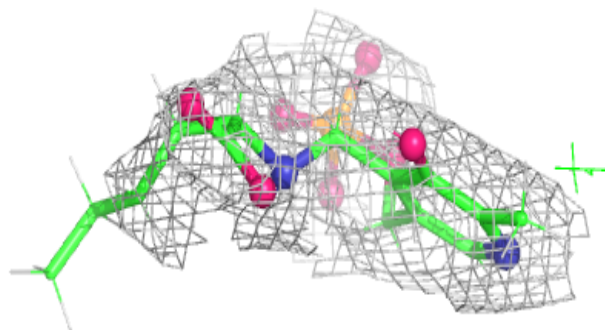
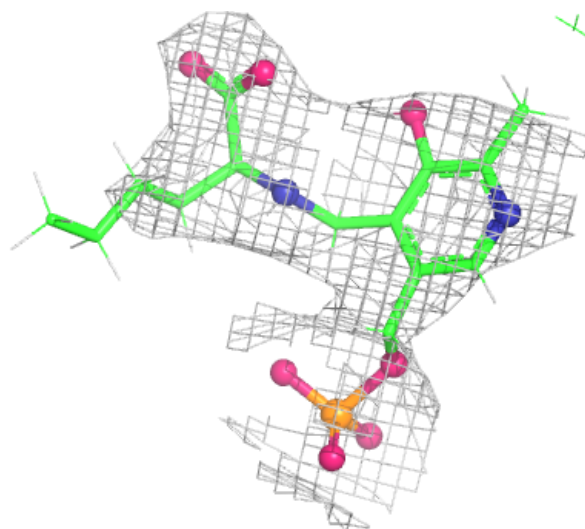
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and green (positive)



**Electron density around PY6 O 401:**

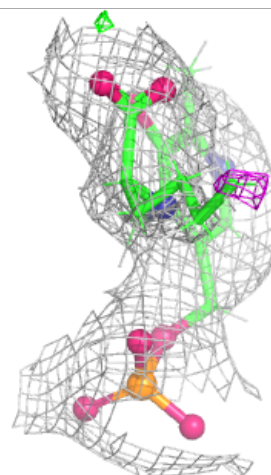
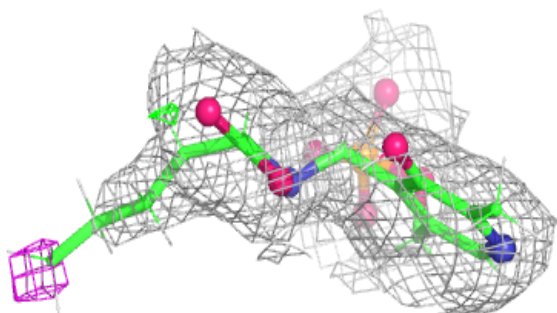
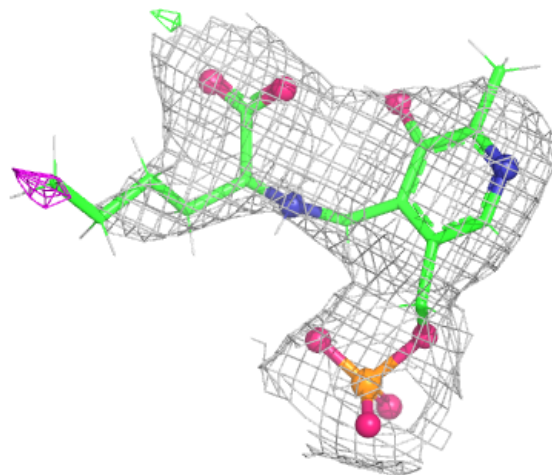
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and green (positive)





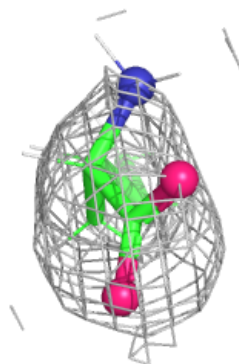
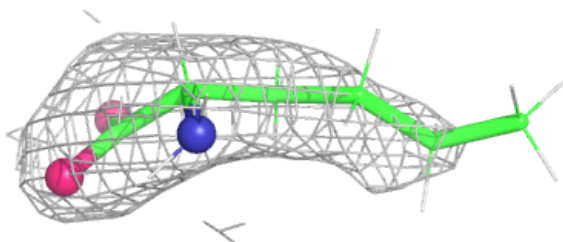
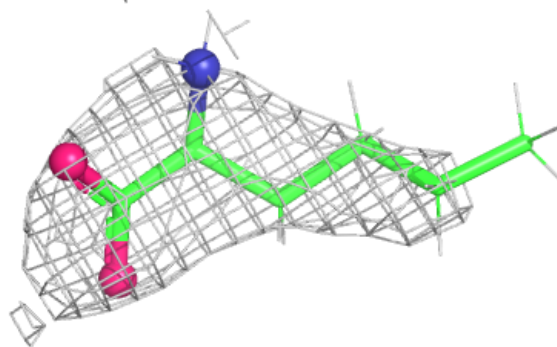
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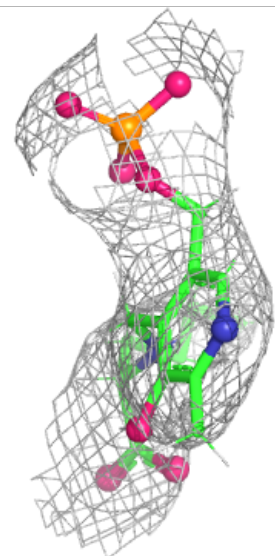
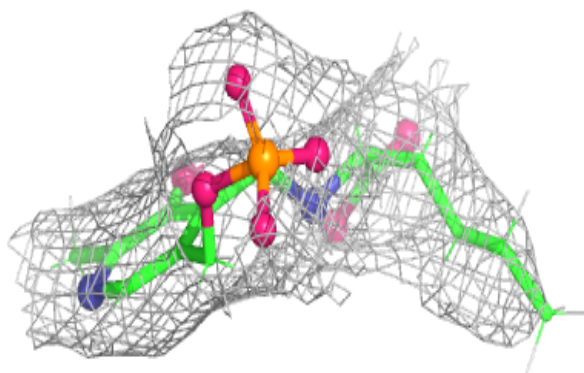
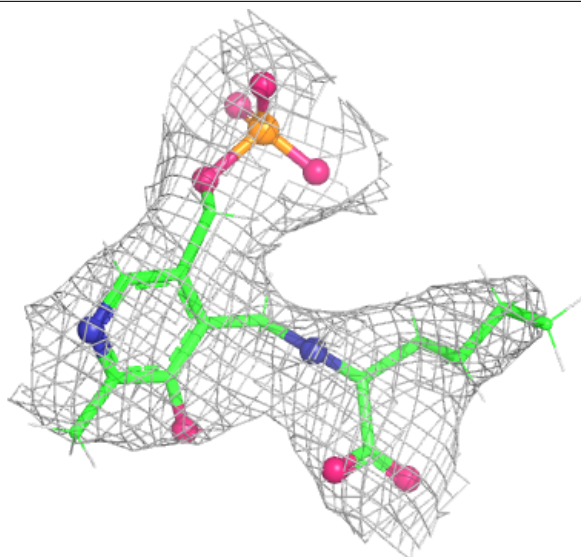
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and green (positive)



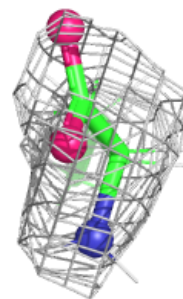
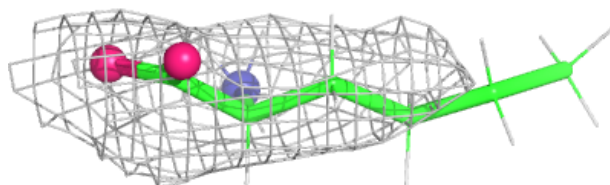
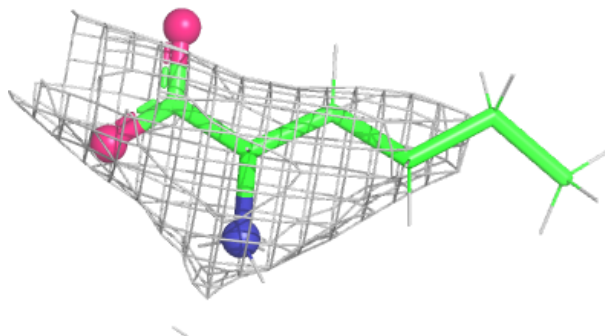
**Electron density around PY6 G 401:**

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and green (positive)



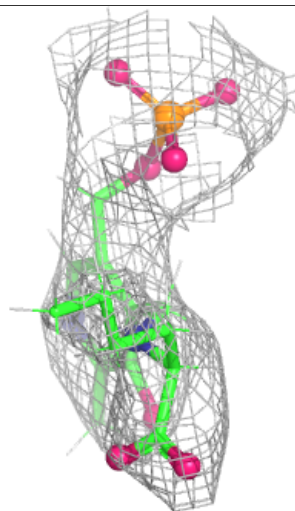
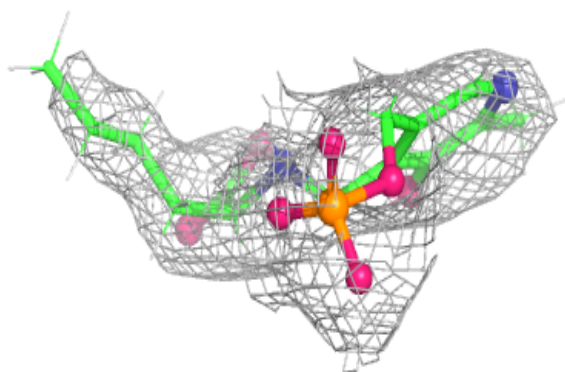
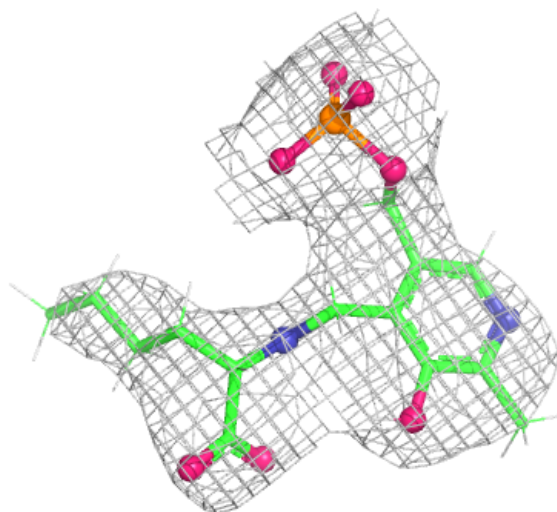
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and green (positive)



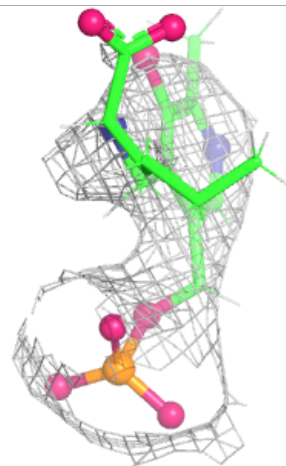
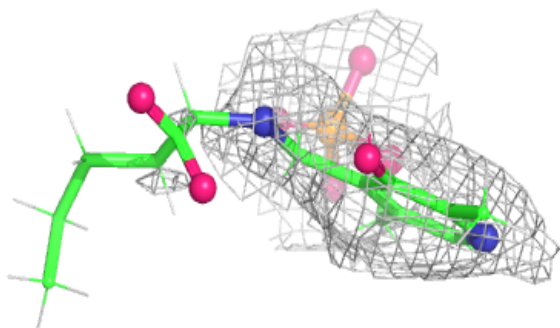
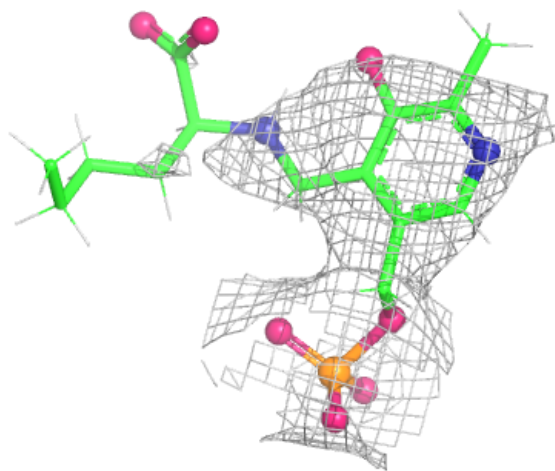
**Electron density around PY6 N 401:**

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and green (positive)



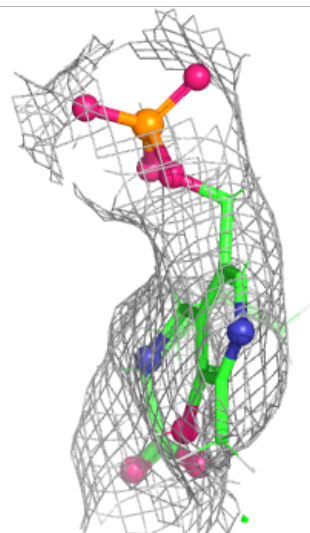
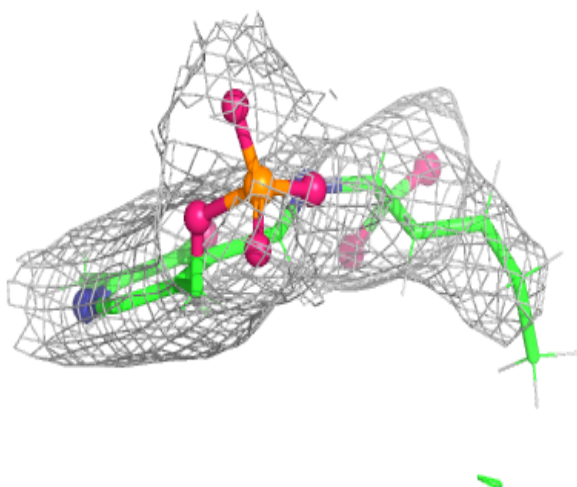
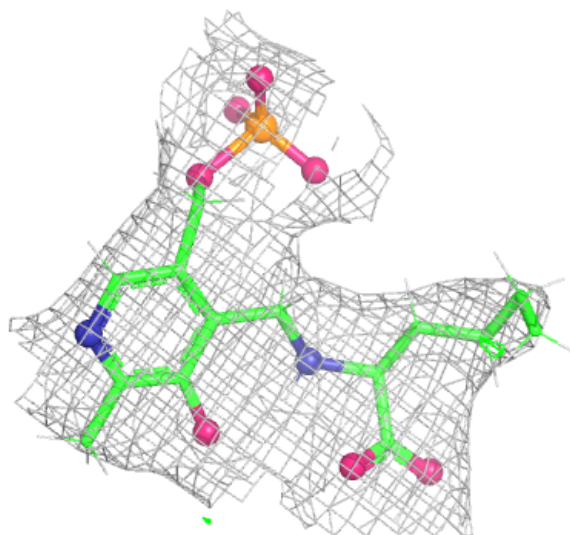
**Electron density around PY6 H 401 (A):**

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



**Electron density around PY6 C 401:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.