



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 15, 2020 – 02:11 PM EST

PDB ID : 4JBI
Title : 2.35Å resolution structure of NADPH bound thermostable alcohol dehydrogenase from *Pyrobaculum aerophilum*
Authors : Lovell, S.; Battaile, K.P.; Vitale, A.; Throne, N.; Hu, X.; Shen, M.; D'Auria, S.; Auld, D.S.
Deposited on : 2013-02-19
Resolution : 2.35 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.0 (224370), CSD as540be (2019)
Xtriage (Phenix) : 1.13
EDS : 2.4
buster-report : 1.1.7 (2018)
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.4

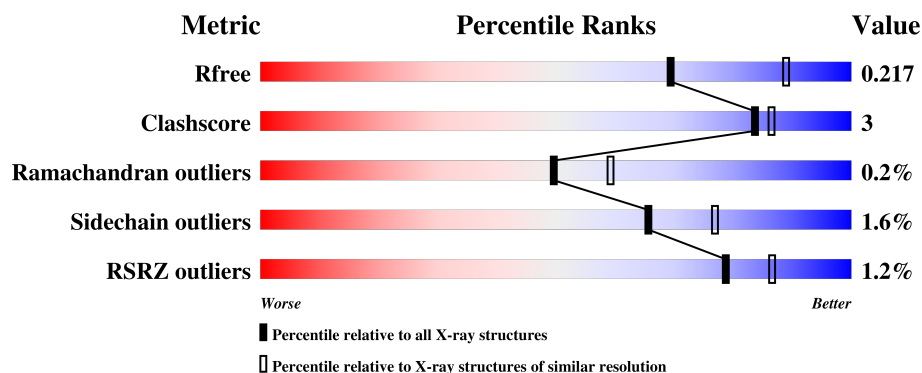
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION






The reported resolution of this entry is 2.35 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}	111664	1015 (2.36-2.36)
Clashscore	122126	1081 (2.36-2.36)
Ramachandran outliers	120053	1066 (2.36-2.36)
Sidechain outliers	120020	1067 (2.36-2.36)
RSRZ outliers	108989	1002 (2.36-2.36)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	370	
1	B	370	
1	C	370	
1	D	370	
1	E	370	

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Mol	Chain	Length	Quality of chain
1	F	370	 84%6%10%
1	G	370	%  85%5%10%
1	H	370	 85%5%10%
1	I	370	 85%5%10%
1	J	370	%  83%7%10%
1	K	370	%  82%8%10%
1	L	370	4%  84%6%10%
1	M	370	2%  85%5%10%
1	N	370	 83%6%10%
1	O	370	3%  78%11%10%
1	P	370	3%  79%10%10%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 40799 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 Alcohol dehydrogenase (Zinc).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	333	Total	C	N	O	S	0	1	0
			2444	1554	428	453	9			
1	B	333	Total	C	N	O	S	0	1	0
			2436	1550	424	453	9			
1	C	333	Total	C	N	O	S	0	1	0
			2452	1556	434	453	9			
1	D	333	Total	C	N	O	S	0	1	0
			2425	1544	421	451	9			
1	E	333	Total	C	N	O	S	0	1	0
			2446	1553	431	453	9			
1	F	333	Total	C	N	O	S	0	1	0
			2448	1553	433	453	9			
1	G	333	Total	C	N	O	S	0	1	0
			2437	1548	427	453	9			
1	H	333	Total	C	N	O	S	0	1	0
			2427	1545	420	453	9			
1	I	333	Total	C	N	O	S	0	1	0
			2430	1545	423	453	9			
1	J	333	Total	C	N	O	S	0	0	0
			2424	1542	420	453	9			
1	K	333	Total	C	N	O	S	0	1	0
			2422	1541	423	449	9			
1	L	333	Total	C	N	O	S	0	1	0
			2432	1546	424	453	9			
1	M	333	Total	C	N	O	S	0	1	0
			2431	1547	424	451	9			
1	N	333	Total	C	N	O	S	0	1	0
			2433	1548	423	453	9			
1	O	333	Total	C	N	O	S	0	1	0
			2406	1532	414	451	9			
1	P	333	Total	C	N	O	S	0	0	0
			2415	1536	417	453	9			

There are 624 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-38	MET	-	expression tag	UNP Q8ZUP0
A	-37	GLY	-	expression tag	UNP Q8ZUP0
A	-36	SER	-	expression tag	UNP Q8ZUP0
A	-35	SER	-	expression tag	UNP Q8ZUP0
A	-34	HIS	-	expression tag	UNP Q8ZUP0
A	-33	HIS	-	expression tag	UNP Q8ZUP0
A	-32	HIS	-	expression tag	UNP Q8ZUP0
A	-31	HIS	-	expression tag	UNP Q8ZUP0
A	-30	HIS	-	expression tag	UNP Q8ZUP0
A	-29	HIS	-	expression tag	UNP Q8ZUP0
A	-28	SER	-	expression tag	UNP Q8ZUP0
A	-27	SER	-	expression tag	UNP Q8ZUP0
A	-26	GLY	-	expression tag	UNP Q8ZUP0
A	-25	LEU	-	expression tag	UNP Q8ZUP0
A	-24	VAL	-	expression tag	UNP Q8ZUP0
A	-23	PRO	-	expression tag	UNP Q8ZUP0
A	-22	ARG	-	expression tag	UNP Q8ZUP0
A	-21	GLY	-	expression tag	UNP Q8ZUP0
A	-20	SER	-	expression tag	UNP Q8ZUP0
A	-19	HIS	-	expression tag	UNP Q8ZUP0
A	-18	MET	-	expression tag	UNP Q8ZUP0
A	-17	ALA	-	expression tag	UNP Q8ZUP0
A	-16	SER	-	expression tag	UNP Q8ZUP0
A	-15	MET	-	expression tag	UNP Q8ZUP0
A	-14	THR	-	expression tag	UNP Q8ZUP0
A	-13	GLY	-	expression tag	UNP Q8ZUP0
A	-12	GLY	-	expression tag	UNP Q8ZUP0
A	-11	GLN	-	expression tag	UNP Q8ZUP0
A	-10	GLN	-	expression tag	UNP Q8ZUP0
A	-9	MET	-	expression tag	UNP Q8ZUP0
A	-8	GLY	-	expression tag	UNP Q8ZUP0
A	-7	ARG	-	expression tag	UNP Q8ZUP0
A	-6	GLY	-	expression tag	UNP Q8ZUP0
A	-5	SER	-	expression tag	UNP Q8ZUP0
A	-4	GLY	-	expression tag	UNP Q8ZUP0
A	-3	GLY	-	expression tag	UNP Q8ZUP0
A	-2	GLY	-	expression tag	UNP Q8ZUP0
A	-1	HIS	-	expression tag	UNP Q8ZUP0
A	0	GLU	-	expression tag	UNP Q8ZUP0
B	-38	MET	-	expression tag	UNP Q8ZUP0
B	-37	GLY	-	expression tag	UNP Q8ZUP0
B	-36	SER	-	expression tag	UNP Q8ZUP0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-35	SER	-	expression tag	UNP Q8ZUP0
B	-34	HIS	-	expression tag	UNP Q8ZUP0
B	-33	HIS	-	expression tag	UNP Q8ZUP0
B	-32	HIS	-	expression tag	UNP Q8ZUP0
B	-31	HIS	-	expression tag	UNP Q8ZUP0
B	-30	HIS	-	expression tag	UNP Q8ZUP0
B	-29	HIS	-	expression tag	UNP Q8ZUP0
B	-28	SER	-	expression tag	UNP Q8ZUP0
B	-27	SER	-	expression tag	UNP Q8ZUP0
B	-26	GLY	-	expression tag	UNP Q8ZUP0
B	-25	LEU	-	expression tag	UNP Q8ZUP0
B	-24	VAL	-	expression tag	UNP Q8ZUP0
B	-23	PRO	-	expression tag	UNP Q8ZUP0
B	-22	ARG	-	expression tag	UNP Q8ZUP0
B	-21	GLY	-	expression tag	UNP Q8ZUP0
B	-20	SER	-	expression tag	UNP Q8ZUP0
B	-19	HIS	-	expression tag	UNP Q8ZUP0
B	-18	MET	-	expression tag	UNP Q8ZUP0
B	-17	ALA	-	expression tag	UNP Q8ZUP0
B	-16	SER	-	expression tag	UNP Q8ZUP0
B	-15	MET	-	expression tag	UNP Q8ZUP0
B	-14	THR	-	expression tag	UNP Q8ZUP0
B	-13	GLY	-	expression tag	UNP Q8ZUP0
B	-12	GLY	-	expression tag	UNP Q8ZUP0
B	-11	GLN	-	expression tag	UNP Q8ZUP0
B	-10	GLN	-	expression tag	UNP Q8ZUP0
B	-9	MET	-	expression tag	UNP Q8ZUP0
B	-8	GLY	-	expression tag	UNP Q8ZUP0
B	-7	ARG	-	expression tag	UNP Q8ZUP0
B	-6	GLY	-	expression tag	UNP Q8ZUP0
B	-5	SER	-	expression tag	UNP Q8ZUP0
B	-4	GLY	-	expression tag	UNP Q8ZUP0
B	-3	GLY	-	expression tag	UNP Q8ZUP0
B	-2	GLY	-	expression tag	UNP Q8ZUP0
B	-1	HIS	-	expression tag	UNP Q8ZUP0
B	0	GLU	-	expression tag	UNP Q8ZUP0
C	-38	MET	-	expression tag	UNP Q8ZUP0
C	-37	GLY	-	expression tag	UNP Q8ZUP0
C	-36	SER	-	expression tag	UNP Q8ZUP0
C	-35	SER	-	expression tag	UNP Q8ZUP0
C	-34	HIS	-	expression tag	UNP Q8ZUP0
C	-33	HIS	-	expression tag	UNP Q8ZUP0

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-32	HIS	-	expression tag	UNP Q8ZUP0
C	-31	HIS	-	expression tag	UNP Q8ZUP0
C	-30	HIS	-	expression tag	UNP Q8ZUP0
C	-29	HIS	-	expression tag	UNP Q8ZUP0
C	-28	SER	-	expression tag	UNP Q8ZUP0
C	-27	SER	-	expression tag	UNP Q8ZUP0
C	-26	GLY	-	expression tag	UNP Q8ZUP0
C	-25	LEU	-	expression tag	UNP Q8ZUP0
C	-24	VAL	-	expression tag	UNP Q8ZUP0
C	-23	PRO	-	expression tag	UNP Q8ZUP0
C	-22	ARG	-	expression tag	UNP Q8ZUP0
C	-21	GLY	-	expression tag	UNP Q8ZUP0
C	-20	SER	-	expression tag	UNP Q8ZUP0
C	-19	HIS	-	expression tag	UNP Q8ZUP0
C	-18	MET	-	expression tag	UNP Q8ZUP0
C	-17	ALA	-	expression tag	UNP Q8ZUP0
C	-16	SER	-	expression tag	UNP Q8ZUP0
C	-15	MET	-	expression tag	UNP Q8ZUP0
C	-14	THR	-	expression tag	UNP Q8ZUP0
C	-13	GLY	-	expression tag	UNP Q8ZUP0
C	-12	GLY	-	expression tag	UNP Q8ZUP0
C	-11	GLN	-	expression tag	UNP Q8ZUP0
C	-10	GLN	-	expression tag	UNP Q8ZUP0
C	-9	MET	-	expression tag	UNP Q8ZUP0
C	-8	GLY	-	expression tag	UNP Q8ZUP0
C	-7	ARG	-	expression tag	UNP Q8ZUP0
C	-6	GLY	-	expression tag	UNP Q8ZUP0
C	-5	SER	-	expression tag	UNP Q8ZUP0
C	-4	GLY	-	expression tag	UNP Q8ZUP0
C	-3	GLY	-	expression tag	UNP Q8ZUP0
C	-2	GLY	-	expression tag	UNP Q8ZUP0
C	-1	HIS	-	expression tag	UNP Q8ZUP0
C	0	GLU	-	expression tag	UNP Q8ZUP0
D	-38	MET	-	expression tag	UNP Q8ZUP0
D	-37	GLY	-	expression tag	UNP Q8ZUP0
D	-36	SER	-	expression tag	UNP Q8ZUP0
D	-35	SER	-	expression tag	UNP Q8ZUP0
D	-34	HIS	-	expression tag	UNP Q8ZUP0
D	-33	HIS	-	expression tag	UNP Q8ZUP0
D	-32	HIS	-	expression tag	UNP Q8ZUP0
D	-31	HIS	-	expression tag	UNP Q8ZUP0
D	-30	HIS	-	expression tag	UNP Q8ZUP0

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-29	HIS	-	expression tag	UNP Q8ZUP0
D	-28	SER	-	expression tag	UNP Q8ZUP0
D	-27	SER	-	expression tag	UNP Q8ZUP0
D	-26	GLY	-	expression tag	UNP Q8ZUP0
D	-25	LEU	-	expression tag	UNP Q8ZUP0
D	-24	VAL	-	expression tag	UNP Q8ZUP0
D	-23	PRO	-	expression tag	UNP Q8ZUP0
D	-22	ARG	-	expression tag	UNP Q8ZUP0
D	-21	GLY	-	expression tag	UNP Q8ZUP0
D	-20	SER	-	expression tag	UNP Q8ZUP0
D	-19	HIS	-	expression tag	UNP Q8ZUP0
D	-18	MET	-	expression tag	UNP Q8ZUP0
D	-17	ALA	-	expression tag	UNP Q8ZUP0
D	-16	SER	-	expression tag	UNP Q8ZUP0
D	-15	MET	-	expression tag	UNP Q8ZUP0
D	-14	THR	-	expression tag	UNP Q8ZUP0
D	-13	GLY	-	expression tag	UNP Q8ZUP0
D	-12	GLY	-	expression tag	UNP Q8ZUP0
D	-11	GLN	-	expression tag	UNP Q8ZUP0
D	-10	GLN	-	expression tag	UNP Q8ZUP0
D	-9	MET	-	expression tag	UNP Q8ZUP0
D	-8	GLY	-	expression tag	UNP Q8ZUP0
D	-7	ARG	-	expression tag	UNP Q8ZUP0
D	-6	GLY	-	expression tag	UNP Q8ZUP0
D	-5	SER	-	expression tag	UNP Q8ZUP0
D	-4	GLY	-	expression tag	UNP Q8ZUP0
D	-3	GLY	-	expression tag	UNP Q8ZUP0
D	-2	GLY	-	expression tag	UNP Q8ZUP0
D	-1	HIS	-	expression tag	UNP Q8ZUP0
D	0	GLU	-	expression tag	UNP Q8ZUP0
E	-38	MET	-	expression tag	UNP Q8ZUP0
E	-37	GLY	-	expression tag	UNP Q8ZUP0
E	-36	SER	-	expression tag	UNP Q8ZUP0
E	-35	SER	-	expression tag	UNP Q8ZUP0
E	-34	HIS	-	expression tag	UNP Q8ZUP0
E	-33	HIS	-	expression tag	UNP Q8ZUP0
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E	-31	HIS	-	expression tag	UNP Q8ZUP0
E	-30	HIS	-	expression tag	UNP Q8ZUP0
E	-29	HIS	-	expression tag	UNP Q8ZUP0
E	-28	SER	-	expression tag	UNP Q8ZUP0
E	-27	SER	-	expression tag	UNP Q8ZUP0

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-26	GLY	-	expression tag	UNP Q8ZUP0
E	-25	LEU	-	expression tag	UNP Q8ZUP0
E	-24	VAL	-	expression tag	UNP Q8ZUP0
E	-23	PRO	-	expression tag	UNP Q8ZUP0
E	-22	ARG	-	expression tag	UNP Q8ZUP0
E	-21	GLY	-	expression tag	UNP Q8ZUP0
E	-20	SER	-	expression tag	UNP Q8ZUP0
E	-19	HIS	-	expression tag	UNP Q8ZUP0
E	-18	MET	-	expression tag	UNP Q8ZUP0
E	-17	ALA	-	expression tag	UNP Q8ZUP0
E	-16	SER	-	expression tag	UNP Q8ZUP0
E	-15	MET	-	expression tag	UNP Q8ZUP0
E	-14	THR	-	expression tag	UNP Q8ZUP0
E	-13	GLY	-	expression tag	UNP Q8ZUP0
E	-12	GLY	-	expression tag	UNP Q8ZUP0
E	-11	GLN	-	expression tag	UNP Q8ZUP0
E	-10	GLN	-	expression tag	UNP Q8ZUP0
E	-9	MET	-	expression tag	UNP Q8ZUP0
E	-8	GLY	-	expression tag	UNP Q8ZUP0
E	-7	ARG	-	expression tag	UNP Q8ZUP0
E	-6	GLY	-	expression tag	UNP Q8ZUP0
E	-5	SER	-	expression tag	UNP Q8ZUP0
E	-4	GLY	-	expression tag	UNP Q8ZUP0
E	-3	GLY	-	expression tag	UNP Q8ZUP0
E	-2	GLY	-	expression tag	UNP Q8ZUP0
E	-1	HIS	-	expression tag	UNP Q8ZUP0
E	0	GLU	-	expression tag	UNP Q8ZUP0
F	-38	MET	-	expression tag	UNP Q8ZUP0
F	-37	GLY	-	expression tag	UNP Q8ZUP0
F	-36	SER	-	expression tag	UNP Q8ZUP0
F	-35	SER	-	expression tag	UNP Q8ZUP0
F	-34	HIS	-	expression tag	UNP Q8ZUP0
F	-33	HIS	-	expression tag	UNP Q8ZUP0
F	-32	HIS	-	expression tag	UNP Q8ZUP0
F	-31	HIS	-	expression tag	UNP Q8ZUP0
F	-30	HIS	-	expression tag	UNP Q8ZUP0
F	-29	HIS	-	expression tag	UNP Q8ZUP0
F	-28	SER	-	expression tag	UNP Q8ZUP0
F	-27	SER	-	expression tag	UNP Q8ZUP0
F	-26	GLY	-	expression tag	UNP Q8ZUP0
F	-25	LEU	-	expression tag	UNP Q8ZUP0
F	-24	VAL	-	expression tag	UNP Q8ZUP0

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Chain	Residue	Modelled	Actual	Comment	Reference
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F	-22	ARG	-	expression tag	UNP Q8ZUP0
F	-21	GLY	-	expression tag	UNP Q8ZUP0
F	-20	SER	-	expression tag	UNP Q8ZUP0
F	-19	HIS	-	expression tag	UNP Q8ZUP0
F	-18	MET	-	expression tag	UNP Q8ZUP0
F	-17	ALA	-	expression tag	UNP Q8ZUP0
F	-16	SER	-	expression tag	UNP Q8ZUP0
F	-15	MET	-	expression tag	UNP Q8ZUP0
F	-14	THR	-	expression tag	UNP Q8ZUP0
F	-13	GLY	-	expression tag	UNP Q8ZUP0
F	-12	GLY	-	expression tag	UNP Q8ZUP0
F	-11	GLN	-	expression tag	UNP Q8ZUP0
F	-10	GLN	-	expression tag	UNP Q8ZUP0
F	-9	MET	-	expression tag	UNP Q8ZUP0
F	-8	GLY	-	expression tag	UNP Q8ZUP0
F	-7	ARG	-	expression tag	UNP Q8ZUP0
F	-6	GLY	-	expression tag	UNP Q8ZUP0
F	-5	SER	-	expression tag	UNP Q8ZUP0
F	-4	GLY	-	expression tag	UNP Q8ZUP0
F	-3	GLY	-	expression tag	UNP Q8ZUP0
F	-2	GLY	-	expression tag	UNP Q8ZUP0
F	-1	HIS	-	expression tag	UNP Q8ZUP0
F	0	GLU	-	expression tag	UNP Q8ZUP0
G	-38	MET	-	expression tag	UNP Q8ZUP0
G	-37	GLY	-	expression tag	UNP Q8ZUP0
G	-36	SER	-	expression tag	UNP Q8ZUP0
G	-35	SER	-	expression tag	UNP Q8ZUP0
G	-34	HIS	-	expression tag	UNP Q8ZUP0
G	-33	HIS	-	expression tag	UNP Q8ZUP0
G	-32	HIS	-	expression tag	UNP Q8ZUP0
G	-31	HIS	-	expression tag	UNP Q8ZUP0
G	-30	HIS	-	expression tag	UNP Q8ZUP0
G	-29	HIS	-	expression tag	UNP Q8ZUP0
G	-28	SER	-	expression tag	UNP Q8ZUP0
G	-27	SER	-	expression tag	UNP Q8ZUP0
G	-26	GLY	-	expression tag	UNP Q8ZUP0
G	-25	LEU	-	expression tag	UNP Q8ZUP0
G	-24	VAL	-	expression tag	UNP Q8ZUP0
G	-23	PRO	-	expression tag	UNP Q8ZUP0
G	-22	ARG	-	expression tag	UNP Q8ZUP0
G	-21	GLY	-	expression tag	UNP Q8ZUP0

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-20	SER	-	expression tag	UNP Q8ZUP0
G	-19	HIS	-	expression tag	UNP Q8ZUP0
G	-18	MET	-	expression tag	UNP Q8ZUP0
G	-17	ALA	-	expression tag	UNP Q8ZUP0
G	-16	SER	-	expression tag	UNP Q8ZUP0
G	-15	MET	-	expression tag	UNP Q8ZUP0
G	-14	THR	-	expression tag	UNP Q8ZUP0
G	-13	GLY	-	expression tag	UNP Q8ZUP0
G	-12	GLY	-	expression tag	UNP Q8ZUP0
G	-11	GLN	-	expression tag	UNP Q8ZUP0
G	-10	GLN	-	expression tag	UNP Q8ZUP0
G	-9	MET	-	expression tag	UNP Q8ZUP0
G	-8	GLY	-	expression tag	UNP Q8ZUP0
G	-7	ARG	-	expression tag	UNP Q8ZUP0
G	-6	GLY	-	expression tag	UNP Q8ZUP0
G	-5	SER	-	expression tag	UNP Q8ZUP0
G	-4	GLY	-	expression tag	UNP Q8ZUP0
G	-3	GLY	-	expression tag	UNP Q8ZUP0
G	-2	GLY	-	expression tag	UNP Q8ZUP0
G	-1	HIS	-	expression tag	UNP Q8ZUP0
G	0	GLU	-	expression tag	UNP Q8ZUP0
H	-38	MET	-	expression tag	UNP Q8ZUP0
H	-37	GLY	-	expression tag	UNP Q8ZUP0
H	-36	SER	-	expression tag	UNP Q8ZUP0
H	-35	SER	-	expression tag	UNP Q8ZUP0
H	-34	HIS	-	expression tag	UNP Q8ZUP0
H	-33	HIS	-	expression tag	UNP Q8ZUP0
H	-32	HIS	-	expression tag	UNP Q8ZUP0
H	-31	HIS	-	expression tag	UNP Q8ZUP0
H	-30	HIS	-	expression tag	UNP Q8ZUP0
H	-29	HIS	-	expression tag	UNP Q8ZUP0
H	-28	SER	-	expression tag	UNP Q8ZUP0
H	-27	SER	-	expression tag	UNP Q8ZUP0
H	-26	GLY	-	expression tag	UNP Q8ZUP0
H	-25	LEU	-	expression tag	UNP Q8ZUP0
H	-24	VAL	-	expression tag	UNP Q8ZUP0
H	-23	PRO	-	expression tag	UNP Q8ZUP0
H	-22	ARG	-	expression tag	UNP Q8ZUP0
H	-21	GLY	-	expression tag	UNP Q8ZUP0
H	-20	SER	-	expression tag	UNP Q8ZUP0
H	-19	HIS	-	expression tag	UNP Q8ZUP0
H	-18	MET	-	expression tag	UNP Q8ZUP0

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-17	ALA	-	expression tag	UNP Q8ZUP0
H	-16	SER	-	expression tag	UNP Q8ZUP0
H	-15	MET	-	expression tag	UNP Q8ZUP0
H	-14	THR	-	expression tag	UNP Q8ZUP0
H	-13	GLY	-	expression tag	UNP Q8ZUP0
H	-12	GLY	-	expression tag	UNP Q8ZUP0
H	-11	GLN	-	expression tag	UNP Q8ZUP0
H	-10	GLN	-	expression tag	UNP Q8ZUP0
H	-9	MET	-	expression tag	UNP Q8ZUP0
H	-8	GLY	-	expression tag	UNP Q8ZUP0
H	-7	ARG	-	expression tag	UNP Q8ZUP0
H	-6	GLY	-	expression tag	UNP Q8ZUP0
H	-5	SER	-	expression tag	UNP Q8ZUP0
H	-4	GLY	-	expression tag	UNP Q8ZUP0
H	-3	GLY	-	expression tag	UNP Q8ZUP0
H	-2	GLY	-	expression tag	UNP Q8ZUP0
H	-1	HIS	-	expression tag	UNP Q8ZUP0
H	0	GLU	-	expression tag	UNP Q8ZUP0
I	-38	MET	-	expression tag	UNP Q8ZUP0
I	-37	GLY	-	expression tag	UNP Q8ZUP0
I	-36	SER	-	expression tag	UNP Q8ZUP0
I	-35	SER	-	expression tag	UNP Q8ZUP0
I	-34	HIS	-	expression tag	UNP Q8ZUP0
I	-33	HIS	-	expression tag	UNP Q8ZUP0
I	-32	HIS	-	expression tag	UNP Q8ZUP0
I	-31	HIS	-	expression tag	UNP Q8ZUP0
I	-30	HIS	-	expression tag	UNP Q8ZUP0
I	-29	HIS	-	expression tag	UNP Q8ZUP0
I	-28	SER	-	expression tag	UNP Q8ZUP0
I	-27	SER	-	expression tag	UNP Q8ZUP0
I	-26	GLY	-	expression tag	UNP Q8ZUP0
I	-25	LEU	-	expression tag	UNP Q8ZUP0
I	-24	VAL	-	expression tag	UNP Q8ZUP0
I	-23	PRO	-	expression tag	UNP Q8ZUP0
I	-22	ARG	-	expression tag	UNP Q8ZUP0
I	-21	GLY	-	expression tag	UNP Q8ZUP0
I	-20	SER	-	expression tag	UNP Q8ZUP0
I	-19	HIS	-	expression tag	UNP Q8ZUP0
I	-18	MET	-	expression tag	UNP Q8ZUP0
I	-17	ALA	-	expression tag	UNP Q8ZUP0
I	-16	SER	-	expression tag	UNP Q8ZUP0
I	-15	MET	-	expression tag	UNP Q8ZUP0

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Chain	Residue	Modelled	Actual	Comment	Reference
I	-14	THR	-	expression tag	UNP Q8ZUP0
I	-13	GLY	-	expression tag	UNP Q8ZUP0
I	-12	GLY	-	expression tag	UNP Q8ZUP0
I	-11	GLN	-	expression tag	UNP Q8ZUP0
I	-10	GLN	-	expression tag	UNP Q8ZUP0
I	-9	MET	-	expression tag	UNP Q8ZUP0
I	-8	GLY	-	expression tag	UNP Q8ZUP0
I	-7	ARG	-	expression tag	UNP Q8ZUP0
I	-6	GLY	-	expression tag	UNP Q8ZUP0
I	-5	SER	-	expression tag	UNP Q8ZUP0
I	-4	GLY	-	expression tag	UNP Q8ZUP0
I	-3	GLY	-	expression tag	UNP Q8ZUP0
I	-2	GLY	-	expression tag	UNP Q8ZUP0
I	-1	HIS	-	expression tag	UNP Q8ZUP0
I	0	GLU	-	expression tag	UNP Q8ZUP0
J	-38	MET	-	expression tag	UNP Q8ZUP0
J	-37	GLY	-	expression tag	UNP Q8ZUP0
J	-36	SER	-	expression tag	UNP Q8ZUP0
J	-35	SER	-	expression tag	UNP Q8ZUP0
J	-34	HIS	-	expression tag	UNP Q8ZUP0
J	-33	HIS	-	expression tag	UNP Q8ZUP0
J	-32	HIS	-	expression tag	UNP Q8ZUP0
J	-31	HIS	-	expression tag	UNP Q8ZUP0
J	-30	HIS	-	expression tag	UNP Q8ZUP0
J	-29	HIS	-	expression tag	UNP Q8ZUP0
J	-28	SER	-	expression tag	UNP Q8ZUP0
J	-27	SER	-	expression tag	UNP Q8ZUP0
J	-26	GLY	-	expression tag	UNP Q8ZUP0
J	-25	LEU	-	expression tag	UNP Q8ZUP0
J	-24	VAL	-	expression tag	UNP Q8ZUP0
J	-23	PRO	-	expression tag	UNP Q8ZUP0
J	-22	ARG	-	expression tag	UNP Q8ZUP0
J	-21	GLY	-	expression tag	UNP Q8ZUP0
J	-20	SER	-	expression tag	UNP Q8ZUP0
J	-19	HIS	-	expression tag	UNP Q8ZUP0
J	-18	MET	-	expression tag	UNP Q8ZUP0
J	-17	ALA	-	expression tag	UNP Q8ZUP0
J	-16	SER	-	expression tag	UNP Q8ZUP0
J	-15	MET	-	expression tag	UNP Q8ZUP0
J	-14	THR	-	expression tag	UNP Q8ZUP0
J	-13	GLY	-	expression tag	UNP Q8ZUP0
J	-12	GLY	-	expression tag	UNP Q8ZUP0

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Chain	Residue	Modelled	Actual	Comment	Reference
J	-11	GLN	-	expression tag	UNP Q8ZUP0
J	-10	GLN	-	expression tag	UNP Q8ZUP0
J	-9	MET	-	expression tag	UNP Q8ZUP0
J	-8	GLY	-	expression tag	UNP Q8ZUP0
J	-7	ARG	-	expression tag	UNP Q8ZUP0
J	-6	GLY	-	expression tag	UNP Q8ZUP0
J	-5	SER	-	expression tag	UNP Q8ZUP0
J	-4	GLY	-	expression tag	UNP Q8ZUP0
J	-3	GLY	-	expression tag	UNP Q8ZUP0
J	-2	GLY	-	expression tag	UNP Q8ZUP0
J	-1	HIS	-	expression tag	UNP Q8ZUP0
J	0	GLU	-	expression tag	UNP Q8ZUP0
K	-38	MET	-	expression tag	UNP Q8ZUP0
K	-37	GLY	-	expression tag	UNP Q8ZUP0
K	-36	SER	-	expression tag	UNP Q8ZUP0
K	-35	SER	-	expression tag	UNP Q8ZUP0
K	-34	HIS	-	expression tag	UNP Q8ZUP0
K	-33	HIS	-	expression tag	UNP Q8ZUP0
K	-32	HIS	-	expression tag	UNP Q8ZUP0
K	-31	HIS	-	expression tag	UNP Q8ZUP0
K	-30	HIS	-	expression tag	UNP Q8ZUP0
K	-29	HIS	-	expression tag	UNP Q8ZUP0
K	-28	SER	-	expression tag	UNP Q8ZUP0
K	-27	SER	-	expression tag	UNP Q8ZUP0
K	-26	GLY	-	expression tag	UNP Q8ZUP0
K	-25	LEU	-	expression tag	UNP Q8ZUP0
K	-24	VAL	-	expression tag	UNP Q8ZUP0
K	-23	PRO	-	expression tag	UNP Q8ZUP0
K	-22	ARG	-	expression tag	UNP Q8ZUP0
K	-21	GLY	-	expression tag	UNP Q8ZUP0
K	-20	SER	-	expression tag	UNP Q8ZUP0
K	-19	HIS	-	expression tag	UNP Q8ZUP0
K	-18	MET	-	expression tag	UNP Q8ZUP0
K	-17	ALA	-	expression tag	UNP Q8ZUP0
K	-16	SER	-	expression tag	UNP Q8ZUP0
K	-15	MET	-	expression tag	UNP Q8ZUP0
K	-14	THR	-	expression tag	UNP Q8ZUP0
K	-13	GLY	-	expression tag	UNP Q8ZUP0
K	-12	GLY	-	expression tag	UNP Q8ZUP0
K	-11	GLN	-	expression tag	UNP Q8ZUP0
K	-10	GLN	-	expression tag	UNP Q8ZUP0
K	-9	MET	-	expression tag	UNP Q8ZUP0

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Chain	Residue	Modelled	Actual	Comment	Reference
K	-8	GLY	-	expression tag	UNP Q8ZUP0
K	-7	ARG	-	expression tag	UNP Q8ZUP0
K	-6	GLY	-	expression tag	UNP Q8ZUP0
K	-5	SER	-	expression tag	UNP Q8ZUP0
K	-4	GLY	-	expression tag	UNP Q8ZUP0
K	-3	GLY	-	expression tag	UNP Q8ZUP0
K	-2	GLY	-	expression tag	UNP Q8ZUP0
K	-1	HIS	-	expression tag	UNP Q8ZUP0
K	0	GLU	-	expression tag	UNP Q8ZUP0
L	-38	MET	-	expression tag	UNP Q8ZUP0
L	-37	GLY	-	expression tag	UNP Q8ZUP0
L	-36	SER	-	expression tag	UNP Q8ZUP0
L	-35	SER	-	expression tag	UNP Q8ZUP0
L	-34	HIS	-	expression tag	UNP Q8ZUP0
L	-33	HIS	-	expression tag	UNP Q8ZUP0
L	-32	HIS	-	expression tag	UNP Q8ZUP0
L	-31	HIS	-	expression tag	UNP Q8ZUP0
L	-30	HIS	-	expression tag	UNP Q8ZUP0
L	-29	HIS	-	expression tag	UNP Q8ZUP0
L	-28	SER	-	expression tag	UNP Q8ZUP0
L	-27	SER	-	expression tag	UNP Q8ZUP0
L	-26	GLY	-	expression tag	UNP Q8ZUP0
L	-25	LEU	-	expression tag	UNP Q8ZUP0
L	-24	VAL	-	expression tag	UNP Q8ZUP0
L	-23	PRO	-	expression tag	UNP Q8ZUP0
L	-22	ARG	-	expression tag	UNP Q8ZUP0
L	-21	GLY	-	expression tag	UNP Q8ZUP0
L	-20	SER	-	expression tag	UNP Q8ZUP0
L	-19	HIS	-	expression tag	UNP Q8ZUP0
L	-18	MET	-	expression tag	UNP Q8ZUP0
L	-17	ALA	-	expression tag	UNP Q8ZUP0
L	-16	SER	-	expression tag	UNP Q8ZUP0
L	-15	MET	-	expression tag	UNP Q8ZUP0
L	-14	THR	-	expression tag	UNP Q8ZUP0
L	-13	GLY	-	expression tag	UNP Q8ZUP0
L	-12	GLY	-	expression tag	UNP Q8ZUP0
L	-11	GLN	-	expression tag	UNP Q8ZUP0
L	-10	GLN	-	expression tag	UNP Q8ZUP0
L	-9	MET	-	expression tag	UNP Q8ZUP0
L	-8	GLY	-	expression tag	UNP Q8ZUP0
L	-7	ARG	-	expression tag	UNP Q8ZUP0
L	-6	GLY	-	expression tag	UNP Q8ZUP0

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Chain	Residue	Modelled	Actual	Comment	Reference
L	-5	SER	-	expression tag	UNP Q8ZUP0
L	-4	GLY	-	expression tag	UNP Q8ZUP0
L	-3	GLY	-	expression tag	UNP Q8ZUP0
L	-2	GLY	-	expression tag	UNP Q8ZUP0
L	-1	HIS	-	expression tag	UNP Q8ZUP0
L	0	GLU	-	expression tag	UNP Q8ZUP0
M	-38	MET	-	expression tag	UNP Q8ZUP0
M	-37	GLY	-	expression tag	UNP Q8ZUP0
M	-36	SER	-	expression tag	UNP Q8ZUP0
M	-35	SER	-	expression tag	UNP Q8ZUP0
M	-34	HIS	-	expression tag	UNP Q8ZUP0
M	-33	HIS	-	expression tag	UNP Q8ZUP0
M	-32	HIS	-	expression tag	UNP Q8ZUP0
M	-31	HIS	-	expression tag	UNP Q8ZUP0
M	-30	HIS	-	expression tag	UNP Q8ZUP0
M	-29	HIS	-	expression tag	UNP Q8ZUP0
M	-28	SER	-	expression tag	UNP Q8ZUP0
M	-27	SER	-	expression tag	UNP Q8ZUP0
M	-26	GLY	-	expression tag	UNP Q8ZUP0
M	-25	LEU	-	expression tag	UNP Q8ZUP0
M	-24	VAL	-	expression tag	UNP Q8ZUP0
M	-23	PRO	-	expression tag	UNP Q8ZUP0
M	-22	ARG	-	expression tag	UNP Q8ZUP0
M	-21	GLY	-	expression tag	UNP Q8ZUP0
M	-20	SER	-	expression tag	UNP Q8ZUP0
M	-19	HIS	-	expression tag	UNP Q8ZUP0
M	-18	MET	-	expression tag	UNP Q8ZUP0
M	-17	ALA	-	expression tag	UNP Q8ZUP0
M	-16	SER	-	expression tag	UNP Q8ZUP0
M	-15	MET	-	expression tag	UNP Q8ZUP0
M	-14	THR	-	expression tag	UNP Q8ZUP0
M	-13	GLY	-	expression tag	UNP Q8ZUP0
M	-12	GLY	-	expression tag	UNP Q8ZUP0
M	-11	GLN	-	expression tag	UNP Q8ZUP0
M	-10	GLN	-	expression tag	UNP Q8ZUP0
M	-9	MET	-	expression tag	UNP Q8ZUP0
M	-8	GLY	-	expression tag	UNP Q8ZUP0
M	-7	ARG	-	expression tag	UNP Q8ZUP0
M	-6	GLY	-	expression tag	UNP Q8ZUP0
M	-5	SER	-	expression tag	UNP Q8ZUP0
M	-4	GLY	-	expression tag	UNP Q8ZUP0
M	-3	GLY	-	expression tag	UNP Q8ZUP0

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Chain	Residue	Modelled	Actual	Comment	Reference
M	-2	GLY	-	expression tag	UNP Q8ZUP0
M	-1	HIS	-	expression tag	UNP Q8ZUP0
M	0	GLU	-	expression tag	UNP Q8ZUP0
N	-38	MET	-	expression tag	UNP Q8ZUP0
N	-37	GLY	-	expression tag	UNP Q8ZUP0
N	-36	SER	-	expression tag	UNP Q8ZUP0
N	-35	SER	-	expression tag	UNP Q8ZUP0
N	-34	HIS	-	expression tag	UNP Q8ZUP0
N	-33	HIS	-	expression tag	UNP Q8ZUP0
N	-32	HIS	-	expression tag	UNP Q8ZUP0
N	-31	HIS	-	expression tag	UNP Q8ZUP0
N	-30	HIS	-	expression tag	UNP Q8ZUP0
N	-29	HIS	-	expression tag	UNP Q8ZUP0
N	-28	SER	-	expression tag	UNP Q8ZUP0
N	-27	SER	-	expression tag	UNP Q8ZUP0
N	-26	GLY	-	expression tag	UNP Q8ZUP0
N	-25	LEU	-	expression tag	UNP Q8ZUP0
N	-24	VAL	-	expression tag	UNP Q8ZUP0
N	-23	PRO	-	expression tag	UNP Q8ZUP0
N	-22	ARG	-	expression tag	UNP Q8ZUP0
N	-21	GLY	-	expression tag	UNP Q8ZUP0
N	-20	SER	-	expression tag	UNP Q8ZUP0
N	-19	HIS	-	expression tag	UNP Q8ZUP0
N	-18	MET	-	expression tag	UNP Q8ZUP0
N	-17	ALA	-	expression tag	UNP Q8ZUP0
N	-16	SER	-	expression tag	UNP Q8ZUP0
N	-15	MET	-	expression tag	UNP Q8ZUP0
N	-14	THR	-	expression tag	UNP Q8ZUP0
N	-13	GLY	-	expression tag	UNP Q8ZUP0
N	-12	GLY	-	expression tag	UNP Q8ZUP0
N	-11	GLN	-	expression tag	UNP Q8ZUP0
N	-10	GLN	-	expression tag	UNP Q8ZUP0
N	-9	MET	-	expression tag	UNP Q8ZUP0
N	-8	GLY	-	expression tag	UNP Q8ZUP0
N	-7	ARG	-	expression tag	UNP Q8ZUP0
N	-6	GLY	-	expression tag	UNP Q8ZUP0
N	-5	SER	-	expression tag	UNP Q8ZUP0
N	-4	GLY	-	expression tag	UNP Q8ZUP0
N	-3	GLY	-	expression tag	UNP Q8ZUP0
N	-2	GLY	-	expression tag	UNP Q8ZUP0
N	-1	HIS	-	expression tag	UNP Q8ZUP0
N	0	GLU	-	expression tag	UNP Q8ZUP0

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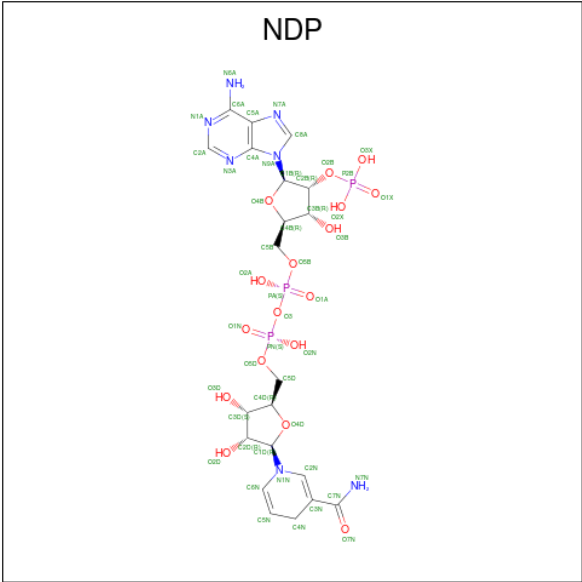
Chain	Residue	Modelled	Actual	Comment	Reference
O	-38	MET	-	expression tag	UNP Q8ZUP0
O	-37	GLY	-	expression tag	UNP Q8ZUP0
O	-36	SER	-	expression tag	UNP Q8ZUP0
O	-35	SER	-	expression tag	UNP Q8ZUP0
O	-34	HIS	-	expression tag	UNP Q8ZUP0
O	-33	HIS	-	expression tag	UNP Q8ZUP0
O	-32	HIS	-	expression tag	UNP Q8ZUP0
O	-31	HIS	-	expression tag	UNP Q8ZUP0
O	-30	HIS	-	expression tag	UNP Q8ZUP0
O	-29	HIS	-	expression tag	UNP Q8ZUP0
O	-28	SER	-	expression tag	UNP Q8ZUP0
O	-27	SER	-	expression tag	UNP Q8ZUP0
O	-26	GLY	-	expression tag	UNP Q8ZUP0
O	-25	LEU	-	expression tag	UNP Q8ZUP0
O	-24	VAL	-	expression tag	UNP Q8ZUP0
O	-23	PRO	-	expression tag	UNP Q8ZUP0
O	-22	ARG	-	expression tag	UNP Q8ZUP0
O	-21	GLY	-	expression tag	UNP Q8ZUP0
O	-20	SER	-	expression tag	UNP Q8ZUP0
O	-19	HIS	-	expression tag	UNP Q8ZUP0
O	-18	MET	-	expression tag	UNP Q8ZUP0
O	-17	ALA	-	expression tag	UNP Q8ZUP0
O	-16	SER	-	expression tag	UNP Q8ZUP0
O	-15	MET	-	expression tag	UNP Q8ZUP0
O	-14	THR	-	expression tag	UNP Q8ZUP0
O	-13	GLY	-	expression tag	UNP Q8ZUP0
O	-12	GLY	-	expression tag	UNP Q8ZUP0
O	-11	GLN	-	expression tag	UNP Q8ZUP0
O	-10	GLN	-	expression tag	UNP Q8ZUP0
O	-9	MET	-	expression tag	UNP Q8ZUP0
O	-8	GLY	-	expression tag	UNP Q8ZUP0
O	-7	ARG	-	expression tag	UNP Q8ZUP0
O	-6	GLY	-	expression tag	UNP Q8ZUP0
O	-5	SER	-	expression tag	UNP Q8ZUP0
O	-4	GLY	-	expression tag	UNP Q8ZUP0
O	-3	GLY	-	expression tag	UNP Q8ZUP0
O	-2	GLY	-	expression tag	UNP Q8ZUP0
O	-1	HIS	-	expression tag	UNP Q8ZUP0
O	0	GLU	-	expression tag	UNP Q8ZUP0
P	-38	MET	-	expression tag	UNP Q8ZUP0
P	-37	GLY	-	expression tag	UNP Q8ZUP0
P	-36	SER	-	expression tag	UNP Q8ZUP0

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Chain	Residue	Modelled	Actual	Comment	Reference
P	-35	SER	-	expression tag	UNP Q8ZUP0
P	-34	HIS	-	expression tag	UNP Q8ZUP0
P	-33	HIS	-	expression tag	UNP Q8ZUP0
P	-32	HIS	-	expression tag	UNP Q8ZUP0
P	-31	HIS	-	expression tag	UNP Q8ZUP0
P	-30	HIS	-	expression tag	UNP Q8ZUP0
P	-29	HIS	-	expression tag	UNP Q8ZUP0
P	-28	SER	-	expression tag	UNP Q8ZUP0
P	-27	SER	-	expression tag	UNP Q8ZUP0
P	-26	GLY	-	expression tag	UNP Q8ZUP0
P	-25	LEU	-	expression tag	UNP Q8ZUP0
P	-24	VAL	-	expression tag	UNP Q8ZUP0
P	-23	PRO	-	expression tag	UNP Q8ZUP0
P	-22	ARG	-	expression tag	UNP Q8ZUP0
P	-21	GLY	-	expression tag	UNP Q8ZUP0
P	-20	SER	-	expression tag	UNP Q8ZUP0
P	-19	HIS	-	expression tag	UNP Q8ZUP0
P	-18	MET	-	expression tag	UNP Q8ZUP0
P	-17	ALA	-	expression tag	UNP Q8ZUP0
P	-16	SER	-	expression tag	UNP Q8ZUP0
P	-15	MET	-	expression tag	UNP Q8ZUP0
P	-14	THR	-	expression tag	UNP Q8ZUP0
P	-13	GLY	-	expression tag	UNP Q8ZUP0
P	-12	GLY	-	expression tag	UNP Q8ZUP0
P	-11	GLN	-	expression tag	UNP Q8ZUP0
P	-10	GLN	-	expression tag	UNP Q8ZUP0
P	-9	MET	-	expression tag	UNP Q8ZUP0
P	-8	GLY	-	expression tag	UNP Q8ZUP0
P	-7	ARG	-	expression tag	UNP Q8ZUP0
P	-6	GLY	-	expression tag	UNP Q8ZUP0
P	-5	SER	-	expression tag	UNP Q8ZUP0
P	-4	GLY	-	expression tag	UNP Q8ZUP0
P	-3	GLY	-	expression tag	UNP Q8ZUP0
P	-2	GLY	-	expression tag	UNP Q8ZUP0
P	-1	HIS	-	expression tag	UNP Q8ZUP0
P	0	GLU	-	expression tag	UNP Q8ZUP0

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).



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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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 ZINC ION (three-letter code: ZN) (formula: Zn).

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

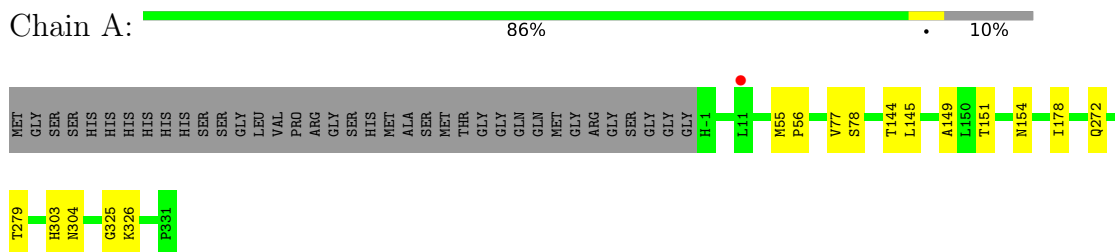
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	101	Total 101	O 101	0	0
4	B	91	Total 91	O 91	0	0
4	C	89	Total 89	O 89	0	0
4	D	81	Total 81	O 81	0	0
4	E	84	Total 84	O 84	0	0
4	F	91	Total 91	O 91	0	0
4	G	67	Total 67	O 67	0	0
4	H	83	Total 83	O 83	0	0
4	I	64	Total 64	O 64	0	0
4	J	68	Total 68	O 68	0	0
4	K	51	Total 51	O 51	0	0
4	L	53	Total 53	O 53	0	0
4	M	44	Total 44	O 44	0	0
4	N	54	Total 54	O 54	0	0
4	O	44	Total 44	O 44	0	0
4	P	42	Total 42	O 42	0	0

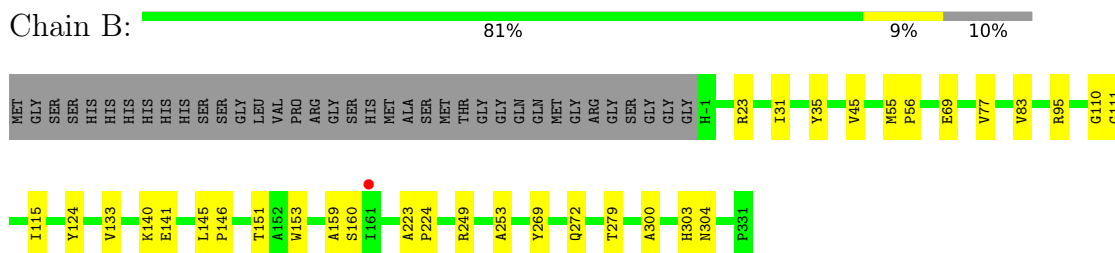
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

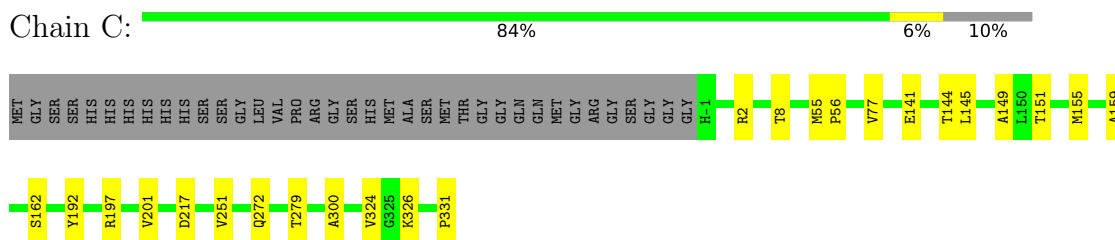
- Molecule 1: Alcohol dehydrogenase (Zinc)



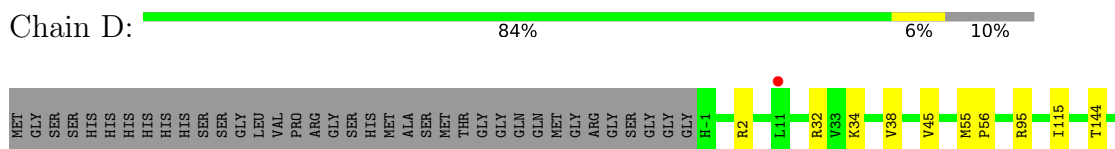
- Molecule 1: Alcohol dehydrogenase (Zinc)



- Molecule 1: Alcohol dehydrogenase (Zinc)



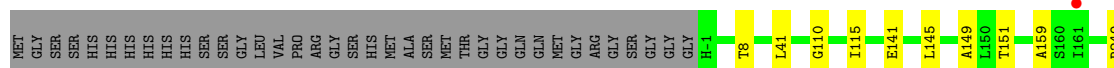
- Molecule 1: Alcohol dehydrogenase (Zinc)





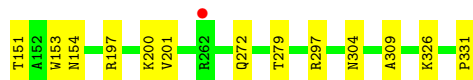
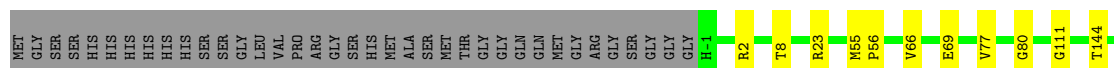
• Molecule 1: Alcohol dehydrogenase (Zinc)

Chain E: 86% 10%



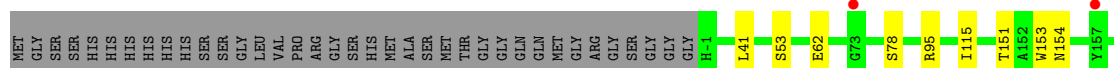
• Molecule 1: Alcohol dehydrogenase (Zinc)

Chain F: 84% 6% 10%



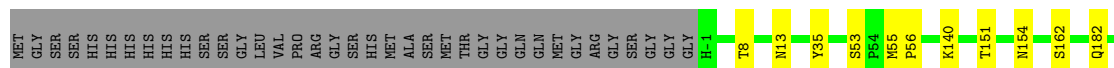
• Molecule 1: Alcohol dehydrogenase (Zinc)

Chain G: 85% 5% 10%



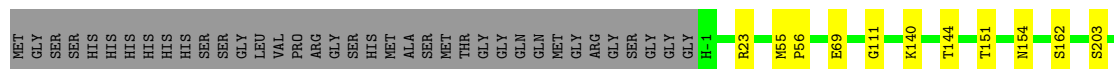
• Molecule 1: Alcohol dehydrogenase (Zinc)

Chain H: 85% 5% 10%



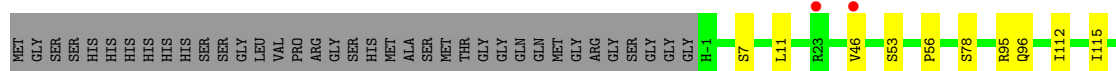
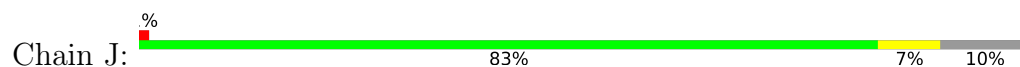
• Molecule 1: Alcohol dehydrogenase (Zinc)

Chain I: 85% 5% 10%

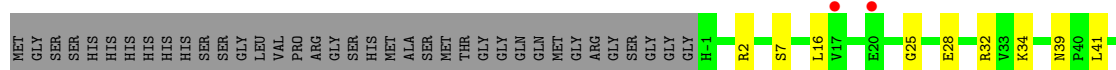
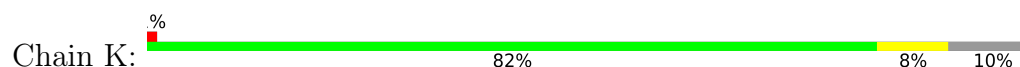




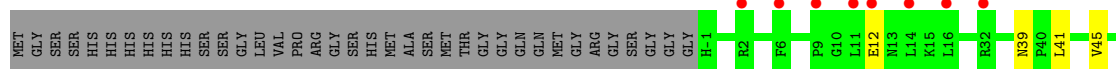
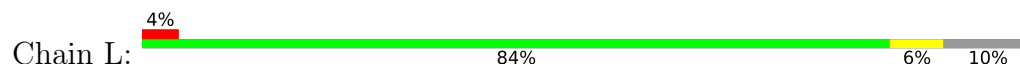
• Molecule 1: Alcohol dehydrogenase (Zinc)



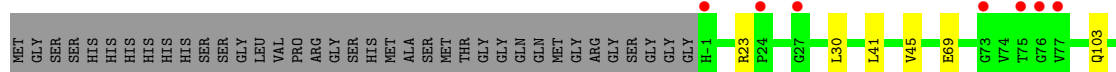
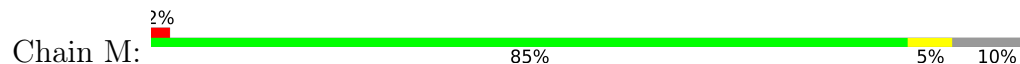
• Molecule 1: Alcohol dehydrogenase (Zinc)



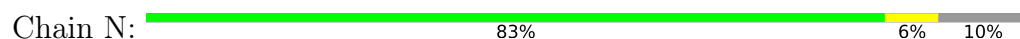
• Molecule 1: Alcohol dehydrogenase (Zinc)

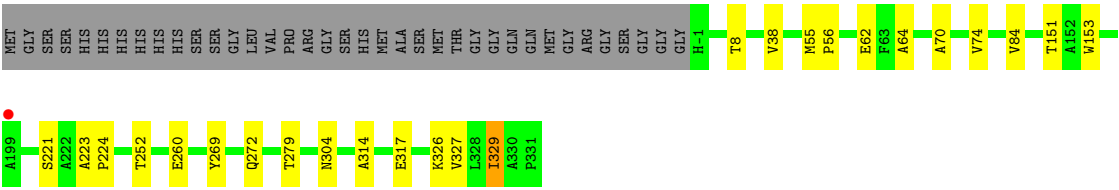


• Molecule 1: Alcohol dehydrogenase (Zinc)

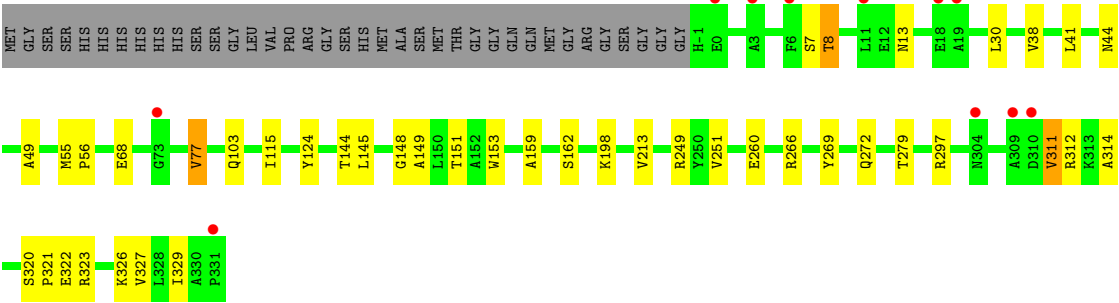
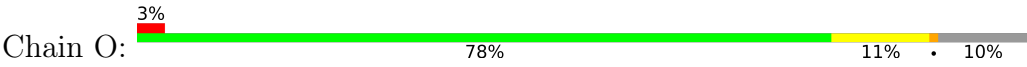


• Molecule 1: Alcohol dehydrogenase (Zinc)

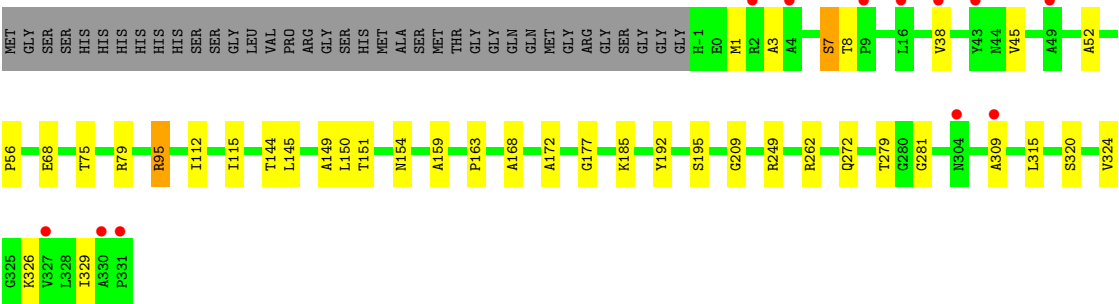
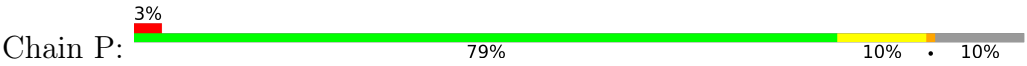




• Molecule 1: Alcohol dehydrogenase (Zinc)



• Molecule 1: Alcohol dehydrogenase (Zinc)



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	138.13Å 169.26Å 149.15Å 90.00° 116.25° 90.00°	Depositor
Resolution (Å)	44.59 – 2.35 49.51 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.9 (44.59-2.35) 99.9 (49.51-2.35)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.97 (at 2.34Å)	Xtriage
Refinement program	PHENIX dev_1241	Depositor
R, R_{free}	0.161 , 0.213 0.168 , 0.217	Depositor DCC
R_{free} test set	12804 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	32.9	Xtriage
Anisotropy	0.222	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 40.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.088 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	40799	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.03% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NDP, ZN

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	0.61	0/2494	0.72	0/3393
1	B	0.58	0/2486	0.73	0/3384
1	C	0.59	0/2502	0.73	0/3403
1	D	0.58	1/2475 (0.0%)	0.73	2/3371 (0.1%)
1	E	0.58	0/2496	0.69	0/3396
1	F	0.58	0/2498	0.72	0/3399
1	G	0.57	0/2487	0.69	0/3386
1	H	0.56	0/2477	0.68	0/3373
1	I	0.55	0/2480	0.69	0/3378
1	J	0.57	0/2470	0.69	0/3363
1	K	0.55	0/2472	0.69	0/3368
1	L	0.53	0/2482	0.68	0/3380
1	M	0.56	0/2481	0.67	0/3378
1	N	0.54	0/2483	0.69	0/3381
1	O	0.55	0/2456	0.67	0/3350
1	P	0.54	0/2460	0.66	1/3352 (0.0%)
All	All	0.56	1/39699 (0.0%)	0.70	3/54055 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	O	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	319	ARG	C-N	7.23	1.50	1.34

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	285	ASP	CB-CG-OD2	-5.78	113.10	118.30
1	P	95	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	D	266	ARG	NE-CZ-NH1	5.33	122.97	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	O	323	ARG	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2444	0	2477	12	0
1	B	2436	0	2459	18	0
1	C	2452	0	2491	13	0
1	D	2425	0	2442	14	0
1	E	2446	0	2477	10	0
1	F	2448	0	2480	16	0
1	G	2437	0	2460	11	0
1	H	2427	0	2446	11	0
1	I	2430	0	2444	10	0
1	J	2424	0	2446	12	0
1	K	2422	0	2436	17	0
1	L	2432	0	2451	12	0
1	M	2431	0	2453	12	0
1	N	2433	0	2450	15	0
1	O	2406	0	2403	27	0
1	P	2415	0	2421	26	0
2	A	48	0	26	1	0
2	B	48	0	26	4	0
2	C	48	0	26	1	0
2	D	48	0	26	2	0
2	E	48	0	26	2	0
2	F	48	0	26	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	48	0	26	1	0
2	H	48	0	26	1	0
2	I	48	0	26	1	0
2	J	48	0	26	0	0
2	K	48	0	26	2	0
2	L	48	0	26	3	0
2	M	48	0	26	1	0
2	N	48	0	26	2	0
2	O	48	0	26	1	0
2	P	48	0	26	4	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
3	K	1	0	0	0	0
3	L	1	0	0	0	0
3	M	1	0	0	0	0
3	N	1	0	0	0	0
3	O	1	0	0	0	0
3	P	1	0	0	0	0
4	A	101	0	0	1	0
4	B	91	0	0	2	0
4	C	89	0	0	0	0
4	D	81	0	0	3	0
4	E	84	0	0	2	0
4	F	91	0	0	2	0
4	G	67	0	0	0	0
4	H	83	0	0	0	0
4	I	64	0	0	0	0
4	J	68	0	0	1	0
4	K	51	0	0	2	0
4	L	53	0	0	0	0
4	M	44	0	0	0	0
4	N	54	0	0	0	0
4	O	44	0	0	1	0
4	P	42	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	40799	0	39652	207	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 3.

The worst 5 of 207 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:D:32:ARG:NH2	4:D:566:HOH:O	2.27	0.68
1:F:23:ARG:NH1	1:F:69:GLU:OE1	2.28	0.67
1:O:151:THR:OG1	2:O:401:NDP:H41N	1.95	0.67
1:L:68:GLU:OE2	1:L:79:ARG:NH2	2.29	0.66
1:P:151:THR:OG1	2:P:401:NDP:H41N	1.97	0.65

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	332/370 (90%)	327 (98%)	5 (2%)	0	100	100
1	B	332/370 (90%)	328 (99%)	3 (1%)	1 (0%)	43	50
1	C	332/370 (90%)	327 (98%)	4 (1%)	1 (0%)	43	50
1	D	332/370 (90%)	324 (98%)	8 (2%)	0	100	100
1	E	332/370 (90%)	325 (98%)	7 (2%)	0	100	100
1	F	332/370 (90%)	325 (98%)	5 (2%)	2 (1%)	27	30
1	G	332/370 (90%)	327 (98%)	5 (2%)	0	100	100
1	H	332/370 (90%)	323 (97%)	9 (3%)	0	100	100
1	I	332/370 (90%)	324 (98%)	7 (2%)	1 (0%)	43	50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	J	331/370 (90%)	324 (98%)	7 (2%)	0	100	100
1	K	332/370 (90%)	323 (97%)	9 (3%)	0	100	100
1	L	332/370 (90%)	320 (96%)	10 (3%)	2 (1%)	27	30
1	M	332/370 (90%)	319 (96%)	13 (4%)	0	100	100
1	N	332/370 (90%)	323 (97%)	9 (3%)	0	100	100
1	O	332/370 (90%)	315 (95%)	15 (4%)	2 (1%)	27	30
1	P	331/370 (90%)	321 (97%)	9 (3%)	1 (0%)	43	50
All	All	5310/5920 (90%)	5175 (98%)	125 (2%)	10 (0%)	49	59

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	111	GLY
1	I	111	GLY
1	B	111	GLY
1	C	77	VAL
1	L	111	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	244/274 (89%)	241 (99%)	3 (1%)	74	84
1	B	242/274 (88%)	237 (98%)	5 (2%)	56	67
1	C	246/274 (90%)	243 (99%)	3 (1%)	74	84
1	D	240/274 (88%)	236 (98%)	4 (2%)	63	75
1	E	244/274 (89%)	243 (100%)	1 (0%)	92	96
1	F	245/274 (89%)	242 (99%)	3 (1%)	74	84
1	G	243/274 (89%)	238 (98%)	5 (2%)	56	67
1	H	241/274 (88%)	239 (99%)	2 (1%)	83	90
1	I	241/274 (88%)	238 (99%)	3 (1%)	74	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	241/274 (88%)	236 (98%)	5 (2%)	56	67
1	K	239/274 (87%)	235 (98%)	4 (2%)	63	75
1	L	242/274 (88%)	236 (98%)	6 (2%)	50	60
1	M	241/274 (88%)	240 (100%)	1 (0%)	92	96
1	N	241/274 (88%)	235 (98%)	6 (2%)	50	60
1	O	237/274 (86%)	232 (98%)	5 (2%)	56	67
1	P	238/274 (87%)	231 (97%)	7 (3%)	45	55
All	All	3865/4384 (88%)	3802 (98%)	63 (2%)	65	77

5 of 63 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	203	SER
1	K	16	LEU
1	P	75	THR
1	J	53	SER
1	J	95	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 47 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	272	GLN
1	K	96	GLN
1	O	131	ASN
1	J	96	GLN
1	K	131	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 32 ligands modelled in this entry, 16 are monoatomic - leaving 16 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NDP	A	401	-	45,52,52	1.60	4 (8%)	54,80,80	1.26	4 (7%)
2	NDP	B	401	-	45,52,52	1.60	4 (8%)	54,80,80	1.17	3 (5%)
2	NDP	C	401	-	45,52,52	1.51	5 (11%)	54,80,80	1.46	7 (12%)
2	NDP	D	401	-	45,52,52	1.69	5 (11%)	54,80,80	1.37	4 (7%)
2	NDP	E	401	-	45,52,52	1.69	6 (13%)	54,80,80	1.26	2 (3%)
2	NDP	F	401	-	45,52,52	1.63	5 (11%)	54,80,80	1.26	3 (5%)
2	NDP	G	401	-	45,52,52	1.68	4 (8%)	54,80,80	1.32	4 (7%)
2	NDP	H	401	-	45,52,52	1.69	6 (13%)	54,80,80	1.47	4 (7%)
2	NDP	I	401	-	45,52,52	1.68	4 (8%)	54,80,80	1.36	6 (11%)
2	NDP	J	401	-	45,52,52	1.67	4 (8%)	54,80,80	1.17	2 (3%)
2	NDP	K	401	-	45,52,52	1.65	5 (11%)	54,80,80	1.28	4 (7%)
2	NDP	L	401	-	45,52,52	1.61	4 (8%)	54,80,80	1.28	3 (5%)
2	NDP	M	401	-	45,52,52	1.72	4 (8%)	54,80,80	1.40	5 (9%)
2	NDP	N	401	-	45,52,52	1.64	5 (11%)	54,80,80	1.42	5 (9%)
2	NDP	O	401	-	45,52,52	1.71	6 (13%)	54,80,80	1.37	3 (5%)
2	NDP	P	401	-	45,52,52	1.69	5 (11%)	54,80,80	1.26	5 (9%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NDP	A	401	-	-	5/30/77/77	0/5/5/5
2	NDP	B	401	-	-	4/30/77/77	0/5/5/5
2	NDP	C	401	-	-	5/30/77/77	0/5/5/5
2	NDP	D	401	-	-	4/30/77/77	0/5/5/5
2	NDP	E	401	-	-	5/30/77/77	0/5/5/5
2	NDP	F	401	-	-	5/30/77/77	0/5/5/5
2	NDP	G	401	-	-	5/30/77/77	0/5/5/5
2	NDP	H	401	-	-	5/30/77/77	0/5/5/5
2	NDP	I	401	-	-	4/30/77/77	0/5/5/5
2	NDP	J	401	-	-	5/30/77/77	0/5/5/5
2	NDP	K	401	-	-	4/30/77/77	0/5/5/5
2	NDP	L	401	-	-	3/30/77/77	0/5/5/5
2	NDP	M	401	-	-	3/30/77/77	0/5/5/5
2	NDP	N	401	-	-	5/30/77/77	0/5/5/5
2	NDP	O	401	-	-	4/30/77/77	0/5/5/5
2	NDP	P	401	-	-	4/30/77/77	0/5/5/5

The worst 5 of 76 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	401	NDP	O7N-C7N	8.12	1.44	1.24
2	H	401	NDP	O7N-C7N	7.83	1.43	1.24
2	O	401	NDP	O7N-C7N	7.51	1.42	1.24
2	K	401	NDP	O7N-C7N	7.38	1.42	1.24
2	G	401	NDP	O7N-C7N	7.38	1.42	1.24

The worst 5 of 64 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	401	NDP	N3A-C2A-N1A	-6.65	117.96	128.68
2	C	401	NDP	N3A-C2A-N1A	-6.51	118.18	128.68
2	O	401	NDP	N3A-C2A-N1A	-6.36	118.43	128.68
2	D	401	NDP	N3A-C2A-N1A	-6.33	118.47	128.68
2	E	401	NDP	N3A-C2A-N1A	-6.11	118.83	128.68

There are no chirality outliers.

5 of 70 torsion outliers are listed below:

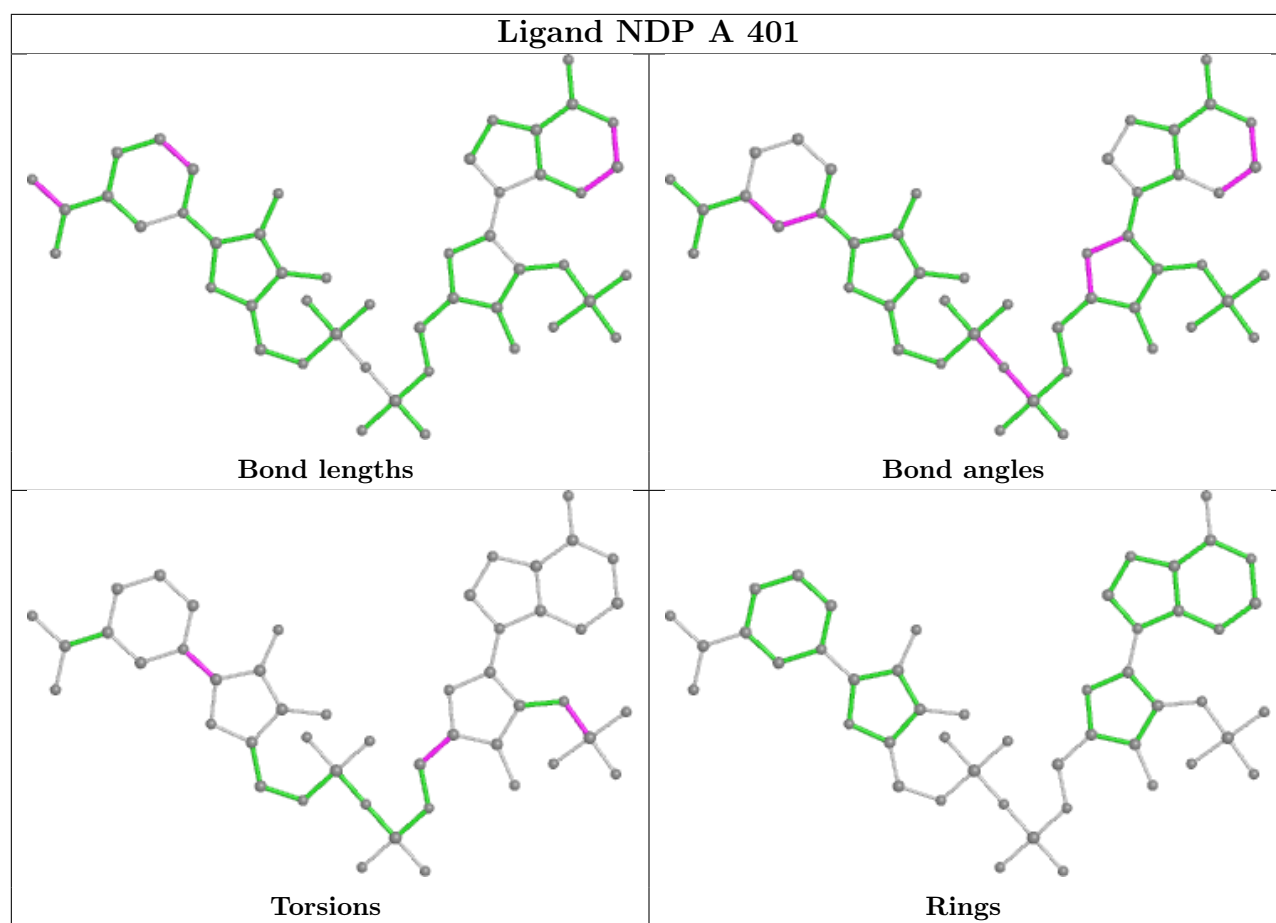
Mol	Chain	Res	Type	Atoms
2	I	401	NDP	C2D-C1D-N1N-C2N
2	L	401	NDP	O4D-C1D-N1N-C2N
2	I	401	NDP	O4D-C1D-N1N-C2N
2	O	401	NDP	C3B-C4B-C5B-O5B
2	H	401	NDP	O4D-C1D-N1N-C2N

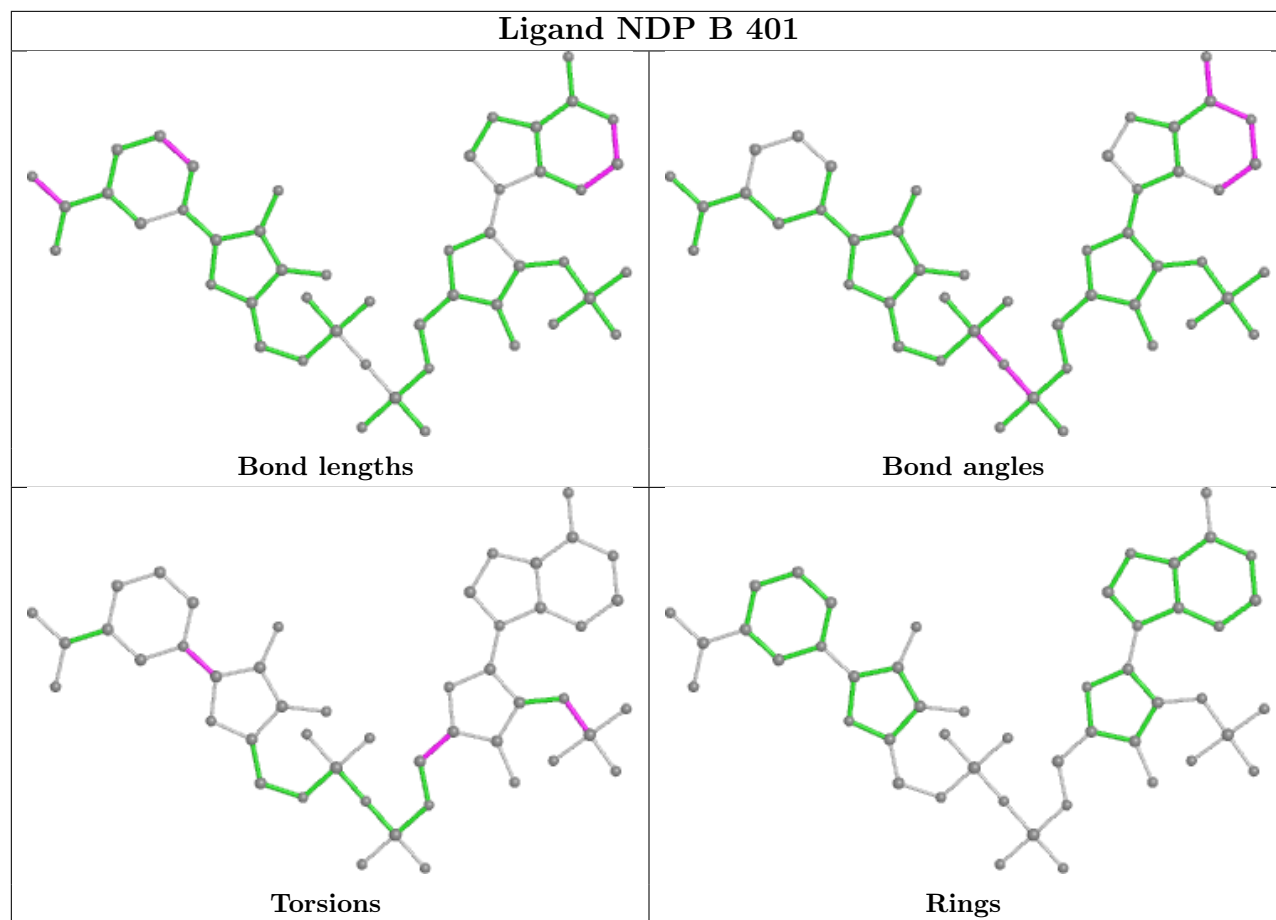
There are no ring outliers.

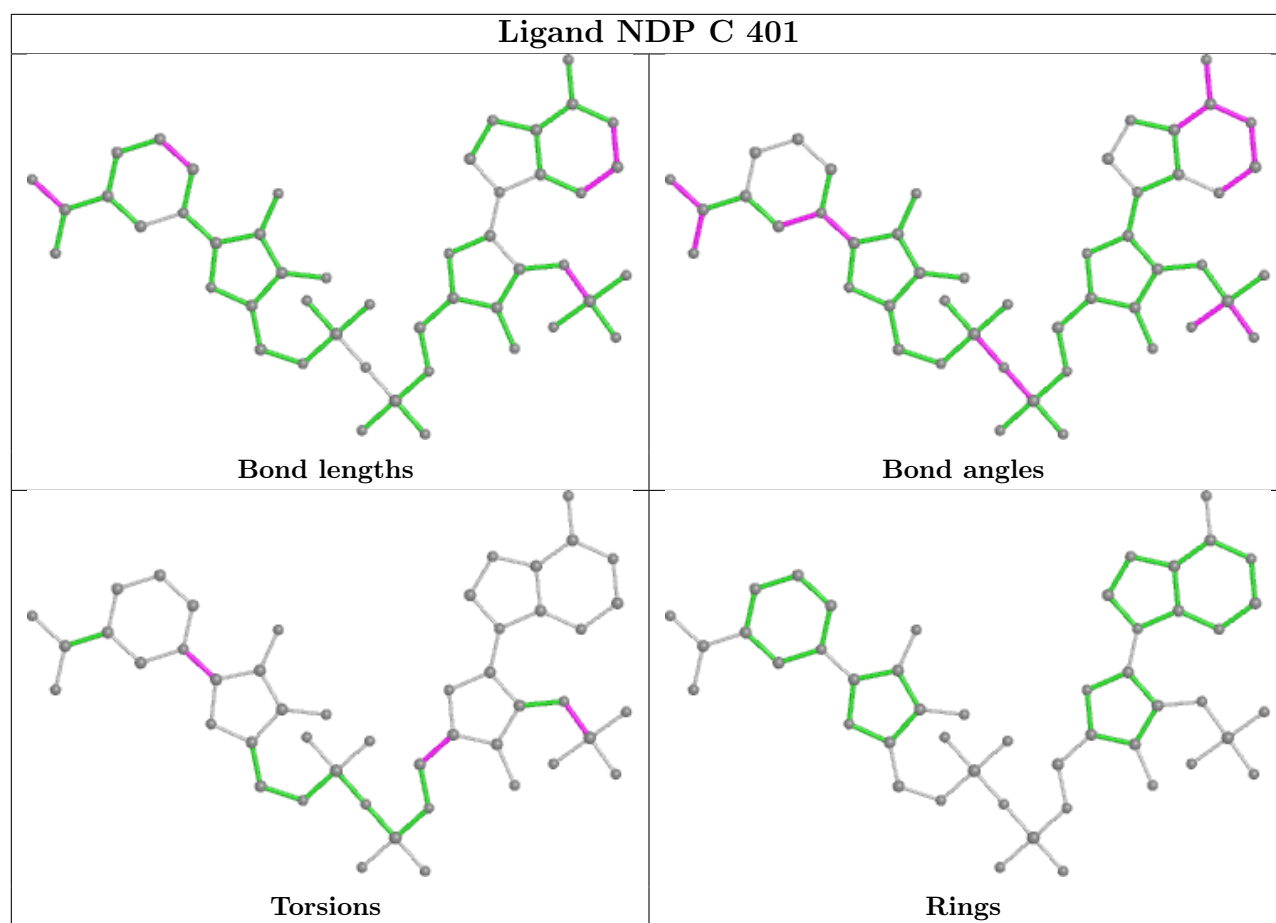
15 monomers are involved in 27 short contacts:

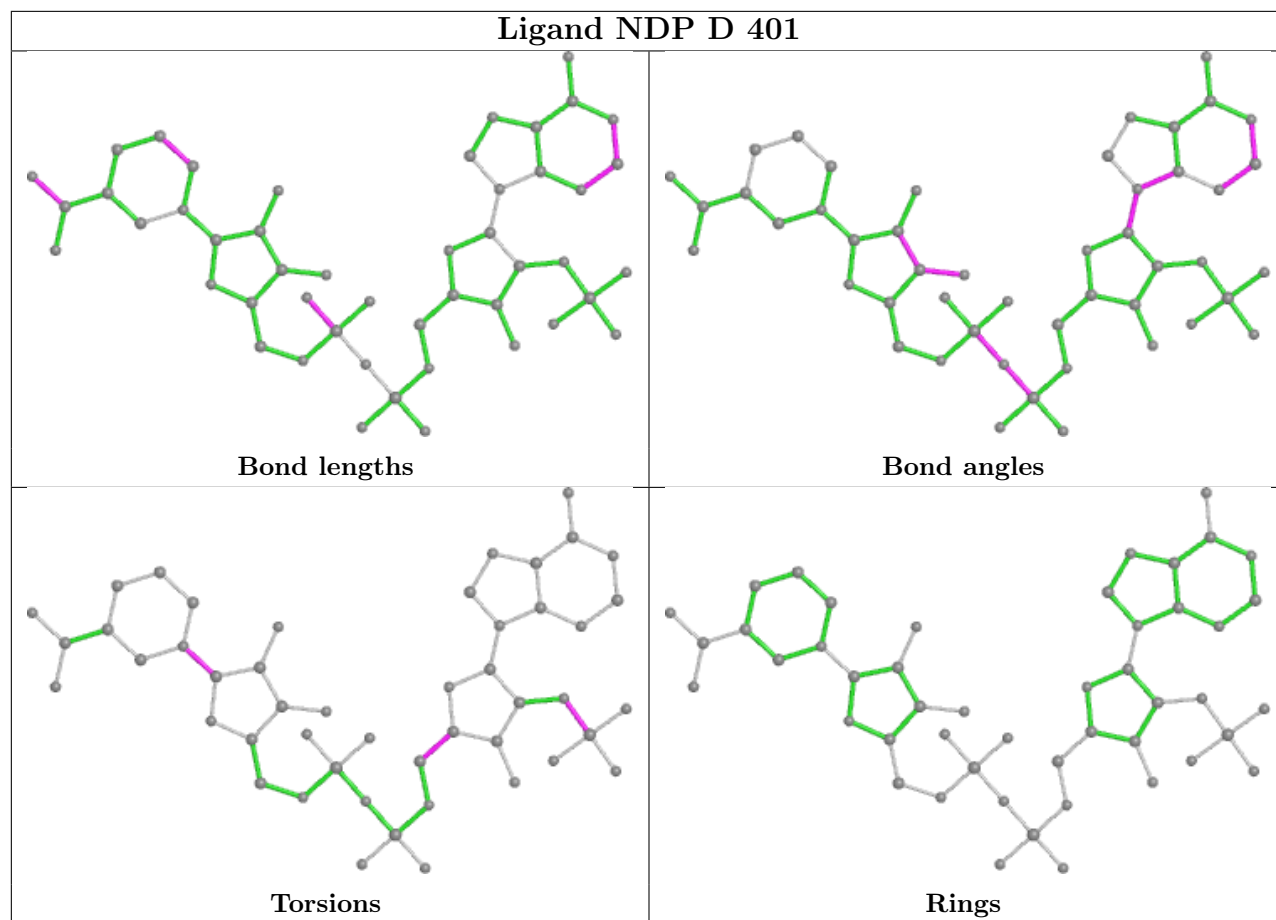
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	NDP	1	0
2	B	401	NDP	4	0
2	C	401	NDP	1	0
2	D	401	NDP	2	0
2	E	401	NDP	2	0
2	F	401	NDP	1	0
2	G	401	NDP	1	0
2	H	401	NDP	1	0
2	I	401	NDP	1	0
2	K	401	NDP	2	0
2	L	401	NDP	3	0
2	M	401	NDP	1	0
2	N	401	NDP	2	0
2	O	401	NDP	1	0
2	P	401	NDP	4	0

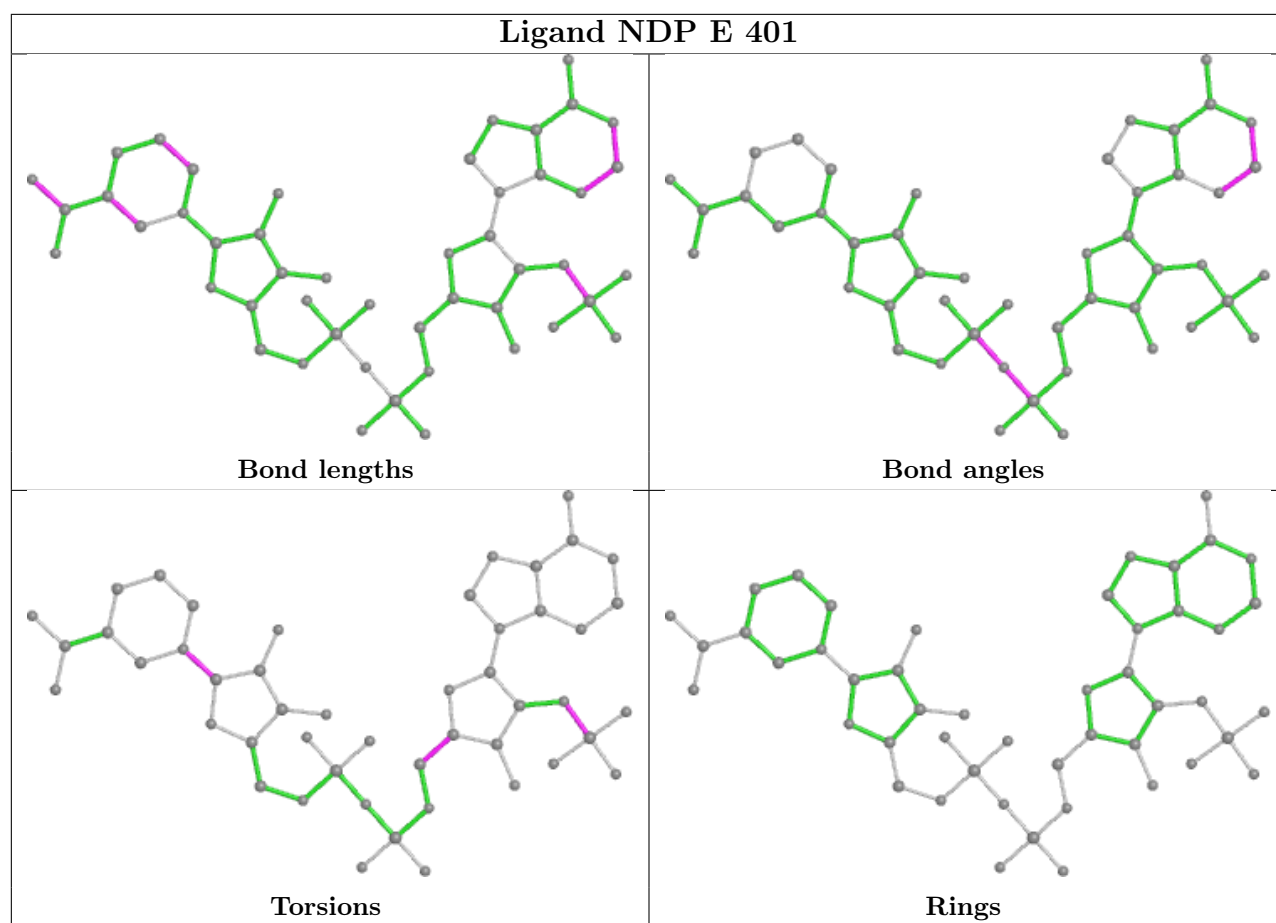
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

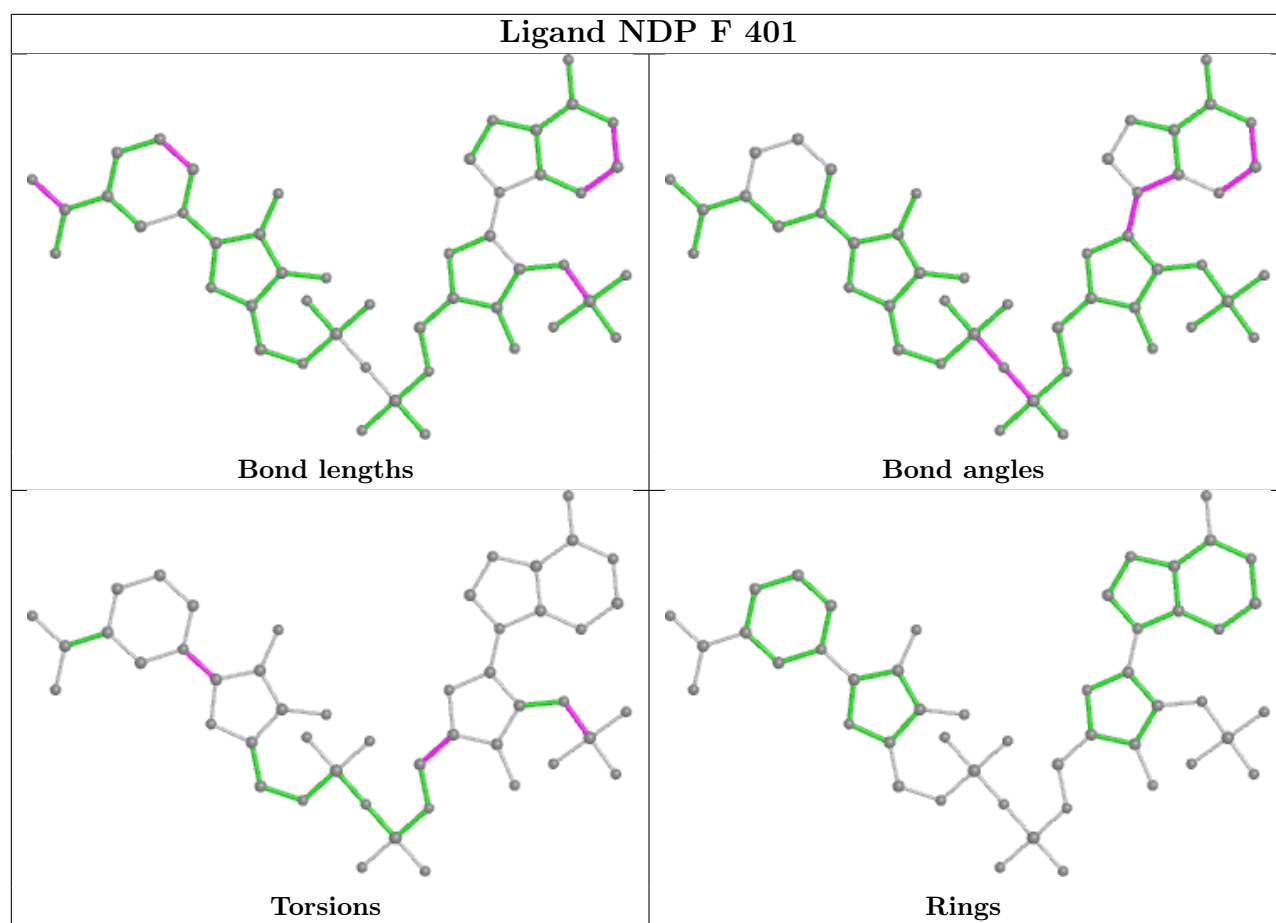


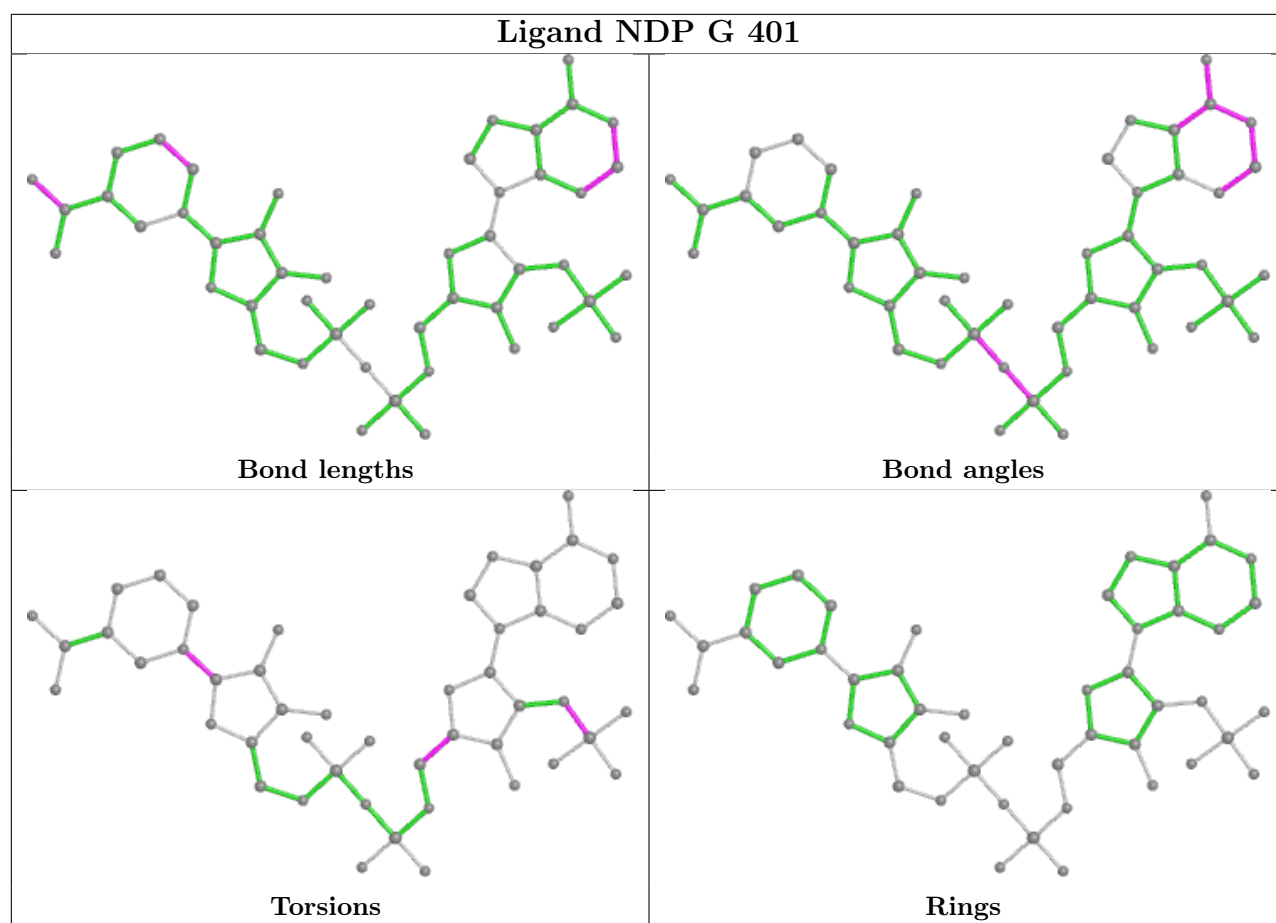


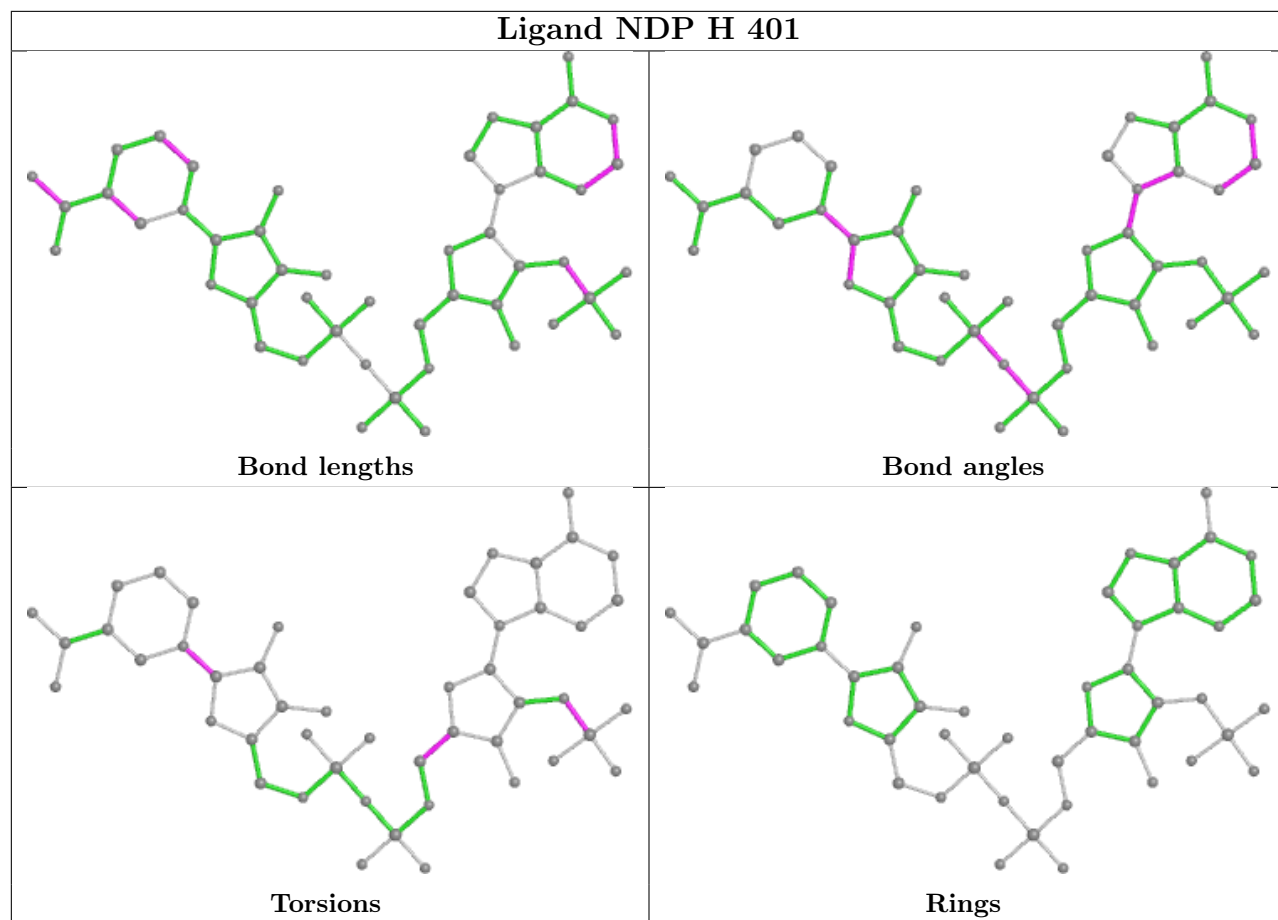


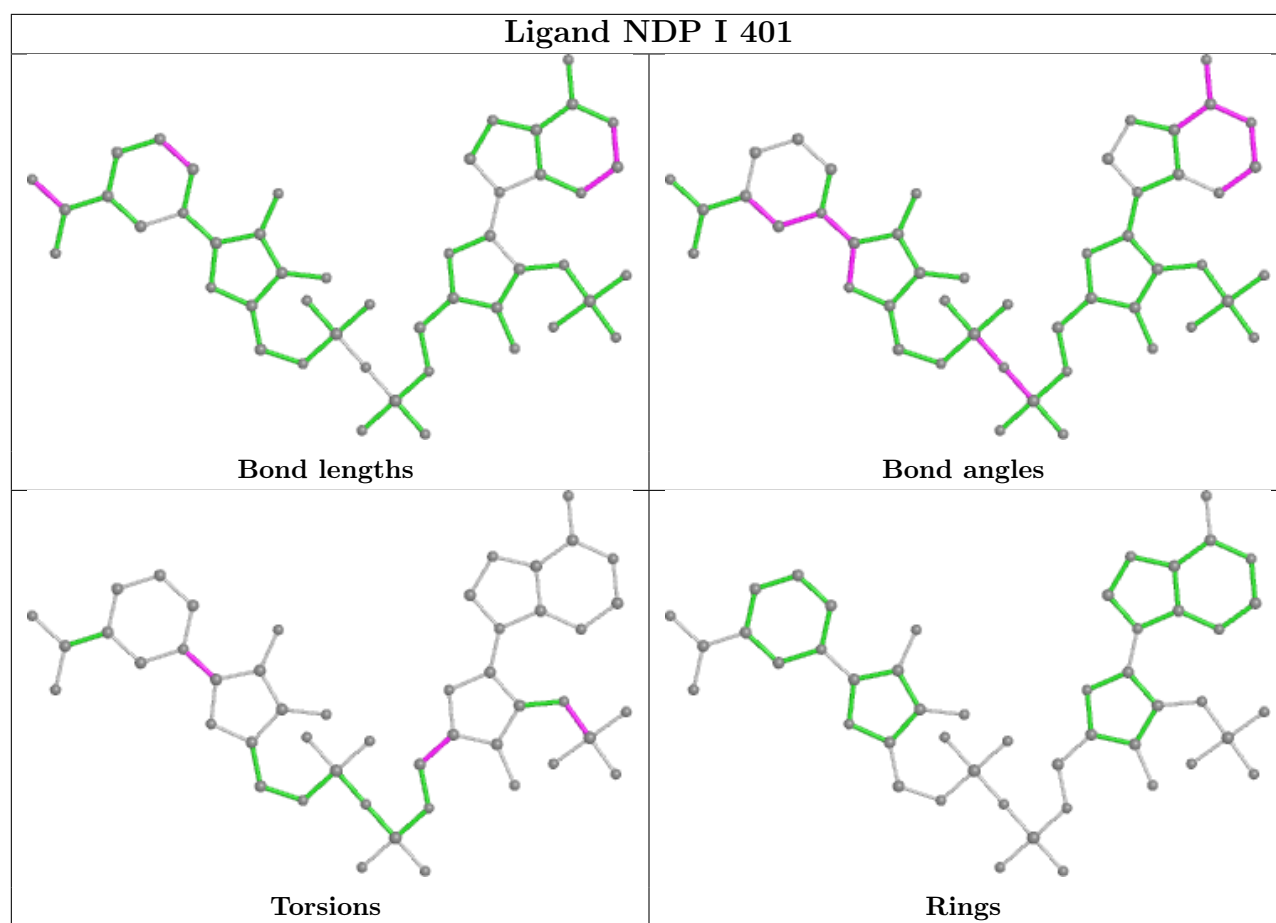


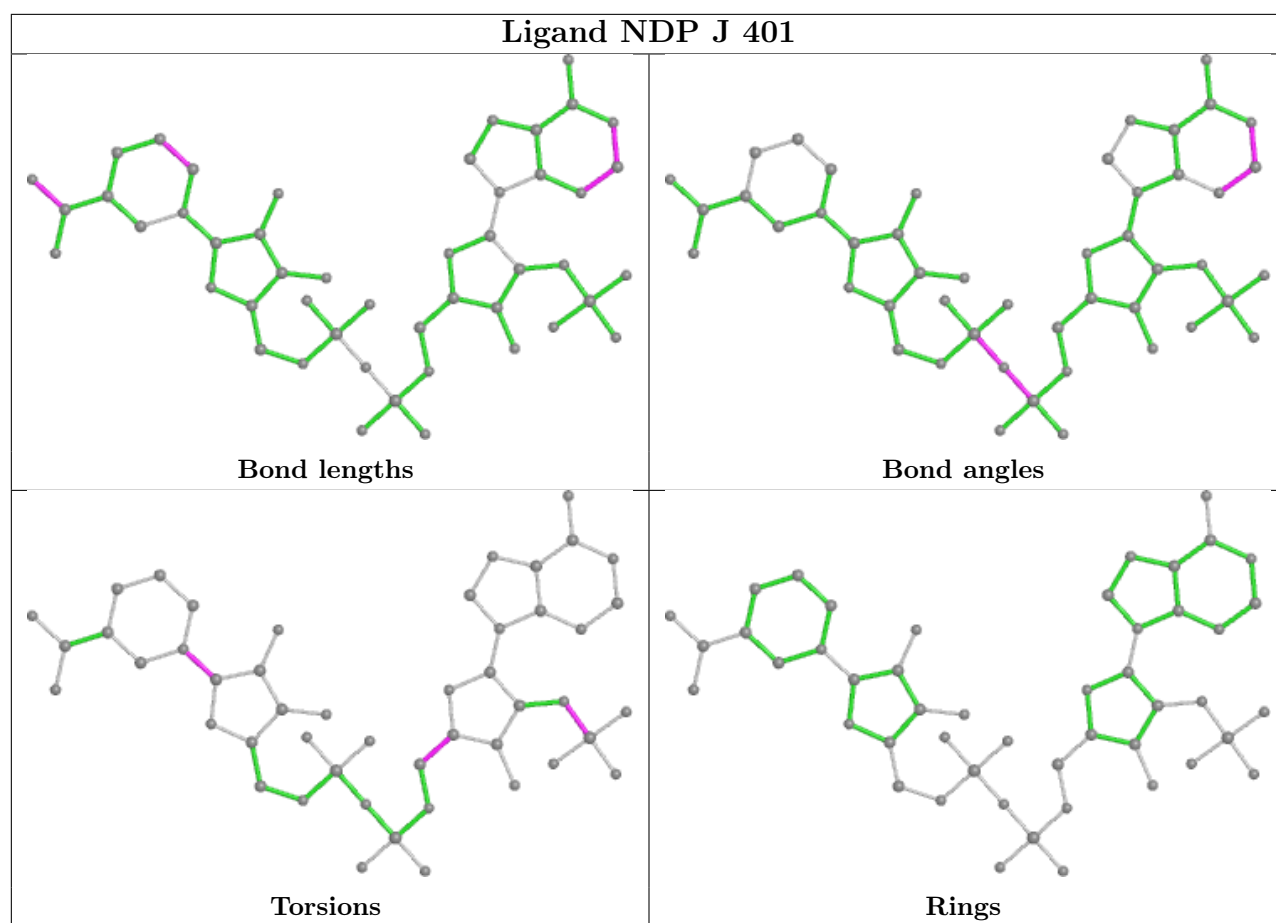


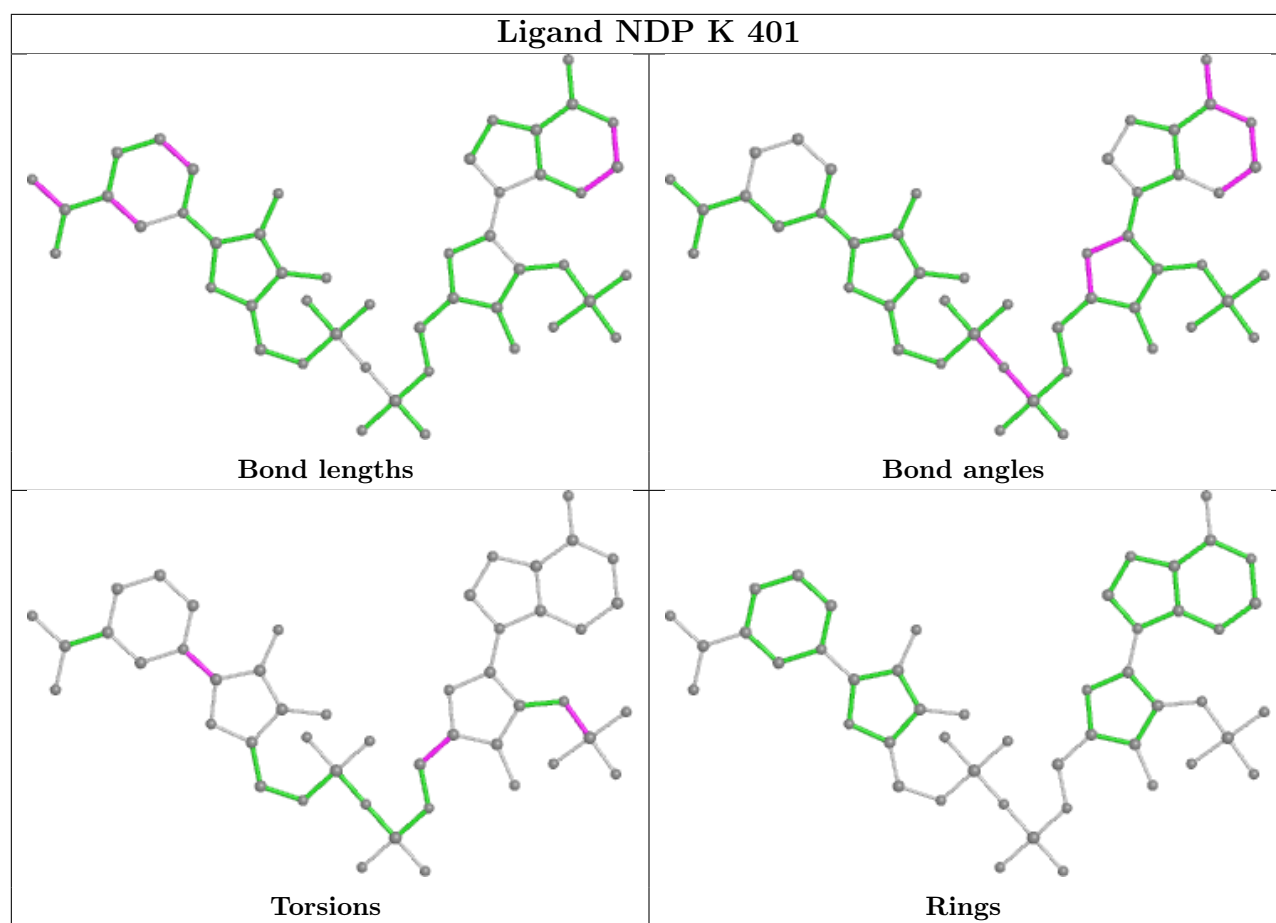


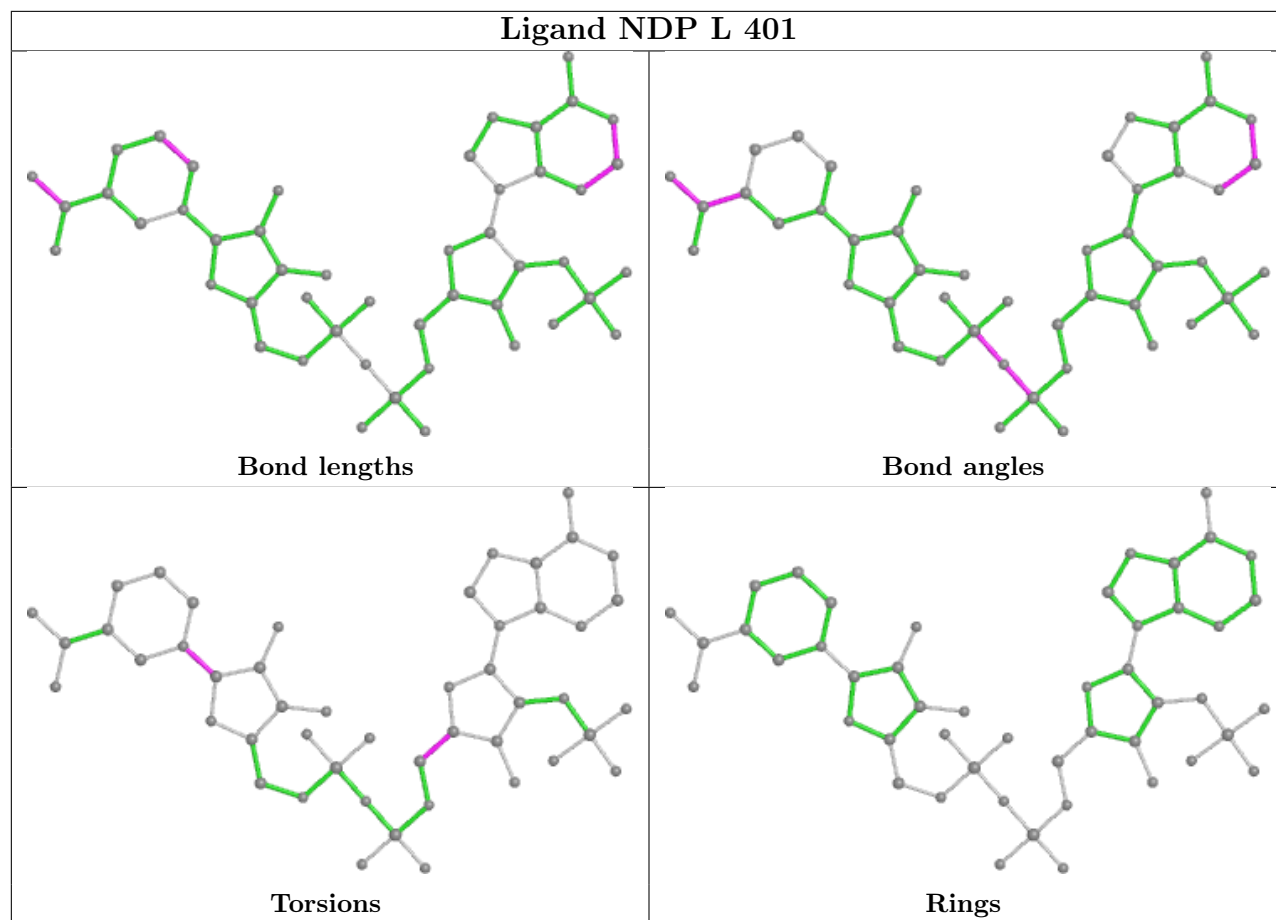


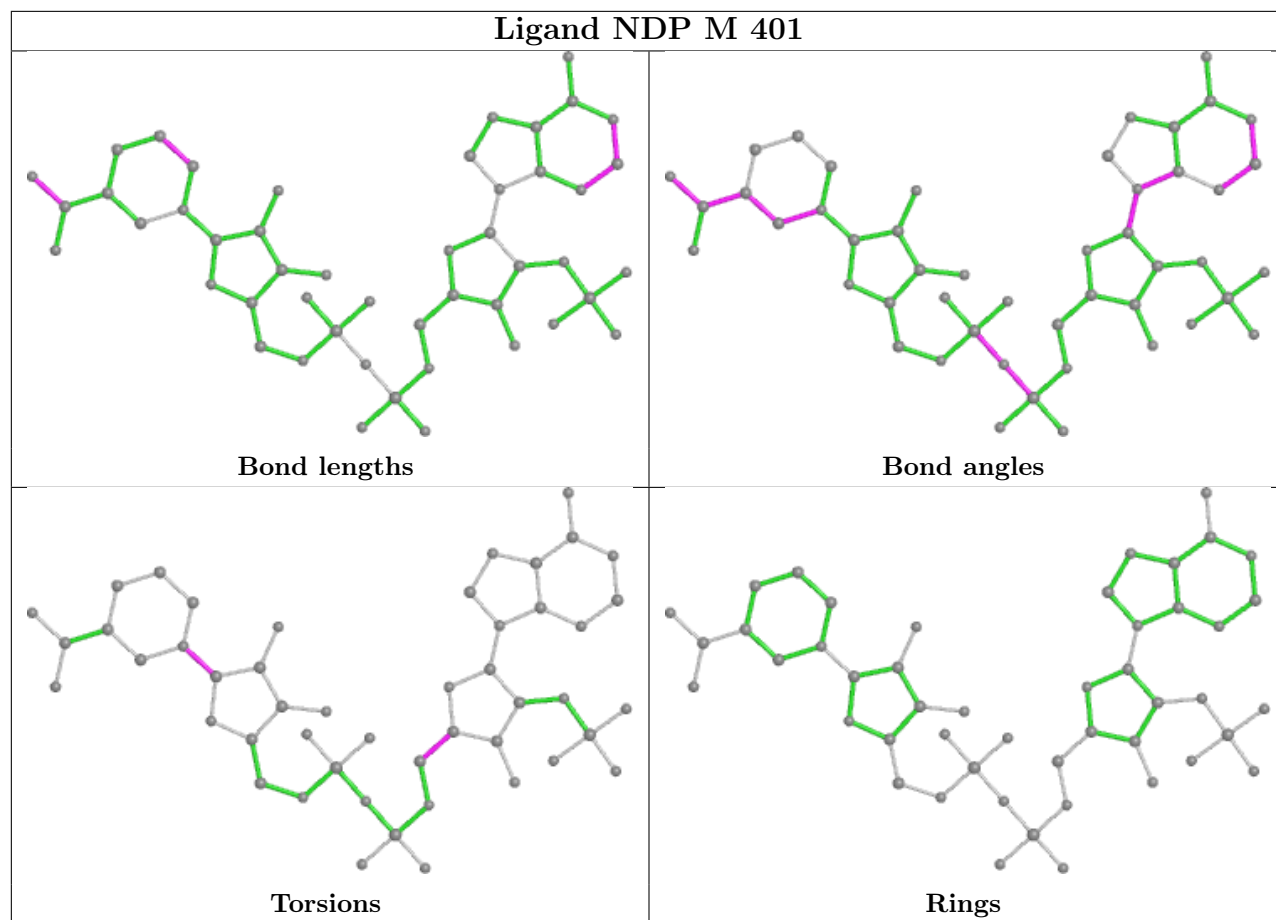


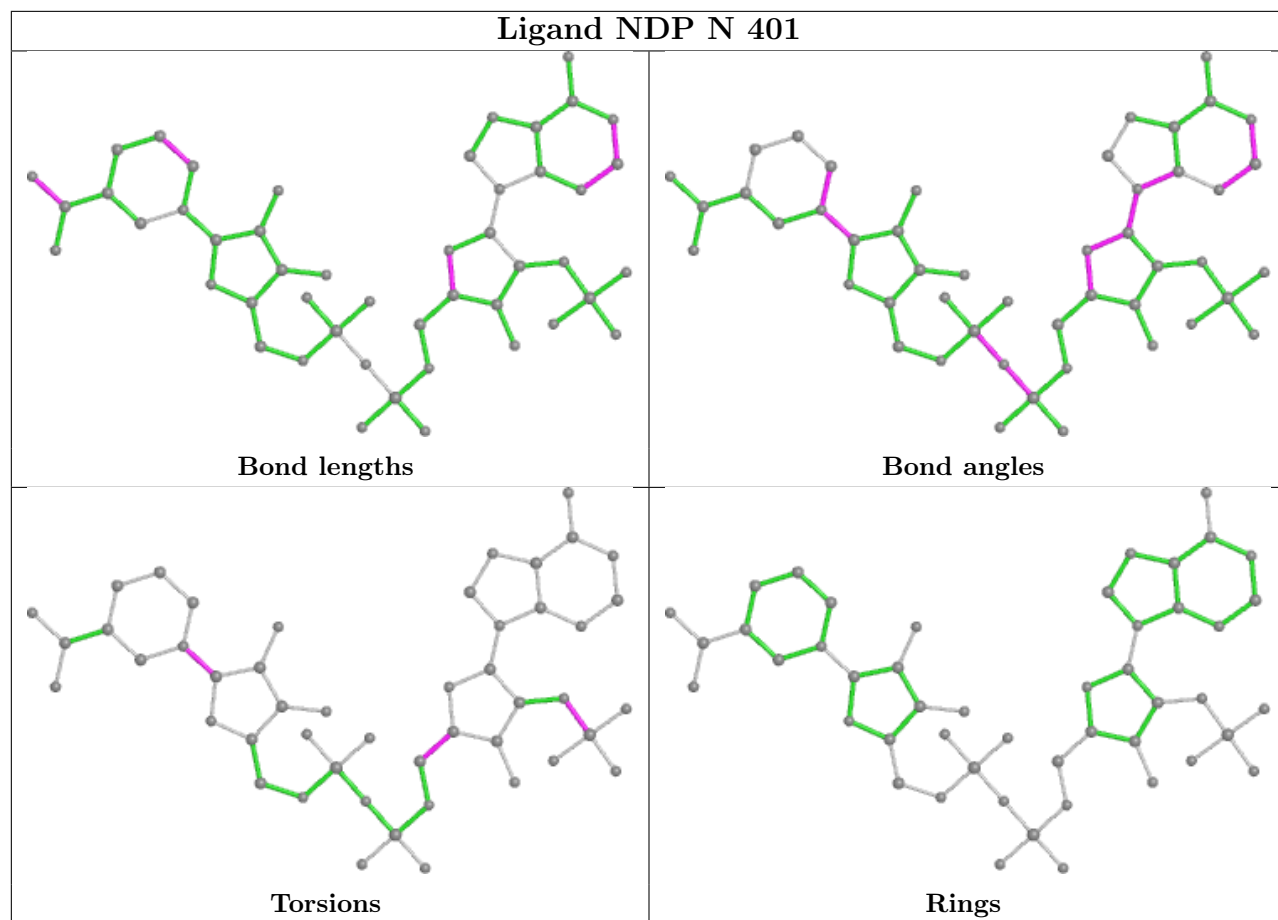


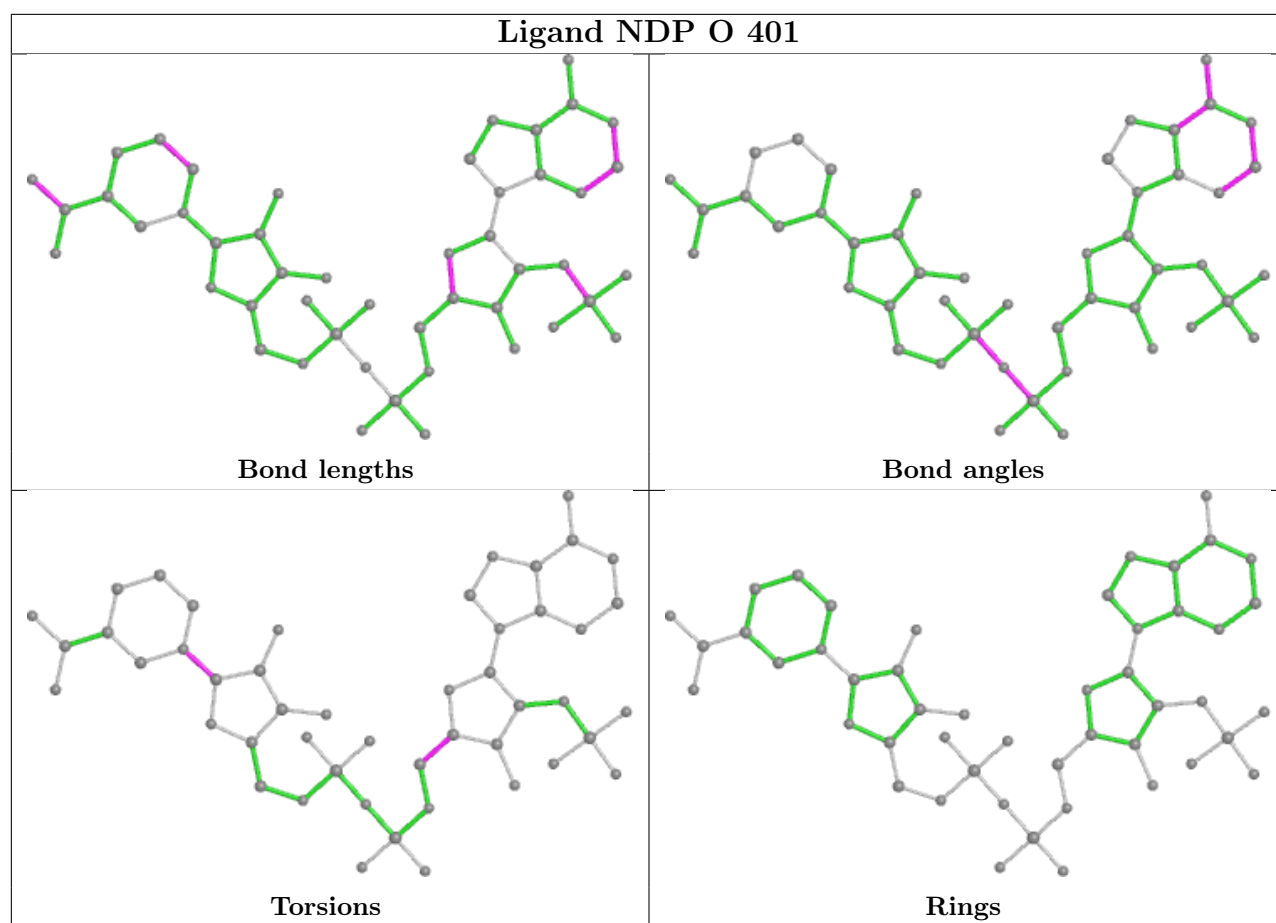


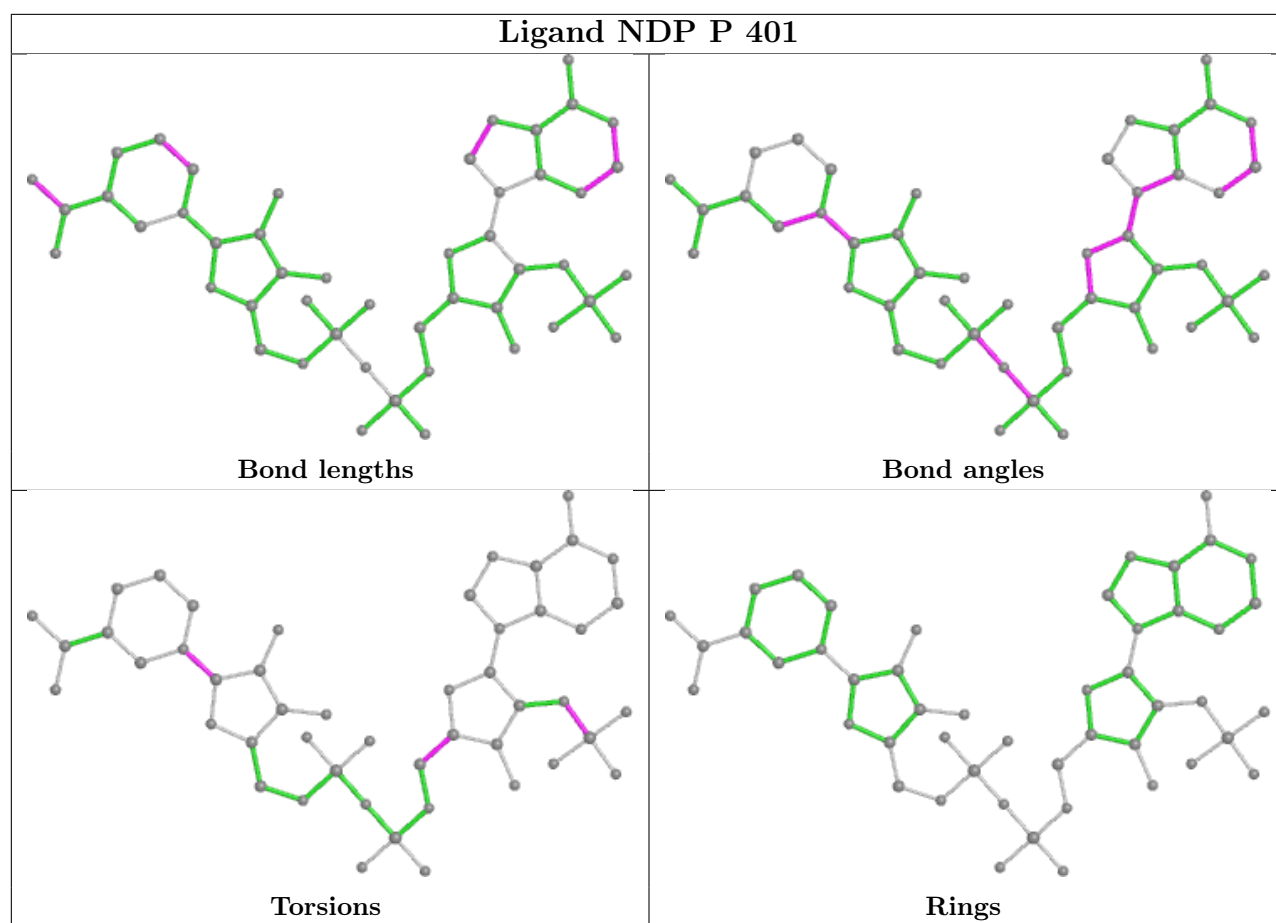












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	333/370 (90%)	-0.23	1 (0%) 93 97	25, 35, 57, 68	0
1	B	333/370 (90%)	-0.24	1 (0%) 93 97	27, 37, 56, 71	0
1	C	333/370 (90%)	-0.28	0 100 100	27, 36, 53, 66	0
1	D	333/370 (90%)	-0.22	1 (0%) 93 97	27, 37, 58, 70	0
1	E	333/370 (90%)	-0.19	1 (0%) 93 97	27, 38, 57, 73	0
1	F	333/370 (90%)	-0.13	1 (0%) 93 97	25, 36, 55, 72	0
1	G	333/370 (90%)	-0.01	4 (1%) 79 86	30, 40, 57, 71	0
1	H	333/370 (90%)	-0.25	0 100 100	27, 38, 55, 71	0
1	I	333/370 (90%)	-0.16	0 100 100	28, 39, 57, 69	0
1	J	333/370 (90%)	-0.19	3 (0%) 84 90	31, 41, 57, 68	0
1	K	333/370 (90%)	-0.12	3 (0%) 84 90	28, 44, 64, 71	0
1	L	333/370 (90%)	0.14	16 (4%) 30 44	29, 45, 68, 76	0
1	M	333/370 (90%)	0.10	7 (2%) 63 75	34, 48, 64, 71	0
1	N	333/370 (90%)	-0.08	1 (0%) 93 97	31, 45, 63, 73	0
1	O	333/370 (90%)	0.11	11 (3%) 46 60	28, 51, 68, 75	0
1	P	333/370 (90%)	0.24	12 (3%) 42 56	30, 50, 68, 75	0
All	All	5328/5920 (90%)	-0.09	62 (1%) 79 86	25, 41, 63, 76	0

The worst 5 of 62 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	P	304	ASN	4.1
1	N	199	ALA	3.8
1	P	327	VAL	3.8
1	L	304	ASN	3.6
1	P	309	ALA	3.6

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

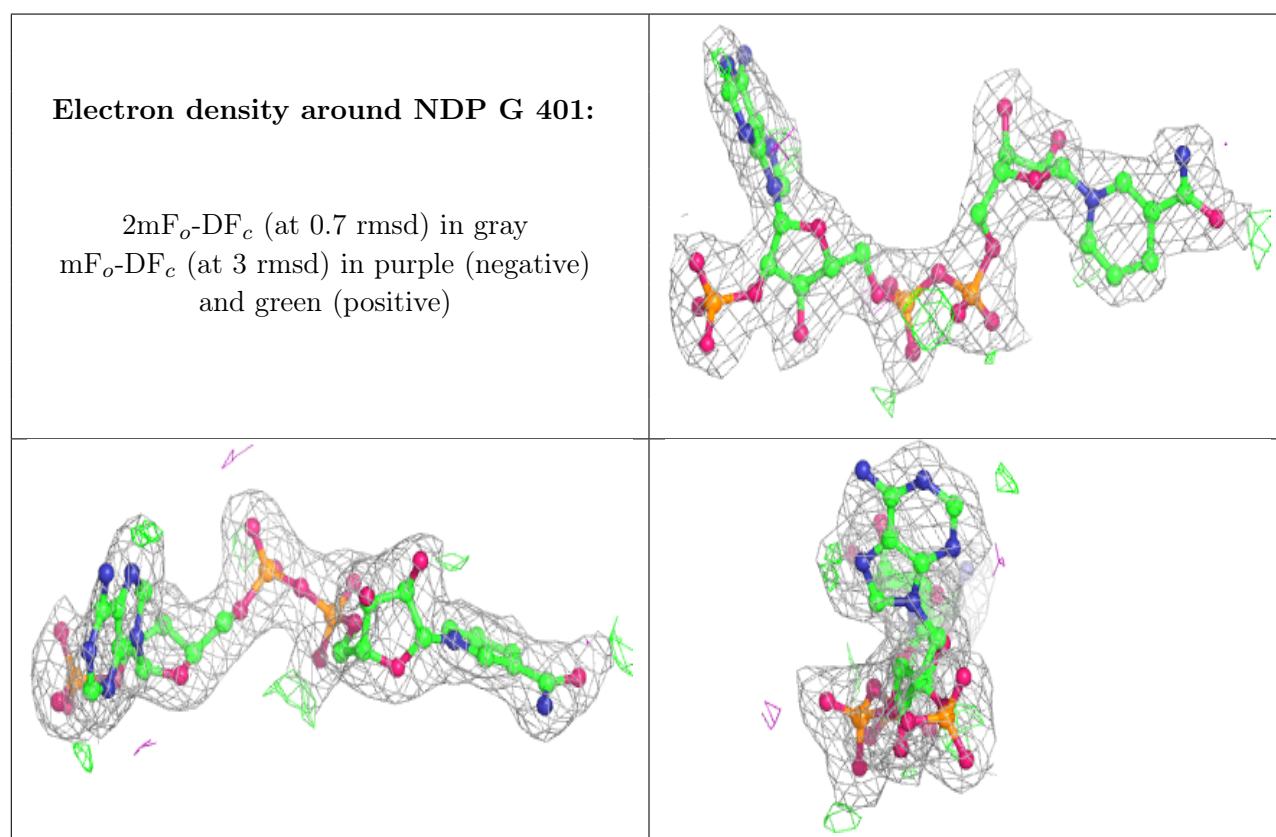
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NDP	G	401	48/48	0.95	0.13	26,38,53,64	0
2	NDP	O	401	48/48	0.96	0.12	35,48,61,64	0
2	NDP	J	401	48/48	0.96	0.11	30,41,51,63	0
2	NDP	M	401	48/48	0.96	0.11	32,47,59,64	0
2	NDP	L	401	48/48	0.97	0.12	28,43,60,68	0
2	NDP	K	401	48/48	0.97	0.12	29,38,53,62	0
2	NDP	I	401	48/48	0.97	0.12	25,36,47,56	0
2	NDP	P	401	48/48	0.97	0.12	35,43,54,60	0
2	NDP	B	401	48/48	0.97	0.11	23,35,50,58	0
2	NDP	E	401	48/48	0.98	0.11	25,35,55,61	0
2	NDP	D	401	48/48	0.98	0.10	23,35,49,58	0
2	NDP	F	401	48/48	0.98	0.11	23,31,36,40	0
2	NDP	C	401	48/48	0.98	0.11	21,30,40,49	0
2	NDP	N	401	48/48	0.98	0.11	21,39,56,62	0
2	NDP	H	401	48/48	0.98	0.12	24,34,50,58	0
2	NDP	A	401	48/48	0.98	0.11	24,32,49,52	0
3	ZN	J	402	1/1	0.99	0.11	33,33,33,33	0
3	ZN	P	402	1/1	0.99	0.08	45,45,45,45	0
3	ZN	L	402	1/1	1.00	0.11	39,39,39,39	0
3	ZN	A	402	1/1	1.00	0.12	30,30,30,30	0
3	ZN	E	402	1/1	1.00	0.12	29,29,29,29	0
3	ZN	D	402	1/1	1.00	0.12	31,31,31,31	0
3	ZN	N	402	1/1	1.00	0.08	46,46,46,46	0
3	ZN	B	402	1/1	1.00	0.11	30,30,30,30	0
3	ZN	F	402	1/1	1.00	0.12	34,34,34,34	0
3	ZN	K	402	1/1	1.00	0.12	36,36,36,36	0
3	ZN	M	402	1/1	1.00	0.07	50,50,50,50	0

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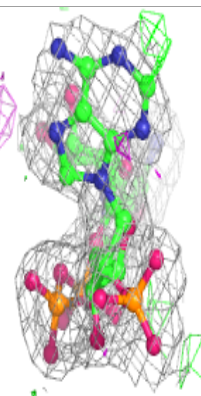
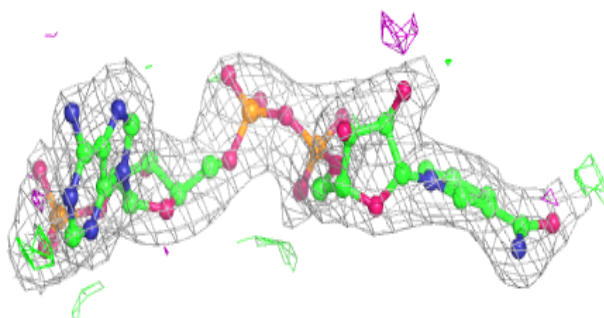
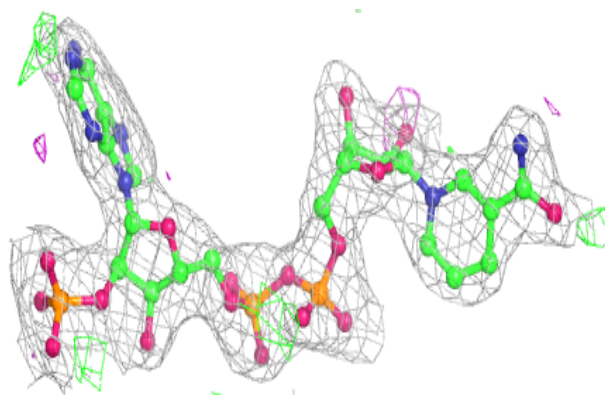
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	ZN	C	402	1/1	1.00	0.11	32,32,32,32	0
3	ZN	O	402	1/1	1.00	0.09	49,49,49,49	0
3	ZN	I	402	1/1	1.00	0.12	32,32,32,32	0
3	ZN	G	402	1/1	1.00	0.11	36,36,36,36	0
3	ZN	H	402	1/1	1.00	0.11	34,34,34,34	0

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.

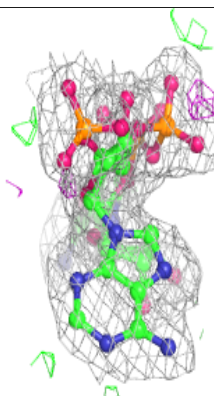
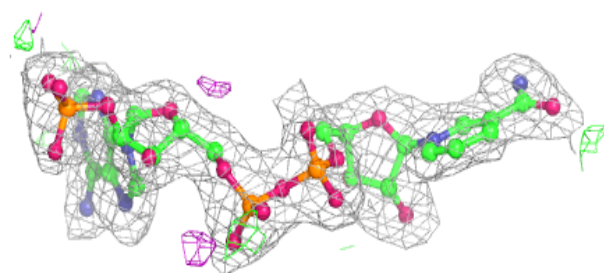
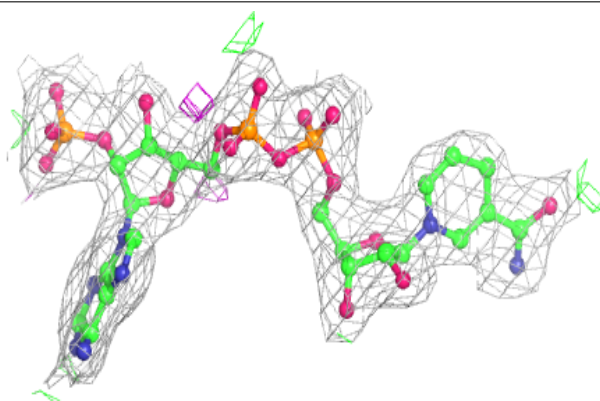


Electron density around NDP O 401:

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

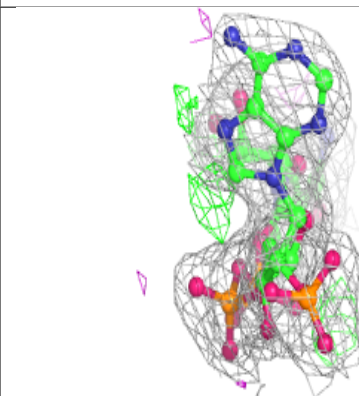
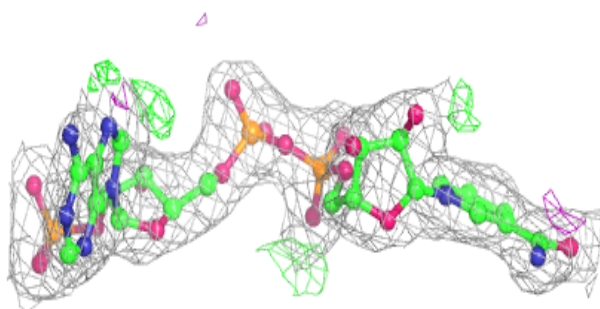
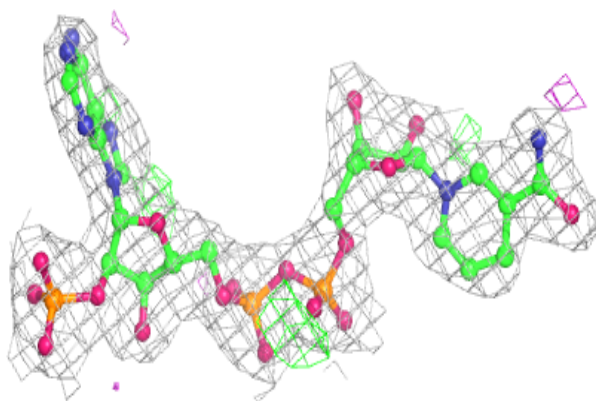
**Electron density around NDP J 401:**

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

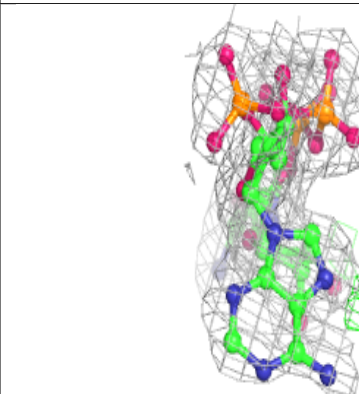
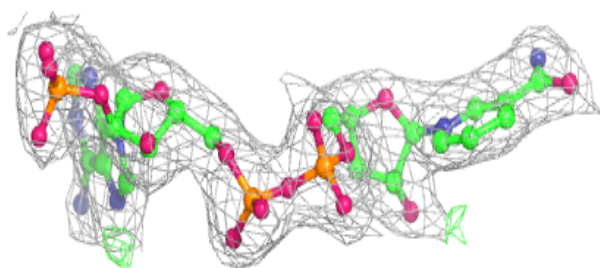
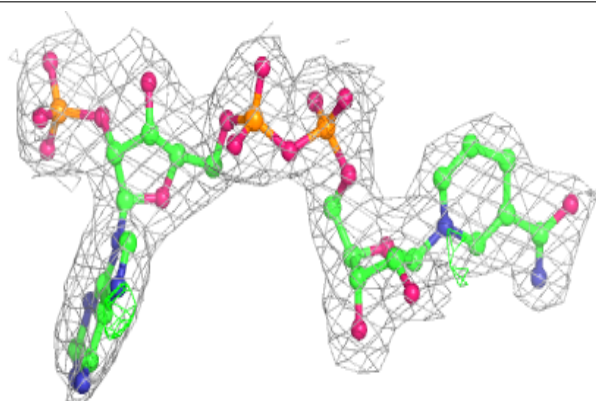


Electron density around NDP M 401:

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

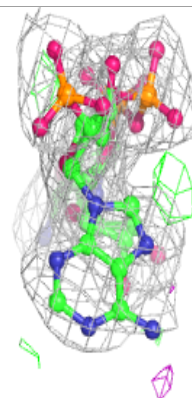
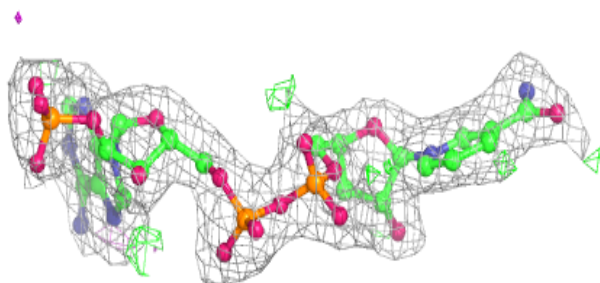
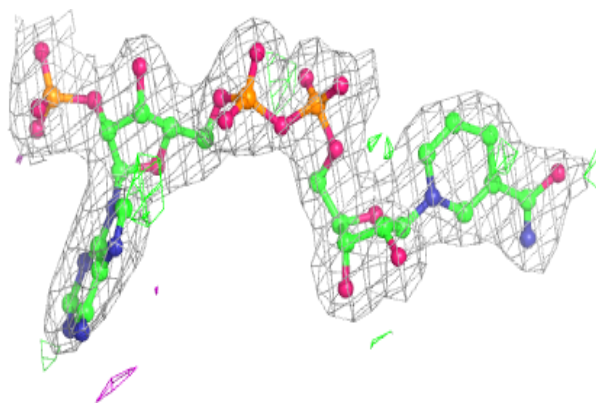
**Electron density around NDP L 401:**

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

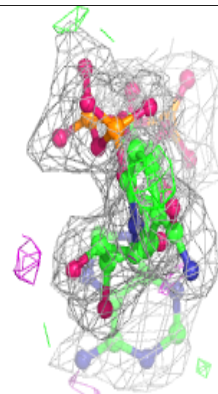
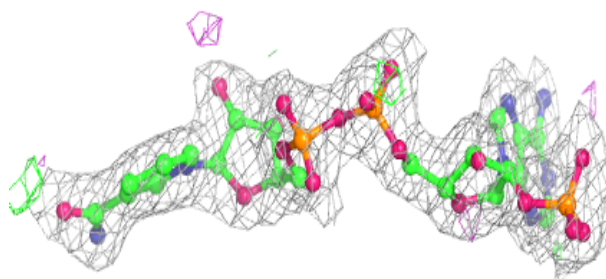
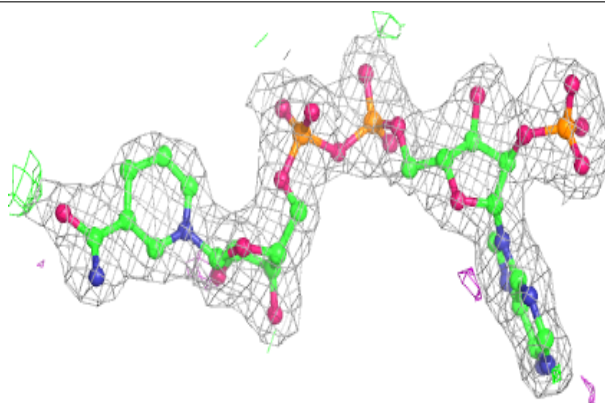


Electron density around NDP K 401:

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

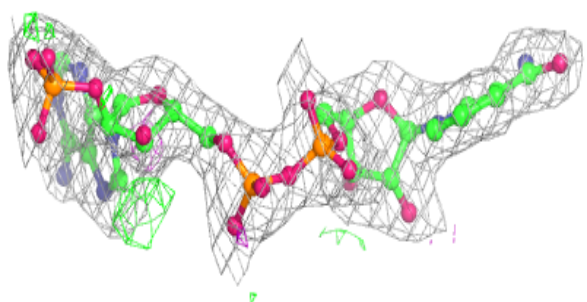
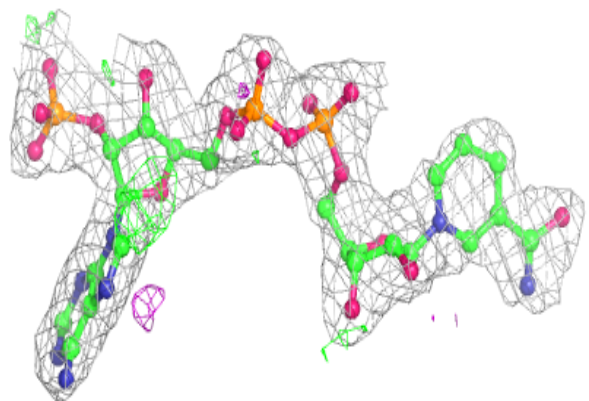
**Electron density around NDP I 401:**

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

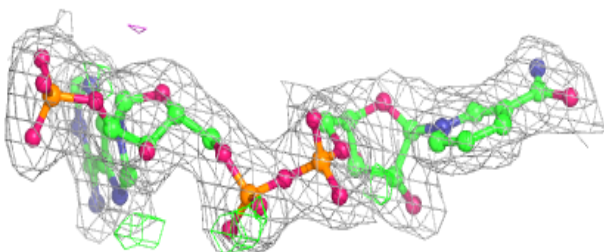
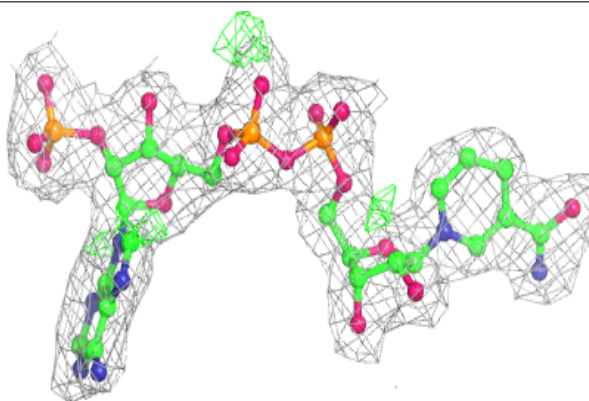


Electron density around NDP P 401:

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

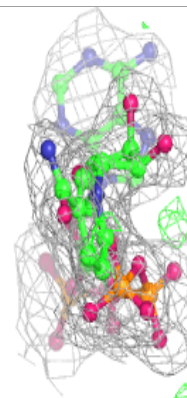
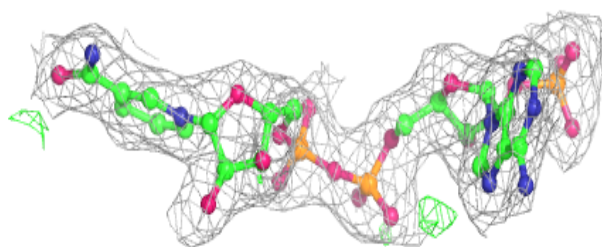
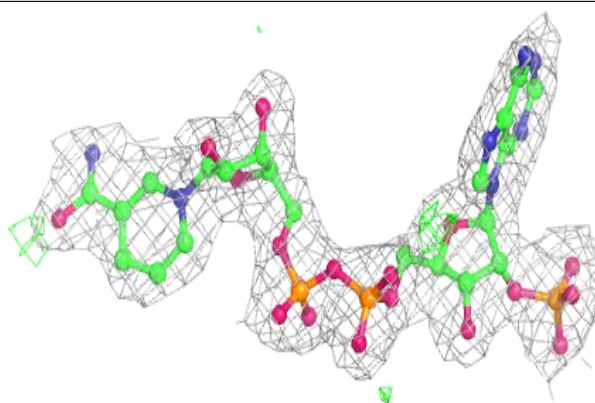
**Electron density around NDP B 401:**

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

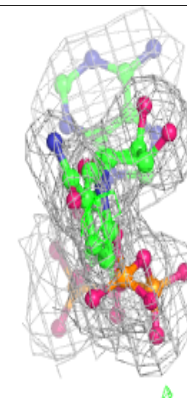
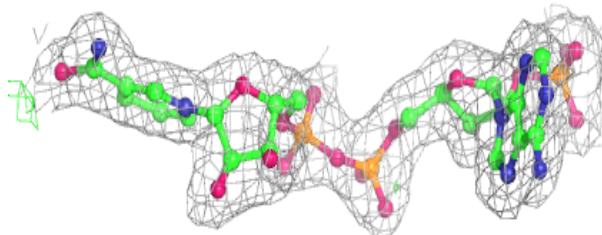
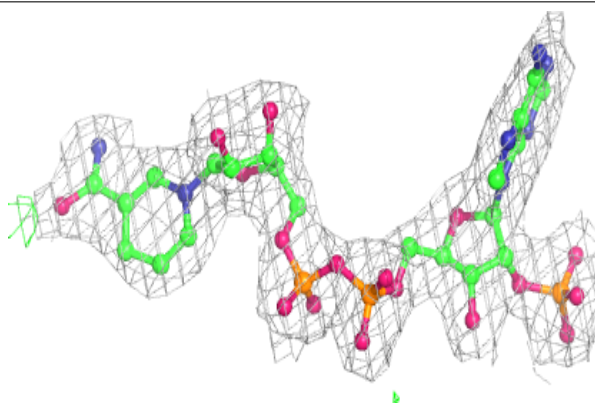


Electron density around NDP E 401:

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

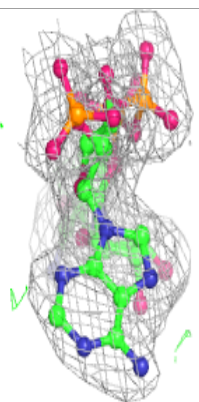
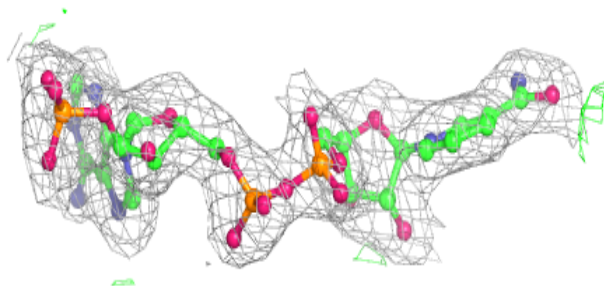
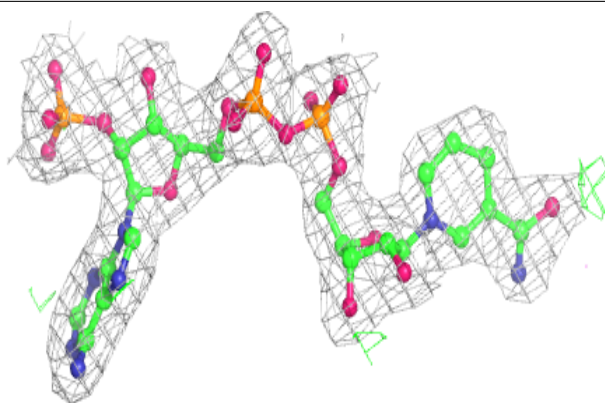
**Electron density around NDP D 401:**

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

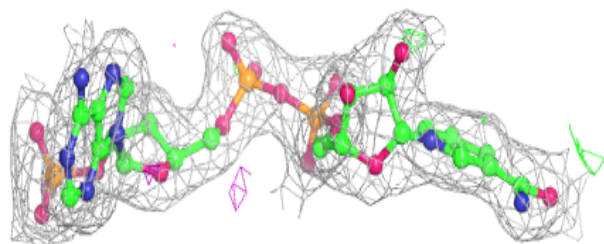
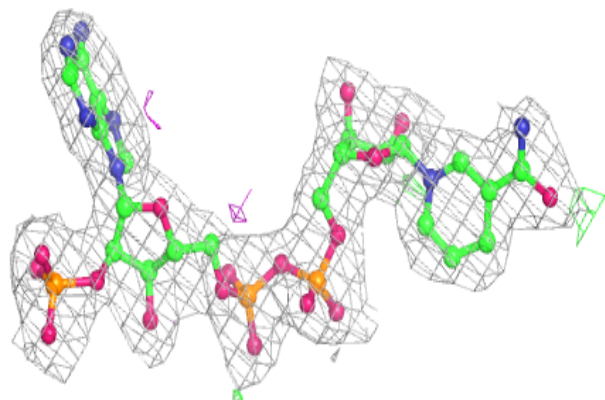


Electron density around NDP F 401:

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

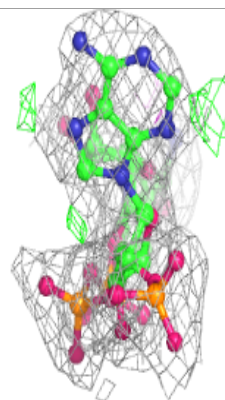
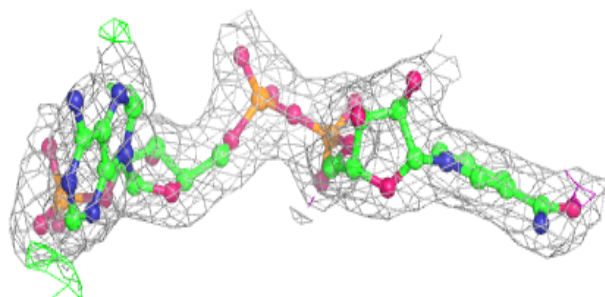
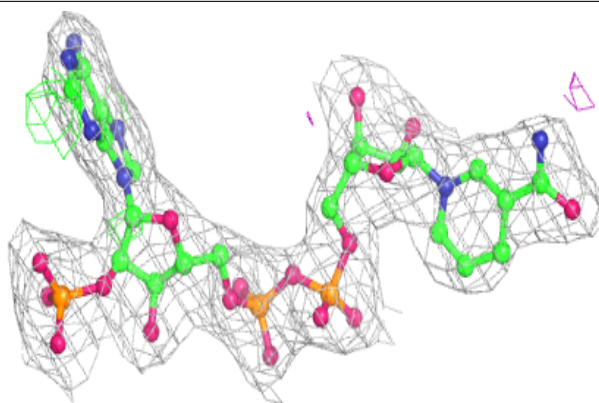
**Electron density around NDP C 401:**

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

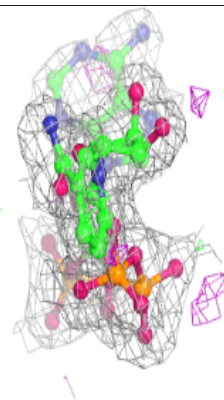
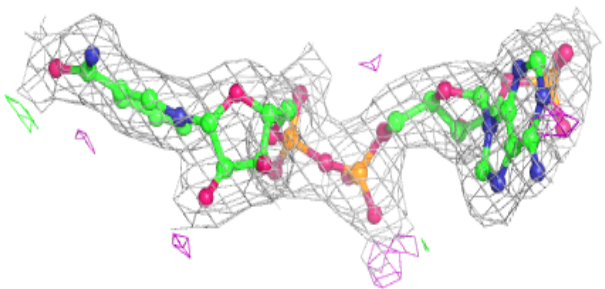
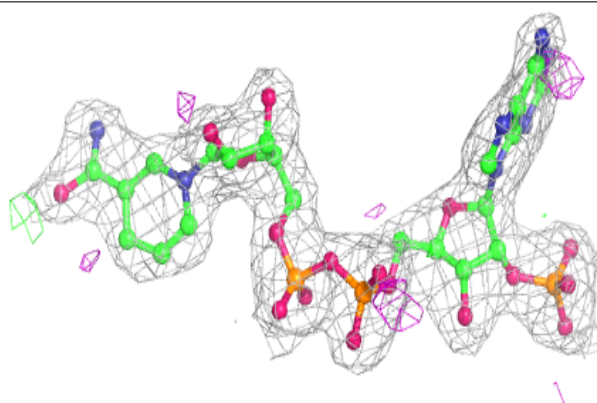


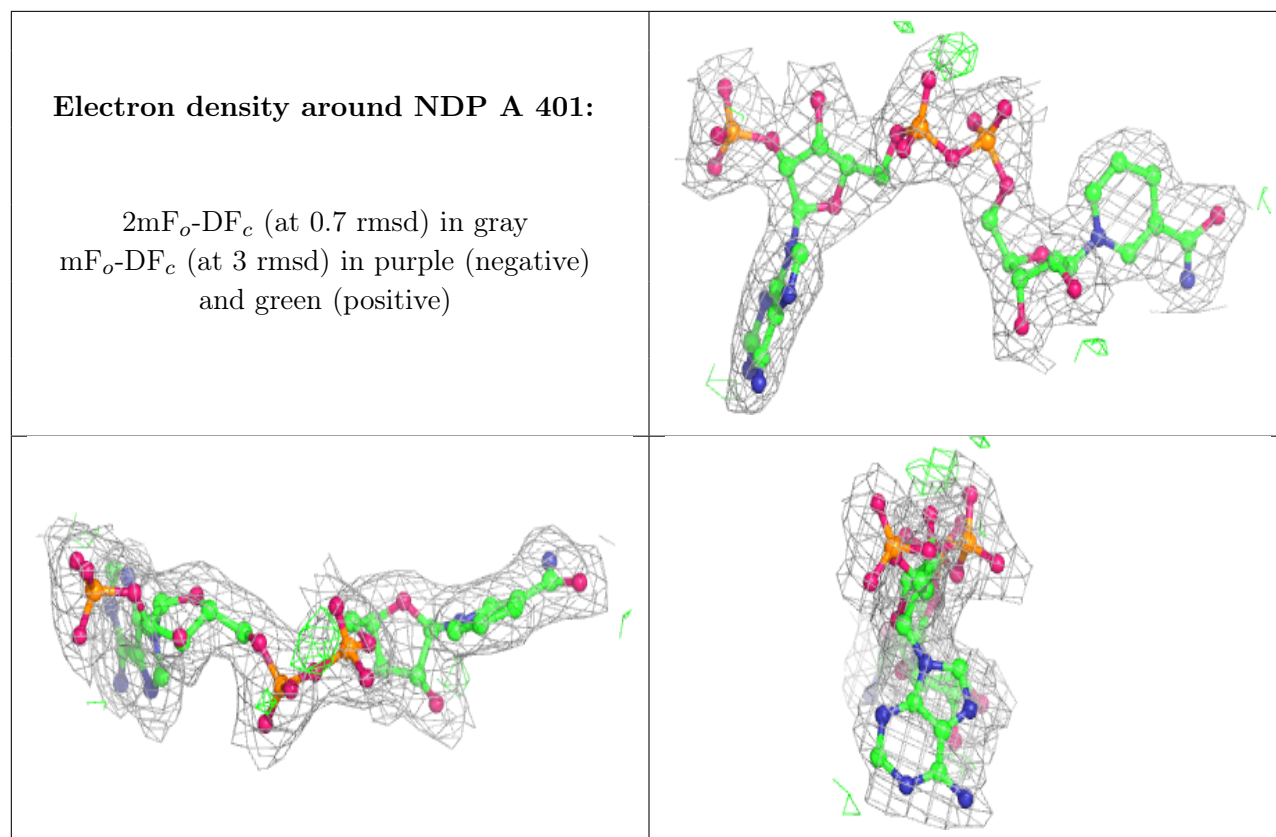
Electron density around NDP N 401:

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

**Electron density around NDP H 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.