



wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 2, 2023 – 02:15 pm GMT

PDB ID : 1H6D
Title : Oxidized Precursor Form of Glucose-Fructose Oxidoreductase from *Zy-*
momonas mobilis complexed with glycerol
Authors : Nurizzo, D.; Baker, E.N.
Deposited on : 2001-06-12
Resolution : 2.05 Å (reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

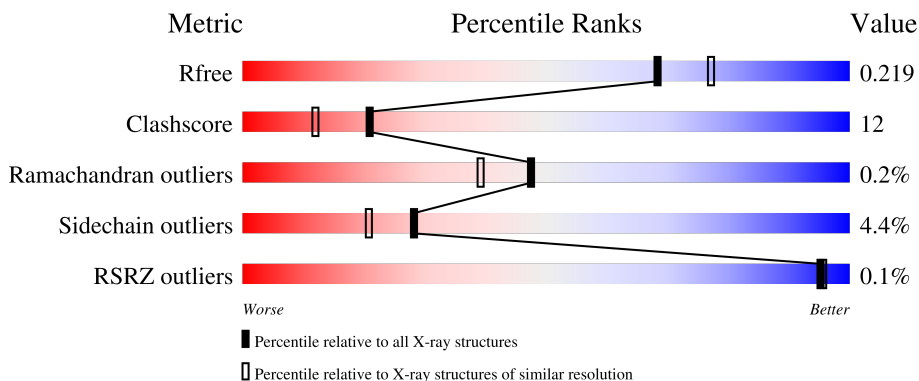
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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}	130704	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	433	
1	B	433	
1	C	433	
1	D	433	
1	E	433	

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Mol	Chain	Length	Quality of chain			
1	F	433				
1	G	433				
1	H	433				
1	I	433				
1	J	433				
1	K	433				
1	L	433				

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	C	600[A]	-	-	X	-
3	GOL	D	600[B]	-	-	X	-
3	GOL	E	600[A]	-	-	X	-
3	GOL	L	600[A]	-	-	X	-

2 Entry composition [i](#)

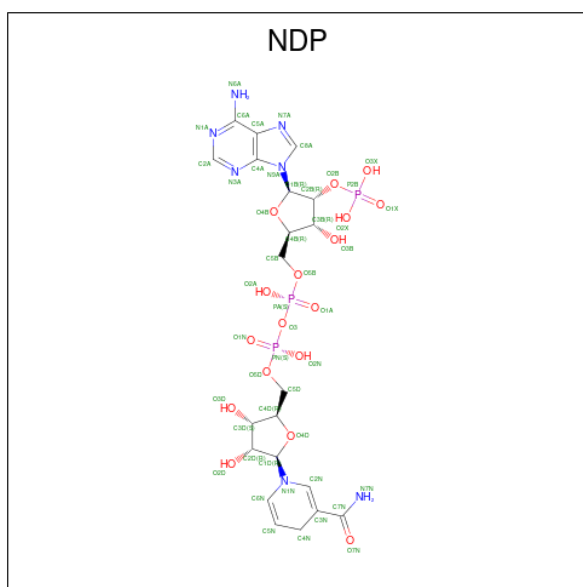
There are 4 unique types of molecules in this entry. The entry contains 40164 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PRECURSOR FORM OF GLUCOSE-FRUCTOSE OXIDOREDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	383	2970	1862	532	556	20	0	0	0
1	B	381	2960	1856	530	554	20	0	0	0
1	C	382	2965	1859	531	555	20	0	0	0
1	D	382	2965	1859	531	555	20	0	0	0
1	E	382	2965	1859	531	555	20	0	0	0
1	F	381	2960	1856	530	554	20	0	0	0
1	G	381	2960	1856	530	554	20	0	0	0
1	H	381	2960	1856	530	554	20	0	0	0
1	I	382	2965	1859	531	555	20	0	0	0
1	J	381	2960	1856	530	554	20	0	0	0
1	K	382	2965	1859	531	555	20	0	0	0
1	L	381	2960	1856	530	554	20	0	0	0

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



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

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 7 3 4	0	1
3	B	1	Total C O 7 3 4	0	1
3	C	1	Total C O 7 3 4	0	1
3	D	1	Total C O 7 3 4	0	1
3	E	1	Total C O 7 3 4	0	1
3	F	1	Total C O 7 3 4	0	1
3	G	1	Total C O 7 3 4	0	1
3	H	1	Total C O 7 3 4	0	1
3	I	1	Total C O 7 3 4	0	1
3	J	1	Total C O 7 3 4	0	1
3	K	1	Total C O 7 3 4	0	1
3	L	1	Total C O 7 3 4	0	1

- Molecule 4 is water.

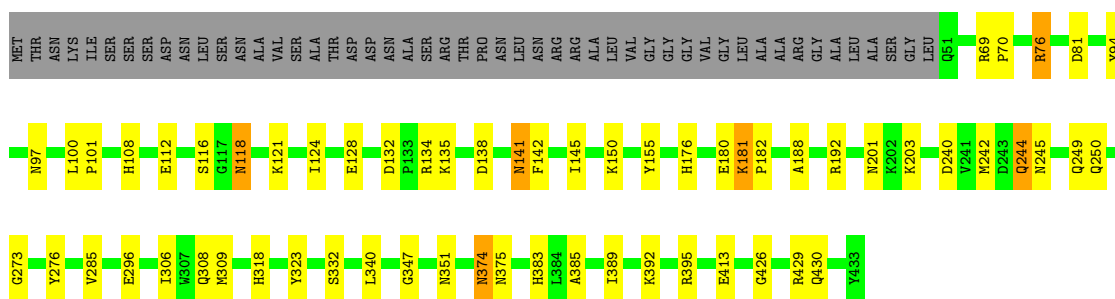
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	390	Total O 390 390	0	0
4	B	295	Total O 295 295	0	0
4	C	320	Total O 320 320	0	0
4	D	213	Total O 213 213	0	0
4	E	341	Total O 341 341	0	0
4	F	219	Total O 219 219	0	0
4	G	371	Total O 371 371	0	0
4	H	289	Total O 289 289	0	0
4	I	391	Total O 391 391	0	0
4	J	377	Total O 377 377	0	0
4	K	386	Total O 386 386	0	0
4	L	357	Total O 357 357	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.

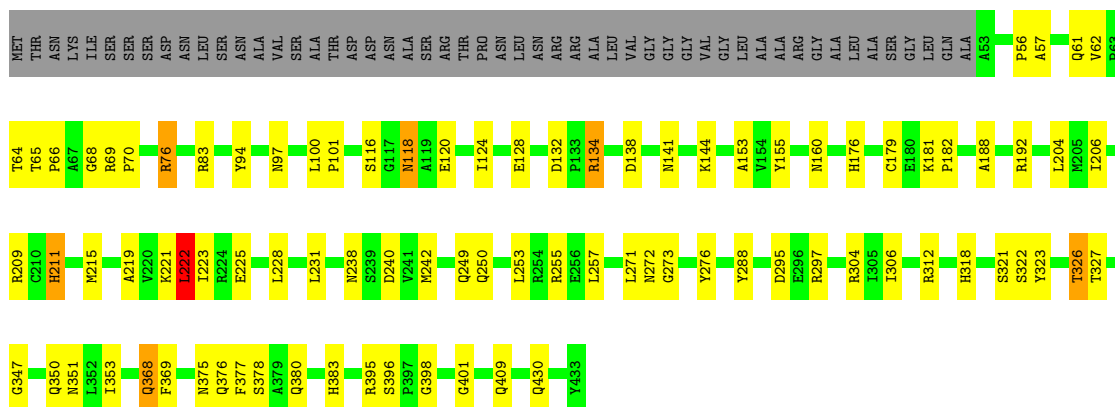
- Molecule 1: PRECURSOR FORM OF GLUCOSE-FRUCTOSE OXIDOREDUCTASE

Chain A: 



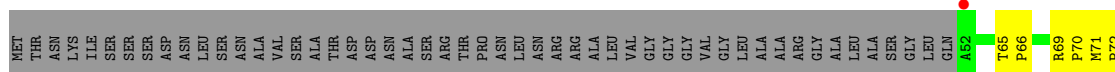
- Molecule 1: PRECURSOR FORM OF GLUCOSE-FRUCTOSE OXIDOREDUCTASE

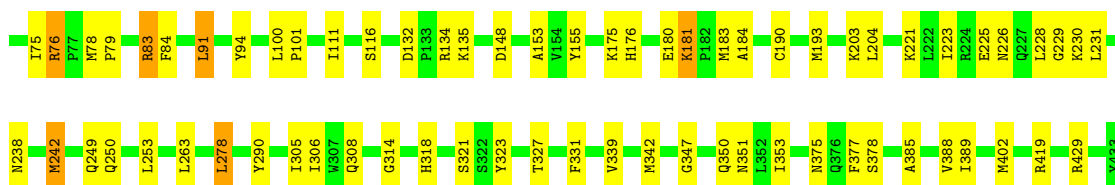
Chain B: 



- Molecule 1: PRECURSOR FORM OF GLUCOSE-FRUCTOSE OXIDOREDUCTASE

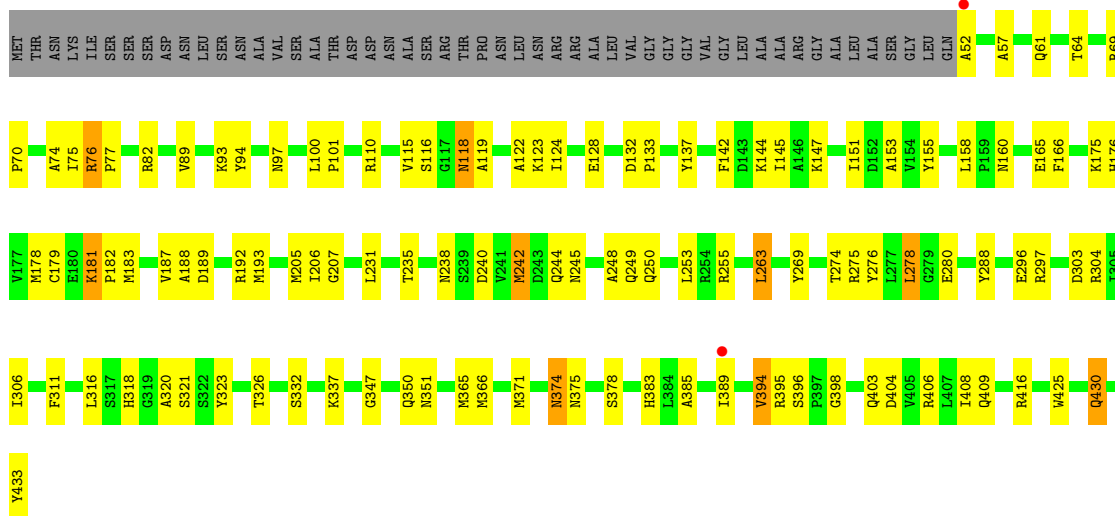
Chain C: 





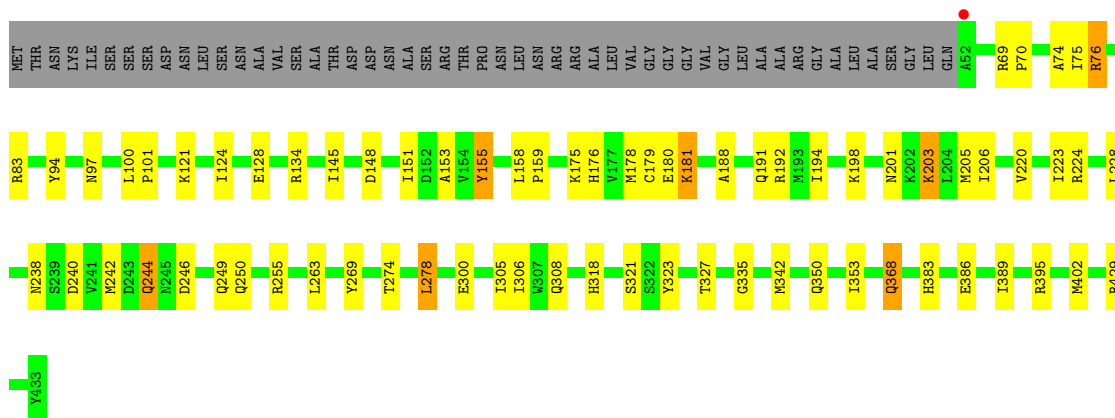
• Molecule 1: PRECURSOR FORM OF GLUCOSE-FRUCTOSE OXIDOREDUCTASE

Chain D: 62% 24% 12%



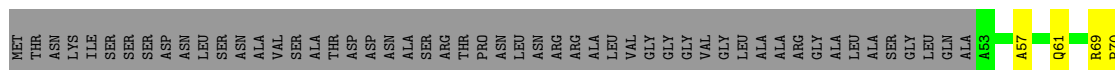
• Molecule 1: PRECURSOR FORM OF GLUCOSE-FRUCTOSE OXIDOREDUCTASE

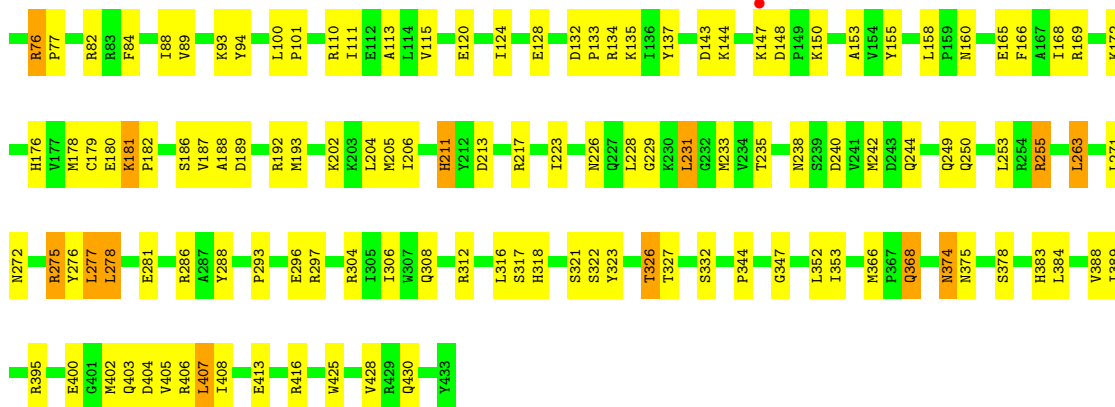
Chain E: 72% 15% 12%



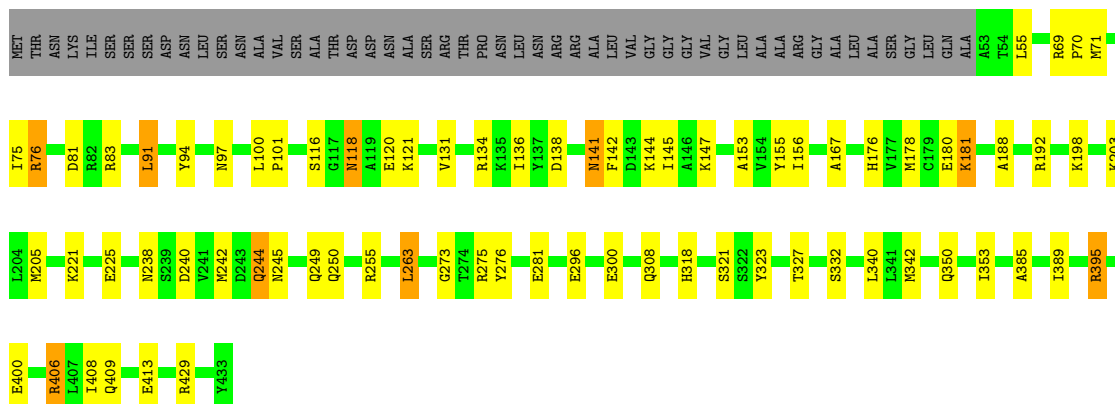
• Molecule 1: PRECURSOR FORM OF GLUCOSE-FRUCTOSE OXIDOREDUCTASE

Chain F: 59% 26% 12%

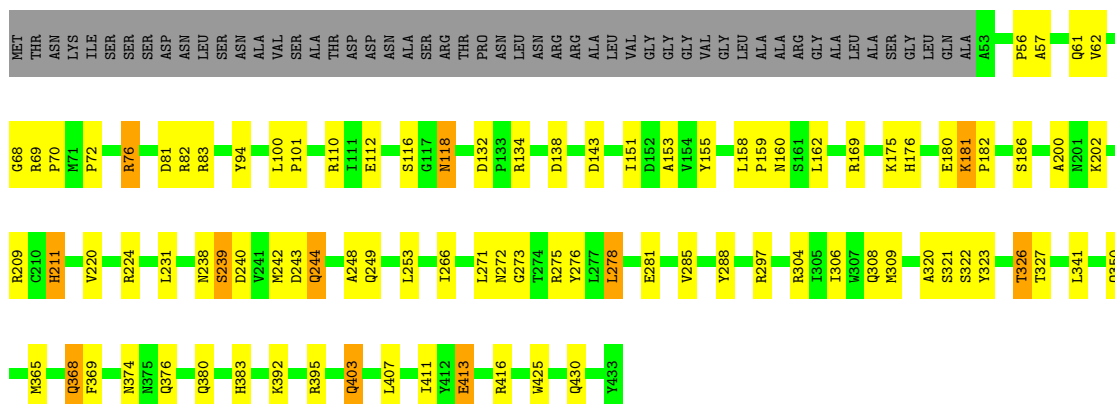




● Molecule 1: PRECURSOR FORM OF GLUCOSE-FRUCTOSE OXIDOREDUCTASE

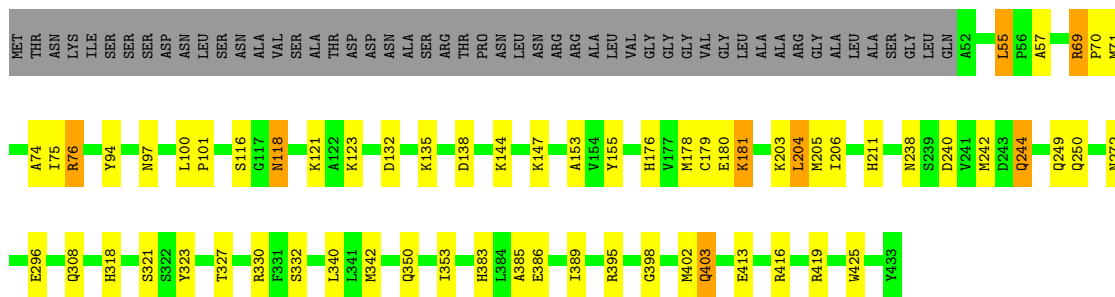


● Molecule 1: PRECURSOR FORM OF GLUCOSE-FRUCTOSE OXIDOREDUCTASE



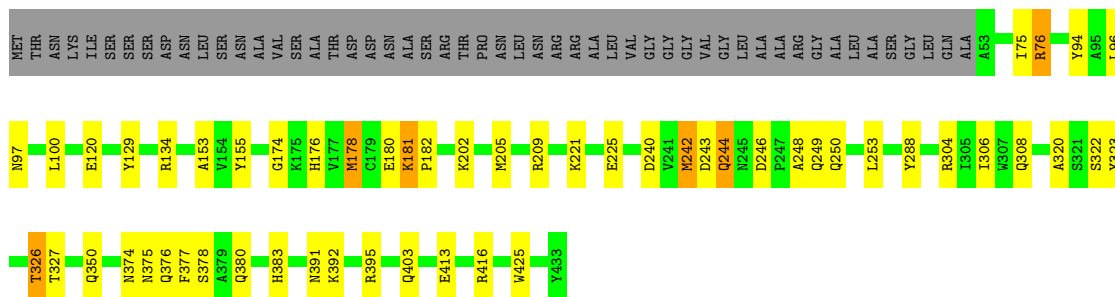
● Molecule 1: PRECURSOR FORM OF GLUCOSE-FRUCTOSE OXIDOREDUCTASE





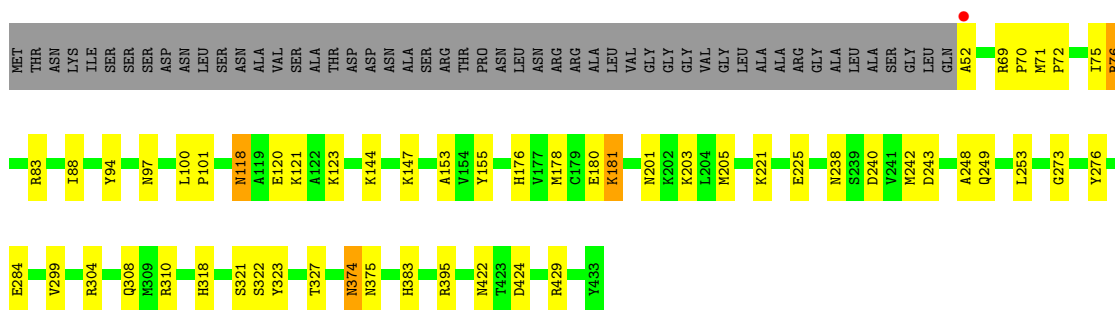
- Molecule 1: PRECURSOR FORM OF GLUCOSE-FRUCTOSE OXIDOREDUCTASE

Chain J: 75% 11% 12%



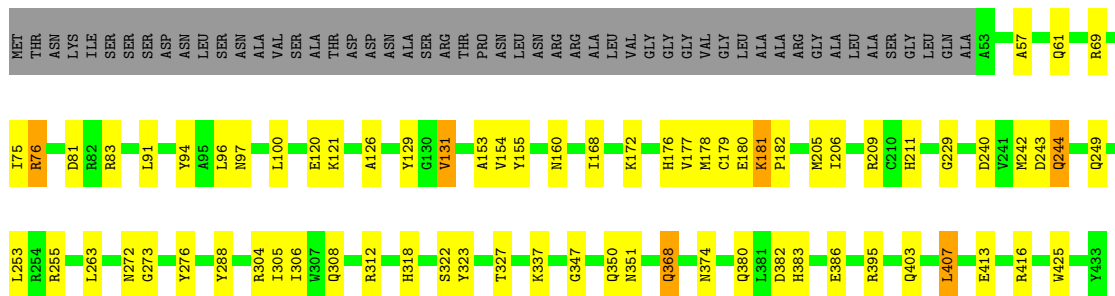
- Molecule 1: PRECURSOR FORM OF GLUCOSE-FRUCTOSE OXIDOREDUCTASE

Chain K: 75% 12% 12%



- Molecule 1: PRECURSOR FORM OF GLUCOSE-FRUCTOSE OXIDOREDUCTASE

Chain L: 71% 15% 12%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	115.72Å 83.75Å 279.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.05 14.99 – 2.05	Depositor EDS
% Data completeness (in resolution range)	95.1 (15.00-2.05) 95.2 (14.99-2.05)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.11 (at 2.05Å)	Xtrriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.197 , 0.228 0.190 , 0.219	Depositor DCC
R_{free} test set	1557 reflections (0.49%)	wwPDB-VP
Wilson B-factor (Å ²)	21.6	Xtrriage
Anisotropy	0.317	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 44.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.476 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	40164	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 56.73 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.6219e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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, GOL

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	0.35	0/3034	0.62	0/4107
1	B	0.31	0/3024	0.59	1/4093 (0.0%)
1	C	0.32	0/3029	0.59	0/4100
1	D	0.30	0/3029	0.58	1/4100 (0.0%)
1	E	0.33	0/3029	0.61	0/4100
1	F	0.30	0/3024	0.59	1/4093 (0.0%)
1	G	0.33	0/3024	0.62	0/4093
1	H	0.31	0/3024	0.59	0/4093
1	I	0.34	0/3029	0.61	0/4100
1	J	0.32	0/3024	0.60	0/4093
1	K	0.35	0/3029	0.62	0/4100
1	L	0.33	0/3024	0.62	0/4093
All	All	0.32	0/36323	0.60	3/49165 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	222	LEU	CA-CB-CG	5.87	128.80	115.30
1	F	275	ARG	NE-CZ-NH2	5.20	122.90	120.30
1	D	275	ARG	NE-CZ-NH2	5.16	122.88	120.30

There are no chirality outliers.

There are no planarity outliers.

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	2970	0	2927	57	0
1	B	2960	0	2920	74	0
1	C	2965	0	2925	72	0
1	D	2965	0	2925	102	0
1	E	2965	0	2925	71	0
1	F	2960	0	2920	109	0
1	G	2960	0	2920	70	0
1	H	2960	0	2920	81	0
1	I	2965	0	2925	67	0
1	J	2960	0	2920	64	0
1	K	2965	0	2925	59	0
1	L	2960	0	2920	70	0
2	A	48	0	26	7	0
2	B	48	0	26	5	0
2	C	48	0	26	10	0
2	D	48	0	26	10	0
2	E	48	0	26	10	0
2	F	48	0	26	10	0
2	G	48	0	26	7	0
2	H	48	0	26	8	0
2	I	48	0	26	6	0
2	J	48	0	26	10	0
2	K	48	0	26	9	0
2	L	48	0	26	10	0
3	A	7	0	6	5	0
3	B	7	0	6	4	0
3	C	7	0	6	7	0
3	D	7	0	6	6	0
3	E	7	0	6	8	0
3	F	7	0	6	6	0
3	G	7	0	6	5	0
3	H	7	0	6	5	0
3	I	7	0	6	4	0
3	J	7	0	6	6	0
3	K	7	0	6	5	0
3	L	7	0	6	7	0
4	A	390	0	0	6	0
4	B	295	0	0	3	0
4	C	320	0	0	6	0
4	D	213	0	0	5	0
4	E	341	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	F	219	0	0	5	0
4	G	371	0	0	7	0
4	H	289	0	0	4	0
4	I	391	0	0	8	0
4	J	377	0	0	4	0
4	K	386	0	0	5	0
4	L	357	0	0	3	0
All	All	40164	0	35456	876	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 12.

The worst 5 of 876 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:K:500:NDP:H42N	3:K:600[B]:GOL:H31	1.20	1.16
2:G:500:NDP:H42N	3:G:600[B]:GOL:H31	1.27	1.15
2:A:500:NDP:H42N	3:A:600[B]:GOL:H31	1.25	1.13
2:K:500:NDP:H42N	3:K:600[A]:GOL:H32	1.14	1.13
2:B:500:NDP:H42N	3:B:600[A]:GOL:H31	1.15	1.13

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	381/433 (88%)	370 (97%)	11 (3%)	0	100 100
1	B	379/433 (88%)	366 (97%)	13 (3%)	0	100 100
1	C	380/433 (88%)	366 (96%)	13 (3%)	1 (0%)	41 31
1	D	380/433 (88%)	364 (96%)	15 (4%)	1 (0%)	41 31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	380/433 (88%)	368 (97%)	11 (3%)	1 (0%)	41	31
1	F	379/433 (88%)	364 (96%)	15 (4%)	0	100	100
1	G	379/433 (88%)	367 (97%)	11 (3%)	1 (0%)	41	31
1	H	379/433 (88%)	365 (96%)	14 (4%)	0	100	100
1	I	380/433 (88%)	369 (97%)	10 (3%)	1 (0%)	41	31
1	J	379/433 (88%)	367 (97%)	12 (3%)	0	100	100
1	K	380/433 (88%)	367 (97%)	12 (3%)	1 (0%)	41	31
1	L	379/433 (88%)	366 (97%)	12 (3%)	1 (0%)	41	31
All	All	4555/5196 (88%)	4399 (97%)	149 (3%)	7 (0%)	47	39

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	327	THR
1	E	327	THR
1	G	327	THR
1	I	327	THR
1	K	327	THR

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	308/345 (89%)	297 (96%)	11 (4%)	35	28
1	B	308/345 (89%)	289 (94%)	19 (6%)	18	10
1	C	308/345 (89%)	299 (97%)	9 (3%)	42	35
1	D	308/345 (89%)	294 (96%)	14 (4%)	27	20
1	E	308/345 (89%)	297 (96%)	11 (4%)	35	28
1	F	308/345 (89%)	288 (94%)	20 (6%)	17	9
1	G	308/345 (89%)	294 (96%)	14 (4%)	27	20
1	H	308/345 (89%)	288 (94%)	20 (6%)	17	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	308/345 (89%)	297 (96%)	11 (4%)	35	28
1	J	308/345 (89%)	297 (96%)	11 (4%)	35	28
1	K	308/345 (89%)	299 (97%)	9 (3%)	42	35
1	L	308/345 (89%)	296 (96%)	12 (4%)	32	25
All	All	3696/4140 (89%)	3535 (96%)	161 (4%)	28	21

5 of 161 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	374	ASN
1	K	155	TYR
1	I	69	ARG
1	J	155	TYR
1	L	131	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 212 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	227	GLN
1	I	227	GLN
1	L	272	ASN
1	G	334	GLN
1	H	294	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

36 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	GOL	L	600[B]	-	5,5,5	0.90	0	5,5,5	0.48	0
2	NDP	B	500	-	45,52,52	1.75	10 (22%)	53,80,80	1.29	5 (9%)
3	GOL	E	600[A]	-	5,5,5	0.94	0	5,5,5	0.49	0
3	GOL	G	600[B]	-	5,5,5	0.94	0	5,5,5	0.49	0
3	GOL	B	600[A]	-	5,5,5	0.97	0	5,5,5	0.48	0
2	NDP	D	500	-	45,52,52	1.78	12 (26%)	53,80,80	1.27	6 (11%)
3	GOL	H	600[A]	-	5,5,5	0.93	0	5,5,5	0.49	0
3	GOL	F	600[A]	-	5,5,5	0.95	0	5,5,5	0.49	0
3	GOL	D	600[A]	-	5,5,5	0.96	0	5,5,5	0.48	0
3	GOL	K	600[A]	-	5,5,5	0.90	0	5,5,5	0.48	0
3	GOL	A	600[A]	-	5,5,5	0.99	0	5,5,5	0.48	0
3	GOL	I	600[B]	-	5,5,5	0.92	0	5,5,5	0.48	0
2	NDP	F	500	-	45,52,52	1.79	12 (26%)	53,80,80	1.28	6 (11%)
3	GOL	C	600[B]	-	5,5,5	0.97	0	5,5,5	0.49	0
3	GOL	J	600[B]	-	5,5,5	0.90	0	5,5,5	0.48	0
2	NDP	H	500	-	45,52,52	1.75	12 (26%)	53,80,80	1.28	5 (9%)
2	NDP	L	500	-	45,52,52	1.74	10 (22%)	53,80,80	1.27	5 (9%)
3	GOL	L	600[A]	-	5,5,5	0.90	0	5,5,5	0.48	0
2	NDP	G	500	-	45,52,52	1.78	12 (26%)	53,80,80	1.27	5 (9%)
3	GOL	G	600[A]	-	5,5,5	0.95	0	5,5,5	0.49	0
2	NDP	E	500	-	45,52,52	1.73	11 (24%)	53,80,80	1.27	5 (9%)
3	GOL	E	600[B]	-	5,5,5	0.94	0	5,5,5	0.49	0
2	NDP	I	500	-	45,52,52	1.75	11 (24%)	53,80,80	1.30	5 (9%)
2	NDP	C	500	-	45,52,52	1.72	9 (20%)	53,80,80	1.27	5 (9%)
2	NDP	J	500	-	45,52,52	1.76	12 (26%)	53,80,80	1.26	5 (9%)
3	GOL	J	600[A]	-	5,5,5	0.91	0	5,5,5	0.48	0
2	NDP	A	500	-	45,52,52	1.78	10 (22%)	53,80,80	1.28	6 (11%)
3	GOL	B	600[B]	-	5,5,5	0.96	0	5,5,5	0.48	0
3	GOL	I	600[A]	-	5,5,5	0.92	0	5,5,5	0.48	0
3	GOL	C	600[A]	-	5,5,5	0.97	0	5,5,5	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GOL	H	600[B]	-	5,5,5	0.93	0	5,5,5	0.49	0
2	NDP	K	500	-	45,52,52	1.75	11 (24%)	53,80,80	1.29	5 (9%)
3	GOL	F	600[B]	-	5,5,5	0.95	0	5,5,5	0.49	0
3	GOL	D	600[B]	-	5,5,5	0.96	0	5,5,5	0.49	0
3	GOL	K	600[B]	-	5,5,5	0.90	0	5,5,5	0.48	0
3	GOL	A	600[B]	-	5,5,5	0.98	0	5,5,5	0.48	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
3	GOL	L	600[B]	-	-	1/4/4/4	-
2	NDP	B	500	-	-	6/30/77/77	0/5/5/5
3	GOL	E	600[A]	-	-	1/4/4/4	-
3	GOL	G	600[B]	-	-	1/4/4/4	-
3	GOL	B	600[A]	-	-	1/4/4/4	-
2	NDP	D	500	-	-	9/30/77/77	0/5/5/5
3	GOL	H	600[A]	-	-	1/4/4/4	-
3	GOL	F	600[A]	-	-	1/4/4/4	-
3	GOL	D	600[A]	-	-	1/4/4/4	-
3	GOL	K	600[A]	-	-	1/4/4/4	-
3	GOL	A	600[A]	-	-	1/4/4/4	-
3	GOL	I	600[B]	-	-	3/4/4/4	-
2	NDP	F	500	-	-	9/30/77/77	0/5/5/5
3	GOL	C	600[B]	-	-	1/4/4/4	-
3	GOL	J	600[B]	-	-	1/4/4/4	-
2	NDP	H	500	-	-	7/30/77/77	0/5/5/5
2	NDP	L	500	-	-	6/30/77/77	0/5/5/5
3	GOL	L	600[A]	-	-	1/4/4/4	-
2	NDP	G	500	-	-	7/30/77/77	0/5/5/5
3	GOL	G	600[A]	-	-	1/4/4/4	-
2	NDP	E	500	-	-	8/30/77/77	0/5/5/5
3	GOL	E	600[B]	-	-	1/4/4/4	-
2	NDP	I	500	-	-	5/30/77/77	0/5/5/5
2	NDP	C	500	-	-	8/30/77/77	0/5/5/5
2	NDP	J	500	-	-	5/30/77/77	0/5/5/5
3	GOL	J	600[A]	-	-	1/4/4/4	-
2	NDP	A	500	-	-	6/30/77/77	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	B	600[B]	-	-	1/4/4/4	-
3	GOL	I	600[A]	-	-	1/4/4/4	-
3	GOL	C	600[A]	-	-	1/4/4/4	-
3	GOL	H	600[B]	-	-	1/4/4/4	-
2	NDP	K	500	-	-	5/30/77/77	0/5/5/5
3	GOL	F	600[B]	-	-	1/4/4/4	-
3	GOL	D	600[B]	-	-	1/4/4/4	-
3	GOL	K	600[B]	-	-	1/4/4/4	-
3	GOL	A	600[B]	-	-	1/4/4/4	-

The worst 5 of 132 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	500	NDP	C6N-C5N	4.77	1.41	1.33
2	K	500	NDP	C6N-C5N	4.77	1.41	1.33
2	L	500	NDP	C6N-C5N	4.76	1.41	1.33
2	G	500	NDP	C6N-C5N	4.72	1.41	1.33
2	H	500	NDP	C6N-C5N	4.68	1.41	1.33

The worst 5 of 63 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	500	NDP	N3A-C2A-N1A	-5.02	120.83	128.68
2	E	500	NDP	N3A-C2A-N1A	-4.98	120.89	128.68
2	H	500	NDP	N3A-C2A-N1A	-4.98	120.90	128.68
2	G	500	NDP	N3A-C2A-N1A	-4.97	120.92	128.68
2	A	500	NDP	N3A-C2A-N1A	-4.96	120.93	128.68

There are no chirality outliers.

5 of 107 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	500	NDP	C5D-O5D-PN-O2N
2	E	500	NDP	C5D-O5D-PN-O2N
3	A	600[A]	GOL	O1-C1-C2-C3
3	A	600[B]	GOL	O1-C1-C2-C3
3	B	600[A]	GOL	O1-C1-C2-C3

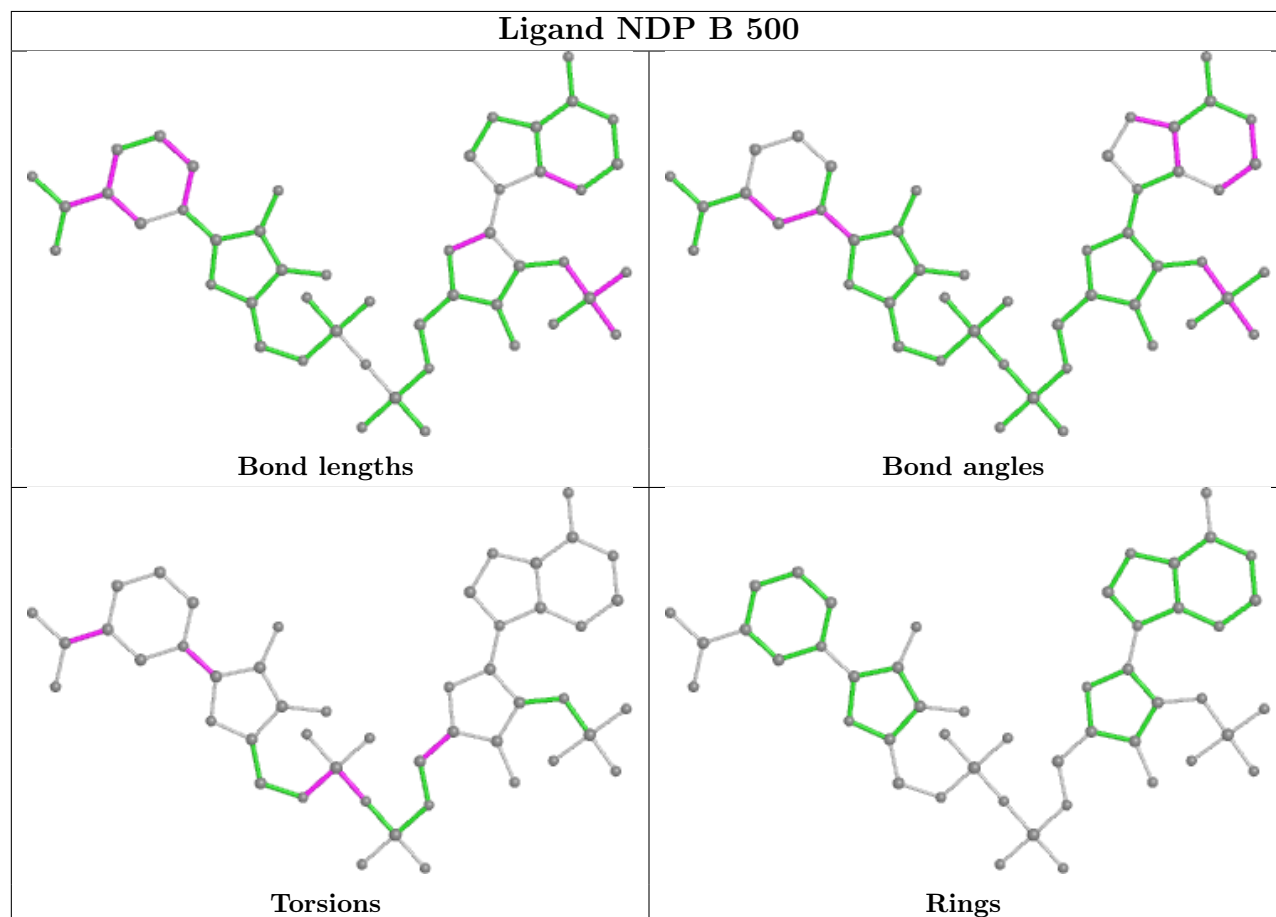
There are no ring outliers.

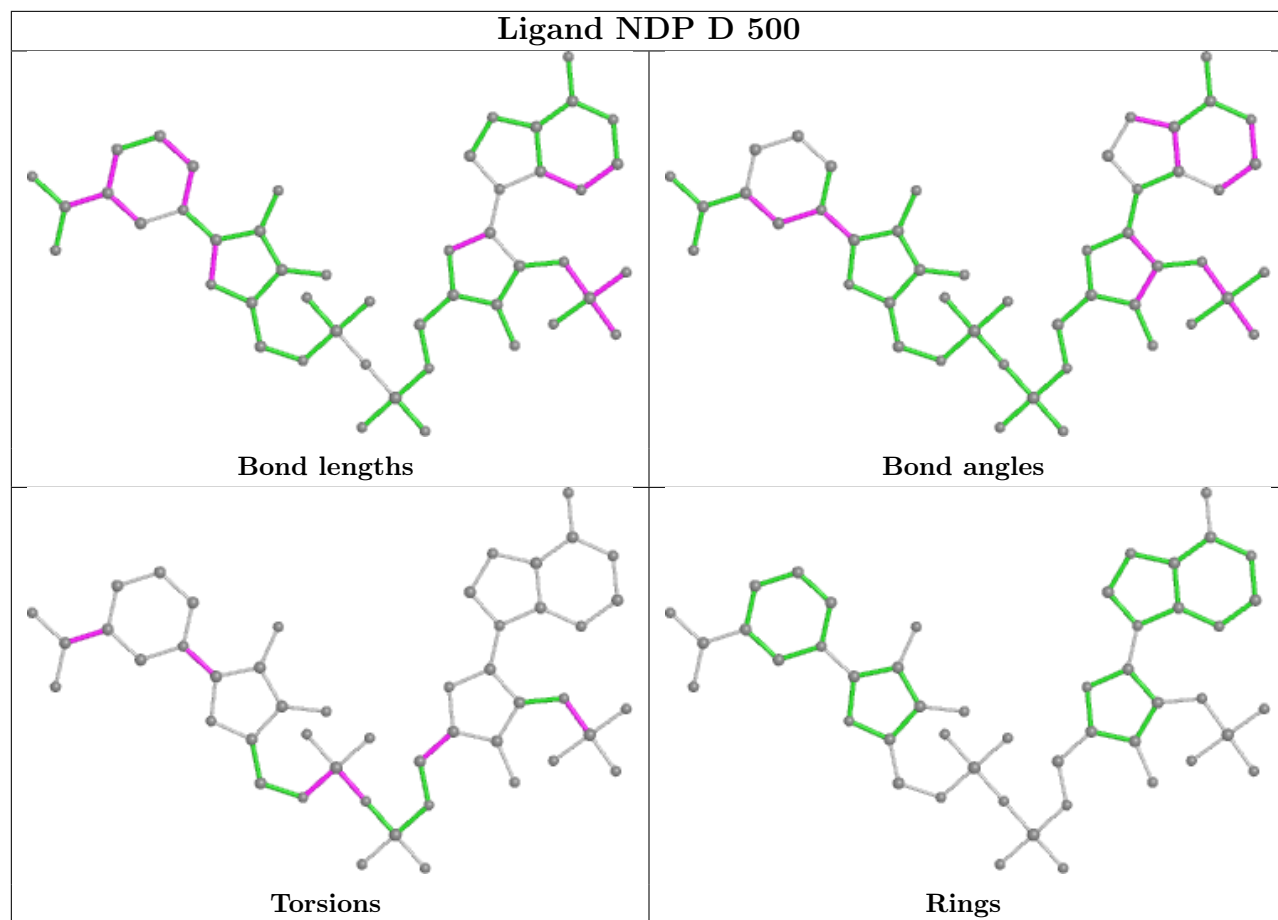
36 monomers are involved in 104 short contacts:

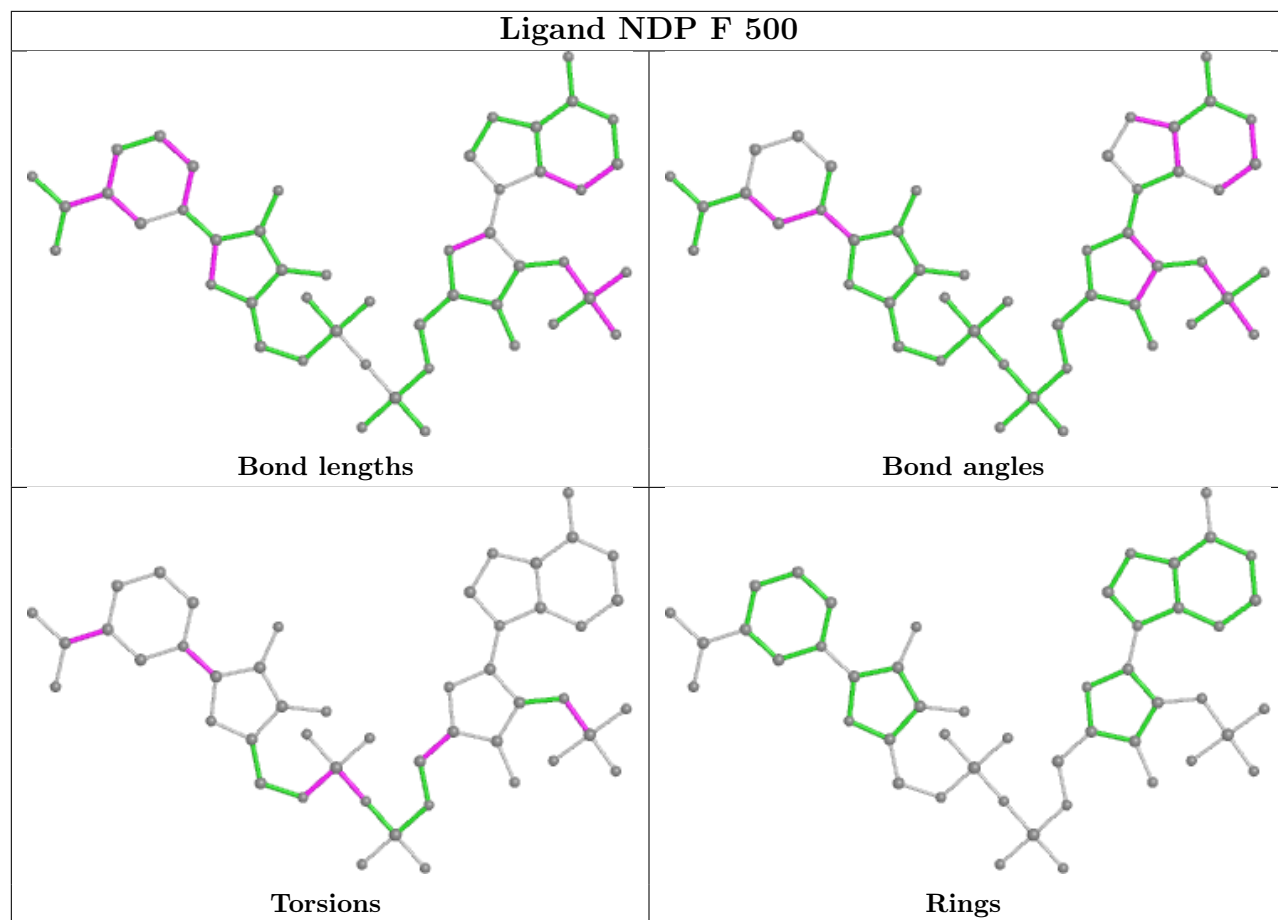
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L	600[B]	GOL	3	0
2	B	500	NDP	5	0
3	E	600[A]	GOL	5	0
3	G	600[B]	GOL	3	0
3	B	600[A]	GOL	2	0
2	D	500	NDP	10	0
3	H	600[A]	GOL	3	0
3	F	600[A]	GOL	3	0
3	D	600[A]	GOL	2	0
3	K	600[A]	GOL	2	0
3	A	600[A]	GOL	2	0
3	I	600[B]	GOL	2	0
2	F	500	NDP	10	0
3	C	600[B]	GOL	3	0
3	J	600[B]	GOL	3	0
2	H	500	NDP	8	0
2	L	500	NDP	10	0
3	L	600[A]	GOL	4	0
2	G	500	NDP	7	0
3	G	600[A]	GOL	2	0
2	E	500	NDP	10	0
3	E	600[B]	GOL	3	0
2	I	500	NDP	6	0
2	C	500	NDP	10	0
2	J	500	NDP	10	0
3	J	600[A]	GOL	3	0
2	A	500	NDP	7	0
3	B	600[B]	GOL	2	0
3	I	600[A]	GOL	2	0
3	C	600[A]	GOL	4	0
3	H	600[B]	GOL	2	0
2	K	500	NDP	9	0
3	F	600[B]	GOL	3	0
3	D	600[B]	GOL	4	0
3	K	600[B]	GOL	3	0
3	A	600[B]	GOL	3	0

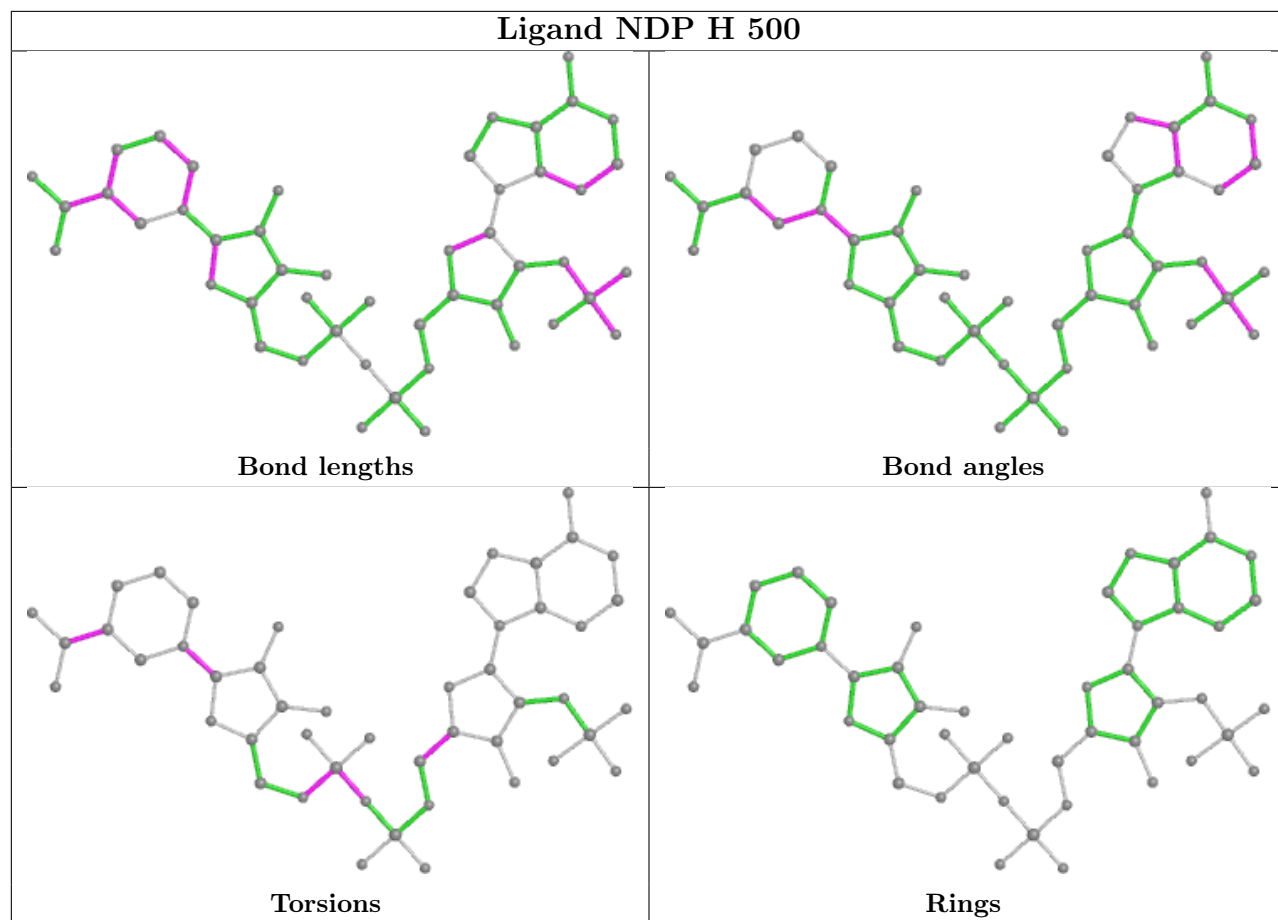
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

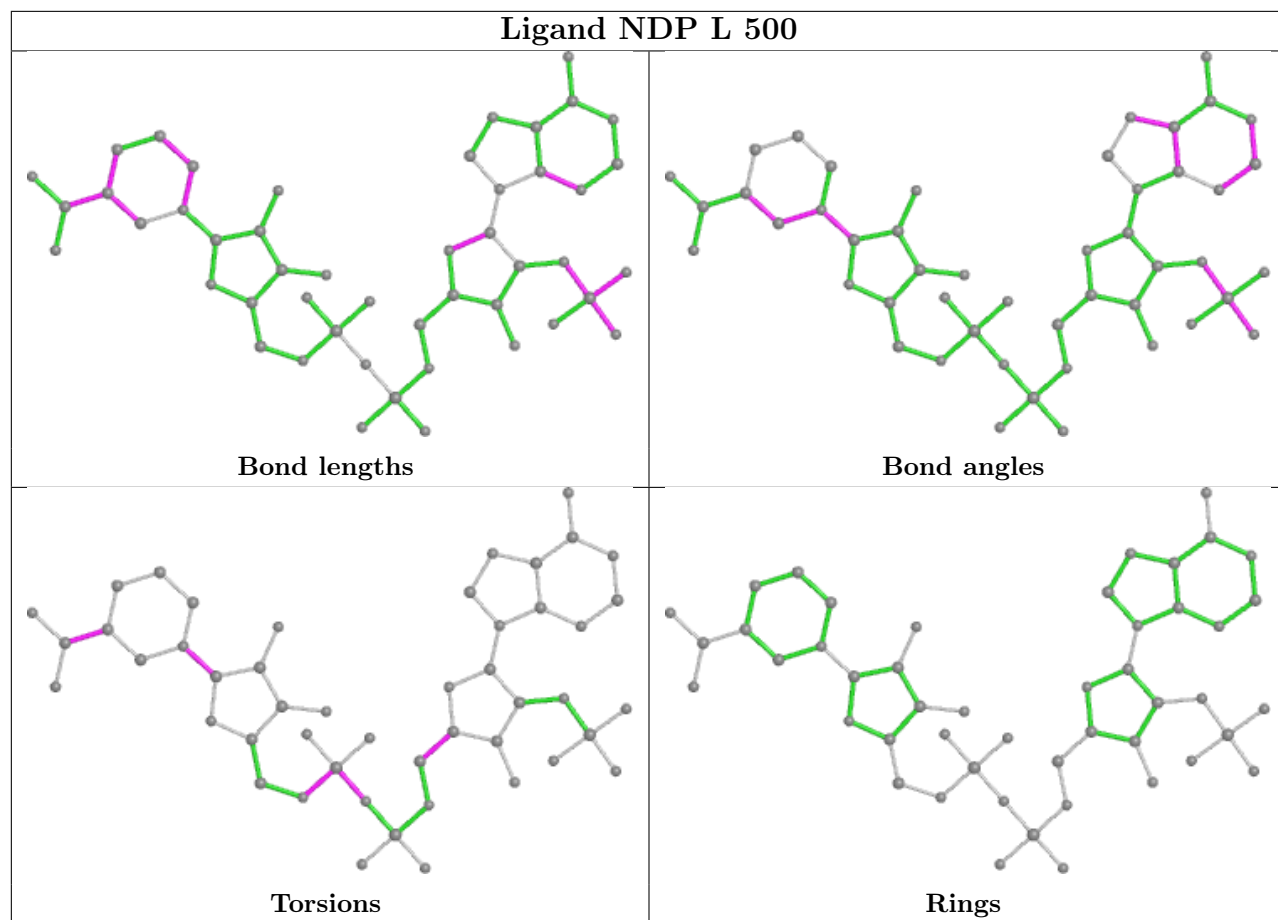
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

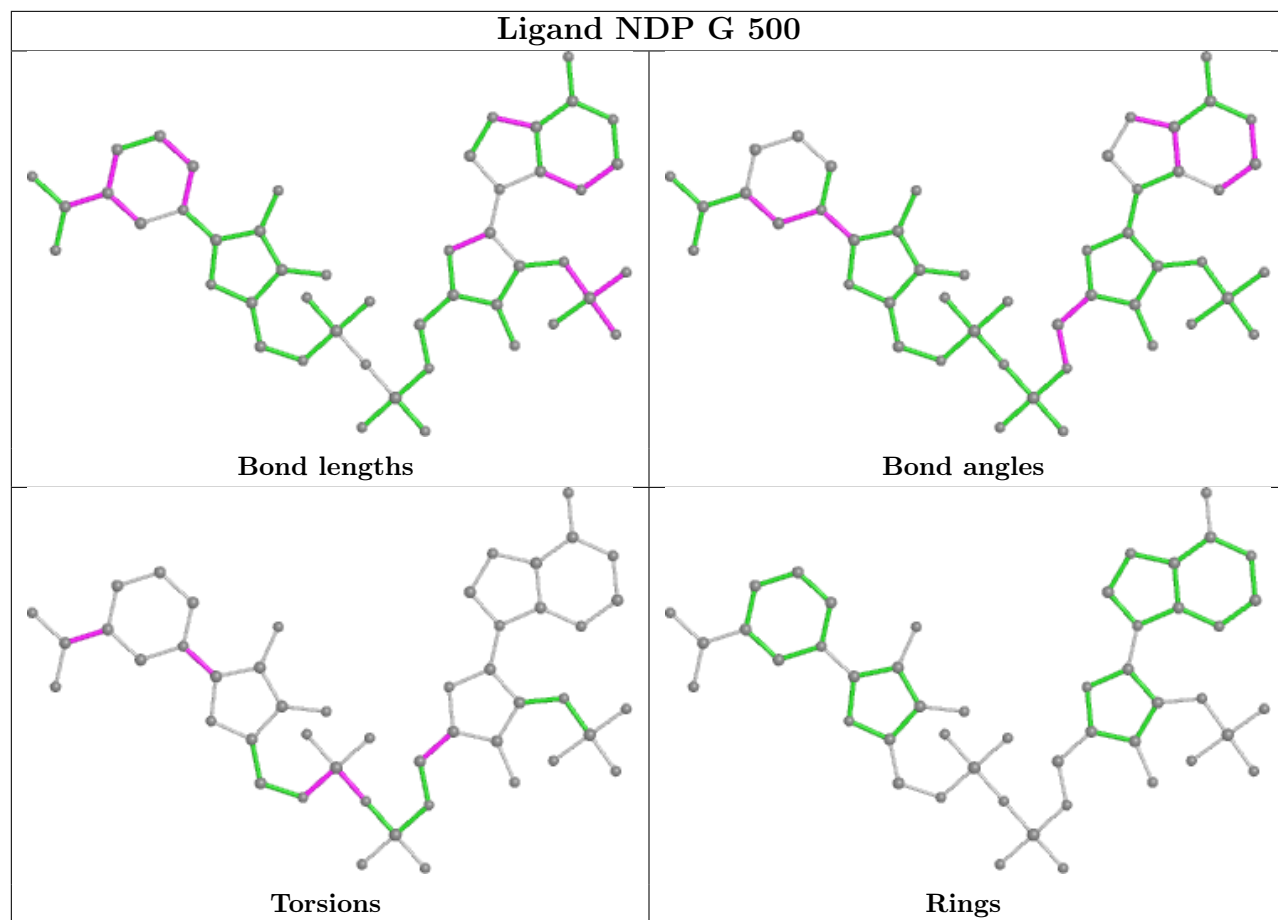


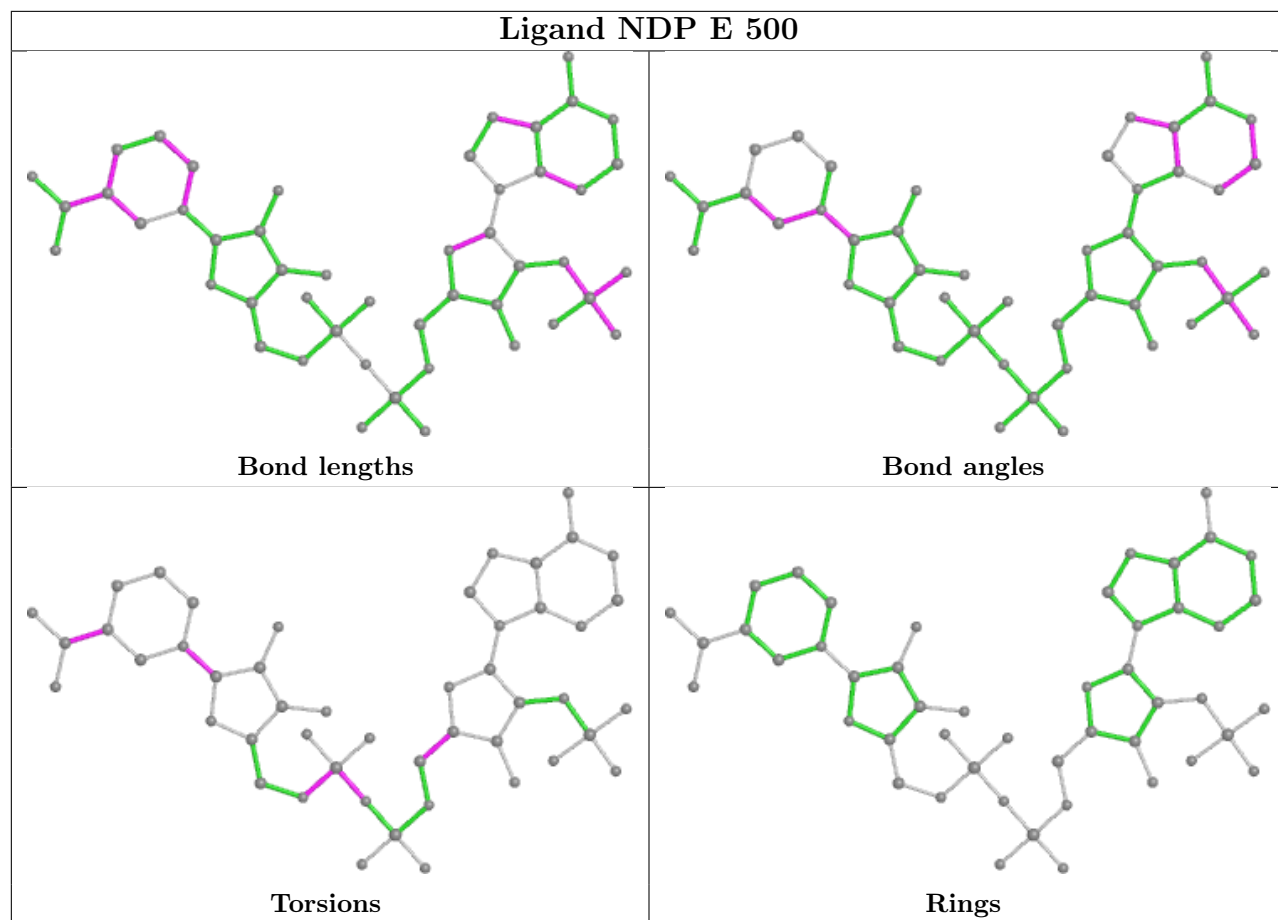


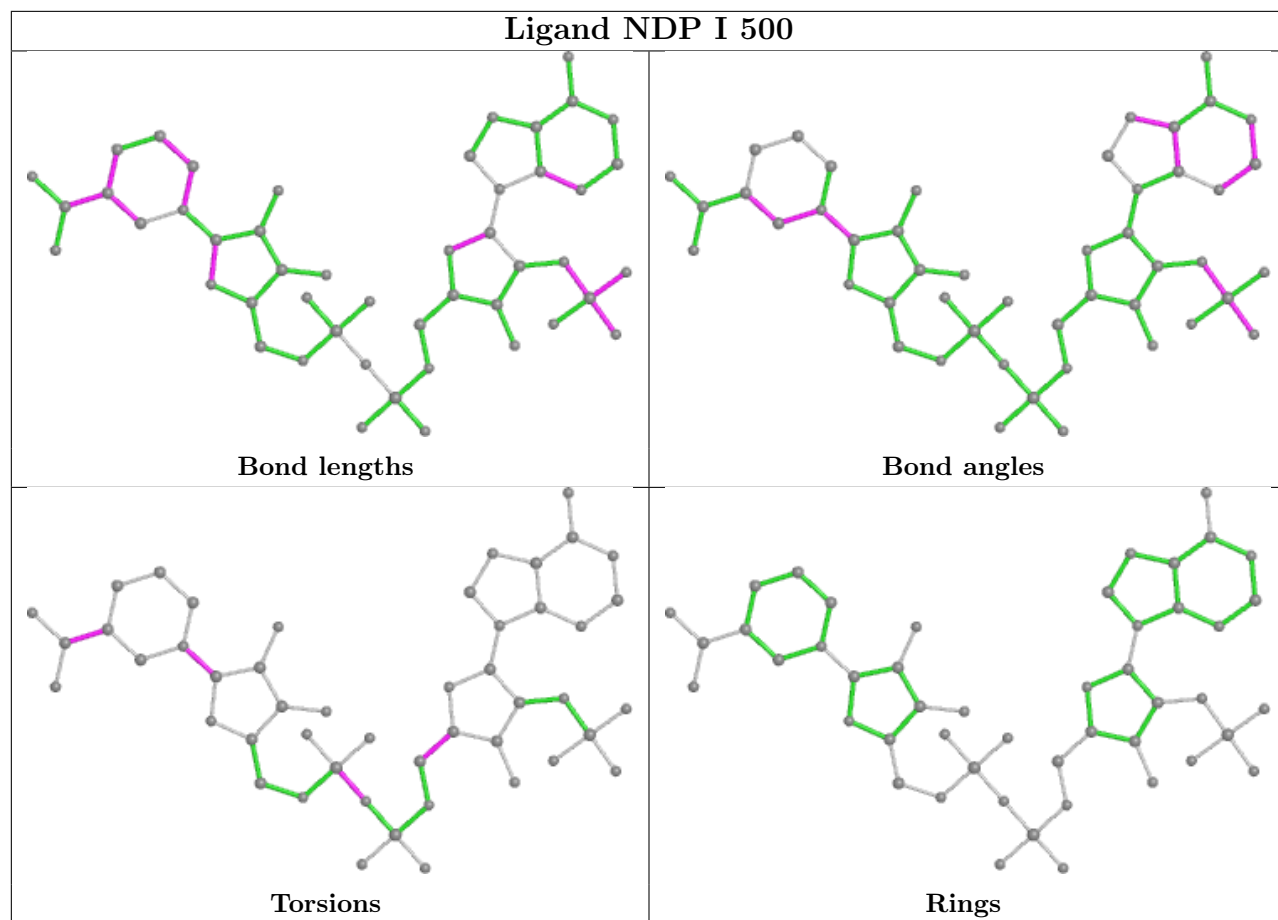


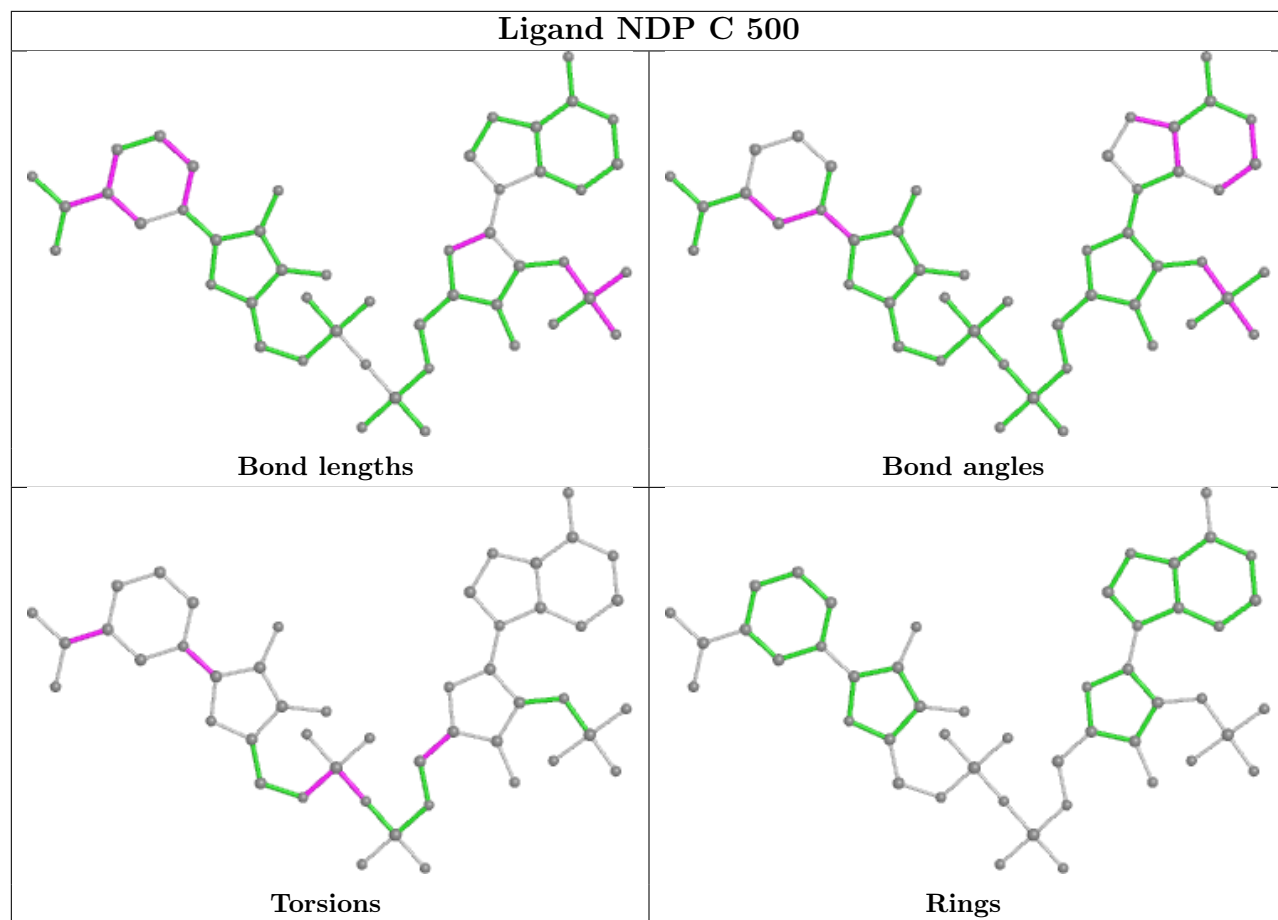


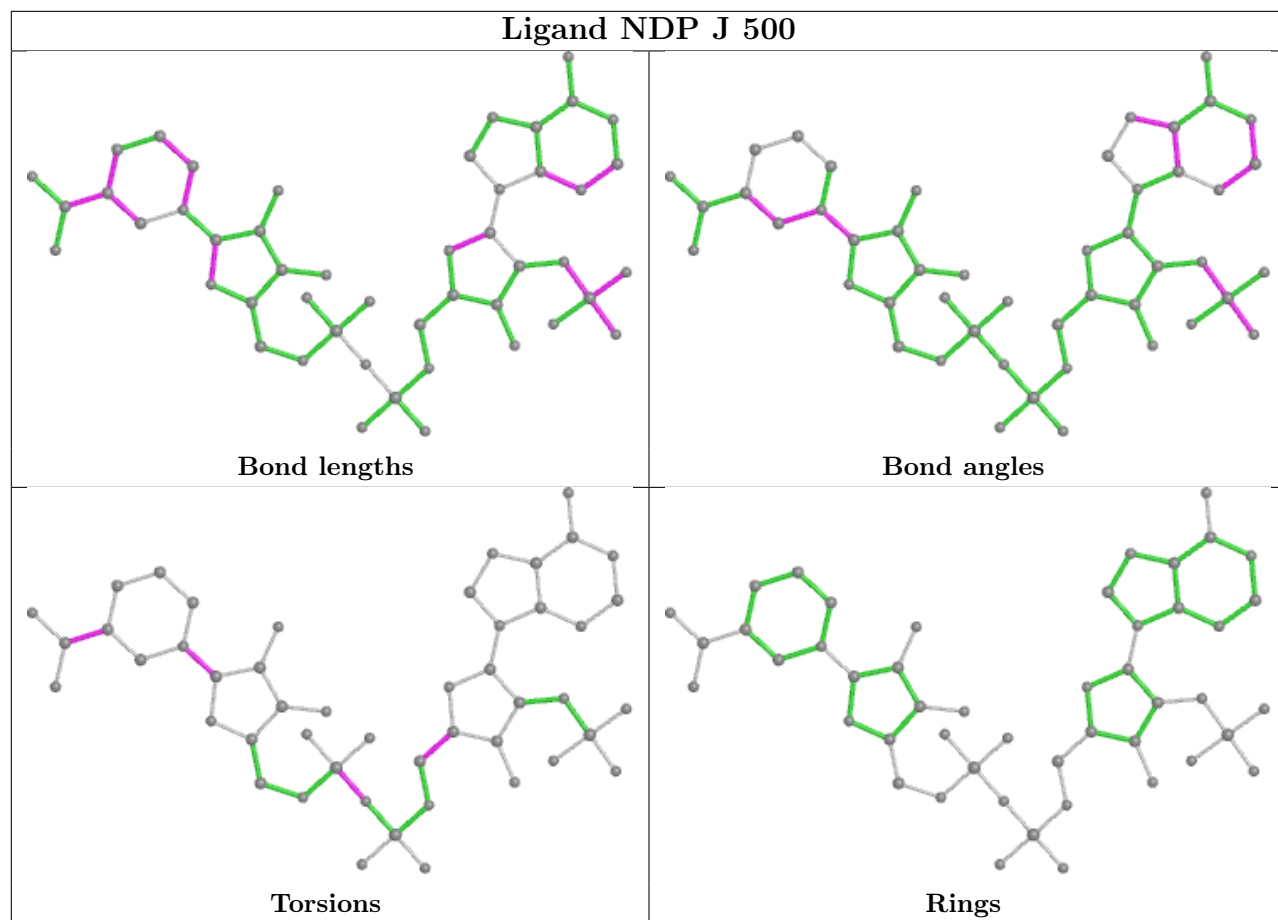


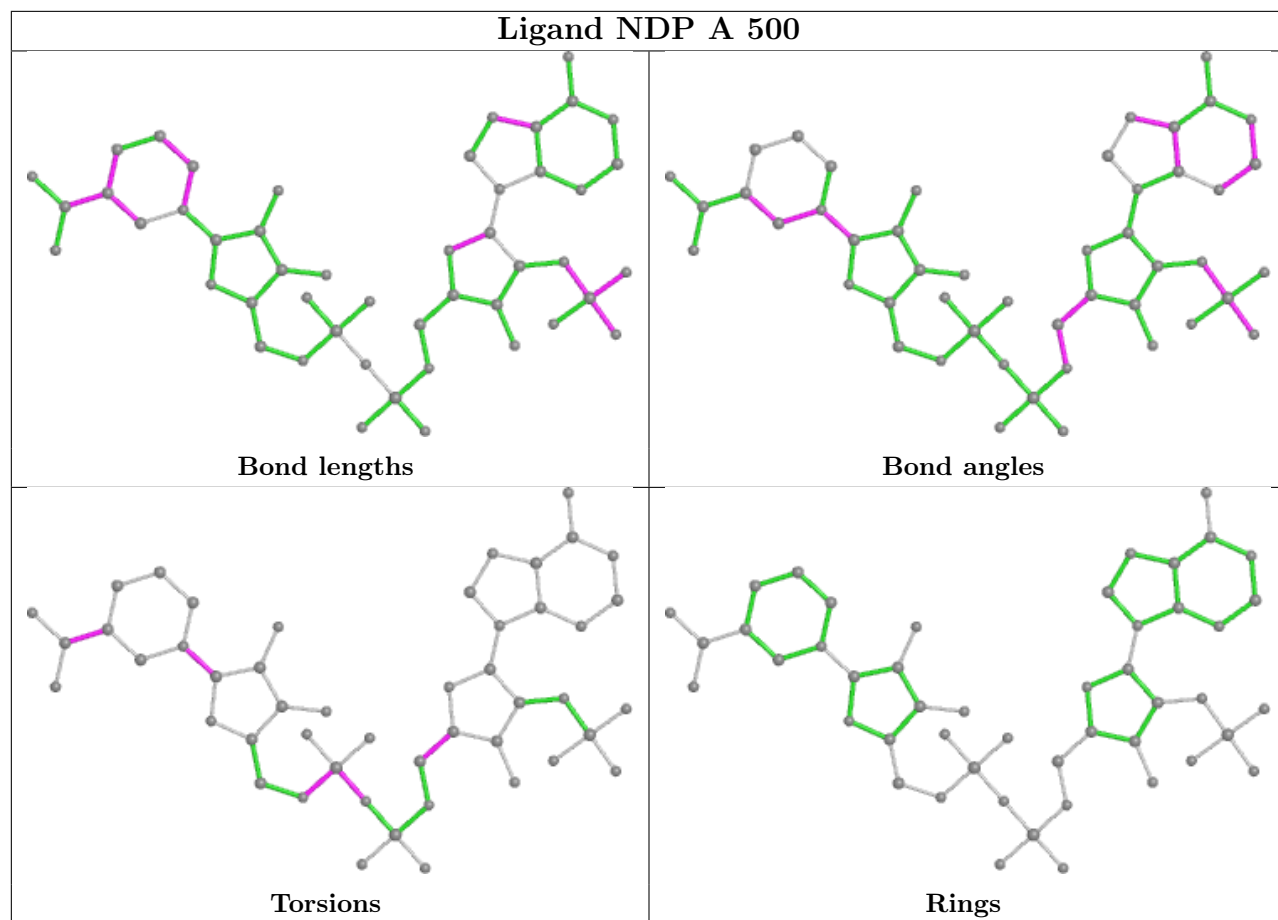


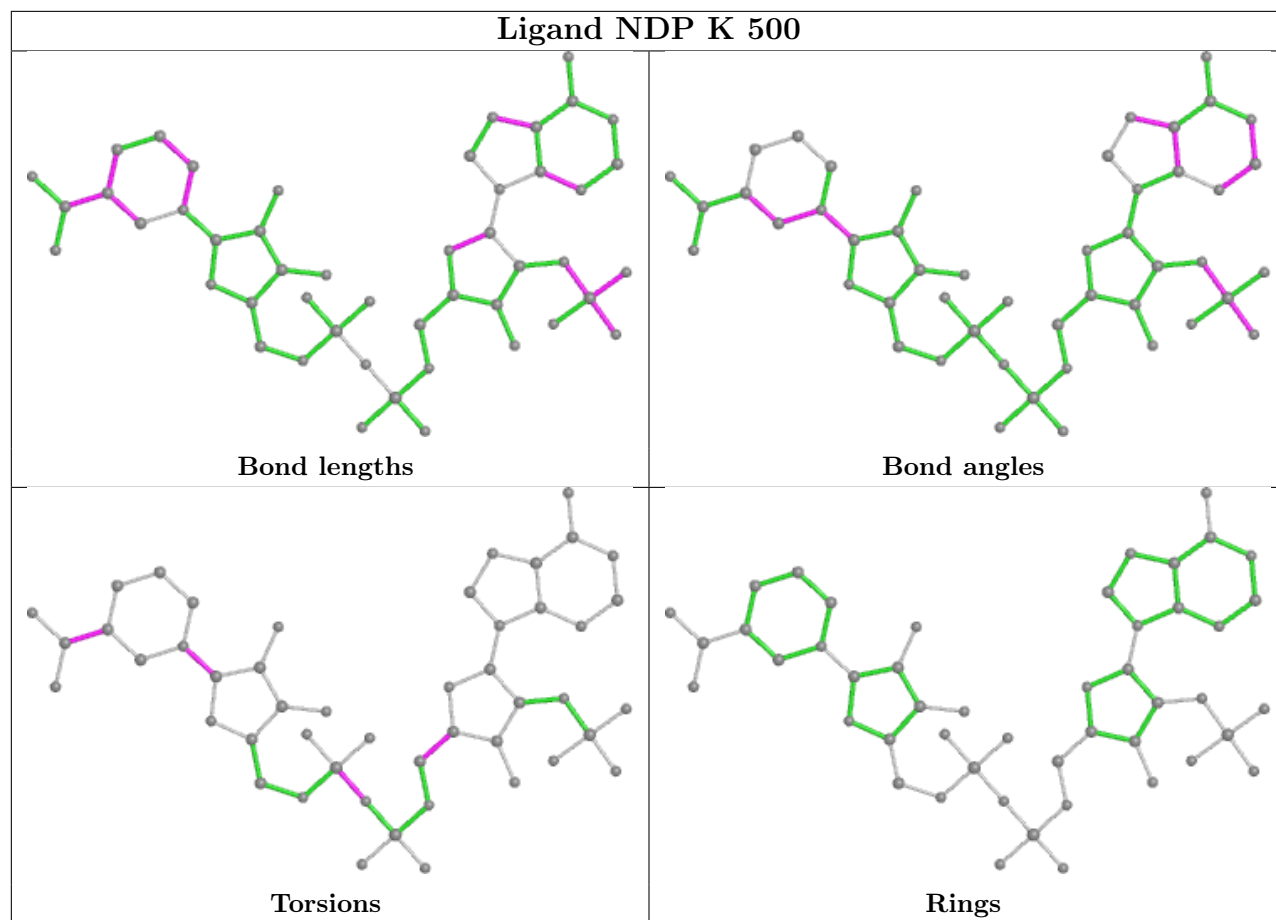












5.7 Other polymers [\(i\)](#)

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	383/433 (88%)	-0.85	0 100 100	12, 18, 30, 48	0
1	B	381/433 (87%)	-0.72	0 100 100	13, 23, 38, 45	0
1	C	382/433 (88%)	-0.77	1 (0%) 94 94	14, 21, 32, 45	0
1	D	382/433 (88%)	-0.47	2 (0%) 91 92	16, 31, 44, 53	0
1	E	382/433 (88%)	-0.75	1 (0%) 94 94	14, 22, 32, 44	0
1	F	381/433 (87%)	-0.47	1 (0%) 94 94	16, 30, 46, 52	0
1	G	381/433 (87%)	-0.86	0 100 100	12, 18, 30, 40	0
1	H	381/433 (87%)	-0.74	0 100 100	14, 23, 39, 46	0
1	I	382/433 (88%)	-0.87	0 100 100	10, 16, 28, 39	0
1	J	381/433 (87%)	-0.84	0 100 100	11, 19, 30, 42	0
1	K	382/433 (88%)	-0.88	1 (0%) 94 94	10, 16, 27, 39	0
1	L	381/433 (87%)	-0.85	0 100 100	11, 19, 29, 40	0
All	All	4579/5196 (88%)	-0.76	6 (0%) 95 95	10, 21, 38, 53	0

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	52	ALA	2.6
1	D	52	ALA	2.3
1	C	52	ALA	2.3
1	F	147	LYS	2.3
1	D	389	ILE	2.2

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

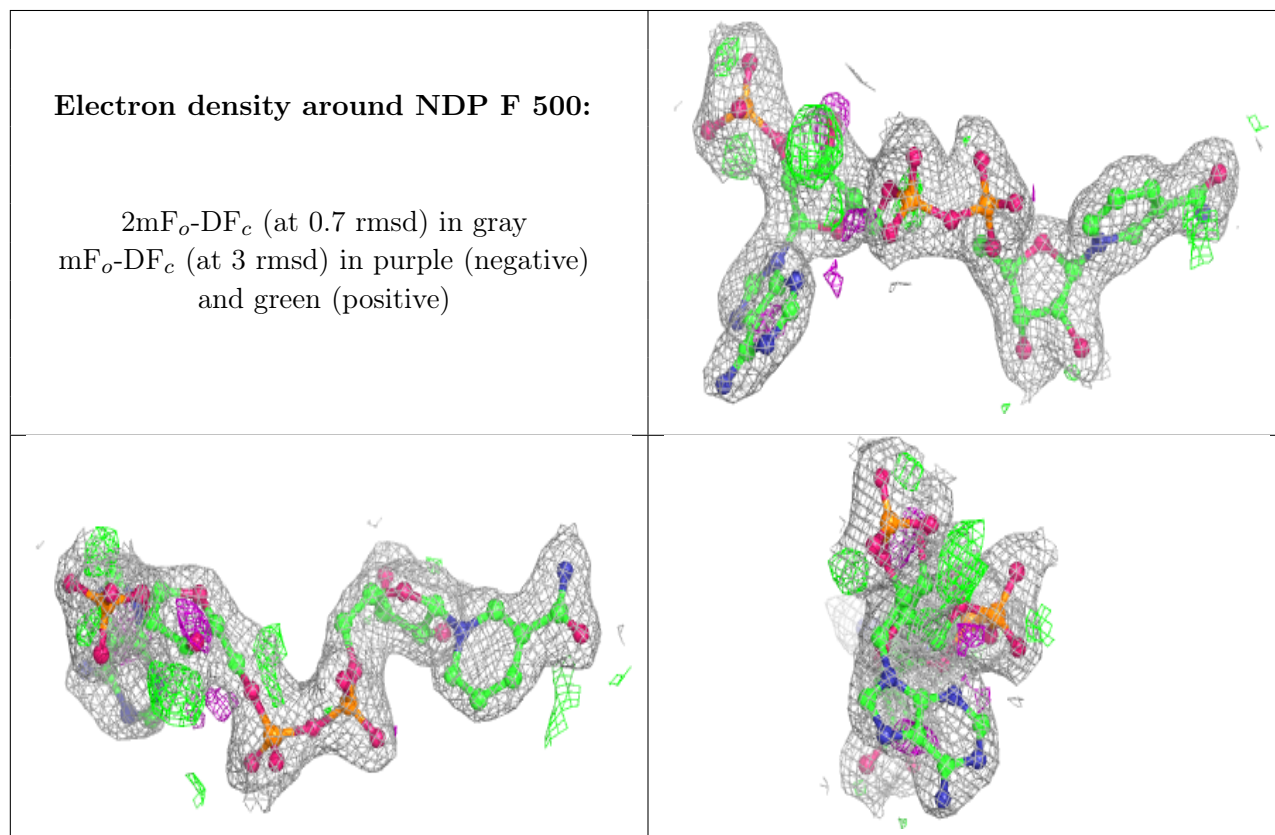
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	GOL	H	600[A]	6/6	0.49	0.26	36,37,38,38	1
3	GOL	H	600[B]	6/6	0.49	0.26	36,37,38,38	1
3	GOL	L	600[A]	6/6	0.49	0.33	32,34,35,35	1
3	GOL	L	600[B]	6/6	0.49	0.33	31,34,35,35	1
3	GOL	F	600[A]	6/6	0.52	0.23	42,43,43,43	1
3	GOL	F	600[B]	6/6	0.52	0.23	42,43,43,43	1
3	GOL	E	600[A]	6/6	0.55	0.29	33,34,34,35	1
3	GOL	E	600[B]	6/6	0.55	0.29	32,34,34,35	1
3	GOL	B	600[A]	6/6	0.55	0.28	33,34,35,35	1
3	GOL	B	600[B]	6/6	0.55	0.28	31,33,35,35	1
3	GOL	D	600[A]	6/6	0.56	0.26	42,44,44,44	1
3	GOL	D	600[B]	6/6	0.56	0.26	43,44,44,44	1
3	GOL	K	600[A]	6/6	0.56	0.29	29,31,32,33	1
3	GOL	K	600[B]	6/6	0.56	0.29	31,31,32,33	1
3	GOL	G	600[A]	6/6	0.56	0.24	25,28,29,31	1
3	GOL	G	600[B]	6/6	0.56	0.24	28,29,30,31	1
3	GOL	J	600[A]	6/6	0.57	0.27	30,30,31,31	1
3	GOL	J	600[B]	6/6	0.57	0.27	27,30,31,31	1
3	GOL	C	600[A]	6/6	0.60	0.27	32,33,33,33	1
3	GOL	C	600[B]	6/6	0.60	0.27	31,33,33,33	1
3	GOL	I	600[A]	6/6	0.66	0.25	29,30,32,33	1
3	GOL	I	600[B]	6/6	0.66	0.25	30,30,32,33	1
3	GOL	A	600[A]	6/6	0.67	0.23	18,22,23,25	1
3	GOL	A	600[B]	6/6	0.67	0.23	21,23,25,25	1
2	NDP	F	500	48/48	0.93	0.12	28,33,42,43	0
2	NDP	D	500	48/48	0.94	0.11	25,34,43,43	0
2	NDP	E	500	48/48	0.96	0.09	15,20,22,23	0
2	NDP	B	500	48/48	0.96	0.09	18,23,26,26	0
2	NDP	H	500	48/48	0.96	0.08	19,22,26,26	0
2	NDP	I	500	48/48	0.97	0.08	10,15,18,18	0
2	NDP	J	500	48/48	0.97	0.09	15,19,22,22	0
2	NDP	K	500	48/48	0.97	0.08	10,16,18,18	0

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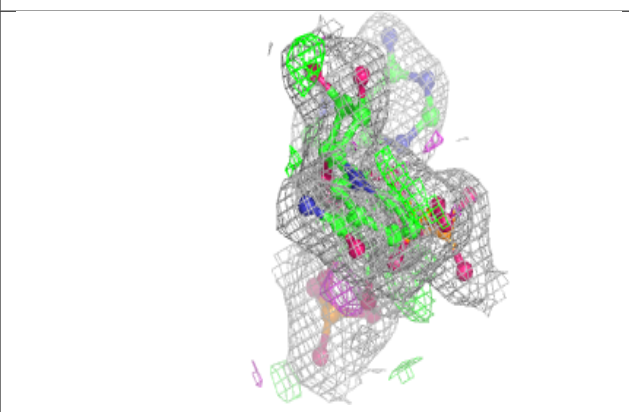
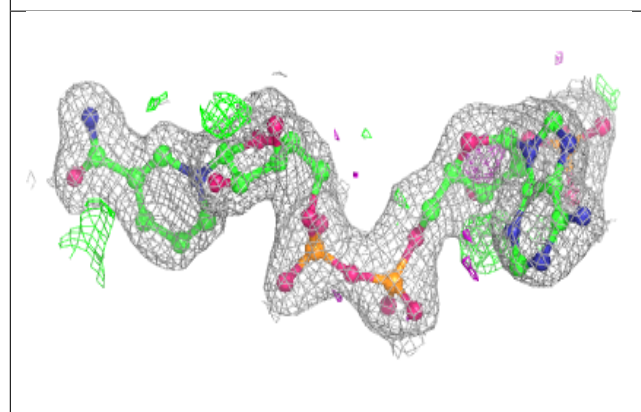
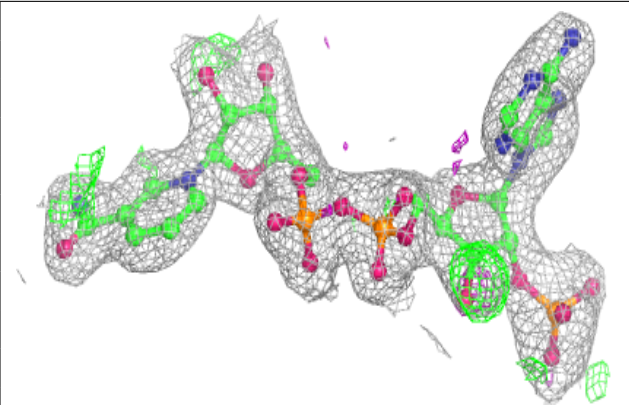
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NDP	L	500	48/48	0.97	0.09	13,19,21,22	0
2	NDP	A	500	48/48	0.97	0.08	12,15,17,17	0
2	NDP	G	500	48/48	0.97	0.08	13,16,18,19	0
2	NDP	C	500	48/48	0.97	0.09	15,19,24,26	0

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.

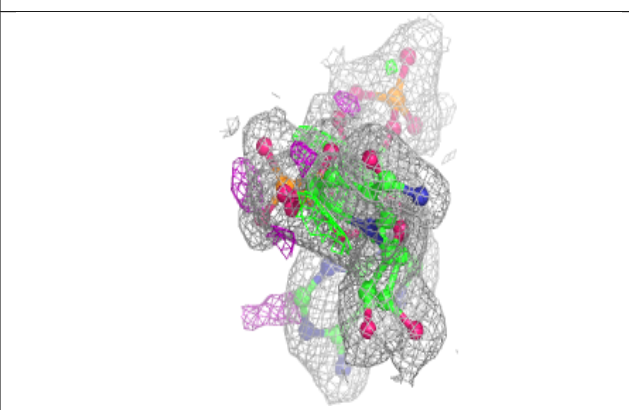
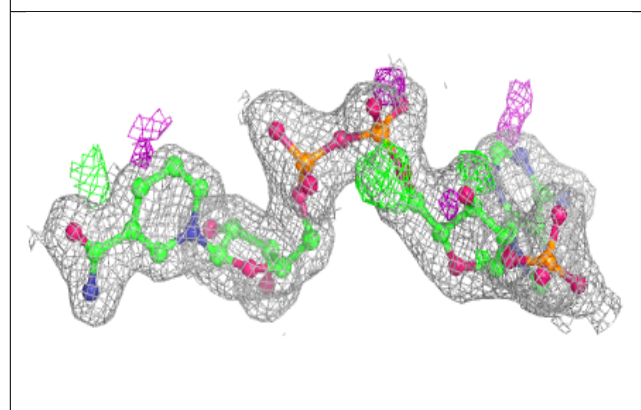
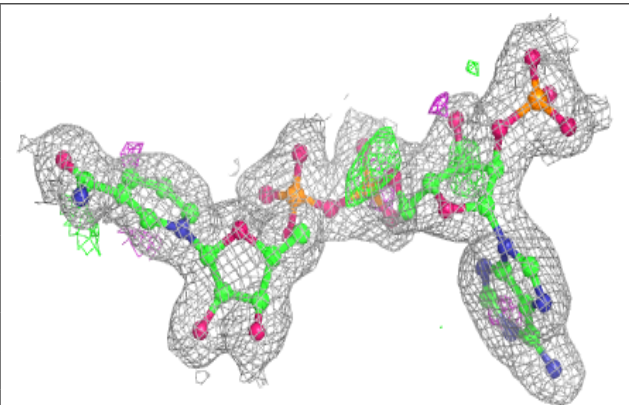


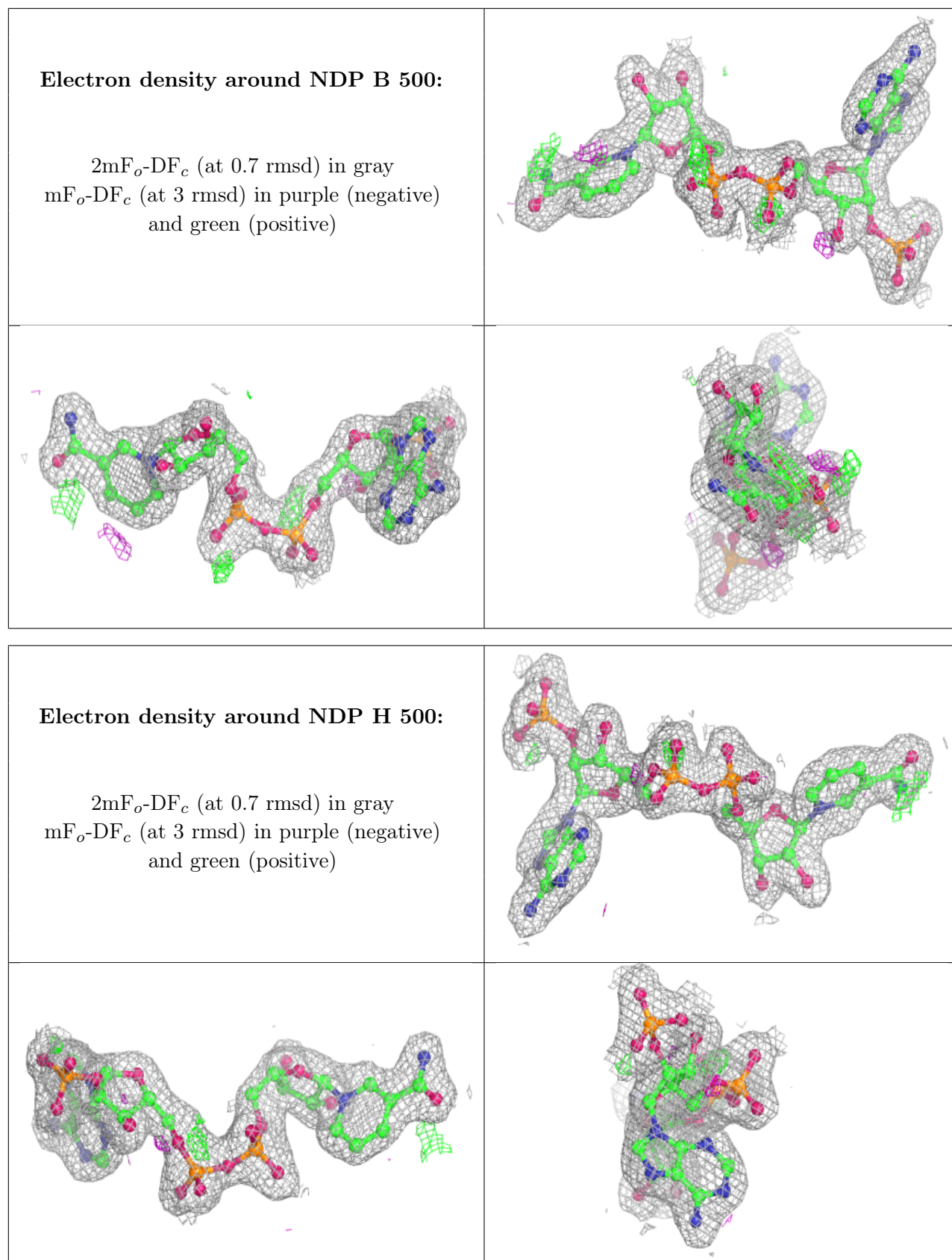
Electron density around NDP D 500:

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

**Electron density around NDP E 500:**

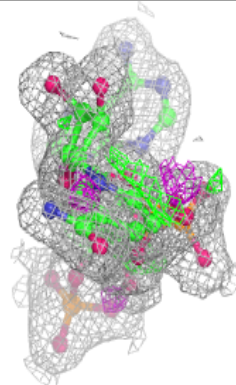
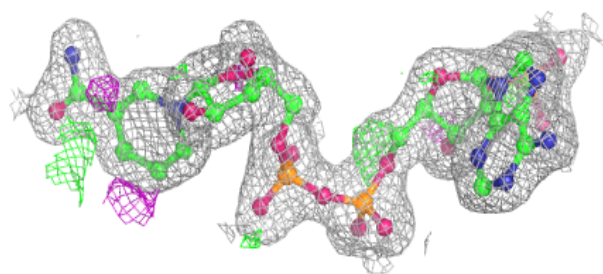
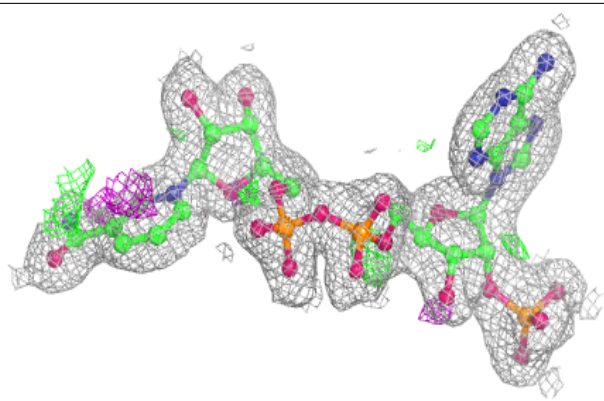
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



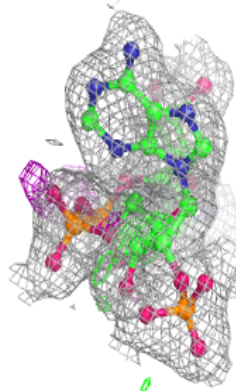
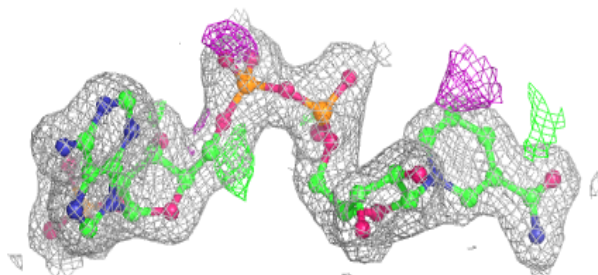
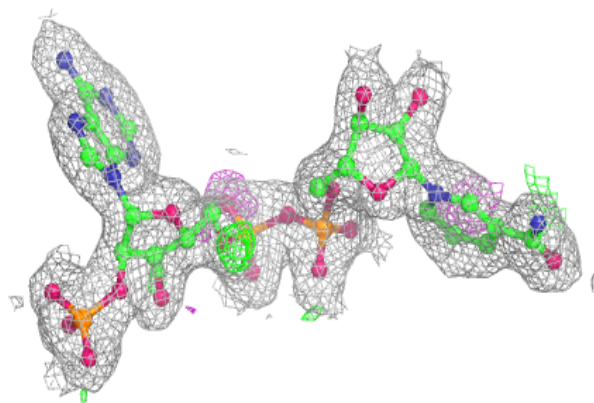


Electron density around NDP I 500:

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

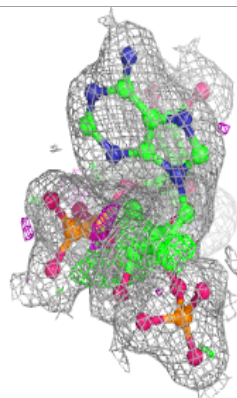
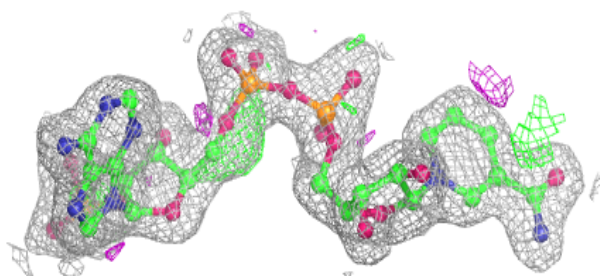
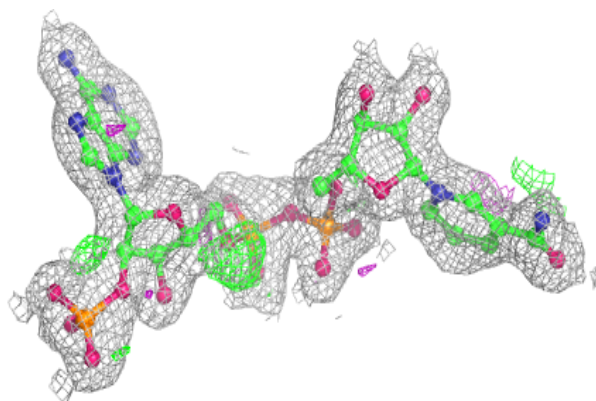
**Electron density around NDP J 500:**

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

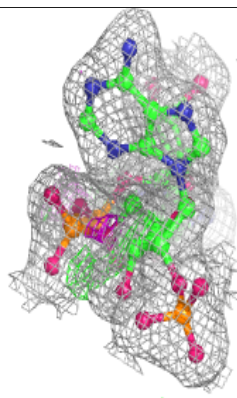
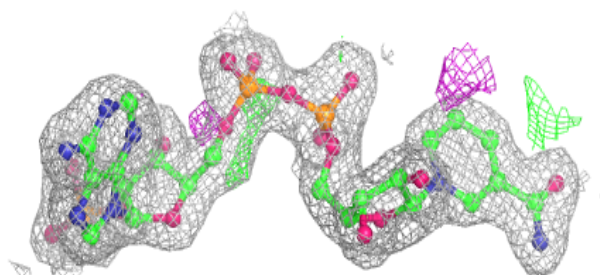
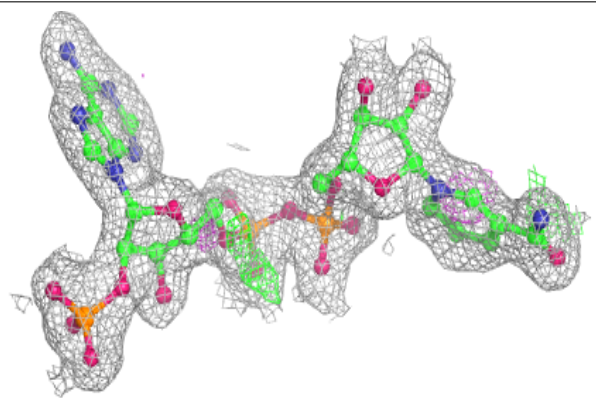


Electron density around NDP K 500:

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

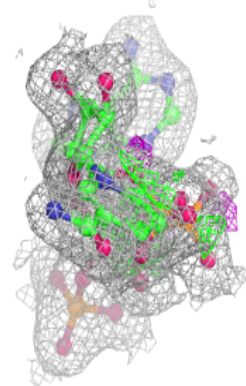
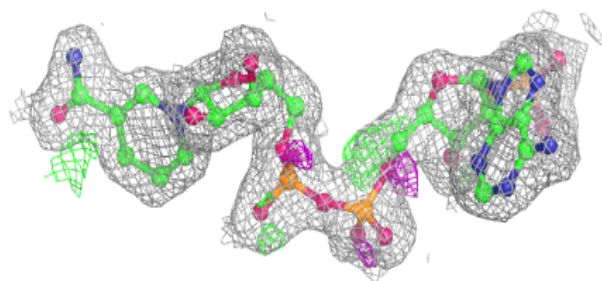
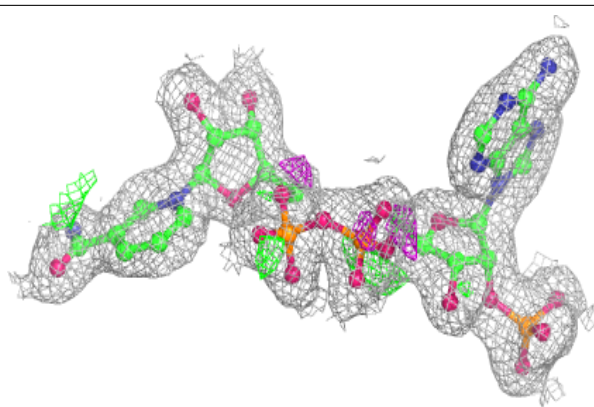
**Electron density around NDP L 500:**

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

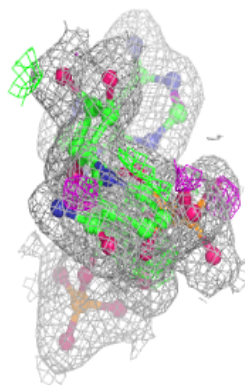
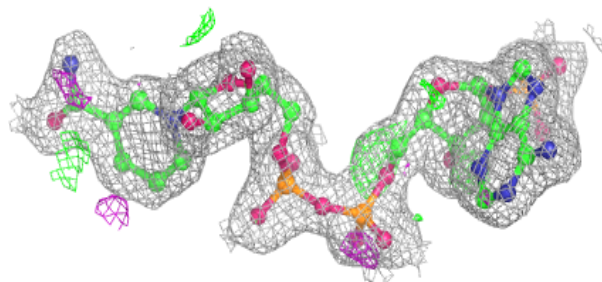
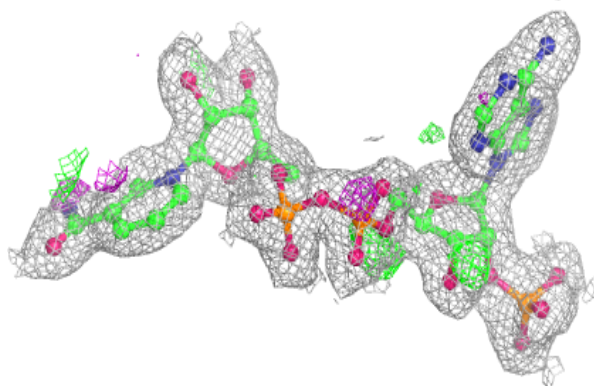


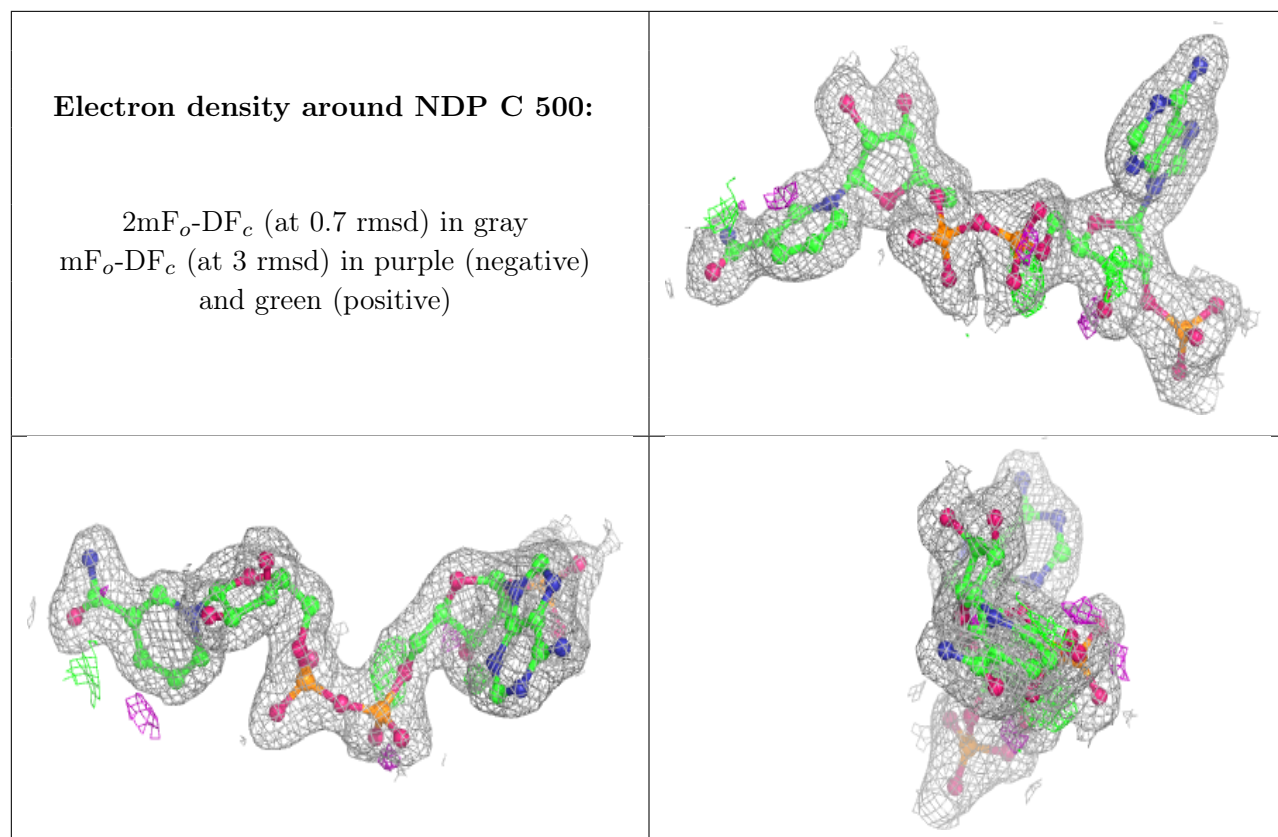
Electron density around NDP A 500:

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

**Electron density around NDP G 500:**

$2mF_o-DF_c$ (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.