



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 12, 2026 – 07:18 PM UTC

PDB ID : 1H6D / pdb_00001h6d
Title : Oxidized Precursor Form of Glucose-Fructose Oxidoreductase from *Zymomonas 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

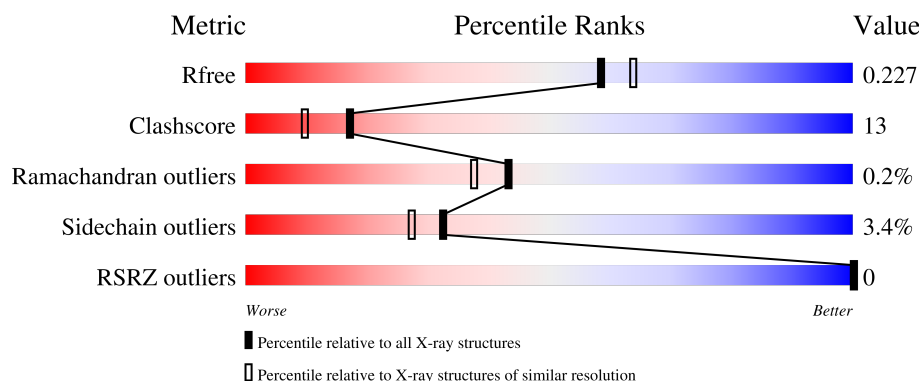
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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}	180053	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (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	 73% 15% • 12%
1	B	433	 67% 20% • 12%
1	C	433	 71% 16% • 12%
1	D	433	 61% 25% • 12%
1	E	433	 70% 16% • 12%

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Mol	Chain	Length	Quality of chain
1	F	433	 58% 28% • 12%
1	G	433	 69% 17% • 12%
1	H	433	 66% 19% • 12%
1	I	433	 72% 14% • 12%
1	J	433	 75% 12% • 12%
1	K	433	 74% 12% • 12%
1	L	433	 71% 15% • 12%

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	E	600[A]	-	-	X	-
3	GOL	L	600[A]	-	-	X	-

2 Entry composition

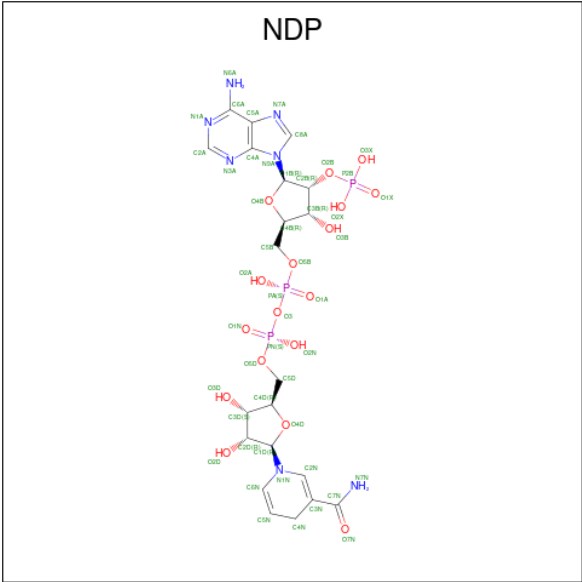
There are 4 unique types of molecules in this entry. The entry contains 40164 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: 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		

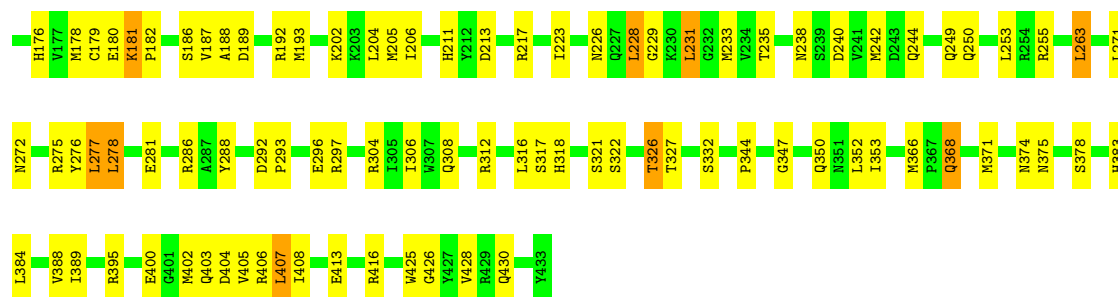
- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

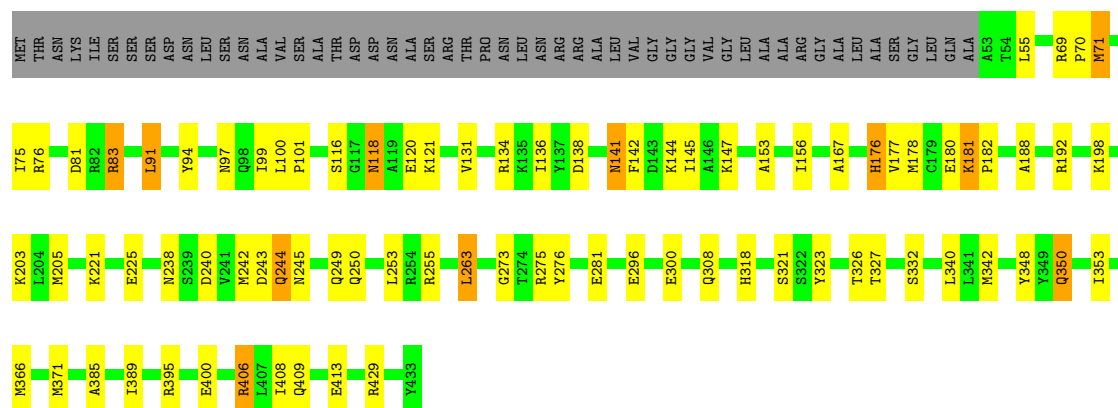
- Molecule 4 is water.

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



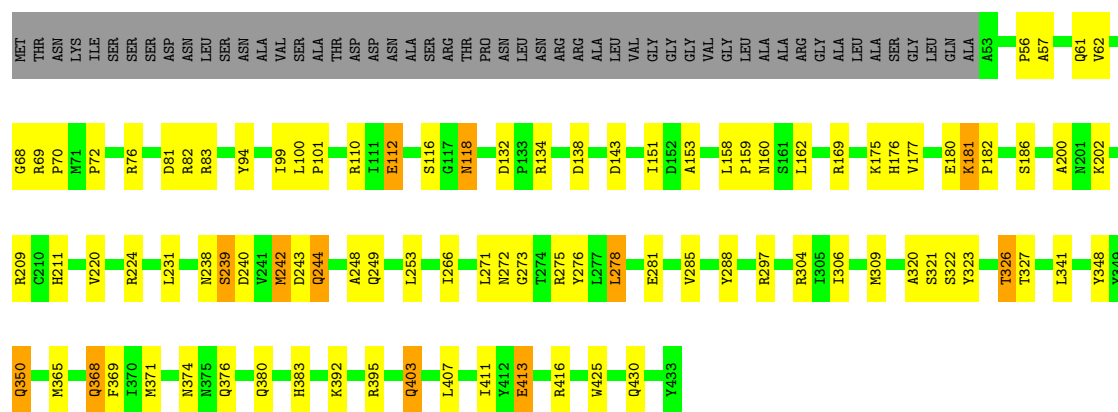
• Molecule 1: PRECURSOR FORM OF GLUCOSE-FRUCTOSE OXIDOREDUCTASE

Chain G: 69% 17% 12%



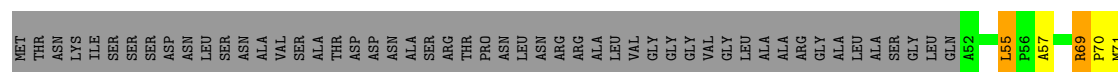
• Molecule 1: PRECURSOR FORM OF GLUCOSE-FRUCTOSE OXIDOREDUCTASE

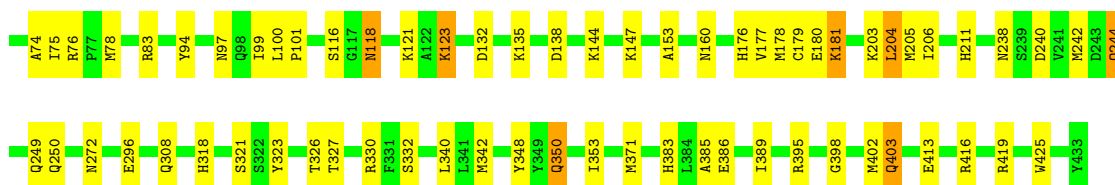
Chain H: 66% 19% 12%



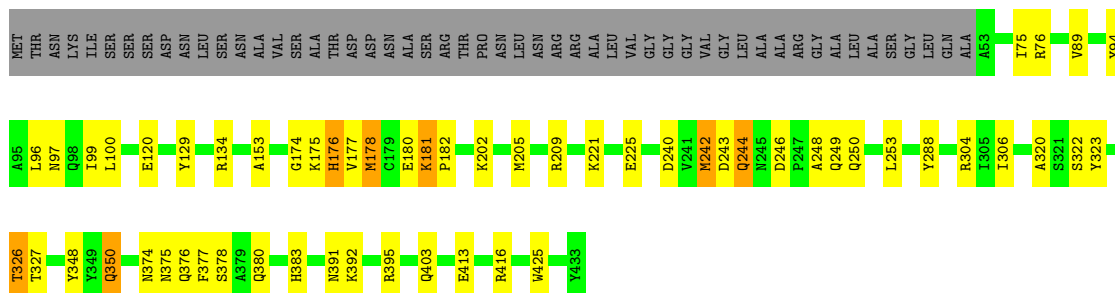
• Molecule 1: PRECURSOR FORM OF GLUCOSE-FRUCTOSE OXIDOREDUCTASE

Chain I: 72% 14% 12%

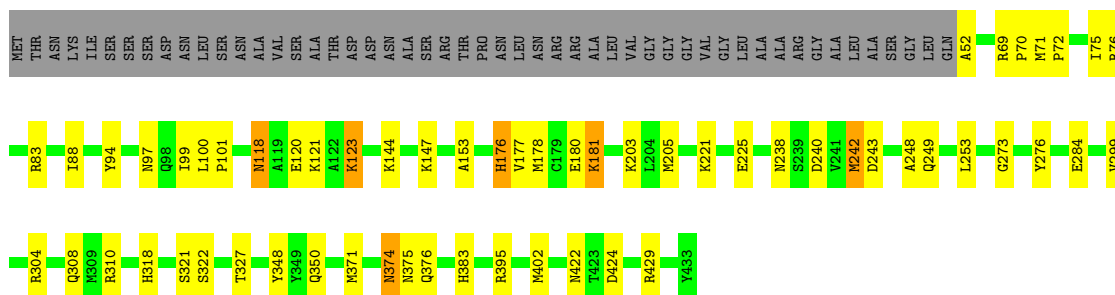




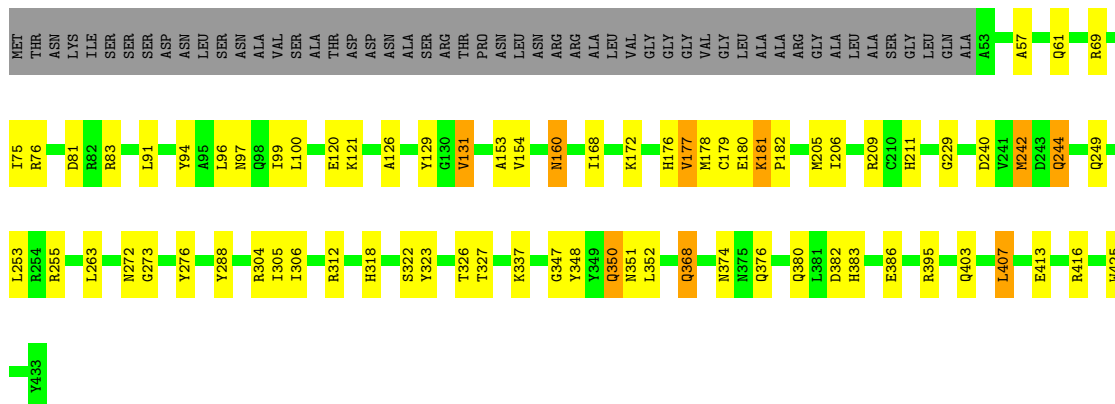
• Molecule 1: PRECURSOR FORM OF GLUCOSE-FRUCTOSE OXIDOREDUCTASE



- Molecule 1: PRECURSOR FORM OF GLUCOSE-FRUCTOSE OXIDOREDUCTASE



- Molecule 1: PRECURSOR FORM OF GLUCOSE-FRUCTOSE OXIDOREDUCTASE



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 15.00 – 2.05	Depositor EDS
% Data completeness (in resolution range)	95.1 (15.00-2.05) 95.2 (15.00-2.05)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.11 (at 2.05Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.197 , 0.228 0.197 , 0.227	Depositor DCC
R_{free} test set	1557 reflections (0.49%)	wwPDB-VP
Wilson B-factor (Å ²)	21.6	Xtriage
Anisotropy	0.317	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 43.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.476 for h,-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	40164	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage'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 ⓘ

5.1 Standard geometry ⓘ

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	0.39	0/3034	0.90	9/4107 (0.2%)
1	B	0.35	0/3024	0.89	7/4093 (0.2%)
1	C	0.38	0/3029	0.88	7/4100 (0.2%)
1	D	0.35	0/3029	0.87	9/4100 (0.2%)
1	E	0.39	0/3029	0.90	11/4100 (0.3%)
1	F	0.35	0/3024	0.90	10/4093 (0.2%)
1	G	0.38	0/3024	0.90	10/4093 (0.2%)
1	H	0.36	1/3024 (0.0%)	0.89	6/4093 (0.1%)
1	I	0.40	0/3029	0.91	9/4100 (0.2%)
1	J	0.38	0/3024	0.90	6/4093 (0.1%)
1	K	0.42	1/3029 (0.0%)	0.91	9/4100 (0.2%)
1	L	0.39	0/3024	0.91	7/4093 (0.2%)
All	All	0.38	2/36323 (0.0%)	0.90	100/49165 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	242	MET	SD-CE	-6.65	1.62	1.79
1	H	242	MET	SD-CE	-5.60	1.65	1.79

The worst 5 of 100 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	99	ILE	N-CA-C	9.04	118.92	110.42
1	F	99	ILE	N-CA-C	8.01	118.06	110.53
1	K	99	ILE	N-CA-C	7.74	117.69	110.42
1	C	99	ILE	N-CA-C	7.50	117.47	110.42
1	E	99	ILE	N-CA-C	7.40	117.37	110.42

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2970	0	2927	60	0
1	B	2960	0	2920	76	0
1	C	2965	0	2925	73	0
1	D	2965	0	2925	100	0
1	E	2965	0	2925	72	0
1	F	2960	0	2920	112	0
1	G	2960	0	2920	72	0
1	H	2960	0	2920	82	0
1	I	2965	0	2925	70	0
1	J	2960	0	2920	67	0
1	K	2965	0	2925	64	0
1	L	2960	0	2920	73	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	5	0
3	E	7	0	6	7	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	4	0
4	E	341	0	0	5	0
4	F	219	0	0	6	0
4	G	371	0	0	8	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	6	0
4	L	357	0	0	3	0
All	All	40164	0	35456	900	0

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

The worst 5 of 900 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:242:MET:HE1	1:H:249:GLN:HB3	1.22	1.17
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

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%)	36	30
1	D	380/433 (88%)	364 (96%)	15 (4%)	1 (0%)	36	30
1	E	380/433 (88%)	368 (97%)	11 (3%)	1 (0%)	36	30
1	F	379/433 (88%)	364 (96%)	15 (4%)	0	100	100
1	G	379/433 (88%)	367 (97%)	11 (3%)	1 (0%)	36	30
1	H	379/433 (88%)	365 (96%)	14 (4%)	0	100	100
1	I	380/433 (88%)	369 (97%)	10 (3%)	1 (0%)	36	30
1	J	379/433 (88%)	367 (97%)	12 (3%)	0	100	100
1	K	380/433 (88%)	367 (97%)	12 (3%)	1 (0%)	36	30
1	L	379/433 (88%)	366 (97%)	12 (3%)	1 (0%)	36	30
All	All	4555/5196 (88%)	4399 (97%)	149 (3%)	7 (0%)	43	37

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 ⓘ

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%)	302 (98%)	6 (2%)	50	50
1	B	308/345 (89%)	291 (94%)	17 (6%)	19	12
1	C	308/345 (89%)	301 (98%)	7 (2%)	44	42
1	D	308/345 (89%)	297 (96%)	11 (4%)	31	26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	308/345 (89%)	301 (98%)	7 (2%)	44	42
1	F	308/345 (89%)	293 (95%)	15 (5%)	22	15
1	G	308/345 (89%)	297 (96%)	11 (4%)	31	26
1	H	308/345 (89%)	291 (94%)	17 (6%)	19	12
1	I	308/345 (89%)	298 (97%)	10 (3%)	34	29
1	J	308/345 (89%)	300 (97%)	8 (3%)	40	37
1	K	308/345 (89%)	303 (98%)	5 (2%)	55	56
1	L	308/345 (89%)	298 (97%)	10 (3%)	34	29
All	All	3696/4140 (89%)	3572 (97%)	124 (3%)	32	27

5 of 124 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	278	LEU
1	K	123	LYS
1	G	323	TYR
1	K	118	ASN
1	L	244	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 210 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	360	HIS
1	I	245	ASN
1	L	318	HIS
1	H	98	GLN
1	H	374	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 oligosaccharides 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	$\# Z > 2$
2	NDP	D	500	-	51,52,52	1.72	14 (27%)	71,80,80	1.67	13 (18%)
3	GOL	A	600[B]	-	5,5,5	1.02	0	5,5,5	0.51	0
3	GOL	L	600[A]	-	5,5,5	0.94	0	5,5,5	0.52	0
3	GOL	C	600[B]	-	5,5,5	1.01	0	5,5,5	0.52	0
2	NDP	G	500	-	51,52,52	1.73	13 (25%)	71,80,80	1.73	13 (18%)
3	GOL	F	600[B]	-	5,5,5	0.99	0	5,5,5	0.52	0
2	NDP	A	500	-	51,52,52	1.73	13 (25%)	71,80,80	1.72	13 (18%)
3	GOL	E	600[B]	-	5,5,5	0.98	0	5,5,5	0.52	0
3	GOL	H	600[A]	-	5,5,5	0.97	0	5,5,5	0.52	0
2	NDP	K	500	-	51,52,52	1.68	12 (23%)	71,80,80	1.73	13 (18%)
3	GOL	I	600[B]	-	5,5,5	0.96	0	5,5,5	0.52	0
3	GOL	K	600[B]	-	5,5,5	0.94	0	5,5,5	0.52	0
3	GOL	A	600[A]	-	5,5,5	1.03	0	5,5,5	0.51	0
3	GOL	B	600[B]	-	5,5,5	1.01	0	5,5,5	0.51	0
3	GOL	C	600[A]	-	5,5,5	1.02	0	5,5,5	0.52	0
3	GOL	G	600[B]	-	5,5,5	0.99	0	5,5,5	0.52	0
3	GOL	J	600[B]	-	5,5,5	0.95	0	5,5,5	0.52	0
3	GOL	F	600[A]	-	5,5,5	0.99	0	5,5,5	0.52	0
3	GOL	E	600[A]	-	5,5,5	0.99	0	5,5,5	0.52	0
3	GOL	I	600[A]	-	5,5,5	0.96	0	5,5,5	0.52	0
3	GOL	D	600[B]	-	5,5,5	1.00	0	5,5,5	0.52	0
2	NDP	E	500	-	51,52,52	1.71	12 (23%)	71,80,80	1.70	12 (16%)
2	NDP	L	500	-	51,52,52	1.69	12 (23%)	71,80,80	1.72	13 (18%)
3	GOL	K	600[A]	-	5,5,5	0.94	0	5,5,5	0.52	0
3	GOL	L	600[B]	-	5,5,5	0.94	0	5,5,5	0.52	0
3	GOL	G	600[A]	-	5,5,5	0.99	0	5,5,5	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GOL	B	600[A]	-	5,5,5	1.01	0	5,5,5	0.51	0
3	GOL	J	600[A]	-	5,5,5	0.95	0	5,5,5	0.52	0
2	NDP	C	500	-	51,52,52	1.68	13 (25%)	71,80,80	1.68	12 (16%)
2	NDP	B	500	-	51,52,52	1.70	13 (25%)	71,80,80	1.71	12 (16%)
2	NDP	J	500	-	51,52,52	1.72	13 (25%)	71,80,80	1.70	12 (16%)
3	GOL	H	600[B]	-	5,5,5	0.97	0	5,5,5	0.52	0
2	NDP	F	500	-	51,52,52	1.73	14 (27%)	71,80,80	1.67	13 (18%)
2	NDP	H	500	-	51,52,52	1.69	14 (27%)	71,80,80	1.69	12 (16%)
3	GOL	D	600[A]	-	5,5,5	1.00	0	5,5,5	0.52	0
2	NDP	I	500	-	51,52,52	1.69	14 (27%)	71,80,80	1.74	12 (16%)

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	D	500	-	-	8/34/77/77	0/5/5/5
3	GOL	A	600[B]	-	-	1/4/4/4	-
3	GOL	L	600[A]	-	-	1/4/4/4	-
3	GOL	C	600[B]	-	-	1/4/4/4	-
2	NDP	G	500	-	-	6/34/77/77	0/5/5/5
3	GOL	F	600[B]	-	-	1/4/4/4	-
2	NDP	A	500	-	-	5/34/77/77	0/5/5/5
3	GOL	E	600[B]	-	-	1/4/4/4	-
3	GOL	H	600[A]	-	-	1/4/4/4	-
2	NDP	K	500	-	-	5/34/77/77	0/5/5/5
3	GOL	I	600[B]	-	-	3/4/4/4	-
3	GOL	K	600[B]	-	-	1/4/4/4	-
3	GOL	A	600[A]	-	-	1/4/4/4	-
3	GOL	B	600[B]	-	-	1/4/4/4	-
3	GOL	C	600[A]	-	-	1/4/4/4	-
3	GOL	G	600[B]	-	-	1/4/4/4	-
3	GOL	J	600[B]	-	-	1/4/4/4	-
3	GOL	F	600[A]	-	-	1/4/4/4	-
3	GOL	E	600[A]	-	-	1/4/4/4	-
3	GOL	I	600[A]	-	-	1/4/4/4	-
3	GOL	D	600[B]	-	-	1/4/4/4	-
2	NDP	E	500	-	-	7/34/77/77	0/5/5/5
2	NDP	L	500	-	-	5/34/77/77	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	K	600[A]	-	-	1/4/4/4	-
3	GOL	L	600[B]	-	-	1/4/4/4	-
3	GOL	G	600[A]	-	-	1/4/4/4	-
3	GOL	B	600[A]	-	-	1/4/4/4	-
3	GOL	J	600[A]	-	-	1/4/4/4	-
2	NDP	C	500	-	-	7/34/77/77	0/5/5/5
2	NDP	B	500	-	-	5/34/77/77	0/5/5/5
2	NDP	J	500	-	-	5/34/77/77	0/5/5/5
3	GOL	H	600[B]	-	-	1/4/4/4	-
2	NDP	F	500	-	-	8/34/77/77	0/5/5/5
2	NDP	H	500	-	-	6/34/77/77	0/5/5/5
3	GOL	D	600[A]	-	-	1/4/4/4	-
2	NDP	I	500	-	-	5/34/77/77	0/5/5/5

The worst 5 of 157 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	500	NDP	P2B-O2X	-4.80	1.37	1.54
2	A	500	NDP	P2B-O2X	-4.76	1.37	1.54
2	D	500	NDP	P2B-O2X	-4.74	1.37	1.54
2	K	500	NDP	P2B-O2X	-4.73	1.37	1.54
2	G	500	NDP	P2B-O2X	-4.67	1.37	1.54

The worst 5 of 150 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	500	NDP	C5A-C4A-N3A	-6.16	118.24	126.72
2	H	500	NDP	C5A-C4A-N3A	-6.15	118.25	126.72
2	K	500	NDP	C5A-C4A-N3A	-6.15	118.25	126.72
2	L	500	NDP	C5A-C4A-N3A	-6.14	118.26	126.72
2	D	500	NDP	C5A-C4A-N3A	-6.14	118.26	126.72

There are no chirality outliers.

5 of 98 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

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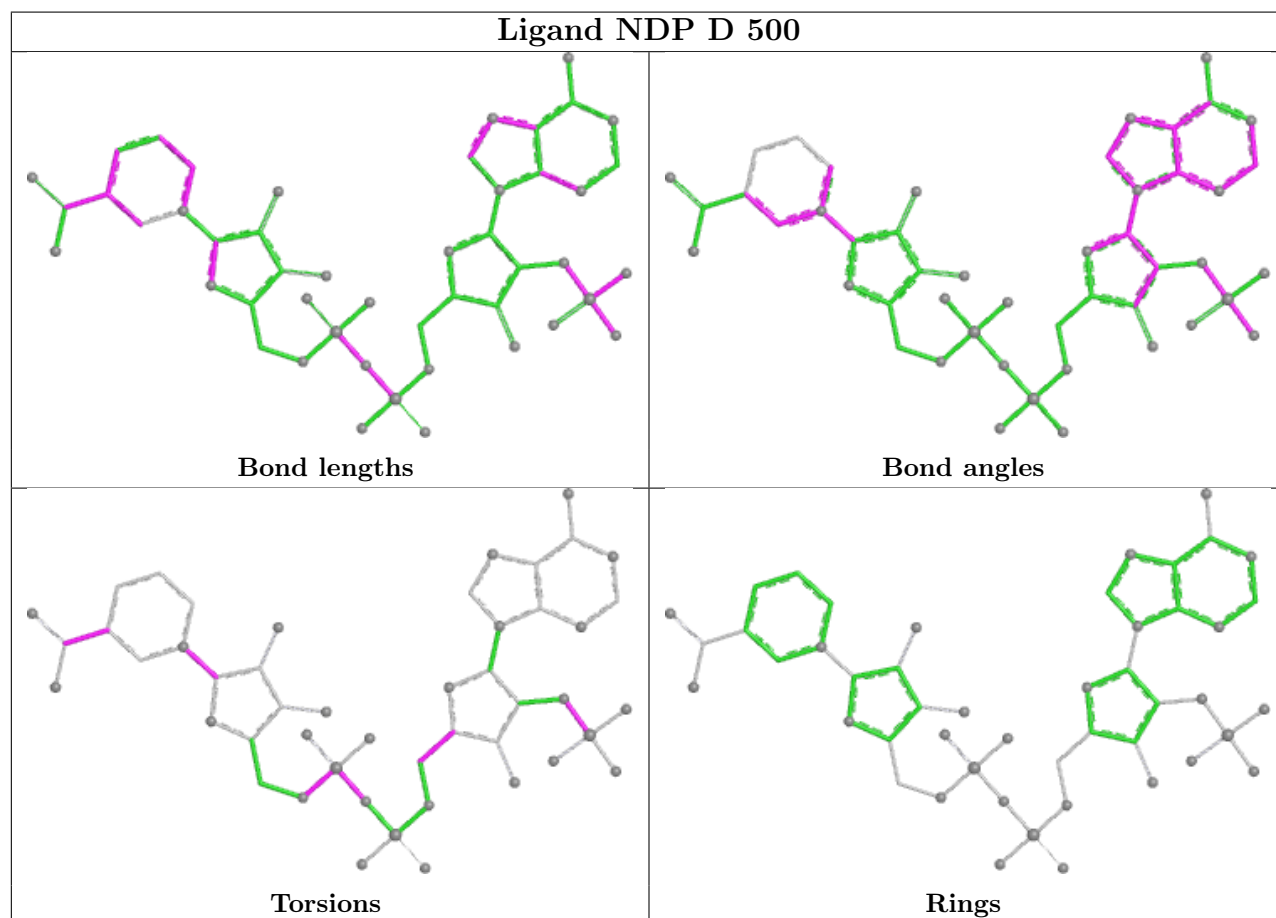
Mol	Chain	Res	Type	Atoms
3	B	600[A]	GOL	O1-C1-C2-C3

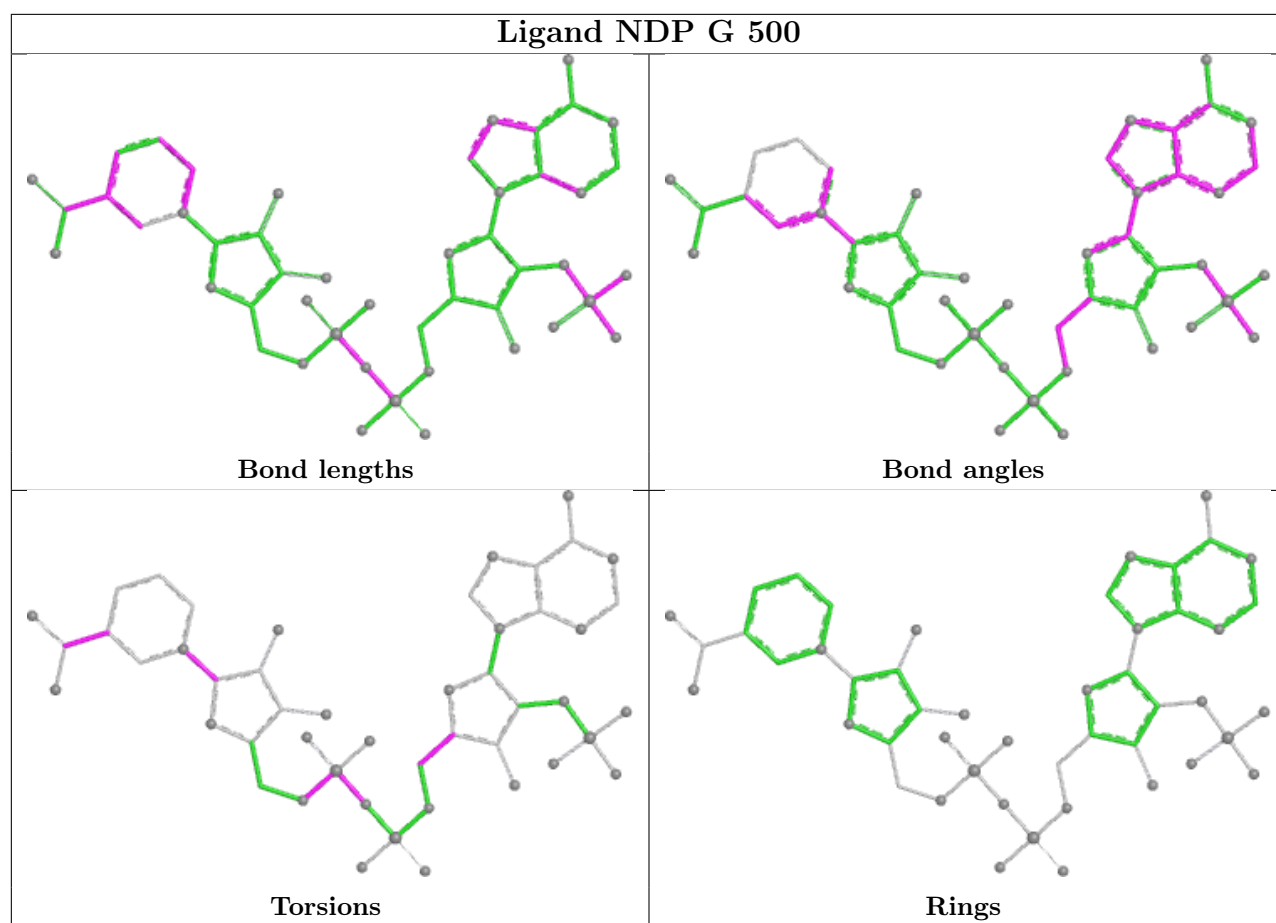
There are no ring outliers.

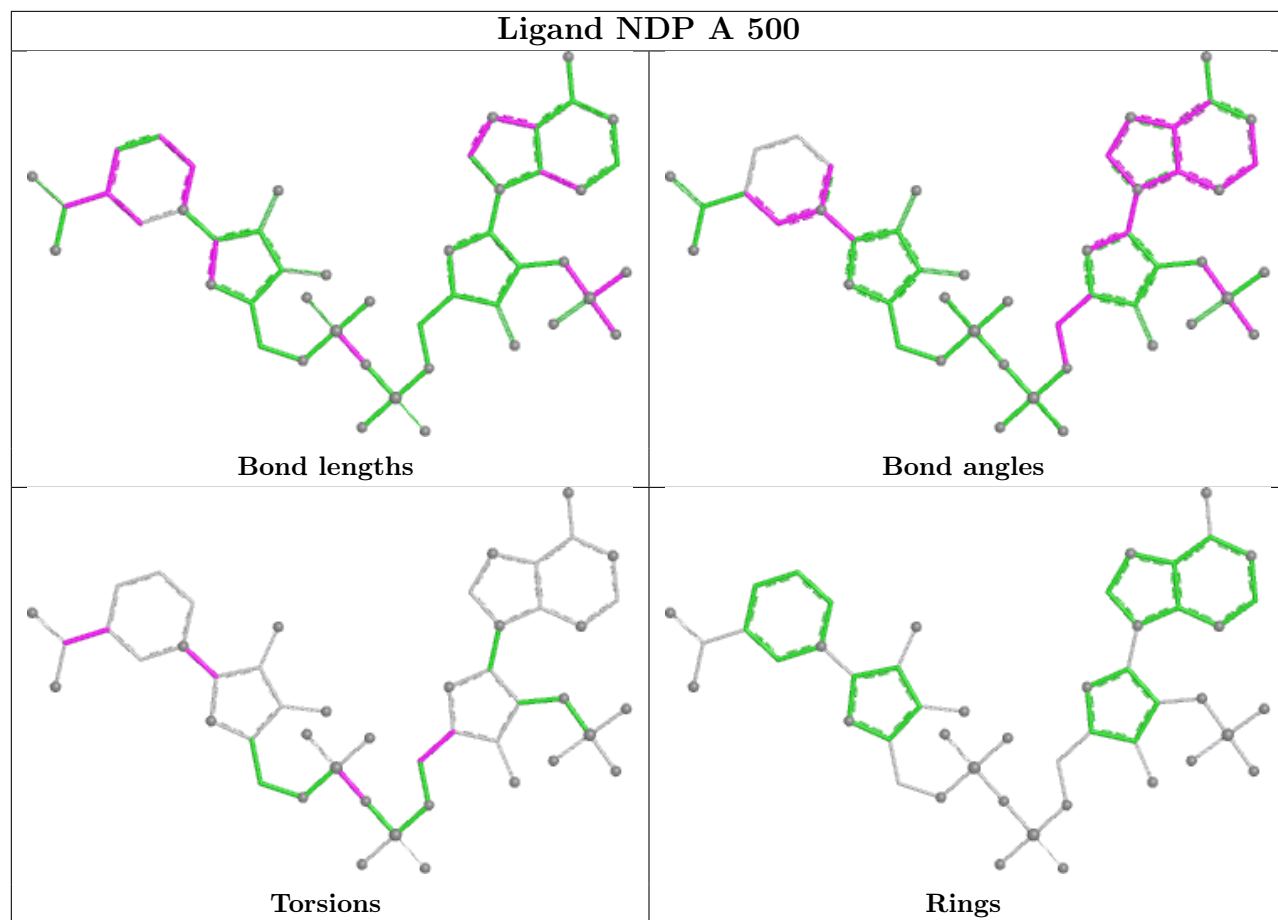
36 monomers are involved in 102 short contacts:

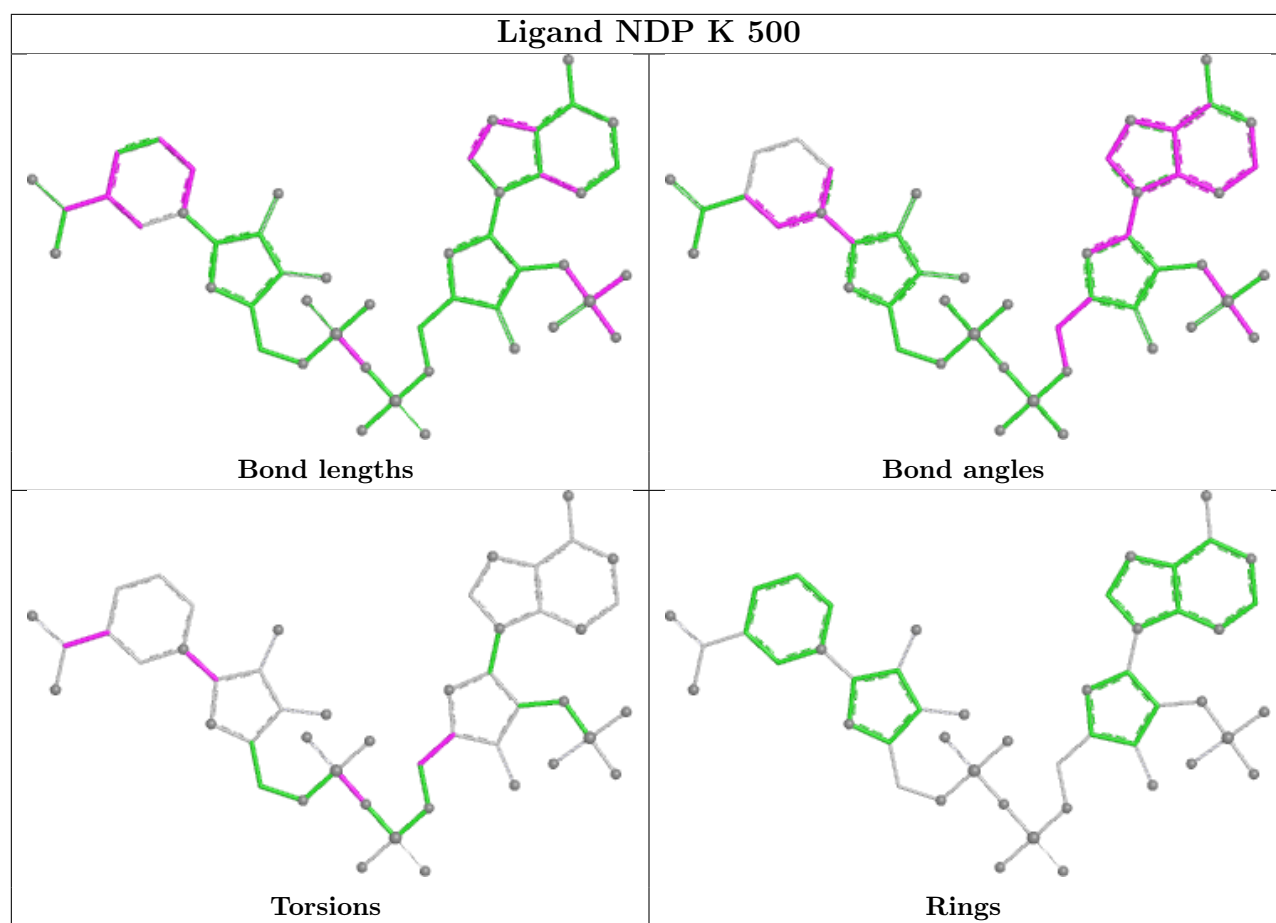
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	500	NDP	10	0
3	A	600[B]	GOL	3	0
3	L	600[A]	GOL	4	0
3	C	600[B]	GOL	3	0
2	G	500	NDP	7	0
3	F	600[B]	GOL	3	0
2	A	500	NDP	7	0
3	E	600[B]	GOL	3	0
3	H	600[A]	GOL	3	0
2	K	500	NDP	9	0
3	I	600[B]	GOL	2	0
3	K	600[B]	GOL	3	0
3	A	600[A]	GOL	2	0
3	B	600[B]	GOL	2	0
3	C	600[A]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

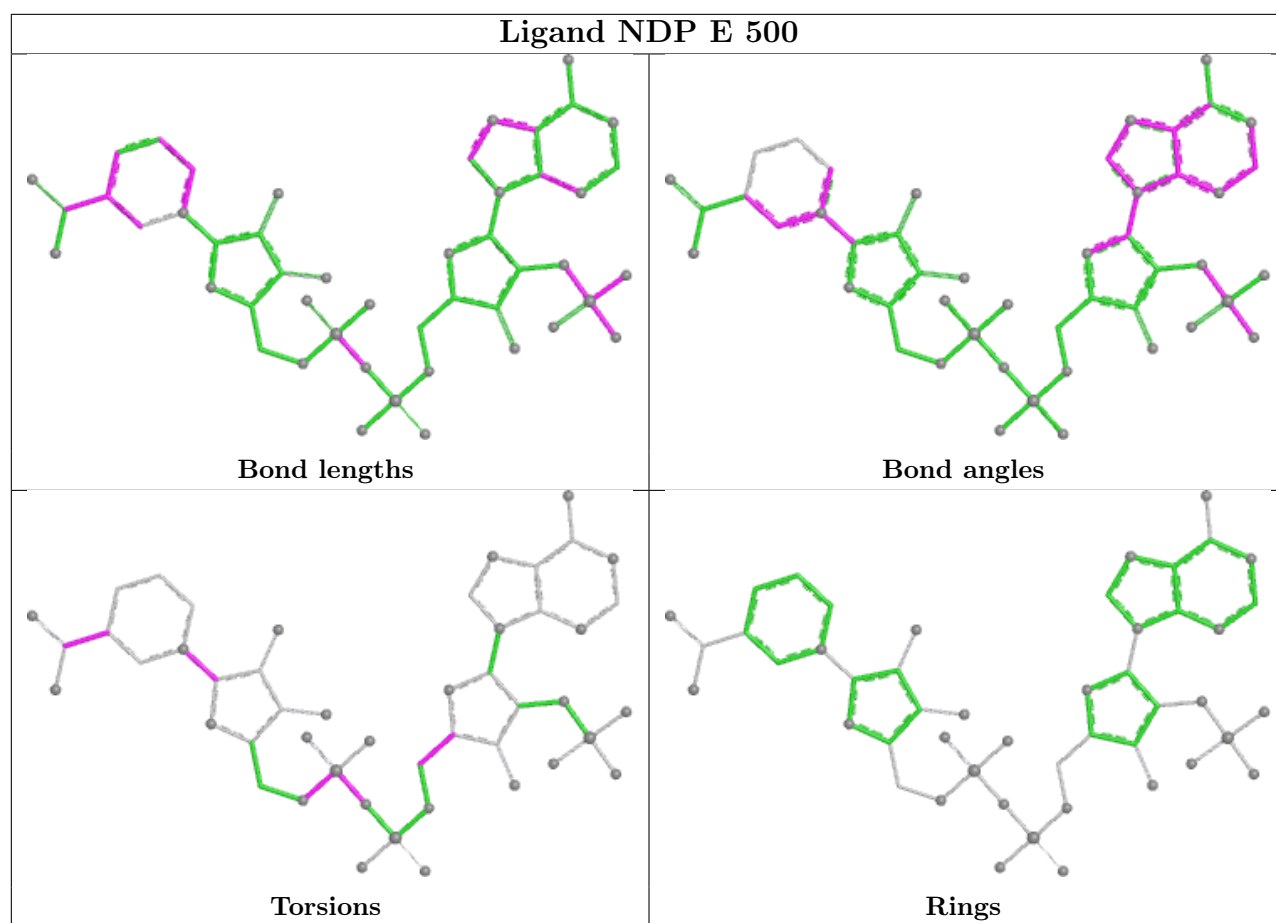
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

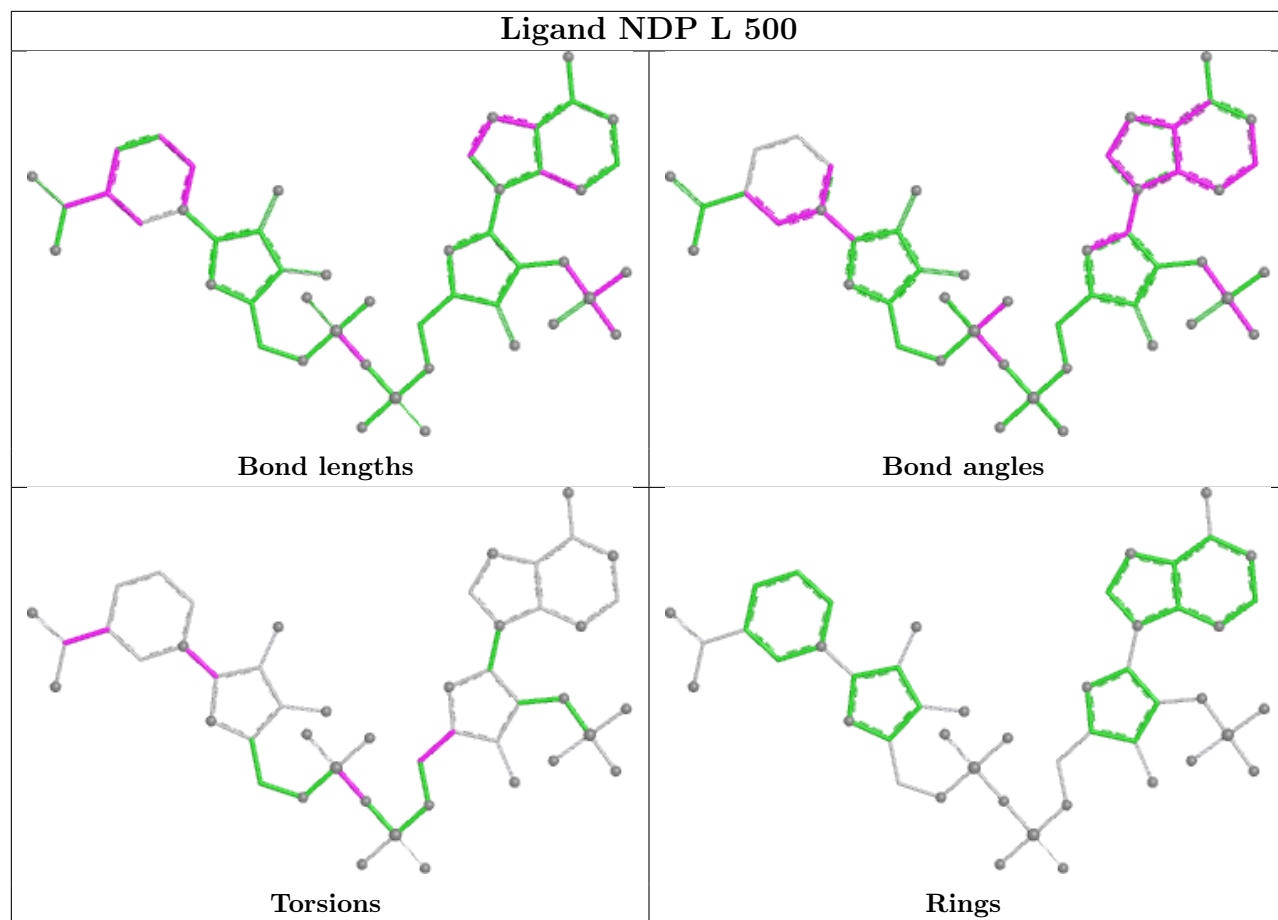


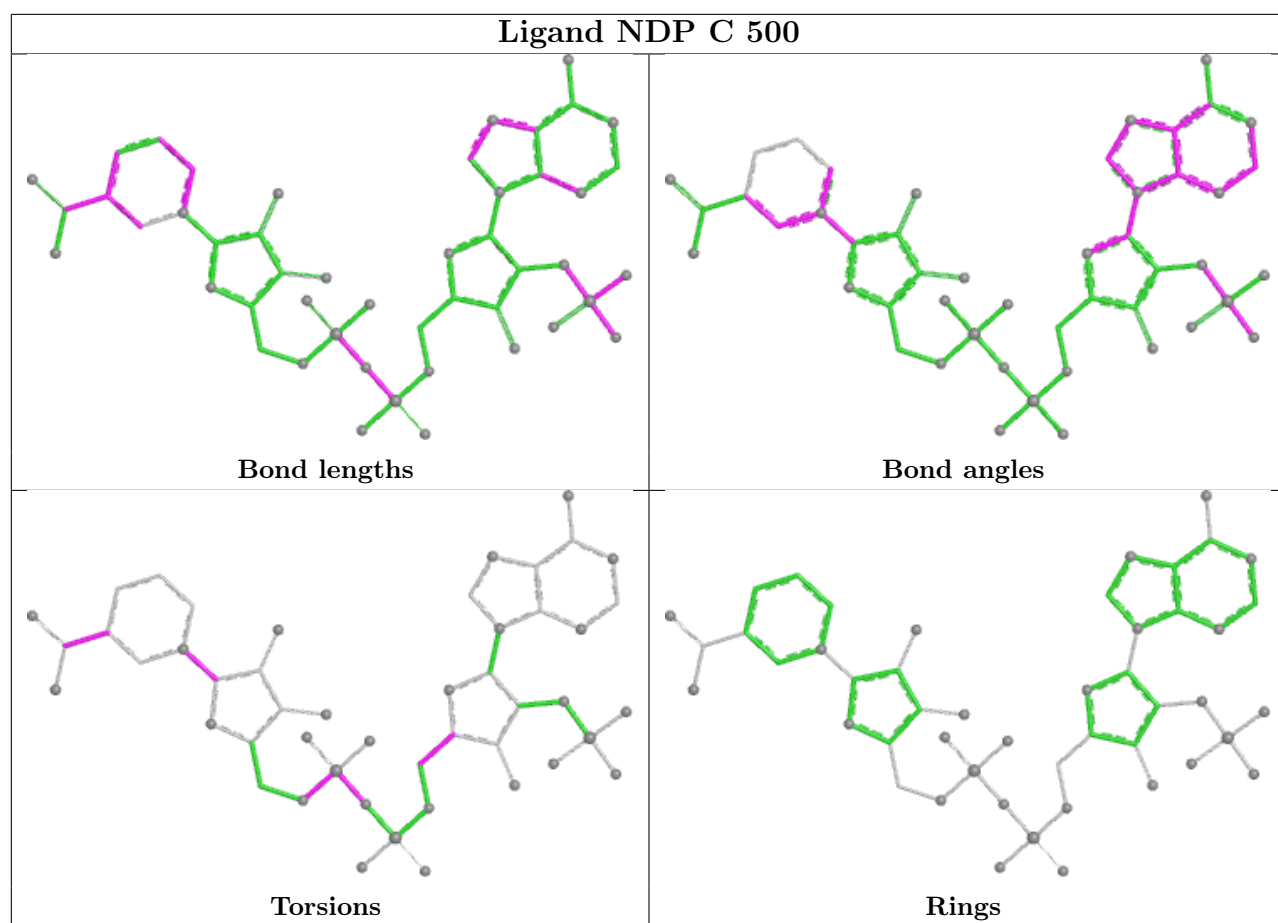


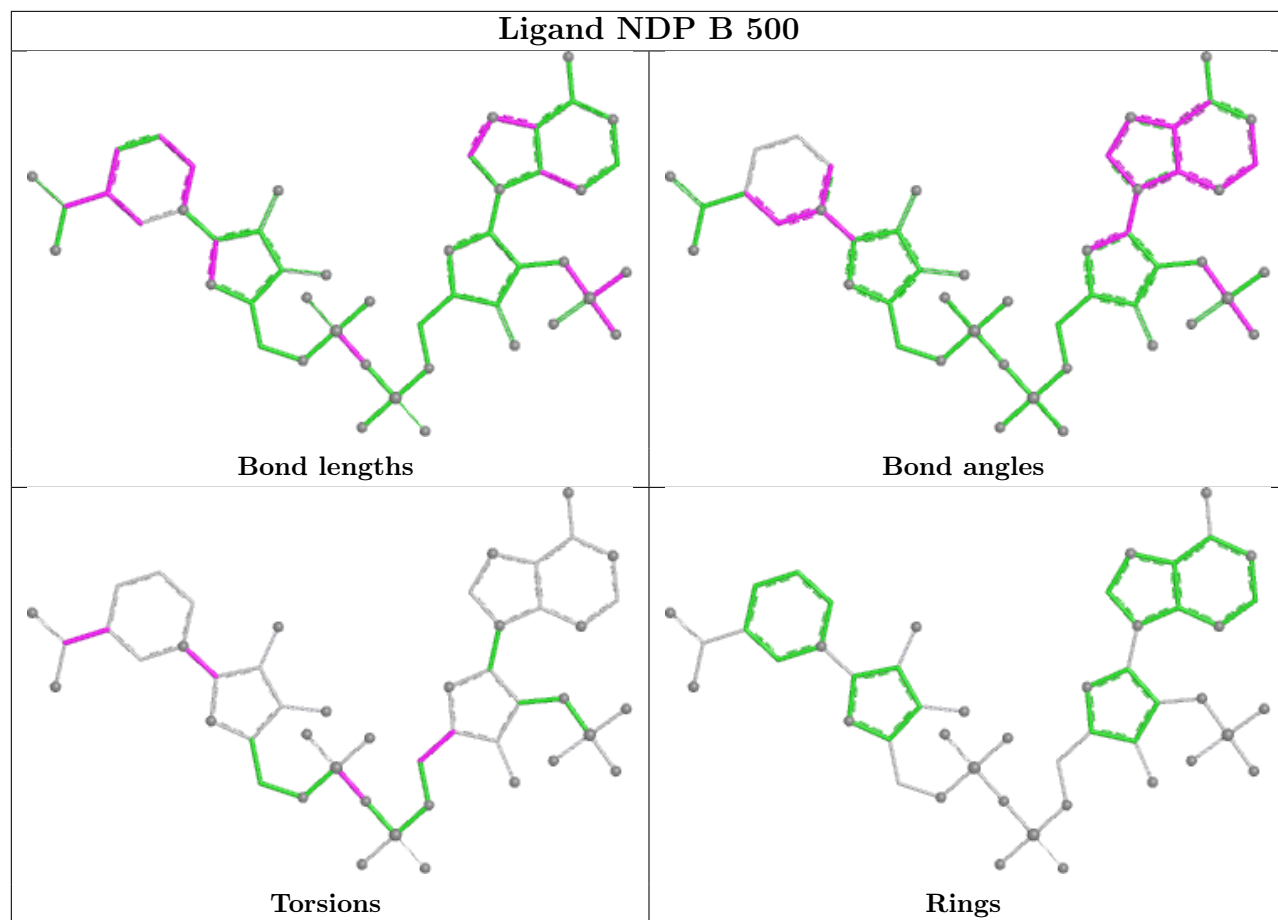


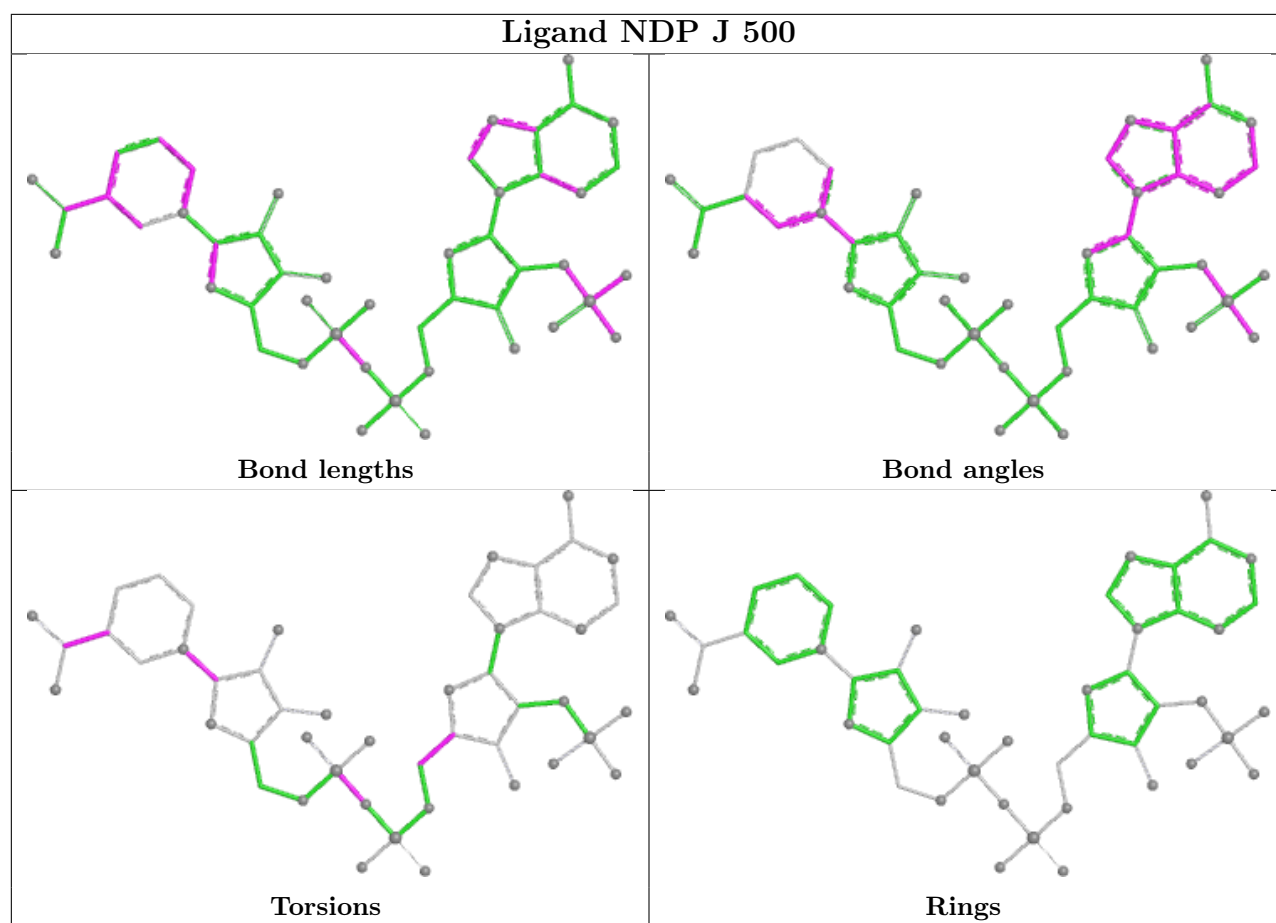


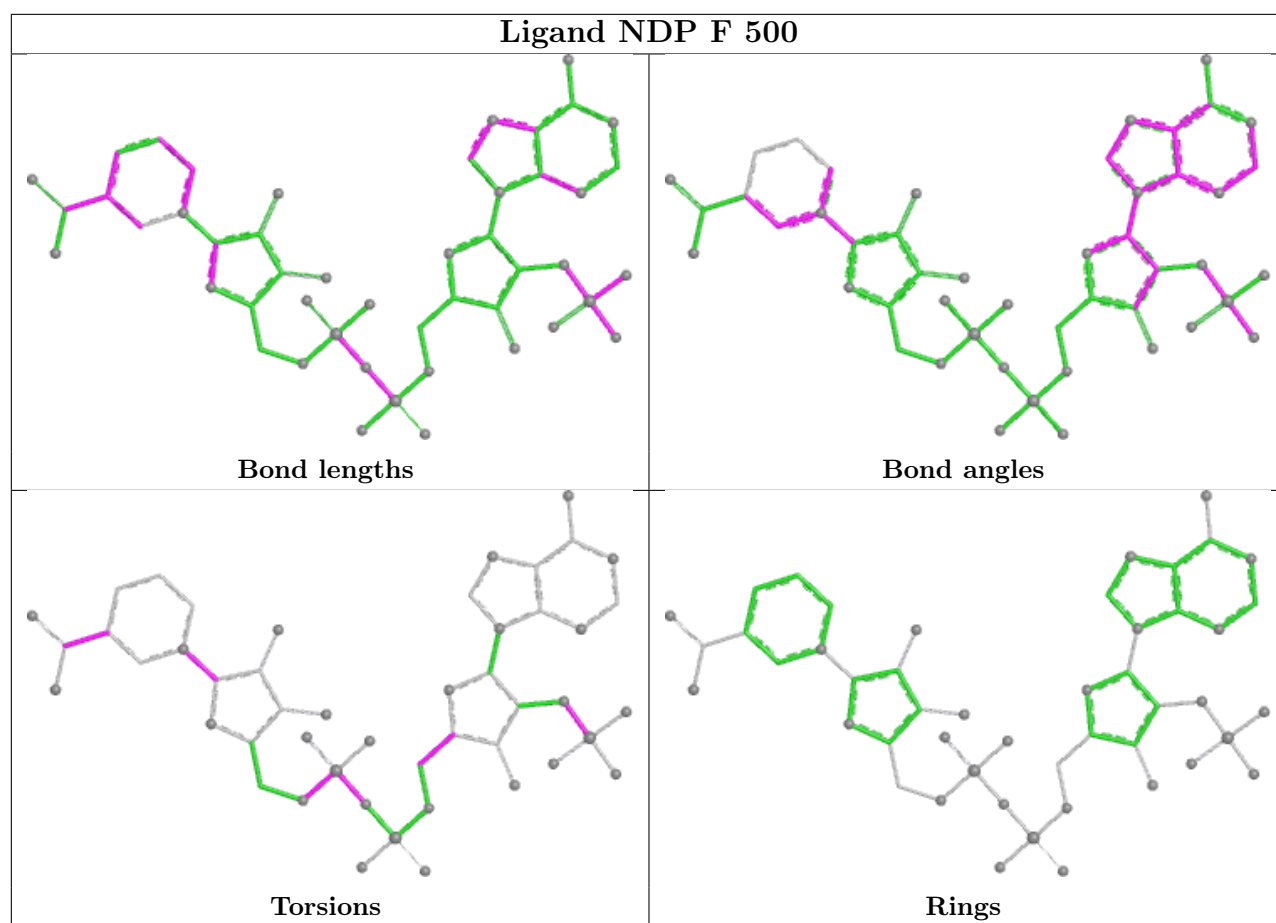


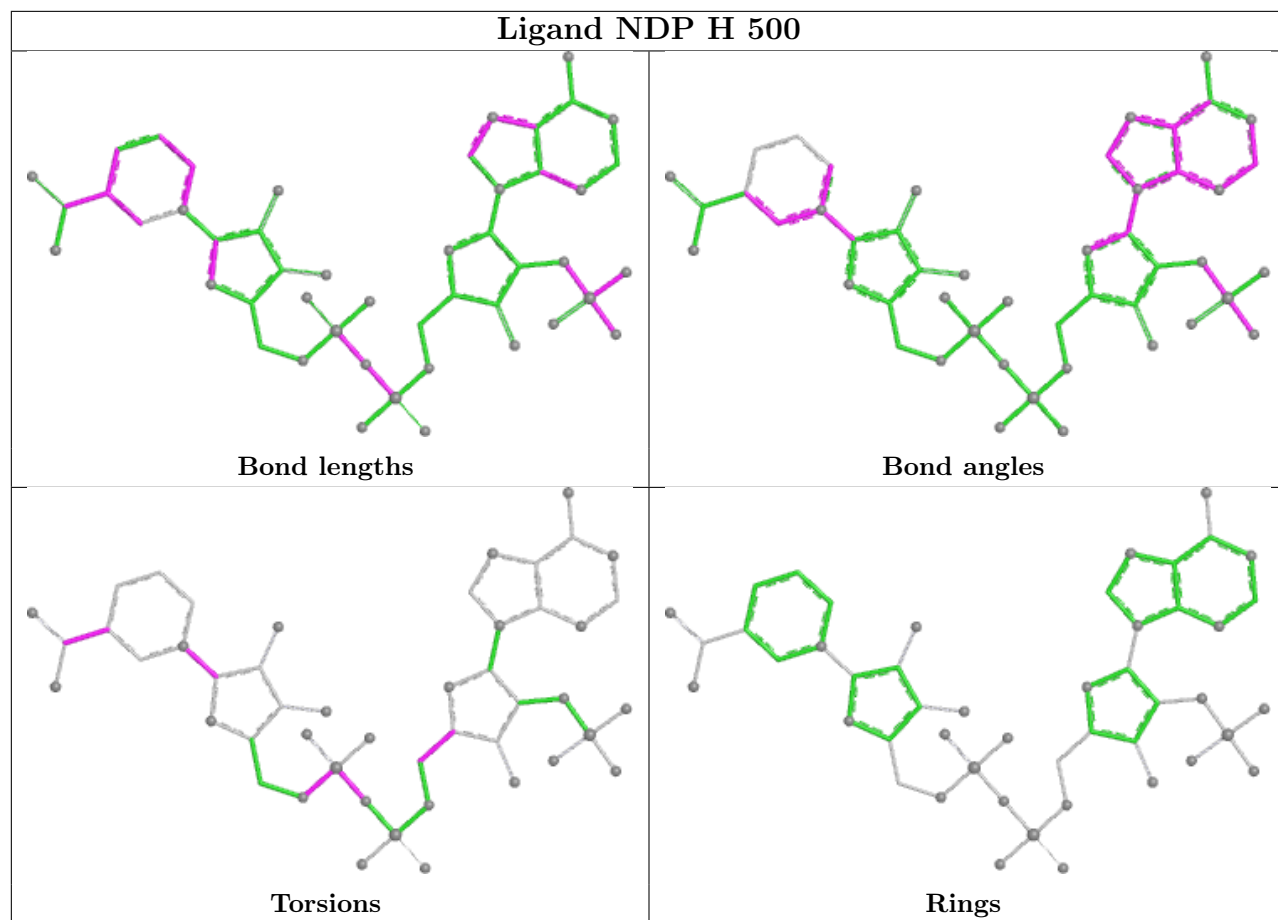


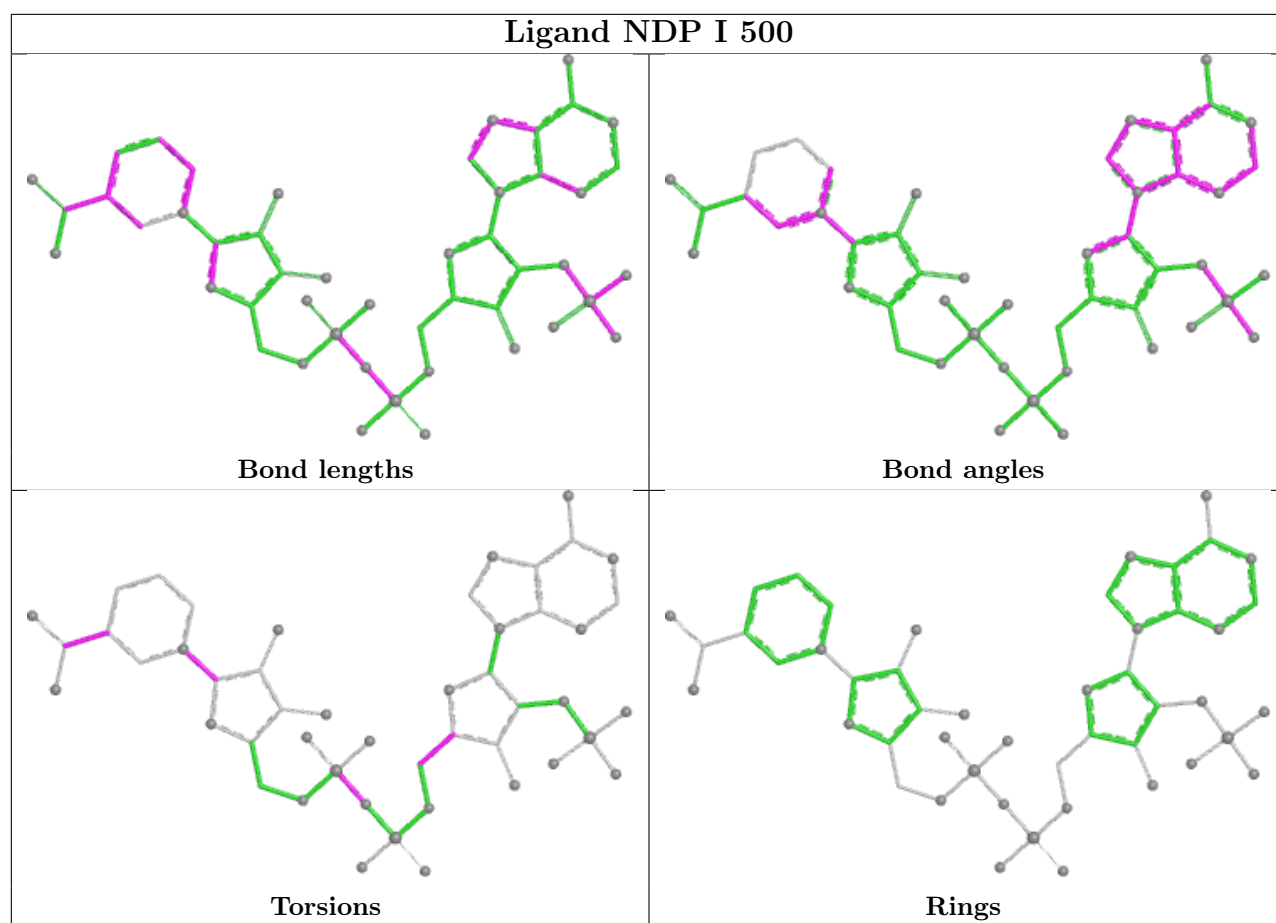












5.7 Other polymers [i](#)

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%)	-1.69	0 100 100	12, 18, 30, 48	0
1	B	381/433 (87%)	-1.64	0 100 100	13, 23, 38, 45	0
1	C	382/433 (88%)	-1.66	0 100 100	14, 21, 32, 45	0
1	D	382/433 (88%)	-1.55	0 100 100	16, 31, 44, 53	0
1	E	382/433 (88%)	-1.66	0 100 100	14, 22, 32, 44	0
1	F	381/433 (87%)	-1.56	0 100 100	16, 30, 46, 52	0
1	G	381/433 (87%)	-1.69	0 100 100	12, 18, 30, 40	0
1	H	381/433 (87%)	-1.64	0 100 100	14, 23, 39, 46	0
1	I	382/433 (88%)	-1.70	0 100 100	10, 16, 28, 39	0
1	J	381/433 (87%)	-1.67	0 100 100	11, 19, 30, 42	0
1	K	382/433 (88%)	-1.70	0 100 100	10, 16, 27, 39	0
1	L	381/433 (87%)	-1.68	0 100 100	11, 19, 29, 40	0
All	All	4579/5196 (88%)	-1.65	0 100 100	10, 21, 38, 53	0

There are no RSRZ outliers to report.

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](#)

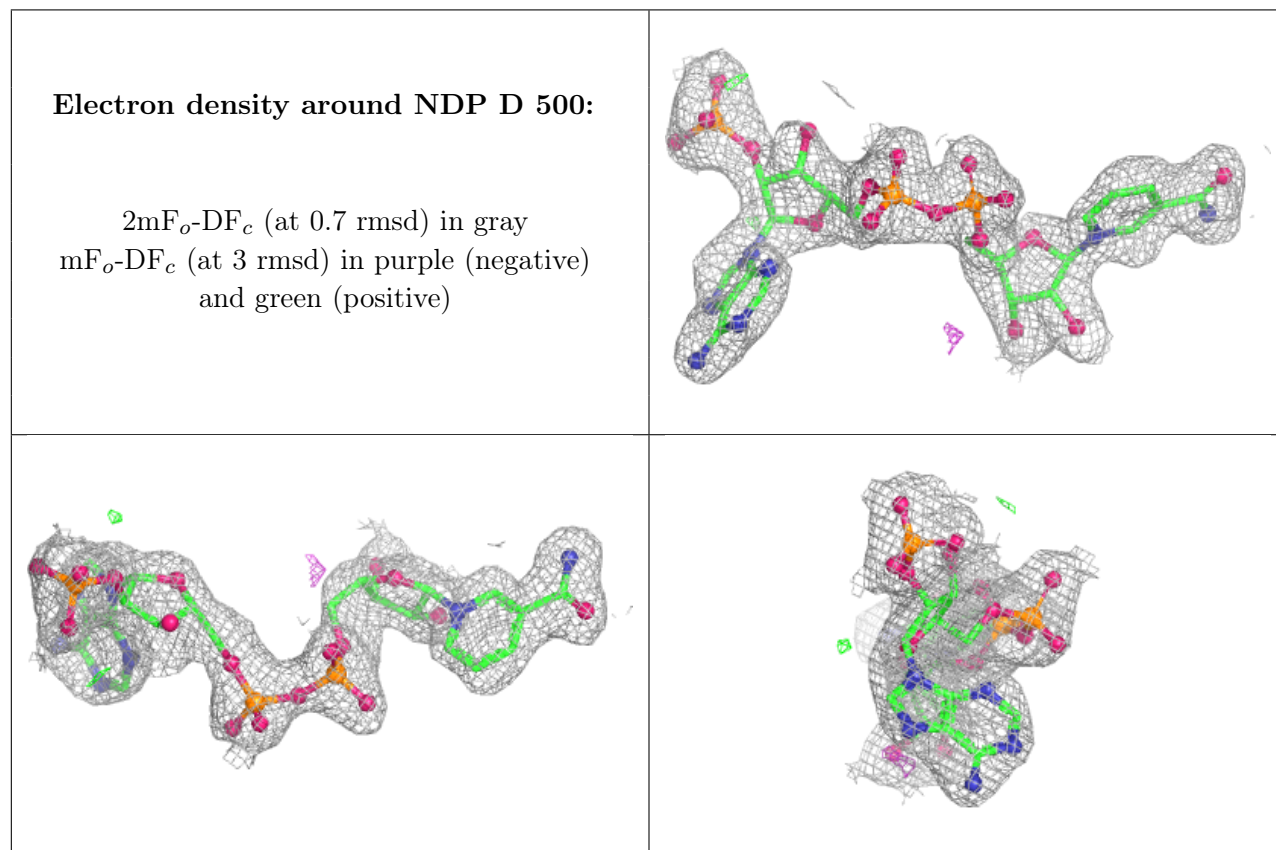
There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

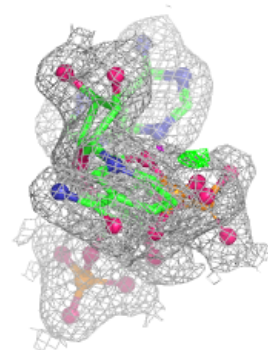
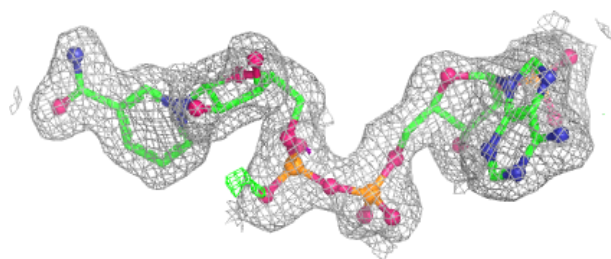
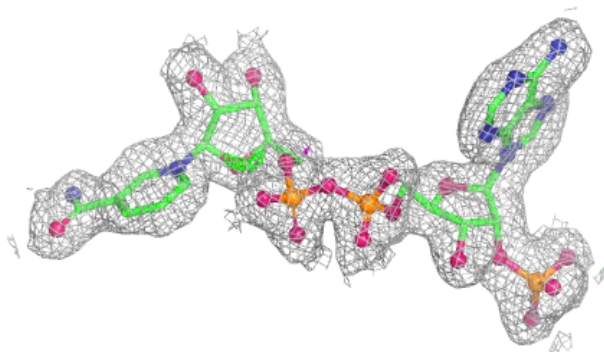
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	GOL	D	600[A]	6/6	0.98	0.05	42,44,44,44	1
3	GOL	D	600[B]	6/6	0.98	0.05	43,44,44,44	1
3	GOL	E	600[A]	6/6	0.98	0.04	33,34,34,35	1
3	GOL	E	600[B]	6/6	0.98	0.04	32,34,34,35	1
3	GOL	F	600[A]	6/6	0.98	0.05	42,43,43,43	1
3	GOL	F	600[B]	6/6	0.98	0.05	42,43,43,43	1
3	GOL	H	600[A]	6/6	0.98	0.05	36,37,38,38	1
3	GOL	H	600[B]	6/6	0.98	0.05	36,37,38,38	1
3	GOL	J	600[A]	6/6	0.98	0.05	30,30,31,31	1
3	GOL	J	600[B]	6/6	0.98	0.05	27,30,31,31	1
3	GOL	L	600[A]	6/6	0.98	0.07	32,34,35,35	1
3	GOL	L	600[B]	6/6	0.98	0.07	31,34,35,35	1
3	GOL	C	600[A]	6/6	0.99	0.04	32,33,33,33	1
3	GOL	G	600[A]	6/6	0.99	0.04	25,28,29,31	1
3	GOL	G	600[B]	6/6	0.99	0.04	28,29,30,31	1
3	GOL	C	600[B]	6/6	0.99	0.04	31,33,33,33	1
2	NDP	D	500	48/48	0.99	0.03	25,34,43,43	0
3	GOL	I	600[A]	6/6	0.99	0.04	29,30,32,33	1
3	GOL	I	600[B]	6/6	0.99	0.04	30,30,32,33	1
3	GOL	A	600[A]	6/6	0.99	0.03	18,22,23,25	1
3	GOL	A	600[B]	6/6	0.99	0.03	21,23,25,25	1
3	GOL	K	600[A]	6/6	0.99	0.04	29,31,32,33	1
3	GOL	K	600[B]	6/6	0.99	0.04	31,31,32,33	1
3	GOL	B	600[A]	6/6	0.99	0.05	33,34,35,35	1
3	GOL	B	600[B]	6/6	0.99	0.05	31,33,35,35	1
2	NDP	A	500	48/48	1.00	0.02	12,15,17,17	0
2	NDP	E	500	48/48	1.00	0.02	15,20,22,23	0
2	NDP	F	500	48/48	1.00	0.02	28,33,42,43	0
2	NDP	G	500	48/48	1.00	0.02	13,16,18,19	0
2	NDP	H	500	48/48	1.00	0.02	19,22,26,26	0
2	NDP	I	500	48/48	1.00	0.02	10,15,18,18	0
2	NDP	J	500	48/48	1.00	0.02	15,19,22,22	0
2	NDP	K	500	48/48	1.00	0.02	10,16,18,18	0
2	NDP	L	500	48/48	1.00	0.02	13,19,21,22	0
2	NDP	B	500	48/48	1.00	0.02	18,23,26,26	0
2	NDP	C	500	48/48	1.00	0.02	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.

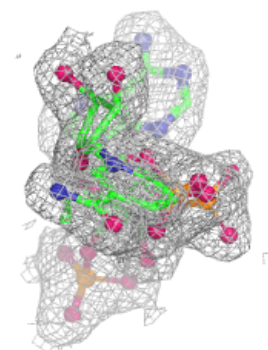
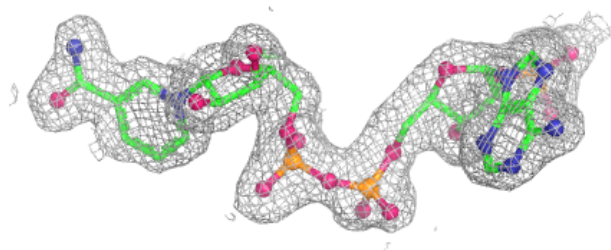
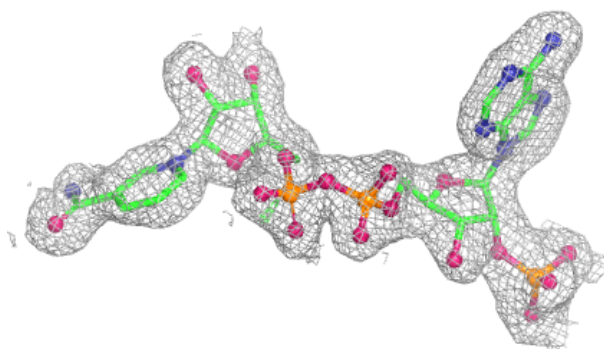


Electron density around NDP A 500:

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

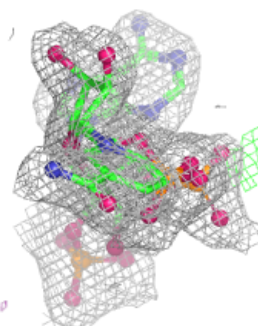
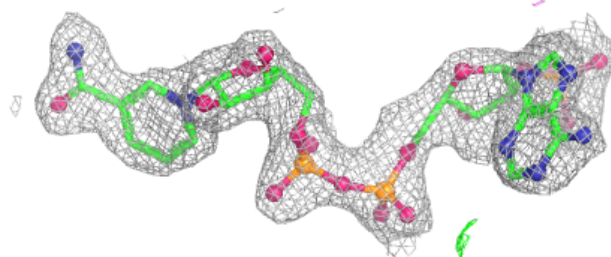
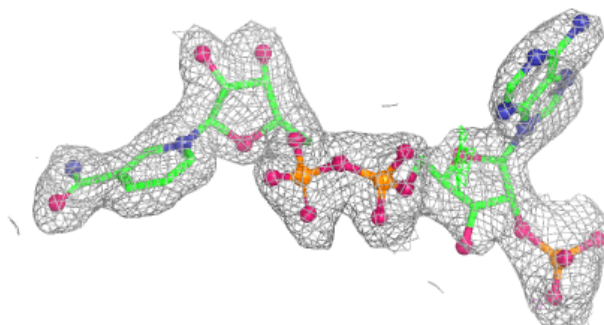
**Electron density around NDP E 500:**

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

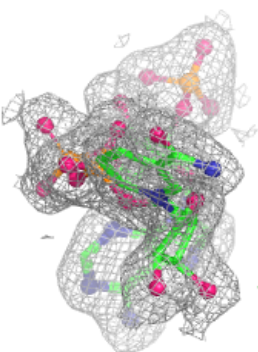
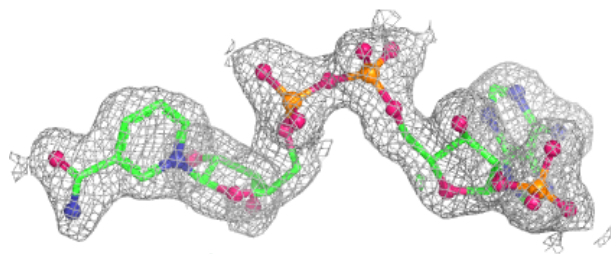
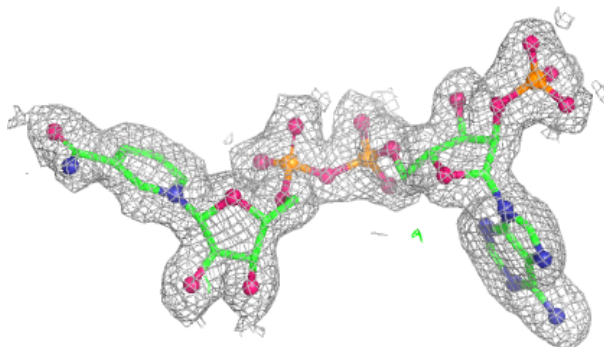


Electron density around NDP F 500:

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

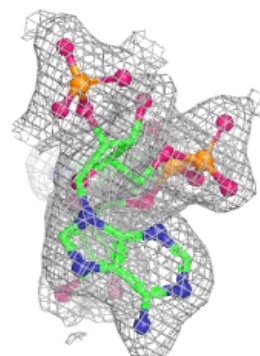
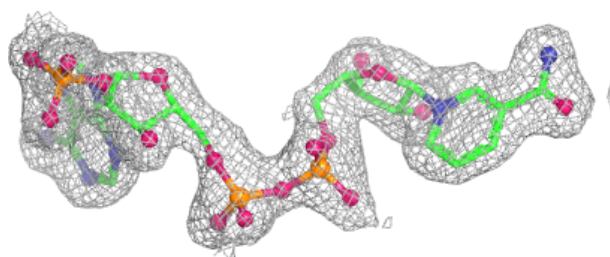
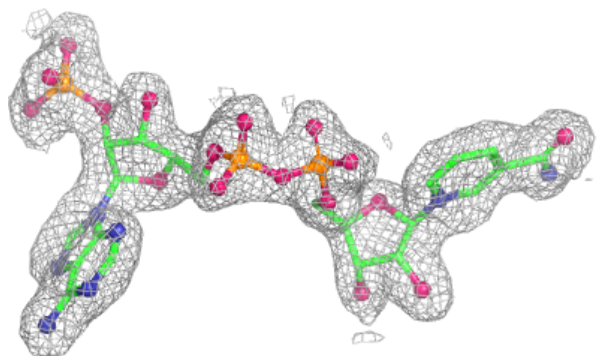
**Electron density around NDP G 500:**

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

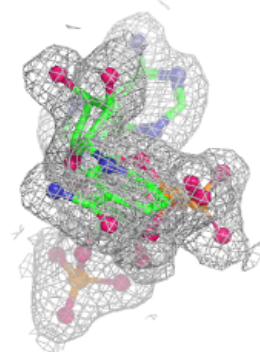
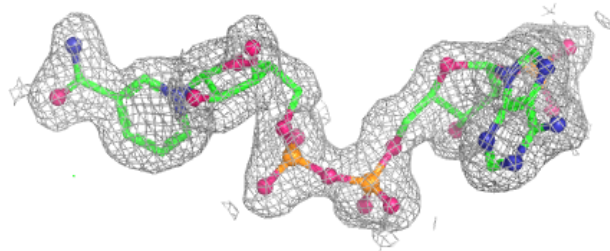
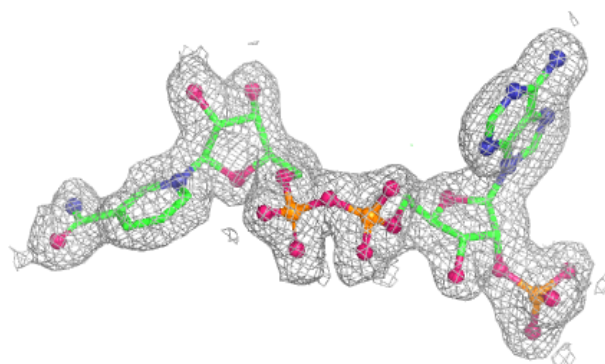


Electron density around NDP H 500:

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

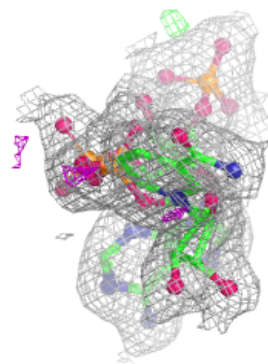
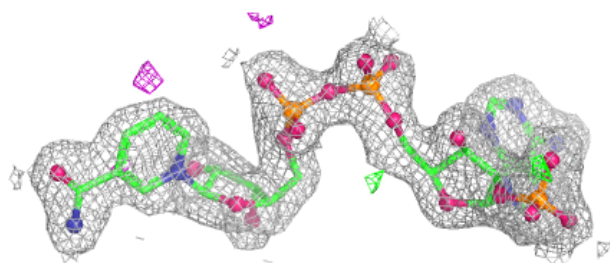
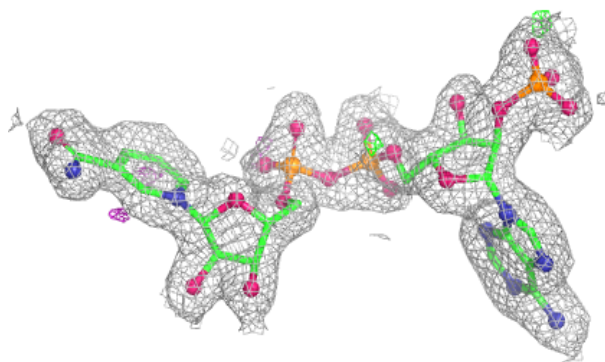
**Electron density around NDP I 500:**

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

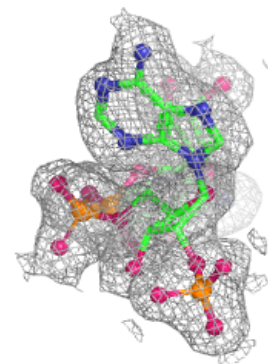
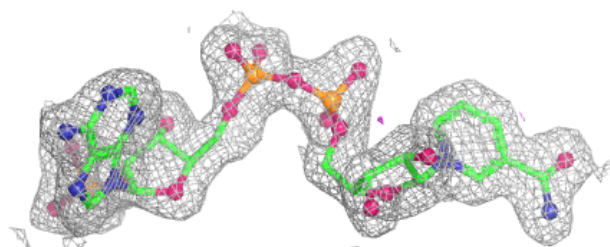
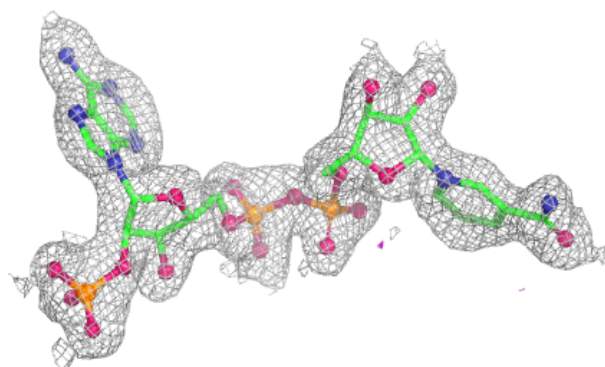


Electron density around NDP J 500:

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

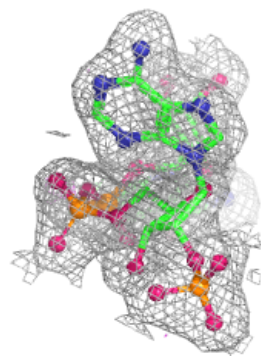
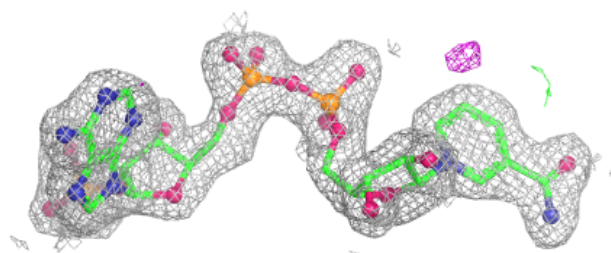
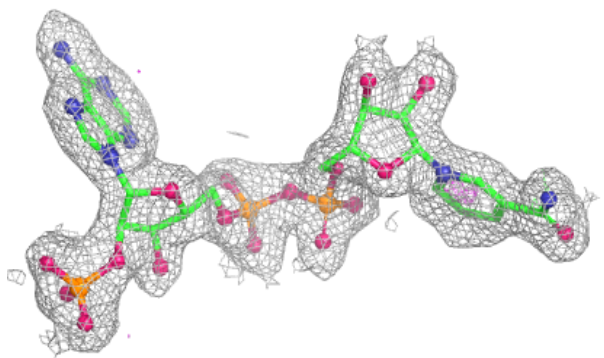
**Electron density around NDP K 500:**

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

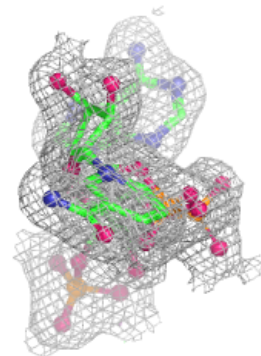
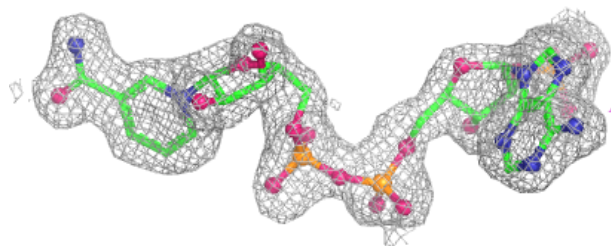
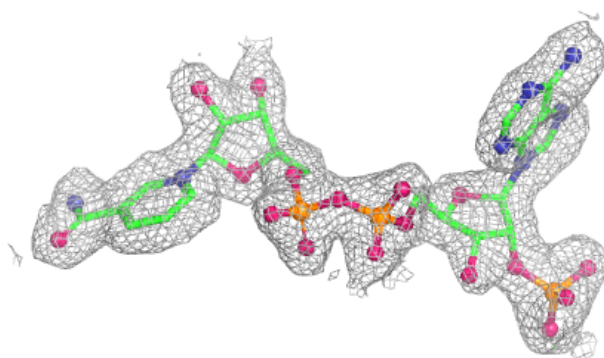


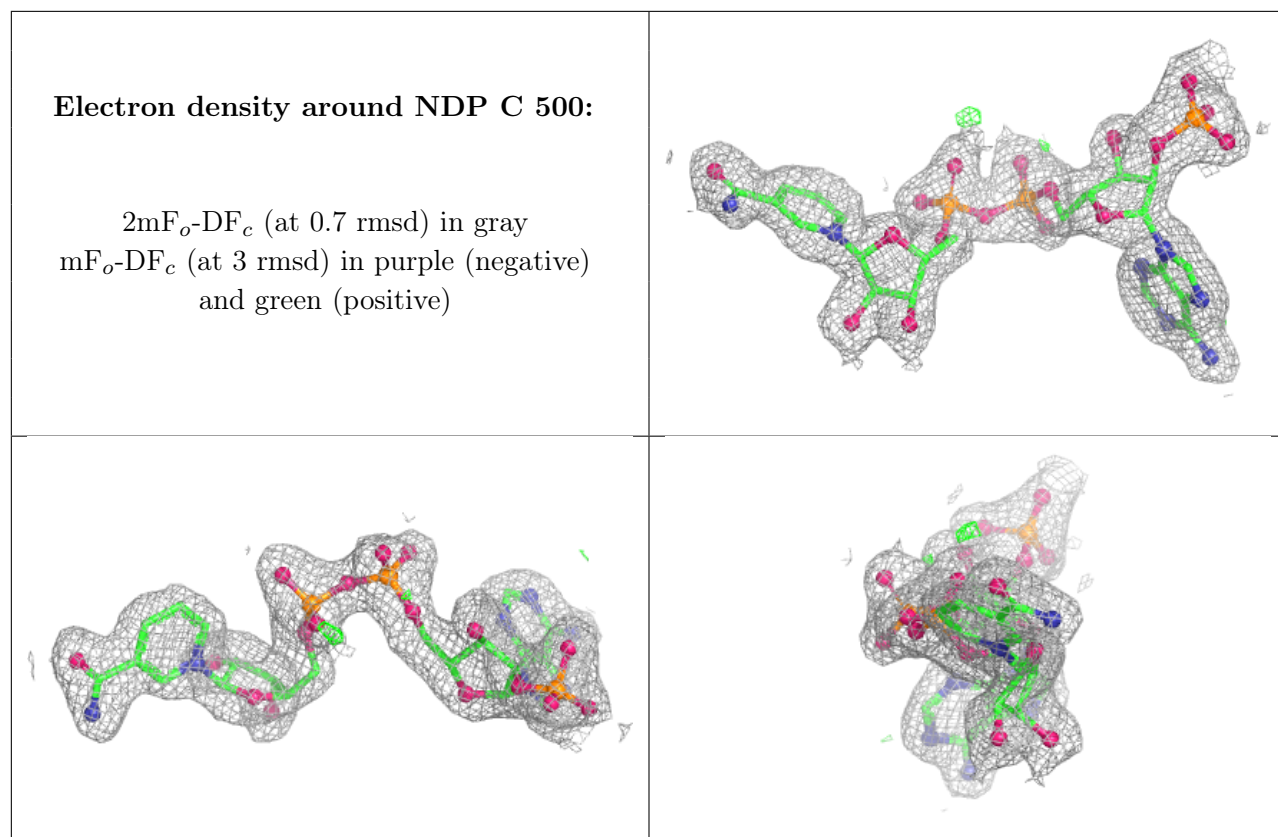
Electron density around NDP L 500:

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

**Electron density around NDP B 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.