



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 04:41 pm BST

PDB ID : 4LK3  
Title : Crystal structure of Human UDP-xylose synthase R236A substitution  
Authors : Walsh Jr., R.M.; Polizzi, S.J.; Wood, Z.A.  
Deposited on : 2013-07-05  
Resolution : 2.64 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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) : 2.11

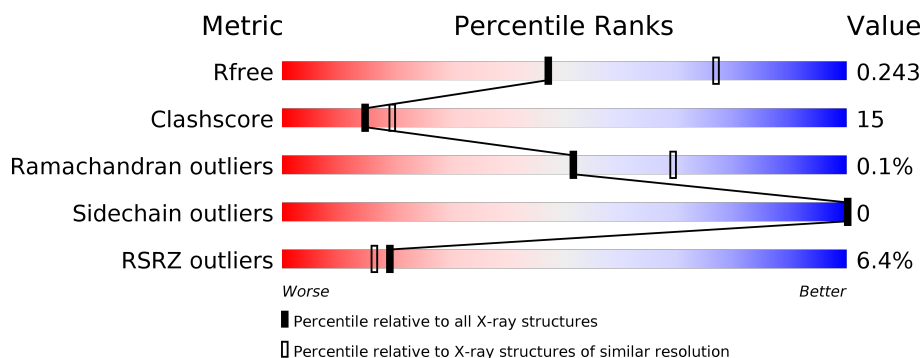
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.64 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	1426 (2.66-2.62)
Clashscore	141614	1472 (2.66-2.62)
Ramachandran outliers	138981	1446 (2.66-2.62)
Sidechain outliers	138945	1446 (2.66-2.62)
RSRZ outliers	127900	1408 (2.66-2.62)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	336	<div> <div>11%</div> <div> <div></div> <div>53%</div> <div>26%</div> <div>21%</div> </div> </div>
1	B	336	<div> <div>3%</div> <div> <div></div> <div>65%</div> <div>16%</div> <div>18%</div> </div> </div>
1	C	336	<div> <div>%</div> <div> <div></div> <div>67%</div> <div>14%</div> <div>19%</div> </div> </div>
1	D	336	<div> <div>%</div> <div> <div></div> <div>61%</div> <div>20%</div> <div>19%</div> </div> </div>
1	E	336	<div> <div>7%</div> <div> <div></div> <div>61%</div> <div>19%</div> <div>20%</div> </div> </div>
1	F	336	<div> <div>8%</div> <div> <div></div> <div>47%</div> <div>31%</div> <div>22%</div> </div> </div>

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
5	SO4	A	505	-	-	X	-

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 13434 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 UDP-glucuronic acid decarboxylase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	267	Total	C	N	O	S	0	0	0
			2113	1349	367	387	10			
1	B	274	Total	C	N	O	S	0	0	0
			2156	1375	374	396	11			
1	C	271	Total	C	N	O	S	0	0	0
			2130	1359	368	393	10			
1	D	273	Total	C	N	O	S	0	0	0
			2148	1370	373	395	10			
1	E	269	Total	C	N	O	S	0	0	0
			2118	1350	369	389	10			
1	F	261	Total	C	N	O	S	0	0	0
			2062	1314	360	378	10			

There are 6 discrepancies between the modelled and reference sequences:

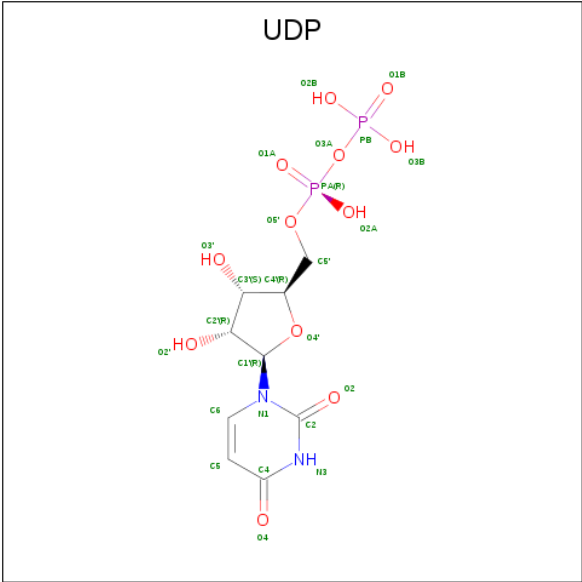
Chain	Residue	Modelled	Actual	Comment	Reference
A	236	ALA	ARG	ENGINEERED MUTATION	UNP Q8NBZ7
B	236	ALA	ARG	ENGINEERED MUTATION	UNP Q8NBZ7
C	236	ALA	ARG	ENGINEERED MUTATION	UNP Q8NBZ7
D	236	ALA	ARG	ENGINEERED MUTATION	UNP Q8NBZ7
E	236	ALA	ARG	ENGINEERED MUTATION	UNP Q8NBZ7
F	236	ALA	ARG	ENGINEERED MUTATION	UNP Q8NBZ7

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C<sub>21</sub>H<sub>27</sub>N<sub>7</sub>O<sub>14</sub>P<sub>2</sub>).



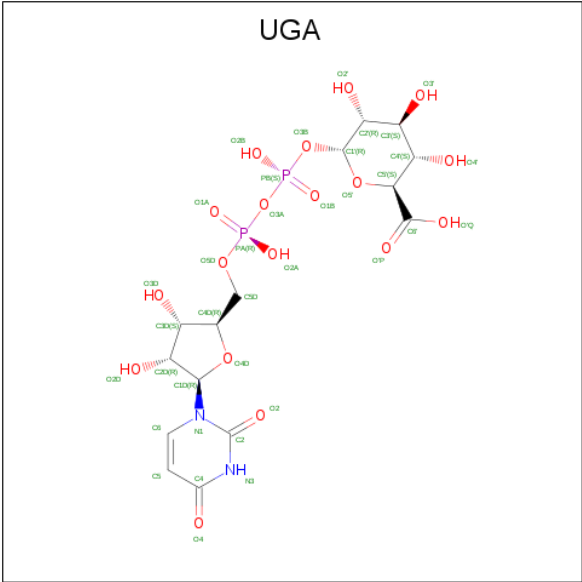
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 44	C 21	N 7	O 14	P 2	0	0
2	B	1	Total 44	C 21	N 7	O 14	P 2	0	0
2	C	1	Total 44	C 21	N 7	O 14	P 2	0	0
2	D	1	Total 44	C 21	N 7	O 14	P 2	0	0
2	E	1	Total 44	C 21	N 7	O 14	P 2	0	0
2	F	1	Total 44	C 21	N 7	O 14	P 2	0	0

- Molecule 3 is URIDINE-5'-DIPHOSPHATE (three-letter code: UDP) (formula:  $\text{C}_9\text{H}_{14}\text{N}_2\text{O}_{12}\text{P}_2$ ).



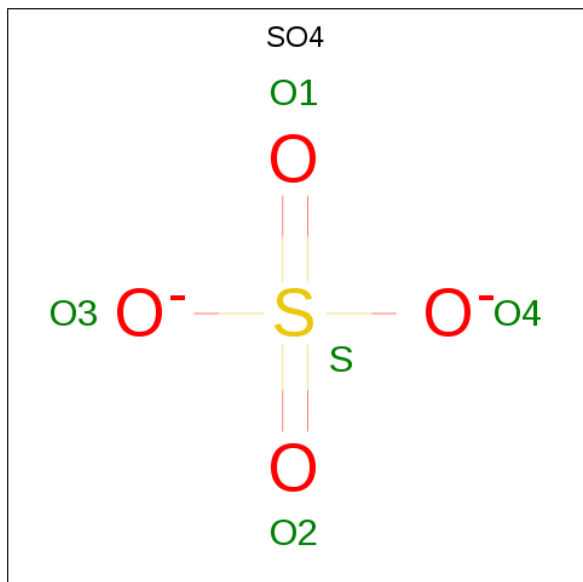
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
3	B	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
3	D	1	Total	C	N	O	P	0	0
			25	9	2	12	2		

- Molecule 4 is URIDINE-5'-DIPHOSPHATE-GLUCURONIC ACID (three-letter code: UGA) (formula: C<sub>15</sub>H<sub>22</sub>N<sub>2</sub>O<sub>18</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			37	15	2	18	2		
4	B	1	Total	C	N	O	P	0	0
			37	15	2	18	2		
4	C	1	Total	C	N	O	P	0	0
			37	15	2	18	2		
4	D	1	Total	C	N	O	P	0	0
			37	15	2	18	2		
4	E	1	Total	C	N	O	P	0	0
			37	15	2	18	2		
4	F	1	Total	C	N	O	P	0	0
			37	15	2	18	2		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



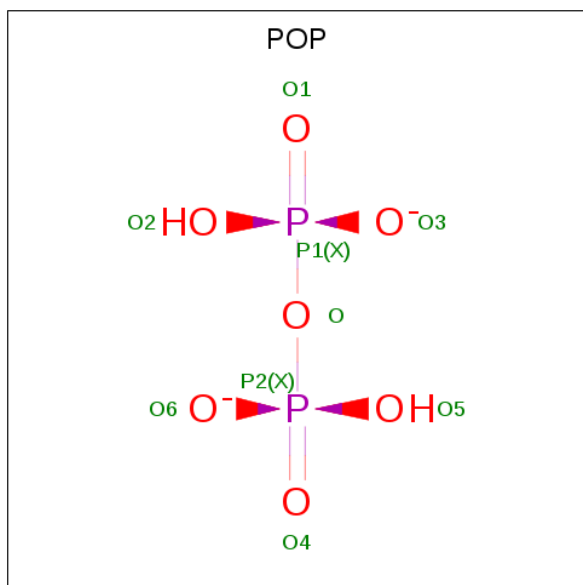
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	O S	0	0
			5 4 1			
5	A	1	Total	O S	0	0
			5 4 1			
5	B	1	Total	O S	0	0
			5 4 1			
5	B	1	Total	O S	0	0
			5 4 1			
5	C	1	Total	O S	0	0
			5 4 1			
5	D	1	Total	O S	0	0
			5 4 1			

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total	O	S	0	0
			5	4	1		
5	E	1	Total	O	S	0	0
			5	4	1		
5	F	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is PYROPHOSPHATE 2- (three-letter code: POP) (formula:  $\text{H}_2\text{O}_7\text{P}_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	O	P	0	0
			9	7	2		
6	E	1	Total	O	P	0	0
			9	7	2		
6	F	1	Total	O	P	0	0
			9	7	2		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	32	Total	O	0	0
			32	32		
7	C	31	Total	O	0	0
			31	31		
7	D	9	Total	O	0	0
			9	9		

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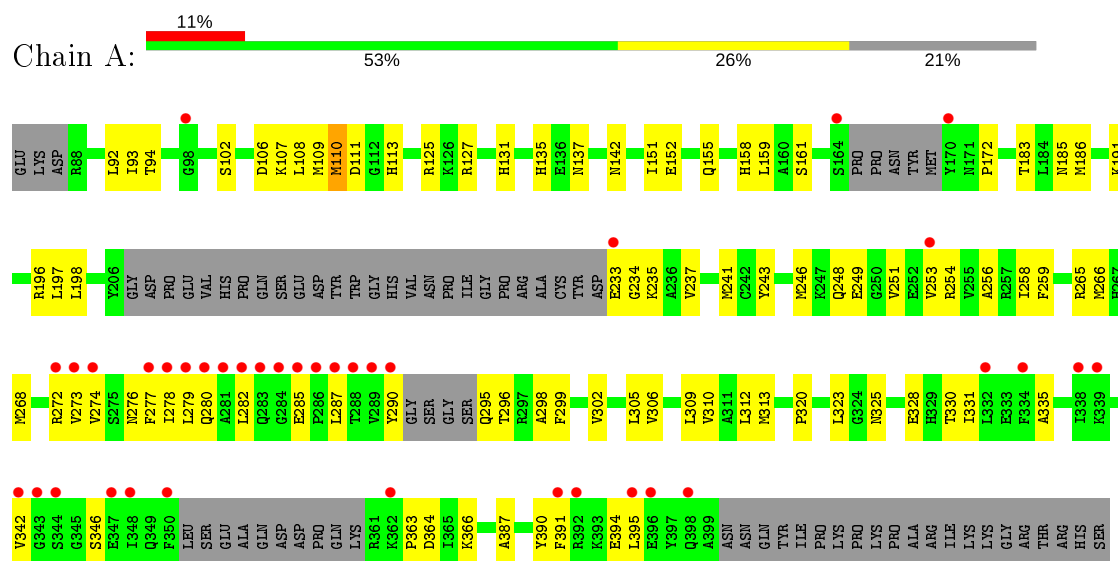
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	E	2	Total	O	0	0
			2	2		

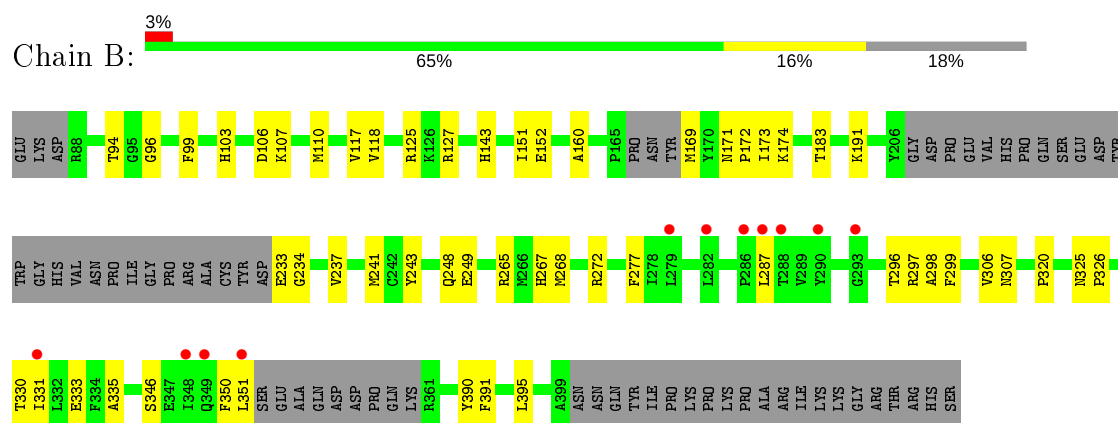
### 3 Residue-property plots

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.

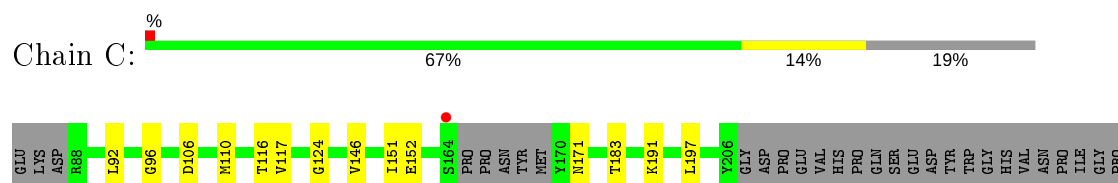
#### • Molecule 1: UDP-glucuronic acid decarboxylase 1

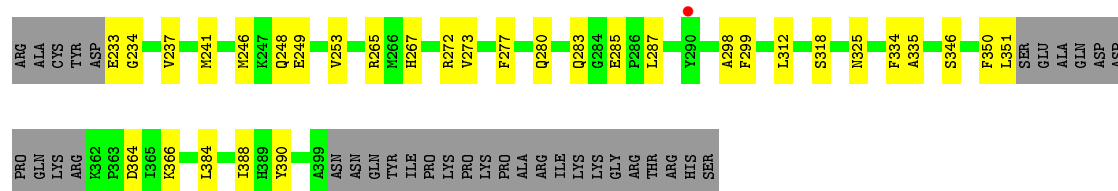


#### • Molecule 1: UDP-glucuronic acid decarboxylase 1

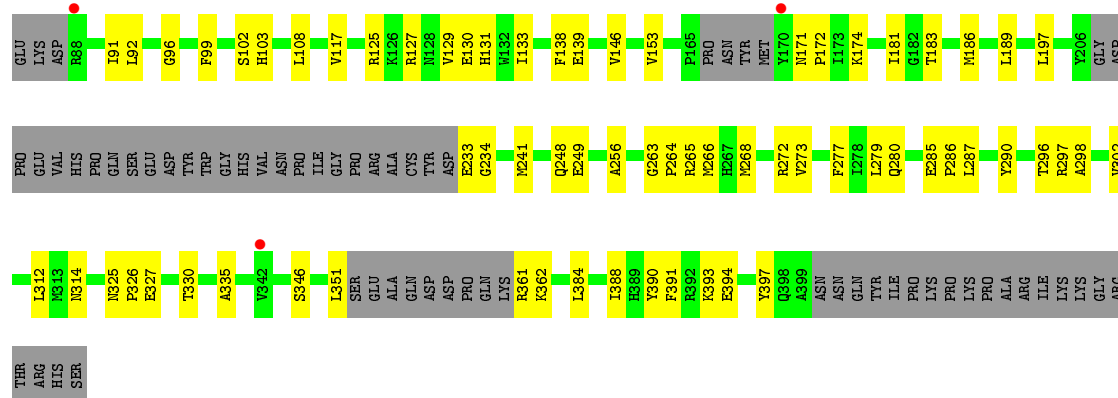


#### • Molecule 1: UDP-glucuronic acid decarboxylase 1

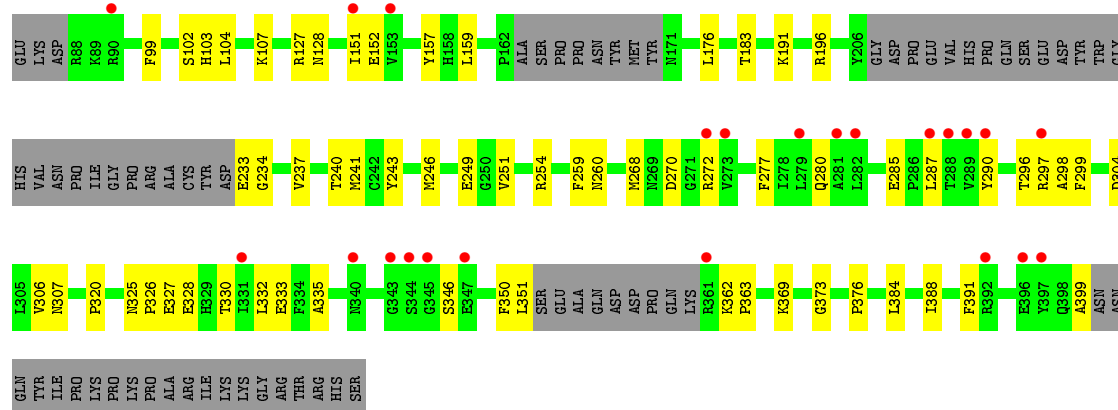




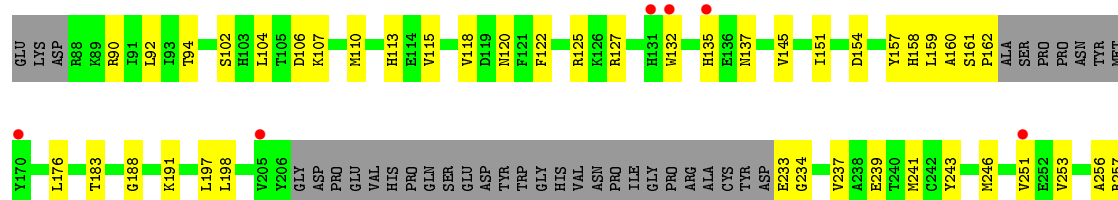
• Molecule 1: UDP-glucuronic acid decarboxylase 1



• Molecule 1: UDP-glucuronic acid decarboxylase 1



• Molecule 1: UDP-glucuronic acid decarboxylase 1



I258	I331	I399
F259	I332	ASN
M260	E333	ASN
T261	F334	GLN
F262	A335	TYR
		ILE
R265	I336	PRO
M266	K339	LYS
E267	K340	PRO
M268	I341	LYS
	V342	PRO
R272	G343	ALA
V273	S344	ARG
V274	G345	ILE
	S346	LYS
F277	E347	LYS
I278	I348	GLY
L279	GLN	ARG
Q280	PHE	THR
A281	LEU	ARG
L282	SER	HIS
Q283	GLU	SER
G284	ALA	
E285	GLN	
E286	ASP	
L287	ASP	
THR	PRO	
VAL	GLN	
TYR	LYS	
GLY	K361	
SER	K362	
GLY	P363	
S294	D364	
Q295	I365	
T296	K366	
R297		
A298	K369	
F299	I370	
Q300		
Y301	G373	
V302		
S303	I380	
D304	E381	
L305	E382	
V306	G383	
N307	I384	
	N385	
L312	K386	
	A387	
V317	I388	
S318	H389	
S319	Y390	
P320	F391	
	K392	
N325	K393	
P326	E394	
E327	I395	
E328	E396	
H329	Y397	
T330	Q398	

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	83.57Å 92.07Å 290.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.37 – 2.64 38.90 – 2.64	Depositor EDS
% Data completeness (in resolution range)	98.4 (36.37-2.64) 95.6 (38.90-2.64)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.21 (at 2.65Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, $R_{free}$	0.198 , 0.245 0.197 , 0.243	Depositor DCC
$R_{free}$ test set	3330 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	55.2	Xtriage
Anisotropy	0.318	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 58.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	13434	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.80% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, UDP, UGA, NAD, POP

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	0.48	0/2152	0.67	0/2905
1	B	0.57	0/2197	0.73	0/2967
1	C	0.56	0/2170	0.72	0/2931
1	D	0.50	0/2189	0.67	1/2957 (0.0%)
1	E	0.48	0/2157	0.66	0/2912
1	F	0.47	0/2099	0.70	0/2832
All	All	0.51	0/12964	0.69	1/17504 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	314	ASN	O-C-N	-5.18	114.41	122.70

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	2113	0	2123	88	0
1	B	2156	0	2167	47	0
1	C	2130	0	2138	46	0
1	D	2148	0	2158	68	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2118	0	2132	57	0
1	F	2062	0	2076	108	0
2	A	44	0	26	0	0
2	B	44	0	26	0	0
2	C	44	0	26	1	0
2	D	44	0	26	0	0
2	E	44	0	26	0	0
2	F	44	0	26	3	0
3	A	25	0	11	1	0
3	B	25	0	11	0	0
3	D	25	0	11	2	0
4	A	37	0	19	2	0
4	B	37	0	19	2	0
4	C	37	0	19	0	0
4	D	37	0	19	1	0
4	E	37	0	19	0	0
4	F	37	0	19	2	0
5	A	10	0	0	3	0
5	B	10	0	0	1	0
5	C	5	0	0	0	0
5	D	10	0	0	0	0
5	E	5	0	0	0	0
5	F	5	0	0	0	0
6	C	9	0	0	2	0
6	E	9	0	0	0	0
6	F	9	0	0	3	0
7	B	32	0	0	2	0
7	C	31	0	0	3	0
7	D	9	0	0	0	0
7	E	2	0	0	0	0
All	All	13434	0	13097	404	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 15.

All (404) 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:F:262:PHE:HE2	1:F:299:PHE:CD1	1.43	1.37
1:F:262:PHE:CE2	1:F:299:PHE:CD1	2.34	1.15
1:B:233:GLU:HG2	1:B:234:GLY:H	1.05	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:233:GLU:HG2	1:F:234:GLY:H	0.94	1.06
1:F:262:PHE:CZ	1:F:272:ARG:HD3	1.90	1.06
1:C:233:GLU:HG2	1:C:234:GLY:H	0.95	1.06
1:E:233:GLU:HG2	1:E:234:GLY:H	0.89	1.05
1:E:233:GLU:CG	1:E:234:GLY:H	1.71	1.01
1:D:130:GLU:HG3	1:D:133:ILE:HD12	1.40	1.00
1:E:233:GLU:HG2	1:E:234:GLY:N	1.74	0.99
1:A:387:ALA:O	1:A:391:PHE:HD1	1.46	0.98
1:F:233:GLU:HG2	1:F:234:GLY:N	1.79	0.97
1:F:233:GLU:CG	1:F:234:GLY:H	1.77	0.97
1:C:233:GLU:HG2	1:C:234:GLY:N	1.78	0.96
1:D:233:GLU:HG2	1:D:234:GLY:H	1.28	0.96
1:F:92:LEU:HD22	1:F:151:ILE:HD11	1.46	0.95
1:E:350:PHE:C	1:E:351:LEU:HD12	1.87	0.95
1:C:233:GLU:CG	1:C:234:GLY:H	1.79	0.94
1:E:280:GLN:OE1	1:E:287:LEU:HA	1.67	0.94
1:C:183:THR:HB	1:C:241:MET:HE1	1.50	0.92
1:B:183:THR:HB	1:B:241:MET:HE1	1.49	0.92
1:C:272:ARG:HG3	6:C:503:POP:O1	1.70	0.92
1:F:243:TYR:OH	1:F:320:PRO:HD3	1.69	0.91
1:A:387:ALA:O	1:A:391:PHE:CD1	2.22	0.91
1:B:183:THR:HB	1:B:241:MET:CE	2.02	0.89
1:D:287:LEU:CD1	1:D:346:SER:HB3	2.05	0.87
1:D:125:ARG:HD3	1:D:127:ARG:NE	1.88	0.87
1:A:155:GLN:HB3	1:A:313:MET:CE	2.05	0.86
1:A:268:MET:HG2	1:A:391:PHE:CE2	2.10	0.85
1:B:233:GLU:HG2	1:B:234:GLY:N	1.89	0.85
1:B:233:GLU:CG	1:B:234:GLY:H	1.87	0.83
1:F:273:VAL:HG12	6:F:503:POP:O1	1.79	0.82
1:A:155:GLN:HB3	1:A:313:MET:HE2	1.62	0.82
1:A:390:TYR:O	1:A:394:GLU:HG2	1.80	0.82
1:B:350:PHE:C	1:B:351:LEU:HD12	1.99	0.81
1:F:328:GLU:OE2	1:F:362:LYS:HB2	1.80	0.81
1:E:270:ASP:OD2	1:E:272:ARG:HG3	1.81	0.81
1:B:107:LYS:HD3	1:B:306:VAL:HG12	1.64	0.80
1:A:243:TYR:OH	1:A:320:PRO:HD3	1.83	0.79
1:C:350:PHE:C	1:C:351:LEU:HD12	2.03	0.79
1:F:260:ASN:HB3	1:F:272:ARG:NH1	1.98	0.79
1:D:393:LYS:NZ	1:E:399:ALA:C	2.37	0.78
1:F:262:PHE:CZ	1:F:272:ARG:CD	2.67	0.78
1:A:127:ARG:HB3	5:A:505:SO4:O1	1.85	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:260:ASN:HB3	1:F:272:ARG:HH12	1.50	0.77
1:A:280:GLN:OE1	1:A:287:LEU:HA	1.84	0.76
1:A:183:THR:HB	1:A:241:MET:HE1	1.66	0.76
1:E:183:THR:HB	1:E:241:MET:HE1	1.67	0.76
1:E:384:LEU:O	1:E:388:ILE:HG13	1.86	0.76
1:C:246:MET:HE3	1:C:318:SER:HB2	1.66	0.75
1:F:262:PHE:HE2	1:F:299:PHE:CE1	2.04	0.74
4:F:502:UGA:O2'	4:F:502:UGA:O3A	2.03	0.74
1:E:350:PHE:O	1:E:351:LEU:HD12	1.88	0.73
1:A:233:GLU:CG	1:A:234:GLY:H	2.01	0.72
1:F:260:ASN:CB	1:F:272:ARG:HH12	2.03	0.72
1:E:328:GLU:OE2	1:E:362:LYS:HB2	1.89	0.71
1:D:125:ARG:HD3	1:D:127:ARG:CZ	2.21	0.71
1:D:125:ARG:HG2	1:D:125:ARG:HH11	1.54	0.71
1:A:161:SER:OG	1:A:235:LYS:NZ	2.21	0.70
1:B:125:ARG:HD3	1:B:127:ARG:NH2	2.06	0.70
1:D:287:LEU:HD11	1:D:346:SER:HB3	1.74	0.69
1:A:268:MET:HG2	1:A:391:PHE:CD2	2.27	0.69
1:F:369:LYS:O	1:F:373:GLY:HA2	1.92	0.69
1:D:393:LYS:HZ2	1:E:399:ALA:C	1.94	0.69
1:F:132:TRP:HA	1:F:135:HIS:HD2	1.56	0.69
1:F:391:PHE:O	1:F:395:LEU:HG	1.93	0.69
1:D:186:MET:HE3	1:D:189:LEU:HD23	1.76	0.68
1:C:272:ARG:CG	6:C:503:POP:O1	2.41	0.68
4:A:503:UGA:H2'1	1:B:173:ILE:HG21	1.75	0.68
1:A:285:GLU:O	1:A:346:SER:HB3	1.94	0.67
1:F:132:TRP:HA	1:F:135:HIS:CD2	2.30	0.67
1:F:262:PHE:CE1	1:F:272:ARG:HD2	2.30	0.67
1:C:299:PHE:HD2	1:C:334:PHE:CZ	2.12	0.66
1:A:266:MET:SD	1:A:391:PHE:HZ	2.19	0.66
1:D:361:ARG:NH1	1:D:362:LYS:O	2.28	0.66
1:F:287:LEU:CD1	1:F:346:SER:HB3	2.25	0.66
1:F:262:PHE:CE2	1:F:299:PHE:CE1	2.81	0.66
1:F:262:PHE:CE1	1:F:272:ARG:CD	2.78	0.66
1:F:262:PHE:CE1	1:F:274:VAL:HB	2.31	0.65
1:F:268:MET:HE2	1:F:391:PHE:CD2	2.32	0.65
1:E:328:GLU:CD	1:E:362:LYS:HB2	2.16	0.65
1:B:277:PHE:CE2	1:B:335:ALA:HB2	2.32	0.65
1:A:233:GLU:CD	1:A:234:GLY:H	2.00	0.64
1:F:243:TYR:OH	1:F:320:PRO:CD	2.44	0.64
1:A:151:ILE:HG12	1:A:152:GLU:H	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:125:ARG:HD3	1:D:127:ARG:HE	1.63	0.64
1:A:102:SER:CB	1:A:265:ARG:HH11	2.11	0.64
1:F:107:LYS:HE3	1:F:307:ASN:OD1	1.97	0.64
1:E:107:LYS:HE3	1:E:307:ASN:OD1	1.98	0.64
1:E:183:THR:HB	1:E:241:MET:CE	2.28	0.63
1:F:273:VAL:CG1	6:F:503:POP:O1	2.46	0.63
1:D:233:GLU:HG2	1:D:234:GLY:N	2.09	0.63
1:C:237:VAL:O	1:C:241:MET:HG3	1.98	0.63
1:C:183:THR:HB	1:C:241:MET:CE	2.25	0.63
1:D:183:THR:HB	1:D:241:MET:HE1	1.80	0.63
1:D:287:LEU:HD12	1:D:346:SER:HB3	1.78	0.62
1:F:239:GLU:OE1	1:F:257:ARG:NH2	2.30	0.62
1:F:301:TYR:CE1	1:F:302:VAL:HG12	2.33	0.62
1:F:262:PHE:CD1	1:F:266:MET:CE	2.83	0.62
1:C:298:ALA:HB1	1:C:325:ASN:O	1.99	0.62
1:E:243:TYR:OH	1:E:320:PRO:HD3	1.99	0.62
1:E:332:LEU:HD13	1:E:350:PHE:HE1	1.64	0.62
1:A:159:LEU:HD12	1:A:159:LEU:N	2.15	0.61
1:A:198:LEU:HD23	1:A:198:LEU:C	2.20	0.61
5:A:505:SO4:O2	1:F:125:ARG:HB3	1.99	0.61
1:B:107:LYS:NZ	1:B:307:ASN:HA	2.15	0.61
1:B:350:PHE:O	1:B:351:LEU:HD12	2.01	0.61
1:F:301:TYR:O	1:F:304:ASP:HB2	2.01	0.61
1:E:104:LEU:CD1	1:E:306:VAL:HG13	2.31	0.61
1:A:93:ILE:HD11	1:A:108:LEU:HD12	1.83	0.60
1:C:246:MET:CE	1:C:318:SER:HB2	2.30	0.60
1:D:326:PRO:O	1:D:362:LYS:HE2	2.02	0.60
1:F:262:PHE:HE2	1:F:299:PHE:HD1	1.33	0.60
1:C:280:GLN:OE1	1:C:287:LEU:HA	2.01	0.59
1:C:248:GLN:OE1	1:D:172:PRO:HG2	2.02	0.59
1:D:393:LYS:HZ1	1:E:399:ALA:C	2.05	0.58
1:E:237:VAL:O	1:E:241:MET:HG3	2.02	0.58
1:F:302:VAL:O	1:F:306:VAL:HG23	2.02	0.58
1:F:259:PHE:CE2	1:F:363:PRO:HB3	2.38	0.58
1:D:91:ILE:HD13	1:D:108:LEU:HD13	1.84	0.58
1:A:151:ILE:HG12	1:A:152:GLU:N	2.18	0.58
1:A:285:GLU:O	1:A:346:SER:CB	2.51	0.58
1:A:282:LEU:HD23	1:A:342:VAL:HG13	1.84	0.58
1:E:260:ASN:HB3	1:E:299:PHE:CE1	2.39	0.57
1:F:329:HIS:CD2	1:F:380:LEU:HD22	2.39	0.57
1:B:249:GLU:OE2	4:B:503:UGA:O3'	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:198:LEU:HD11	1:F:312:LEU:HD23	1.85	0.57
1:C:287:LEU:N	1:C:287:LEU:HD12	2.19	0.57
1:A:233:GLU:CG	1:A:234:GLY:N	2.67	0.57
1:F:159:LEU:HD12	1:F:159:LEU:N	2.20	0.56
1:F:183:THR:HB	1:F:241:MET:HE1	1.87	0.56
1:D:268:MET:HG2	1:D:391:PHE:CE2	2.40	0.56
1:D:130:GLU:HG3	1:D:133:ILE:CD1	2.27	0.56
1:A:237:VAL:O	1:A:241:MET:HG3	2.05	0.56
1:A:131:HIS:O	1:A:135:HIS:CE1	2.58	0.56
1:B:125:ARG:HD3	1:B:127:ARG:CZ	2.36	0.56
1:D:92:LEU:HD21	1:D:186:MET:HE1	1.88	0.56
1:E:328:GLU:OE1	1:E:362:LYS:HE3	2.06	0.56
1:F:183:THR:HB	1:F:241:MET:CE	2.36	0.56
1:A:155:GLN:HB3	1:A:313:MET:HE3	1.88	0.55
1:F:325:ASN:OD1	1:F:327:GLU:HB3	2.06	0.55
1:A:107:LYS:O	1:A:107:LYS:HG3	2.04	0.55
1:A:233:GLU:HG2	1:A:234:GLY:H	1.71	0.55
1:B:267:HIS:HB3	5:B:504:SO4:O1	2.06	0.55
1:E:298:ALA:HB1	1:E:325:ASN:O	2.07	0.55
1:F:301:TYR:HD1	1:F:303:SER:H	1.53	0.55
1:F:259:PHE:CZ	1:F:363:PRO:HB3	2.42	0.55
1:A:273:VAL:HG21	1:A:331:ILE:HD12	1.87	0.55
1:C:312:LEU:HD11	7:C:606:HOH:O	2.06	0.55
1:D:297:ARG:NE	3:D:502:UDP:H5'1	2.21	0.55
1:D:277:PHE:CE2	1:D:335:ALA:HB2	2.41	0.54
1:E:240:THR:HG22	1:F:176:LEU:HD11	1.87	0.54
1:F:262:PHE:HD1	1:F:266:MET:CE	2.20	0.54
1:F:287:LEU:N	1:F:347:GLU:O	2.24	0.54
1:D:189:LEU:HD12	1:D:189:LEU:O	2.06	0.54
1:E:330:THR:OG1	1:E:333:GLU:HB2	2.08	0.54
1:B:330:THR:OG1	1:B:333:GLU:HB2	2.06	0.54
1:C:106:ASP:O	1:C:110:MET:HG2	2.08	0.54
1:B:298:ALA:HB1	1:B:325:ASN:O	2.07	0.54
4:B:503:UGA:H1'1	4:B:503:UGA:O2A	2.08	0.54
1:D:102:SER:HB2	1:D:265:ARG:NH1	2.23	0.54
1:D:280:GLN:OE1	1:D:287:LEU:HA	2.07	0.54
1:F:282:LEU:CD1	1:F:391:PHE:HB3	2.38	0.54
1:E:325:ASN:OD1	1:E:327:GLU:HB3	2.08	0.54
1:A:277:PHE:CE2	1:A:335:ALA:HB2	2.43	0.53
1:C:364:ASP:OD2	1:C:366:LYS:HE2	2.07	0.53
1:C:350:PHE:O	1:C:351:LEU:HD12	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:104:LEU:HD21	1:F:157:TYR:CD2	2.43	0.53
1:F:390:TYR:CE1	1:F:394:GLU:OE2	2.61	0.53
1:A:364:ASP:OD2	1:A:366:LYS:HE2	2.08	0.53
1:F:280:GLN:OE1	1:F:287:LEU:HA	2.09	0.53
1:F:296:THR:O	1:F:297:ARG:HD3	2.09	0.53
1:D:290:TYR:CD1	1:D:351:LEU:HD22	2.44	0.53
1:F:295:GLN:O	1:F:330:THR:HA	2.08	0.53
1:E:104:LEU:HD12	1:E:306:VAL:HG13	1.91	0.53
1:F:125:ARG:HB3	1:F:127:ARG:HG2	1.91	0.53
1:A:248:GLN:NE2	1:B:171:ASN:OD1	2.42	0.52
1:D:183:THR:HB	1:D:241:MET:CE	2.38	0.52
1:C:171:ASN:OD1	1:D:248:GLN:NE2	2.40	0.52
1:F:102:SER:CB	1:F:265:ARG:HH11	2.22	0.52
1:F:277:PHE:CE2	1:F:335:ALA:HB2	2.43	0.52
1:F:287:LEU:HD13	1:F:346:SER:HB3	1.92	0.52
1:B:107:LYS:HD3	1:B:306:VAL:CG1	2.37	0.52
1:C:248:GLN:OE1	1:D:172:PRO:HD2	2.09	0.52
1:D:183:THR:CG2	1:D:241:MET:CE	2.87	0.52
1:F:301:TYR:CD1	1:F:302:VAL:N	2.77	0.52
1:D:96:GLY:HA3	1:D:117:VAL:HG13	1.91	0.52
1:E:332:LEU:HD13	1:E:350:PHE:CE1	2.45	0.52
1:F:92:LEU:HD11	1:F:118:VAL:HG23	1.90	0.52
1:F:256:ALA:HB2	1:F:312:LEU:CD2	2.40	0.52
1:B:106:ASP:O	1:B:110:MET:HG2	2.09	0.52
1:C:151:ILE:HG12	1:C:152:GLU:N	2.24	0.52
1:F:262:PHE:HZ	1:F:272:ARG:HD3	1.64	0.52
1:E:104:LEU:HA	1:E:306:VAL:CG1	2.40	0.52
1:A:158:HIS:C	1:A:159:LEU:HD12	2.31	0.52
1:F:132:TRP:CA	1:F:135:HIS:HD2	2.23	0.51
1:A:391:PHE:O	1:A:395:LEU:HG	2.10	0.51
1:B:237:VAL:O	1:B:241:MET:HG3	2.10	0.51
1:F:102:SER:OG	1:F:265:ARG:NH1	2.41	0.51
1:B:191:LYS:HE3	1:B:249:GLU:OE1	2.10	0.51
1:D:130:GLU:CG	1:D:133:ILE:HD12	2.26	0.51
1:E:290:TYR:N	1:E:290:TYR:CD1	2.77	0.51
1:A:161:SER:CB	1:A:235:LYS:HZ3	2.23	0.51
1:D:287:LEU:HD11	1:D:346:SER:CB	2.40	0.51
1:A:298:ALA:HB1	1:A:325:ASN:O	2.11	0.51
1:A:387:ALA:HB1	1:A:391:PHE:HE1	1.75	0.51
1:B:107:LYS:HZ3	1:B:307:ASN:HA	1.76	0.50
1:A:102:SER:CB	1:A:265:ARG:NH1	2.73	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:LEU:HD21	1:A:186:MET:HE1	1.94	0.50
1:B:265:ARG:HA	1:B:390:TYR:CZ	2.47	0.50
1:C:96:GLY:HA3	1:C:117:VAL:HG13	1.94	0.50
1:D:285:GLU:HB3	1:D:286:PRO:HD2	1.93	0.50
1:A:268:MET:HG2	1:A:391:PHE:HE2	1.72	0.50
1:E:259:PHE:CE2	1:E:363:PRO:HB3	2.46	0.50
1:F:107:LYS:CE	1:F:307:ASN:OD1	2.59	0.50
1:A:191:LYS:HE3	1:A:249:GLU:OE1	2.11	0.50
1:A:268:MET:O	1:A:279:LEU:HD11	2.12	0.50
1:D:298:ALA:HB1	1:D:325:ASN:O	2.11	0.50
1:A:185:ASN:HA	4:A:503:UGA:O4D	2.12	0.50
1:A:309:LEU:HD23	1:A:323:LEU:CD1	2.42	0.50
1:E:246:MET:HA	1:E:251:VAL:O	2.11	0.50
1:F:301:TYR:CE2	1:F:383:GLY:HA2	2.47	0.50
1:A:258:ILE:HG12	1:A:305:LEU:HD11	1.94	0.50
1:D:125:ARG:CG	1:D:125:ARG:HH11	2.19	0.49
1:F:262:PHE:CD1	1:F:266:MET:HE1	2.46	0.49
1:A:106:ASP:O	1:A:110:MET:HG2	2.11	0.49
1:A:102:SER:HB2	1:A:265:ARG:NH1	2.28	0.49
1:D:390:TYR:O	1:D:394:GLU:HG2	2.12	0.49
1:B:243:TYR:OH	1:B:320:PRO:HD3	2.12	0.49
1:A:113:HIS:O	1:A:137:ASN:HB3	2.11	0.49
1:A:92:LEU:HD21	1:A:186:MET:CE	2.43	0.49
1:E:260:ASN:HB3	1:E:299:PHE:CD1	2.47	0.49
1:F:102:SER:HB2	1:F:265:ARG:NH1	2.28	0.49
1:F:94:THR:HB	1:F:160:ALA:HB2	1.95	0.49
1:E:259:PHE:CD2	1:E:363:PRO:HB3	2.48	0.49
1:A:197:LEU:O	1:A:253:VAL:HA	2.12	0.49
1:A:302:VAL:O	1:A:306:VAL:HG23	2.12	0.49
1:F:102:SER:CB	1:F:265:ARG:NH1	2.76	0.49
1:A:285:GLU:O	1:A:346:SER:OG	2.30	0.49
1:C:384:LEU:O	1:C:388:ILE:HG13	2.13	0.48
1:D:272:ARG:HG2	1:D:273:VAL:N	2.28	0.48
1:F:158:HIS:C	1:F:159:LEU:HD12	2.34	0.48
1:C:277:PHE:CE2	1:C:335:ALA:HB2	2.48	0.48
1:E:233:GLU:CG	1:E:234:GLY:N	2.46	0.48
1:F:278:ILE:O	1:F:282:LEU:HG	2.14	0.48
1:B:169:MET:HE2	1:B:172:PRO:HB3	1.96	0.48
1:D:146:VAL:HG13	1:D:181:ILE:HG21	1.95	0.48
1:F:106:ASP:O	1:F:110:MET:HG2	2.13	0.48
1:C:233:GLU:CG	1:C:234:GLY:N	2.50	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:THR:HB	1:A:328:GLU:HB3	1.95	0.47
4:F:502:UGA:PA	4:F:502:UGA:HO'2	2.36	0.47
1:A:256:ALA:HB2	1:A:312:LEU:CD2	2.43	0.47
1:C:146:VAL:O	1:C:146:VAL:HG12	2.14	0.47
1:E:107:LYS:CE	1:E:307:ASN:OD1	2.62	0.47
1:E:104:LEU:HD13	1:E:306:VAL:HG13	1.95	0.47
1:F:92:LEU:HD11	1:F:118:VAL:CG2	2.45	0.47
1:B:297:ARG:HG2	1:B:331:ILE:HD11	1.96	0.47
1:E:285:GLU:O	1:E:346:SER:HB3	2.15	0.47
1:A:295:GLN:N	1:A:295:GLN:OE1	2.48	0.47
1:A:125:ARG:HD3	1:A:127:ARG:NH2	2.30	0.47
1:A:125:ARG:HD3	1:A:127:ARG:CZ	2.45	0.47
1:F:390:TYR:O	1:F:394:GLU:HG2	2.15	0.47
1:A:233:GLU:HG2	1:A:234:GLY:N	2.30	0.47
1:F:273:VAL:HG13	1:F:274:VAL:N	2.29	0.47
1:A:390:TYR:CE1	1:A:394:GLU:OE2	2.68	0.46
1:F:237:VAL:O	1:F:241:MET:N	2.43	0.46
1:F:384:LEU:O	1:F:388:ILE:HG13	2.15	0.46
1:A:259:PHE:CD2	1:A:363:PRO:HB3	2.51	0.46
1:B:151:ILE:HG12	1:B:152:GLU:H	1.79	0.46
1:E:196:ARG:CZ	1:E:254:ARG:NH2	2.79	0.46
1:F:90:ARG:NH2	1:F:154:ASP:OD1	2.33	0.46
1:F:268:MET:HB3	1:F:268:MET:HE2	1.72	0.46
1:F:325:ASN:HA	1:F:326:PRO:HD2	1.81	0.46
1:D:268:MET:HG2	1:D:391:PHE:CZ	2.51	0.46
1:C:151:ILE:HG12	1:C:152:GLU:H	1.79	0.46
1:A:131:HIS:O	1:A:135:HIS:HE1	1.99	0.46
1:B:183:THR:CB	1:B:241:MET:CE	2.84	0.46
1:D:263:GLY:O	1:D:266:MET:HG2	2.16	0.46
1:A:259:PHE:CE2	1:A:363:PRO:HB3	2.51	0.46
1:E:369:LYS:O	1:E:373:GLY:HA2	2.15	0.46
1:F:326:PRO:HG3	1:F:365:ILE:HD11	1.98	0.46
6:F:503:POP:O6	6:F:503:POP:O2	2.34	0.46
1:E:277:PHE:CE2	1:E:335:ALA:HB2	2.51	0.46
1:C:267:HIS:HD2	7:C:607:HOH:O	1.99	0.46
1:D:138:PHE:CG	1:D:139:GLU:N	2.84	0.45
1:D:297:ARG:HE	3:D:502:UDP:H5'1	1.80	0.45
1:B:94:THR:HB	1:B:160:ALA:HB2	1.99	0.45
1:C:265:ARG:HA	1:C:390:TYR:CZ	2.51	0.45
1:E:151:ILE:HG12	1:E:152:GLU:H	1.81	0.45
1:F:297:ARG:HG2	1:F:331:ILE:HD11	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:ASN:ND2	3:A:502:UDP:O4	2.49	0.45
1:E:99:PHE:O	1:E:103:HIS:HD2	1.98	0.45
1:F:246:MET:HA	1:F:251:VAL:O	2.17	0.45
1:A:183:THR:HB	1:A:241:MET:CE	2.41	0.45
1:D:327:GLU:O	1:D:327:GLU:HG2	2.17	0.45
1:B:125:ARG:HD3	1:B:127:ARG:HH21	1.80	0.45
1:D:197:LEU:C	1:D:197:LEU:HD23	2.37	0.45
1:D:249:GLU:OE2	4:D:503:UGA:O3'	2.31	0.45
1:F:197:LEU:O	1:F:253:VAL:HA	2.17	0.45
1:F:113:HIS:O	1:F:137:ASN:HB3	2.16	0.45
1:D:129:VAL:O	1:D:131:HIS:N	2.50	0.45
1:F:297:ARG:CG	1:F:331:ILE:HD11	2.47	0.45
1:F:299:PHE:HD2	1:F:334:PHE:CZ	2.35	0.44
1:A:266:MET:CG	1:A:391:PHE:HZ	2.30	0.44
1:D:290:TYR:N	1:D:290:TYR:CD1	2.85	0.44
1:F:260:ASN:CG	1:F:272:ARG:HH12	2.21	0.44
1:F:330:THR:OG1	1:F:333:GLU:HB2	2.16	0.44
1:A:172:PRO:HD2	1:B:248:GLN:OE1	2.17	0.44
1:C:366:LYS:NZ	7:C:610:HOH:O	2.49	0.44
1:F:319:SER:HB2	1:F:320:PRO:HD2	1.99	0.44
1:C:248:GLN:OE1	1:D:172:PRO:CD	2.65	0.44
1:C:246:MET:CE	1:C:318:SER:CB	2.95	0.44
1:B:151:ILE:HG12	1:B:152:GLU:N	2.32	0.44
1:E:296:THR:O	1:E:297:ARG:HD3	2.17	0.44
1:B:272:ARG:HH11	1:B:299:PHE:HE1	1.64	0.44
1:B:268:MET:HG2	1:B:391:PHE:CZ	2.52	0.44
1:D:92:LEU:HB2	1:D:153:VAL:HG11	2.00	0.44
1:D:102:SER:CB	1:D:265:ARG:HH11	2.31	0.44
1:A:306:VAL:O	1:A:310:VAL:HG23	2.18	0.43
1:B:325:ASN:HA	1:B:326:PRO:HD3	1.84	0.43
1:B:287:LEU:CD1	1:B:346:SER:HB3	2.48	0.43
1:D:129:VAL:O	1:D:130:GLU:C	2.56	0.43
1:D:171:ASN:ND2	1:D:174:LYS:HB2	2.33	0.43
1:C:124:GLY:HA3	2:C:501:NAD:O3B	2.18	0.43
1:A:161:SER:CB	1:A:235:LYS:NZ	2.80	0.43
1:E:304:ASP:CG	1:E:376:PRO:HA	2.39	0.43
1:A:159:LEU:N	1:A:159:LEU:CD1	2.81	0.43
1:A:394:GLU:OE1	1:F:397:TYR:HE1	2.01	0.43
1:B:169:MET:CE	1:B:172:PRO:HB3	2.48	0.43
1:F:145:VAL:HG22	2:F:501:NAD:N1A	2.34	0.43
1:A:394:GLU:HA	1:A:394:GLU:OE1	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118:VAL:HG13	1:B:143:HIS:HB3	2.00	0.43
1:B:296:THR:O	1:B:297:ARG:HD3	2.19	0.43
1:B:174:LYS:CE	7:B:616:HOH:O	2.66	0.43
1:B:233:GLU:CG	1:B:234:GLY:N	2.60	0.43
1:F:394:GLU:HA	1:F:394:GLU:OE1	2.18	0.43
1:D:256:ALA:HB2	1:D:312:LEU:HD23	2.01	0.43
1:F:273:VAL:HG21	1:F:331:ILE:HD12	2.01	0.43
1:A:295:GLN:O	1:A:330:THR:HA	2.19	0.43
1:E:104:LEU:HA	1:E:306:VAL:HG11	1.99	0.43
1:F:188:GLY:O	1:F:191:LYS:HB3	2.19	0.43
1:A:256:ALA:HB2	1:A:312:LEU:HD23	2.00	0.43
1:E:157:TYR:HB3	1:E:159:LEU:CD1	2.48	0.43
1:D:103:HIS:HE1	1:D:264:PRO:O	2.02	0.43
1:D:287:LEU:N	1:D:287:LEU:HD12	2.34	0.43
1:D:265:ARG:HA	1:D:390:TYR:CZ	2.52	0.43
1:E:191:LYS:HE3	1:E:249:GLU:OE1	2.18	0.43
1:E:243:TYR:OH	1:E:320:PRO:CD	2.65	0.43
1:A:246:MET:HA	1:A:251:VAL:O	2.19	0.42
1:B:96:GLY:HA3	1:B:117:VAL:HG13	2.00	0.42
1:C:283:GLN:C	1:C:285:GLU:H	2.23	0.42
1:E:176:LEU:HD13	1:F:241:MET:HA	2.02	0.42
1:D:125:ARG:NH1	1:D:125:ARG:HG2	2.30	0.42
1:E:102:SER:HB3	1:E:128:ASN:HB3	2.02	0.42
1:F:301:TYR:CD2	1:F:383:GLY:HA2	2.54	0.42
1:A:102:SER:HB2	1:A:265:ARG:HH11	1.84	0.42
1:A:274:VAL:O	1:A:278:ILE:HG13	2.20	0.42
1:D:103:HIS:CE1	1:D:265:ARG:HD2	2.54	0.42
1:D:125:ARG:HD3	1:D:127:ARG:NH2	2.35	0.42
1:E:268:MET:HG2	1:E:391:PHE:CE2	2.55	0.42
1:A:243:TYR:OH	1:A:320:PRO:CD	2.61	0.42
1:F:262:PHE:HD1	1:F:266:MET:SD	2.43	0.42
1:F:282:LEU:HD21	1:F:388:ILE:HG23	2.02	0.42
1:C:287:LEU:N	1:C:287:LEU:CD1	2.83	0.42
1:F:161:SER:HB3	2:F:501:NAD:O3D	2.20	0.42
1:F:347:GLU:CG	1:F:348:ILE:N	2.83	0.42
1:A:272:ARG:HH11	1:A:299:PHE:HE1	1.67	0.41
1:A:290:TYR:N	1:A:290:TYR:CD1	2.86	0.41
1:B:99:PHE:O	1:B:103:HIS:HD2	2.03	0.41
1:D:130:GLU:HA	1:D:133:ILE:CD1	2.50	0.41
1:D:397:TYR:OH	1:E:127:ARG:NH1	2.42	0.41
1:D:99:PHE:CZ	1:D:302:VAL:HB	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:MET:SD	1:A:391:PHE:CZ	3.07	0.41
1:C:191:LYS:HE3	1:C:249:GLU:OE1	2.20	0.41
1:C:272:ARG:HG2	1:C:273:VAL:N	2.35	0.41
1:F:122:PHE:HD2	1:F:162:PRO:HB3	1.84	0.41
1:B:174:LYS:HE2	7:B:616:HOH:O	2.20	0.41
1:A:109:MET:C	1:A:111:ASP:N	2.74	0.41
1:C:92:LEU:HD12	1:C:116:THR:O	2.20	0.41
1:C:285:GLU:O	1:C:346:SER:HB3	2.21	0.41
1:C:151:ILE:CG1	1:C:152:GLU:H	2.34	0.41
1:C:299:PHE:CD2	1:C:334:PHE:CZ	3.00	0.41
1:B:395:LEU:HA	1:B:395:LEU:HD23	1.74	0.41
1:C:151:ILE:CG1	1:C:152:GLU:N	2.84	0.41
1:C:197:LEU:O	1:C:253:VAL:HA	2.20	0.41
1:D:384:LEU:O	1:D:388:ILE:HG13	2.21	0.41
1:E:104:LEU:HA	1:E:306:VAL:HG13	2.02	0.41
1:E:151:ILE:HG12	1:E:152:GLU:N	2.36	0.41
1:D:296:THR:HG22	1:D:330:THR:HG22	2.03	0.41
1:E:104:LEU:HD12	1:E:306:VAL:CG1	2.51	0.41
1:F:145:VAL:HG22	2:F:501:NAD:C6A	2.52	0.40
1:F:364:ASP:OD2	1:F:366:LYS:HE2	2.21	0.40
1:A:106:ASP:OD2	1:A:265:ARG:NH2	2.39	0.40
1:C:287:LEU:CD1	1:C:346:SER:HB3	2.51	0.40
1:F:387:ALA:O	1:F:391:PHE:HD1	2.04	0.40
1:B:297:ARG:HD3	1:B:297:ARG:HA	1.80	0.40
1:A:142:ASN:ND2	1:F:120:ASN:O	2.51	0.40
1:A:94:THR:O	1:A:159:LEU:HB2	2.21	0.40
1:A:196:ARG:CZ	1:A:254:ARG:NH2	2.85	0.40
1:A:127:ARG:NH2	5:A:505:SO4:O4	2.52	0.40
1:D:279:LEU:HD23	1:D:279:LEU:HA	1.78	0.40
1:E:325:ASN:HA	1:E:326:PRO:HD2	1.89	0.40
1:F:115:VAL:N	1:F:137:ASN:O	2.53	0.40
1:F:341:LEU:HD22	1:F:385:ASN:OD1	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	257/336 (76%)	249 (97%)	7 (3%)	1 (0%)	34	48
1	B	266/336 (79%)	260 (98%)	6 (2%)	0	100	100
1	C	263/336 (78%)	254 (97%)	9 (3%)	0	100	100
1	D	265/336 (79%)	252 (95%)	13 (5%)	0	100	100
1	E	261/336 (78%)	255 (98%)	6 (2%)	0	100	100
1	F	251/336 (75%)	242 (96%)	9 (4%)	0	100	100
All	All	1563/2016 (78%)	1512 (97%)	50 (3%)	1 (0%)	51	69

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	110	MET

### 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	229/289 (79%)	229 (100%)	0	100	100
1	B	234/289 (81%)	234 (100%)	0	100	100
1	C	231/289 (80%)	231 (100%)	0	100	100
1	D	233/289 (81%)	233 (100%)	0	100	100
1	E	230/289 (80%)	230 (100%)	0	100	100
1	F	224/289 (78%)	224 (100%)	0	100	100
All	All	1381/1734 (80%)	1381 (100%)	0	100	100

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

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	135	HIS
1	A	295	GLN
1	F	135	HIS

### 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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

27 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	NAD	B	501	-	42,48,48	0.88	3 (7%)	50,73,73	1.20	2 (4%)
5	SO4	D	504	-	4,4,4	0.15	0	6,6,6	0.49	0
5	SO4	F	504	-	4,4,4	0.18	0	6,6,6	0.17	0
2	NAD	F	501	-	42,48,48	0.82	1 (2%)	50,73,73	1.15	2 (4%)
4	UGA	C	502	-	33,39,39	2.11	6 (18%)	46,60,60	1.74	8 (17%)
5	SO4	A	504	-	4,4,4	0.17	0	6,6,6	0.28	0
2	NAD	C	501	-	42,48,48	0.91	2 (4%)	50,73,73	1.27	6 (12%)
3	UDP	D	502	-	20,26,26	0.83	0	25,40,40	1.15	1 (4%)
3	UDP	A	502	-	20,26,26	0.79	0	25,40,40	1.25	2 (8%)
6	POP	C	503	-	6,8,8	0.69	0	13,13,13	1.30	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAD	D	501	-	42,48,48	0.78	0	50,73,73	1.24	3 (6%)
5	SO4	B	504	-	4,4,4	0.12	0	6,6,6	0.62	0
5	SO4	D	505	-	4,4,4	0.36	0	6,6,6	0.49	0
4	UGA	D	503	-	33,39,39	2.08	6 (18%)	46,60,60	1.42	6 (13%)
5	SO4	E	504	-	4,4,4	0.15	0	6,6,6	0.31	0
6	POP	F	503	-	6,8,8	0.72	0	13,13,13	1.36	1 (7%)
4	UGA	A	503	-	33,39,39	1.97	6 (18%)	46,60,60	1.56	6 (13%)
3	UDP	B	502	-	20,26,26	0.80	0	25,40,40	1.30	4 (16%)
4	UGA	E	503	-	33,39,39	2.08	5 (15%)	46,60,60	1.59	5 (10%)
4	UGA	F	502	-	33,39,39	1.99	6 (18%)	46,60,60	1.86	9 (19%)
5	SO4	A	505	-	4,4,4	0.15	0	6,6,6	0.18	0
6	POP	E	502	-	6,8,8	1.15	0	13,13,13	1.91	3 (23%)
2	NAD	E	501	-	42,48,48	0.80	0	50,73,73	1.22	5 (10%)
5	SO4	B	505	-	4,4,4	0.20	0	6,6,6	0.41	0
2	NAD	A	501	-	42,48,48	0.80	1 (2%)	50,73,73	1.27	3 (6%)
4	UGA	B	503	-	33,39,39	2.05	6 (18%)	46,60,60	1.47	6 (13%)
5	SO4	C	504	-	4,4,4	0.12	0	6,6,6	0.39	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
2	NAD	B	501	-	-	3/26/62/62	0/5/5/5
3	UDP	D	502	-	-	5/14/32/32	0/2/2/2
4	UGA	F	502	-	-	6/21/61/61	0/3/3/3
6	POP	F	503	-	-	4/6/6/6	-
6	POP	E	502	-	-	0/6/6/6	-
2	NAD	F	501	-	-	1/26/62/62	0/5/5/5
4	UGA	C	502	-	-	4/21/61/61	0/3/3/3
4	UGA	D	503	-	-	3/21/61/61	0/3/3/3
2	NAD	E	501	-	-	1/26/62/62	0/5/5/5
2	NAD	C	501	-	-	4/26/62/62	0/5/5/5
2	NAD	A	501	-	-	3/26/62/62	0/5/5/5
4	UGA	B	503	-	-	3/21/61/61	0/3/3/3
4	UGA	A	503	-	-	1/21/61/61	0/3/3/3
3	UDP	B	502	-	-	6/14/32/32	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	UGA	E	503	-	-	6/21/61/61	0/3/3/3
3	UDP	A	502	-	-	2/14/32/32	0/2/2/2
6	POP	C	503	-	-	2/6/6/6	-
2	NAD	D	501	-	-	5/26/62/62	0/5/5/5

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	503	UGA	C6-N1	-7.57	1.33	1.47
4	D	503	UGA	C6-N1	-7.51	1.33	1.47
4	B	503	UGA	C6-N1	-7.46	1.33	1.47
4	F	502	UGA	C6-N1	-7.43	1.33	1.47
4	A	503	UGA	C6-N1	-7.02	1.34	1.47
4	C	502	UGA	C6-N1	-7.00	1.34	1.47
4	C	502	UGA	C2-N1	5.98	1.44	1.35
4	E	503	UGA	C6-C5	-5.31	1.38	1.52
4	D	503	UGA	C6-C5	-5.25	1.38	1.52
4	B	503	UGA	C6-C5	-5.05	1.39	1.52
4	A	503	UGA	C6-C5	-5.03	1.39	1.52
4	D	503	UGA	C5-C4	-5.03	1.38	1.50
4	F	502	UGA	C6-C5	-4.86	1.39	1.52
4	C	502	UGA	C6-C5	-4.80	1.39	1.52
4	E	503	UGA	C5-C4	-4.76	1.39	1.50
4	F	502	UGA	C5-C4	-4.63	1.39	1.50
4	B	503	UGA	C5-C4	-4.53	1.39	1.50
4	A	503	UGA	C5-C4	-4.48	1.39	1.50
4	C	502	UGA	C5-C4	-4.47	1.39	1.50
4	E	503	UGA	C2-N1	3.93	1.41	1.35
4	B	503	UGA	C2-N1	3.84	1.41	1.35
4	A	503	UGA	C2-N1	3.73	1.41	1.35
4	F	502	UGA	C2-N1	3.50	1.40	1.35
4	D	503	UGA	C2-N1	3.23	1.40	1.35
2	B	501	NAD	O4B-C1B	2.75	1.44	1.41
4	B	503	UGA	C2-N3	-2.68	1.33	1.38
4	B	503	UGA	C4-N3	-2.61	1.33	1.37
4	D	503	UGA	C4-N3	-2.41	1.33	1.37
4	F	502	UGA	C2-N3	-2.40	1.33	1.38
2	A	501	NAD	C5A-C4A	2.38	1.47	1.40
4	A	503	UGA	C2-N3	-2.34	1.33	1.38
4	D	503	UGA	C2-N3	-2.33	1.33	1.38
2	F	501	NAD	C5A-C4A	2.31	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	NAD	C5A-C4A	2.28	1.47	1.40
4	E	503	UGA	C2-N3	-2.28	1.33	1.38
2	B	501	NAD	C5A-N7A	-2.16	1.31	1.39
2	B	501	NAD	C5A-C4A	2.16	1.46	1.40
4	F	502	UGA	C4-N3	-2.15	1.33	1.37
4	C	502	UGA	C2-N3	-2.15	1.34	1.38
2	C	501	NAD	C2A-N3A	2.07	1.35	1.32
4	A	503	UGA	C4-N3	-2.07	1.34	1.37
4	C	502	UGA	C4-N3	-2.03	1.34	1.37

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	502	UGA	C4-N3-C2	-6.87	120.09	125.79
4	F	502	UGA	C4-N3-C2	-6.79	120.16	125.79
4	A	503	UGA	C4-N3-C2	-6.62	120.30	125.79
4	E	503	UGA	C4-N3-C2	-5.93	120.87	125.79
4	D	503	UGA	C4-N3-C2	-5.01	121.64	125.79
6	E	502	POP	P2-O-P1	-4.95	115.83	132.83
4	F	502	UGA	O3A-PB-O3B	-4.90	92.60	102.48
4	B	503	UGA	C4-N3-C2	-4.68	121.91	125.79
4	E	503	UGA	C5-C4-N3	4.08	121.23	116.65
4	A	503	UGA	C5-C4-N3	4.02	121.17	116.65
4	C	502	UGA	C5-C4-N3	3.92	121.06	116.65
2	F	501	NAD	N3A-C2A-N1A	-3.87	122.63	128.68
4	F	502	UGA	N3-C2-N1	3.76	120.62	116.65
4	C	502	UGA	N3-C2-N1	3.64	120.50	116.65
4	F	502	UGA	C5-C4-N3	3.63	120.73	116.65
2	C	501	NAD	C4A-C5A-N7A	-3.59	105.66	109.40
4	D	503	UGA	C5-C4-N3	3.58	120.67	116.65
4	F	502	UGA	O4D-C1D-N1	-3.46	104.58	109.30
2	D	501	NAD	N3A-C2A-N1A	-3.46	123.28	128.68
2	E	501	NAD	N3A-C2A-N1A	-3.33	123.47	128.68
4	C	502	UGA	PA-O3A-PB	-3.29	121.53	132.83
4	E	503	UGA	PA-O3A-PB	-3.28	121.57	132.83
2	A	501	NAD	PN-O3-PA	-3.21	121.81	132.83
4	B	503	UGA	PA-O3A-PB	-3.19	121.86	132.83
3	A	502	UDP	PA-O3A-PB	-3.14	122.05	132.83
4	F	502	UGA	O2-C2-N1	-3.09	119.23	123.11
3	A	502	UDP	C3'-C2'-C1'	3.04	105.56	100.98
2	A	501	NAD	N3A-C2A-N1A	-3.03	123.95	128.68
2	D	501	NAD	PN-O3-PA	-3.02	122.47	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	502	UDP	PA-O3A-PB	-2.99	122.56	132.83
2	B	501	NAD	N3A-C2A-N1A	-2.98	124.02	128.68
6	F	503	POP	P2-O-P1	-2.94	122.75	132.83
4	D	503	UGA	O2-C2-N1	-2.93	119.43	123.11
2	E	501	NAD	PN-O3-PA	-2.87	122.99	132.83
2	A	501	NAD	O4B-C1B-C2B	-2.86	102.74	106.93
4	B	503	UGA	N3-C2-N1	2.86	119.68	116.65
6	C	503	POP	P2-O-P1	-2.85	123.06	132.83
4	B	503	UGA	C5-C4-N3	2.83	119.83	116.65
2	C	501	NAD	C2N-C3N-C4N	2.70	121.31	118.26
4	A	503	UGA	N3-C2-N1	2.67	119.48	116.65
2	C	501	NAD	N3A-C2A-N1A	-2.65	124.53	128.68
4	A	503	UGA	O2-C2-N1	-2.64	119.79	123.11
3	D	502	UDP	PA-O3A-PB	-2.60	123.91	132.83
4	D	503	UGA	C5-C6-N1	2.60	120.17	111.61
4	B	503	UGA	C5-C6-N1	2.55	120.02	111.61
4	C	502	UGA	O2-C2-N3	-2.55	116.76	121.50
4	C	502	UGA	O3B-C1'-C2'	2.53	113.02	108.38
3	B	502	UDP	C3'-C2'-C1'	2.53	104.78	100.98
2	F	501	NAD	C4A-C5A-N7A	-2.52	106.77	109.40
2	C	501	NAD	C5B-C4B-C3B	-2.51	105.78	115.18
2	C	501	NAD	PN-O3-PA	-2.48	124.31	132.83
4	A	503	UGA	O3A-PB-O3B	-2.47	97.50	102.48
3	B	502	UDP	O3B-PB-O2B	2.45	116.99	107.64
4	A	503	UGA	PA-O3A-PB	-2.41	124.55	132.83
4	E	503	UGA	C5-C6-N1	2.38	119.47	111.61
2	E	501	NAD	C4A-C5A-N7A	-2.37	106.93	109.40
6	E	502	POP	O-P2-O4	-2.36	98.09	111.19
2	E	501	NAD	C1B-N9A-C4A	-2.32	122.57	126.64
4	C	502	UGA	C5-C6-N1	2.29	119.14	111.61
4	D	503	UGA	C3D-C2D-C1D	2.28	105.76	101.43
6	E	502	POP	O3-P1-O2	2.27	116.30	107.64
4	F	502	UGA	C5-C6-N1	2.25	119.03	111.61
2	D	501	NAD	N6A-C6A-N1A	2.24	123.22	118.57
4	C	502	UGA	C3D-C2D-C1D	2.23	105.67	101.43
4	E	503	UGA	O5'-C1'-O3B	-2.23	108.46	111.36
2	B	501	NAD	N6A-C6A-N1A	2.15	123.04	118.57
4	F	502	UGA	C3D-C2D-C1D	2.14	105.49	101.43
2	E	501	NAD	C3D-C2D-C1D	2.14	104.19	100.98
4	F	502	UGA	O3B-C1'-C2'	2.11	112.24	108.38
3	B	502	UDP	O3B-PB-O3A	-2.04	97.80	104.64
4	B	503	UGA	C2D-C3D-C4D	2.03	106.59	102.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	503	UGA	O2B-PB-O1B	2.03	122.26	112.24
2	C	501	NAD	O2A-PA-O1A	2.02	122.23	112.24

There are no chirality outliers.

All (59) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	502	UGA	C5D-O5D-PA-O2A
2	C	501	NAD	C5D-O5D-PN-O1N
3	D	502	UDP	O4'-C1'-N1-C6
3	D	502	UDP	C5'-O5'-PA-O1A
3	D	502	UDP	C5'-O5'-PA-O2A
3	D	502	UDP	PA-O3A-PB-O3B
3	A	502	UDP	C2'-C1'-N1-C6
3	A	502	UDP	O4'-C1'-N1-C6
6	C	503	POP	P1-O-P2-O6
2	D	501	NAD	C5B-O5B-PA-O2A
2	D	501	NAD	C5D-O5D-PN-O1N
6	F	503	POP	P2-O-P1-O2
3	B	502	UDP	C2'-C1'-N1-C6
3	B	502	UDP	O4'-C1'-N1-C6
3	B	502	UDP	C5'-O5'-PA-O1A
3	B	502	UDP	C5'-O5'-PA-O2A
3	B	502	UDP	PA-O3A-PB-O2B
4	F	502	UGA	O5'-C1'-O3B-PB
4	F	502	UGA	PB-O3A-PA-O5D
4	D	503	UGA	C1'-O3B-PB-O3A
4	C	502	UGA	C1'-O3B-PB-O3A
4	E	503	UGA	C1'-O3B-PB-O3A
4	B	503	UGA	C1'-O3B-PB-O3A
6	F	503	POP	P1-O-P2-O4
6	F	503	POP	P1-O-P2-O6
4	C	502	UGA	C5D-O5D-PA-O3A
2	D	501	NAD	C5D-O5D-PN-O3
4	E	503	UGA	C5D-O5D-PA-O3A
4	D	503	UGA	PB-O3A-PA-O1A
4	F	502	UGA	C1'-O3B-PB-O3A
2	B	501	NAD	C5D-O5D-PN-O1N
4	C	502	UGA	C5D-O5D-PA-O1A
2	C	501	NAD	C5D-O5D-PN-O2N
2	D	501	NAD	C5D-O5D-PN-O2N
6	C	503	POP	P1-O-P2-O4

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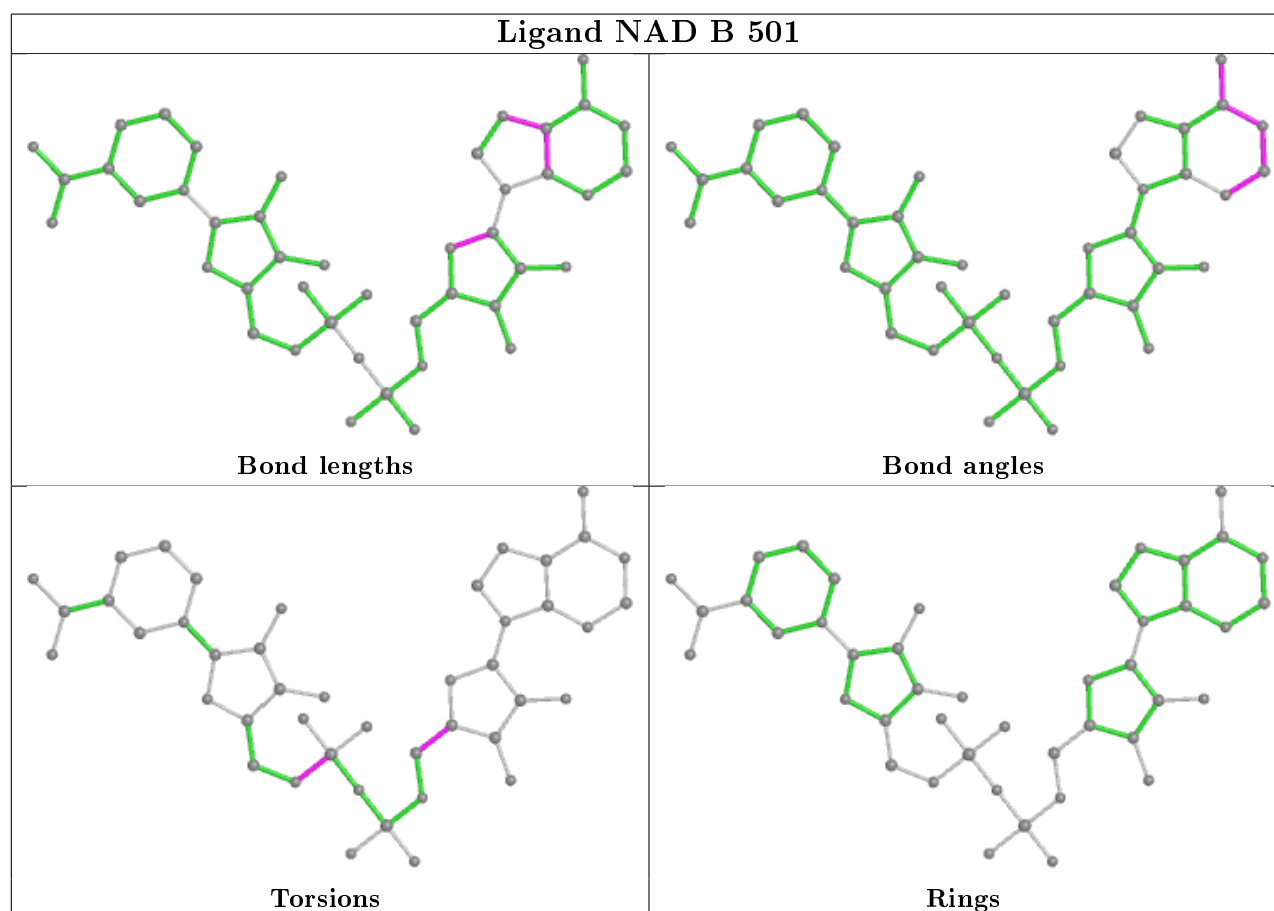
Mol	Chain	Res	Type	Atoms
4	E	503	UGA	PB-O3A-PA-O1A
4	B	503	UGA	PB-O3A-PA-O2A
4	F	502	UGA	C2D-C1D-N1-C6
2	B	501	NAD	O4B-C4B-C5B-O5B
2	C	501	NAD	O4B-C4B-C5B-O5B
2	A	501	NAD	C4N-C3N-C7N-N7N
4	D	503	UGA	PB-O3A-PA-O2A
2	D	501	NAD	O4B-C4B-C5B-O5B
4	F	502	UGA	C2D-C1D-N1-C2
2	F	501	NAD	O4B-C4B-C5B-O5B
6	F	503	POP	P2-O-P1-O3
2	A	501	NAD	C4N-C3N-C7N-O7N
2	B	501	NAD	C5D-O5D-PN-O3
2	C	501	NAD	C5D-O5D-PN-O3
3	D	502	UDP	C5'-O5'-PA-O3A
3	B	502	UDP	C5'-O5'-PA-O3A
4	F	502	UGA	O4D-C1D-N1-C2
2	A	501	NAD	O4B-C4B-C5B-O5B
4	A	503	UGA	PB-O3A-PA-O2A
4	E	503	UGA	PB-O3A-PA-O2A
4	B	503	UGA	PB-O3A-PA-O1A
4	E	503	UGA	C5D-O5D-PA-O1A
4	E	503	UGA	C5D-O5D-PA-O2A
2	E	501	NAD	O4B-C4B-C5B-O5B

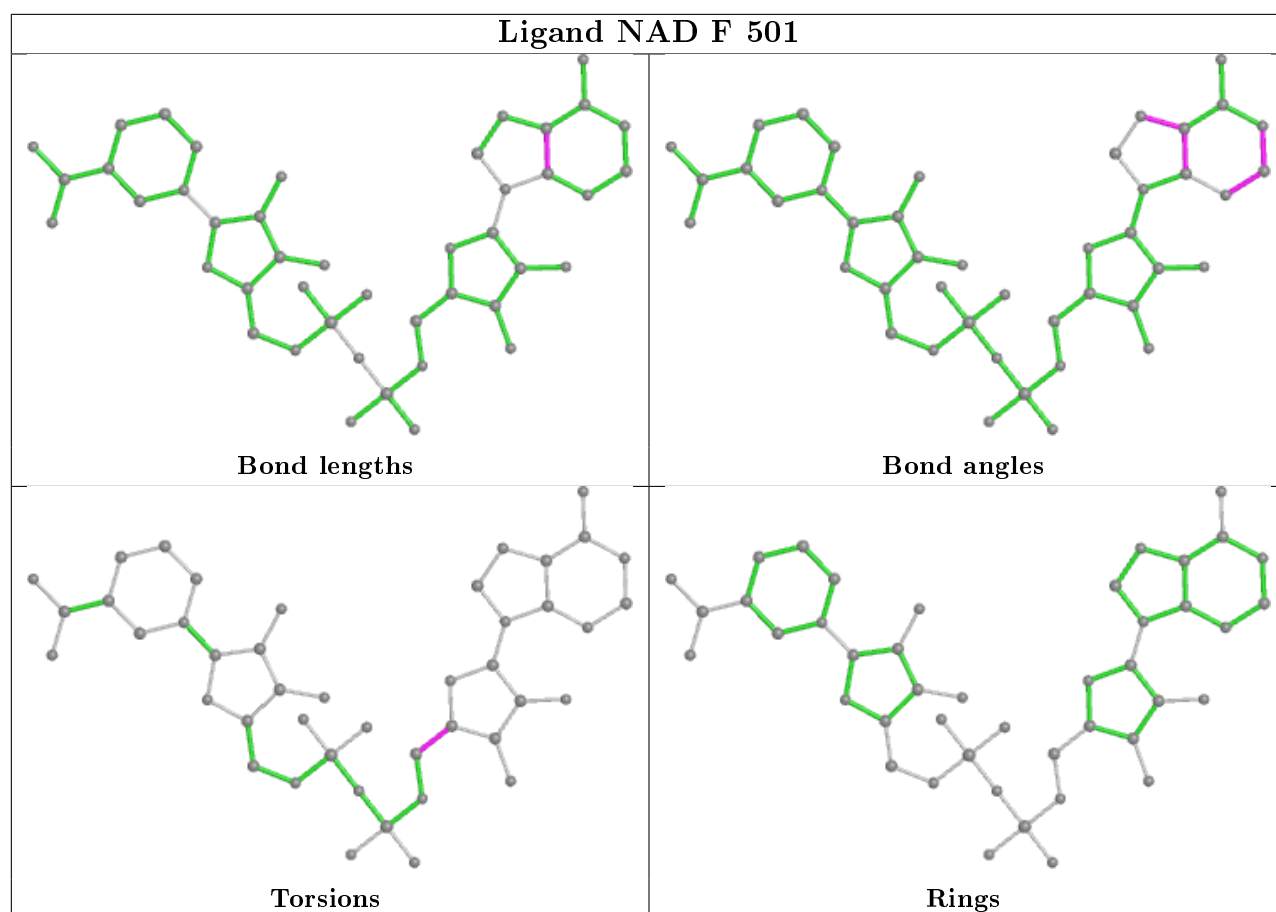
There are no ring outliers.

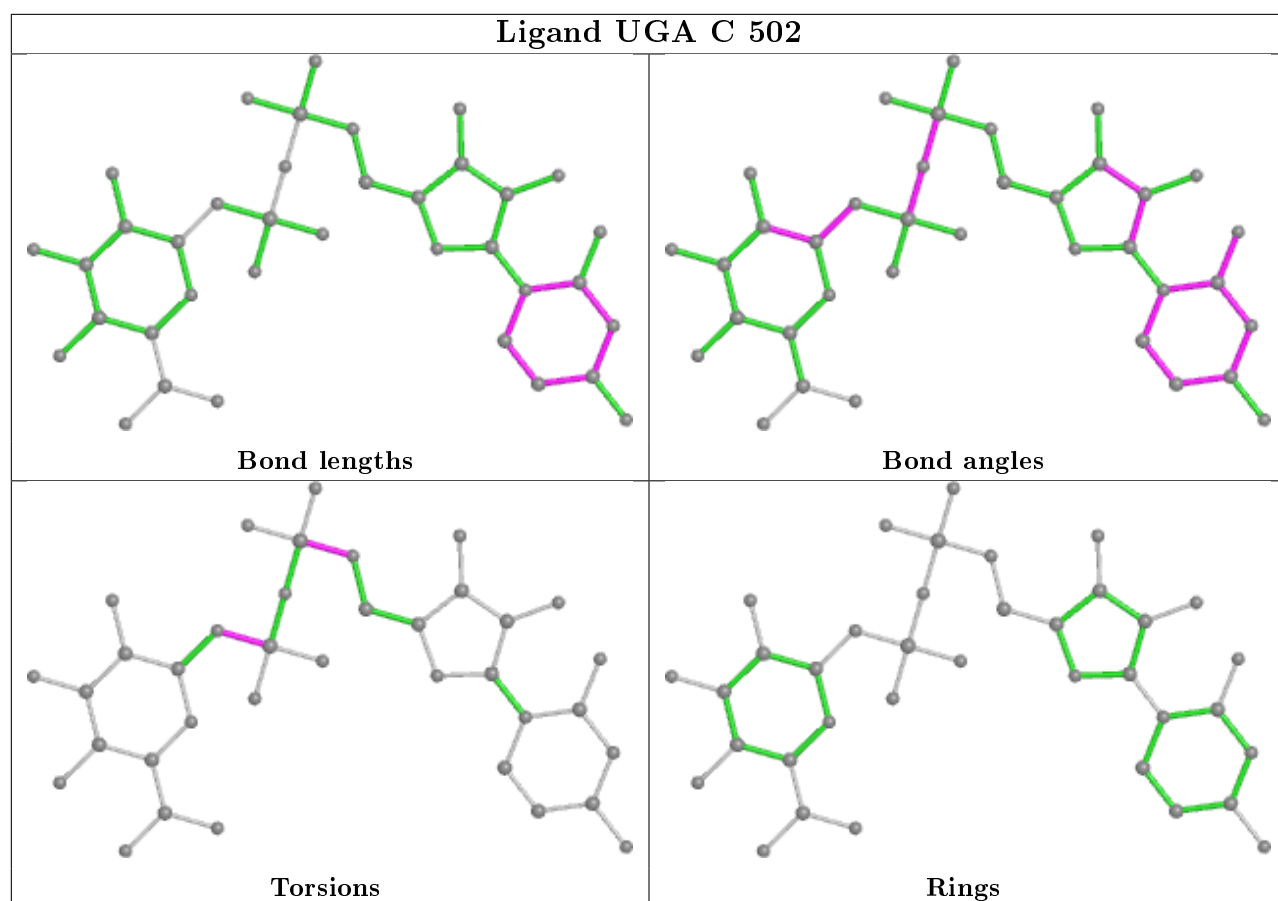
12 monomers are involved in 23 short contacts:

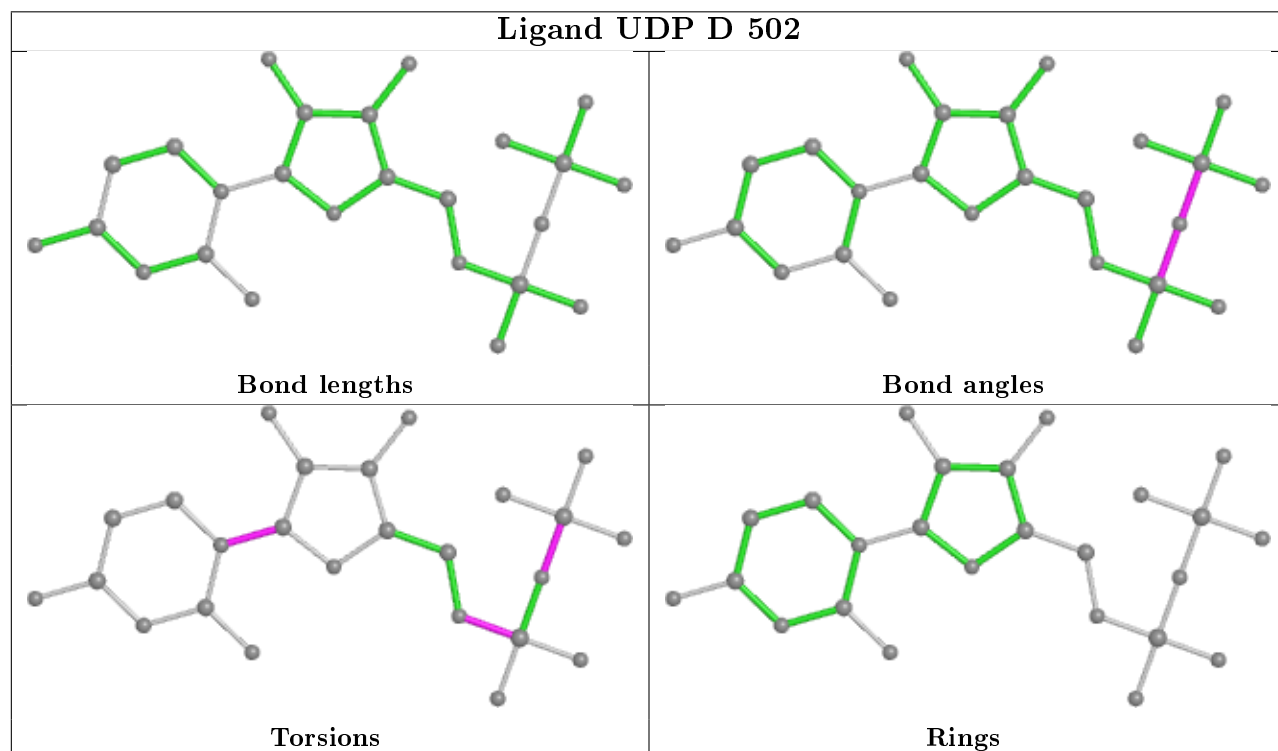
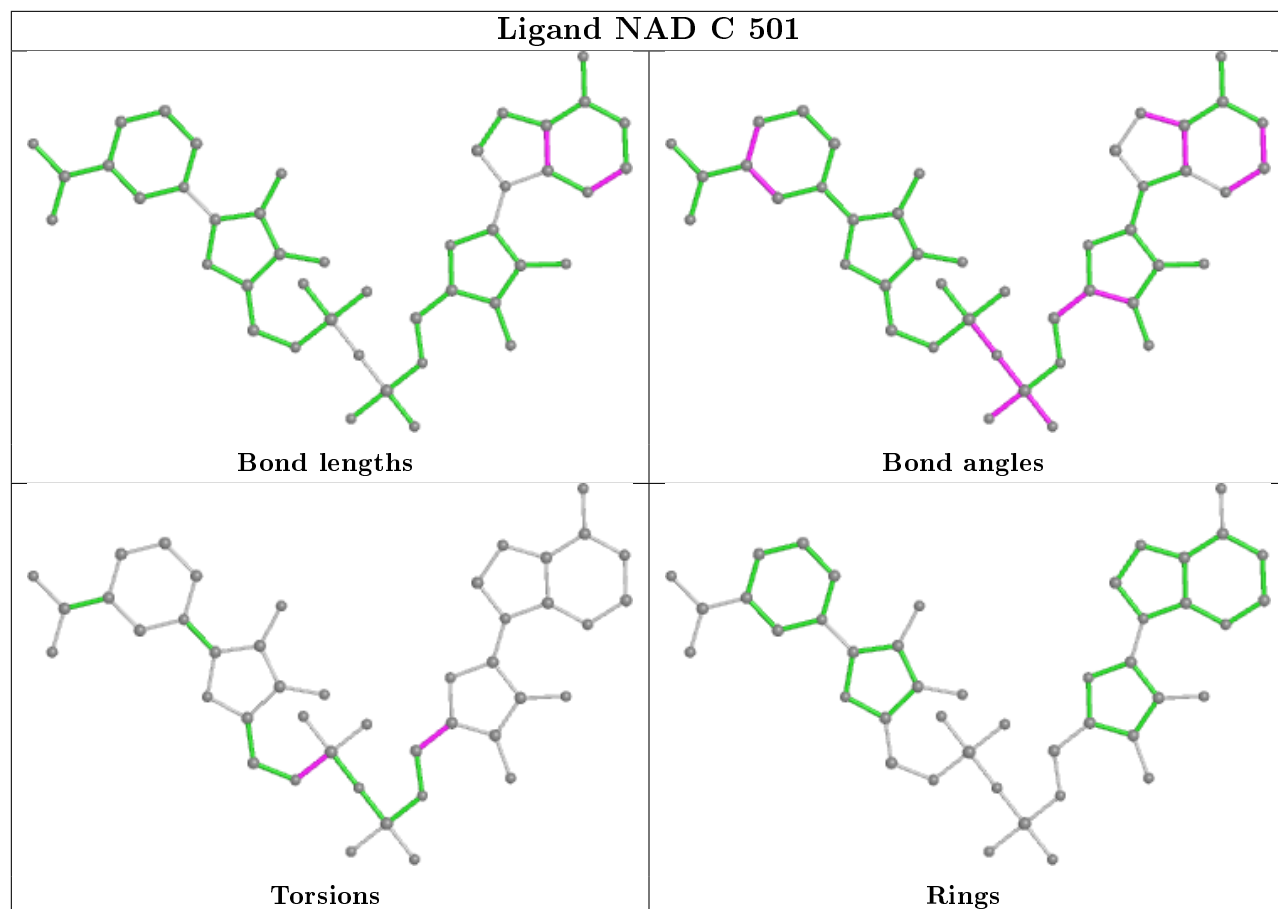
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	501	NAD	3	0
2	C	501	NAD	1	0
3	D	502	UDP	2	0
3	A	502	UDP	1	0
6	C	503	POP	2	0
5	B	504	SO4	1	0
4	D	503	UGA	1	0
6	F	503	POP	3	0
4	A	503	UGA	2	0
4	F	502	UGA	2	0
5	A	505	SO4	3	0
4	B	503	UGA	2	0

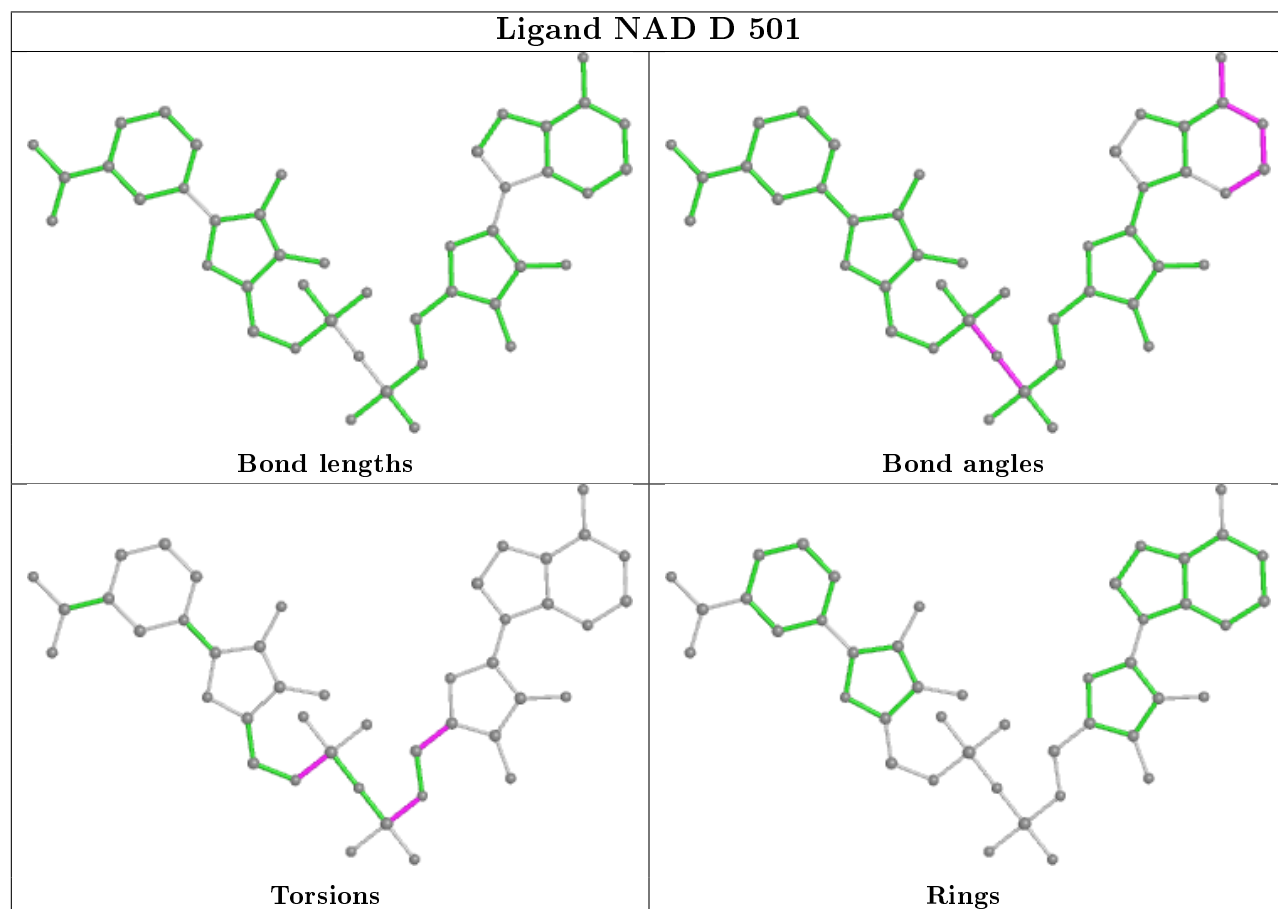
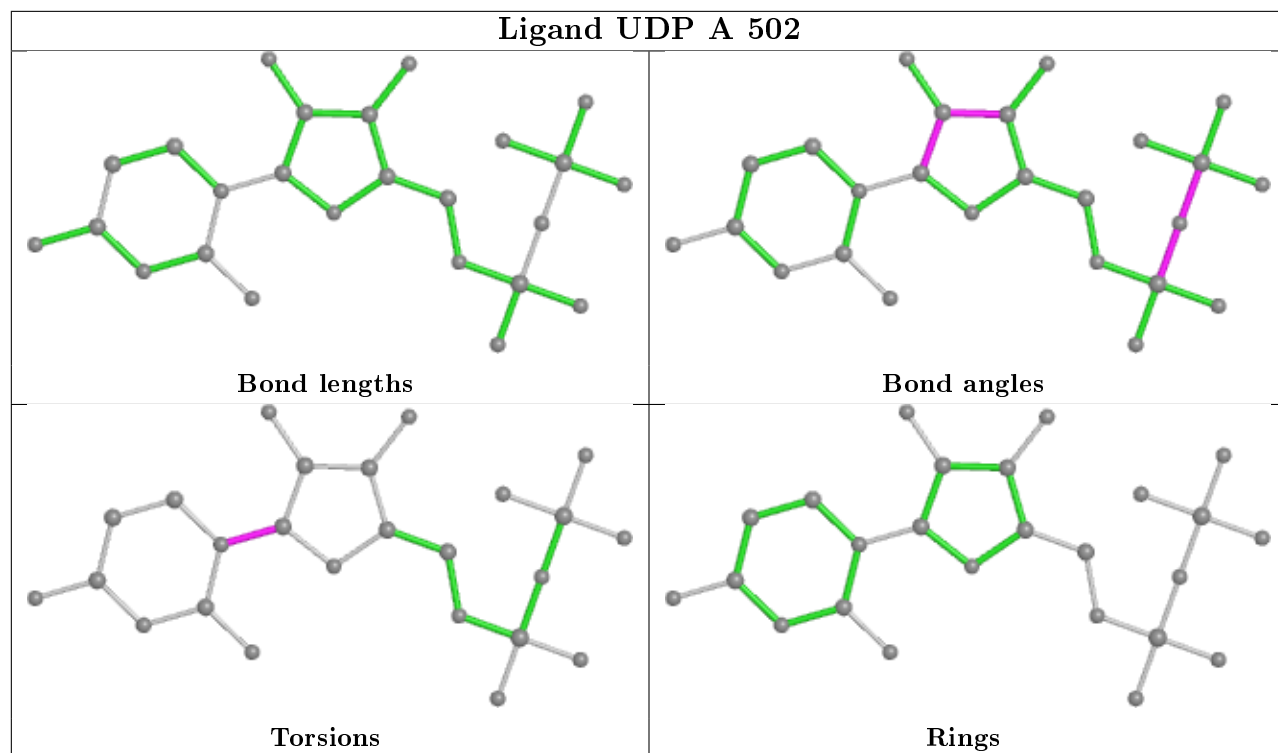
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

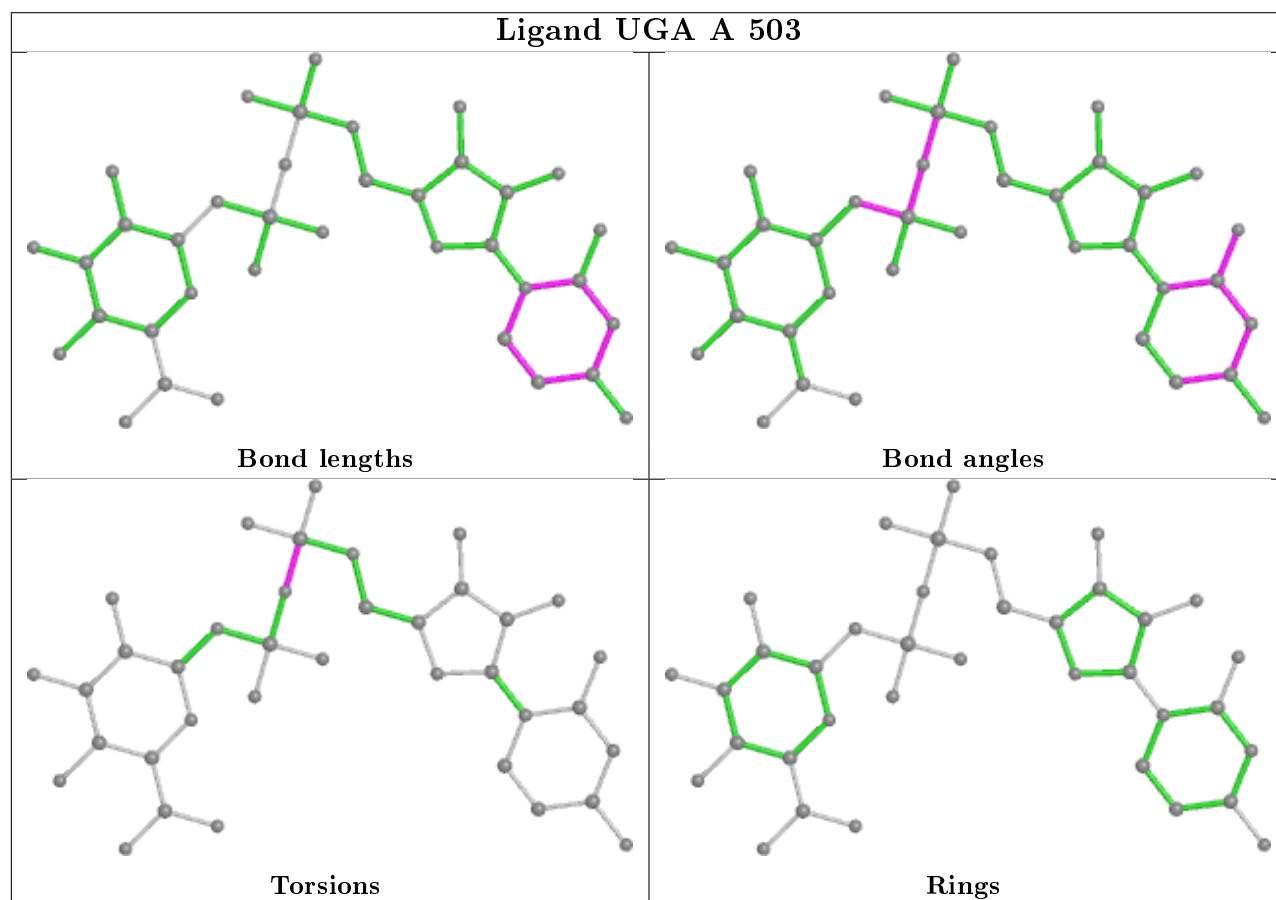
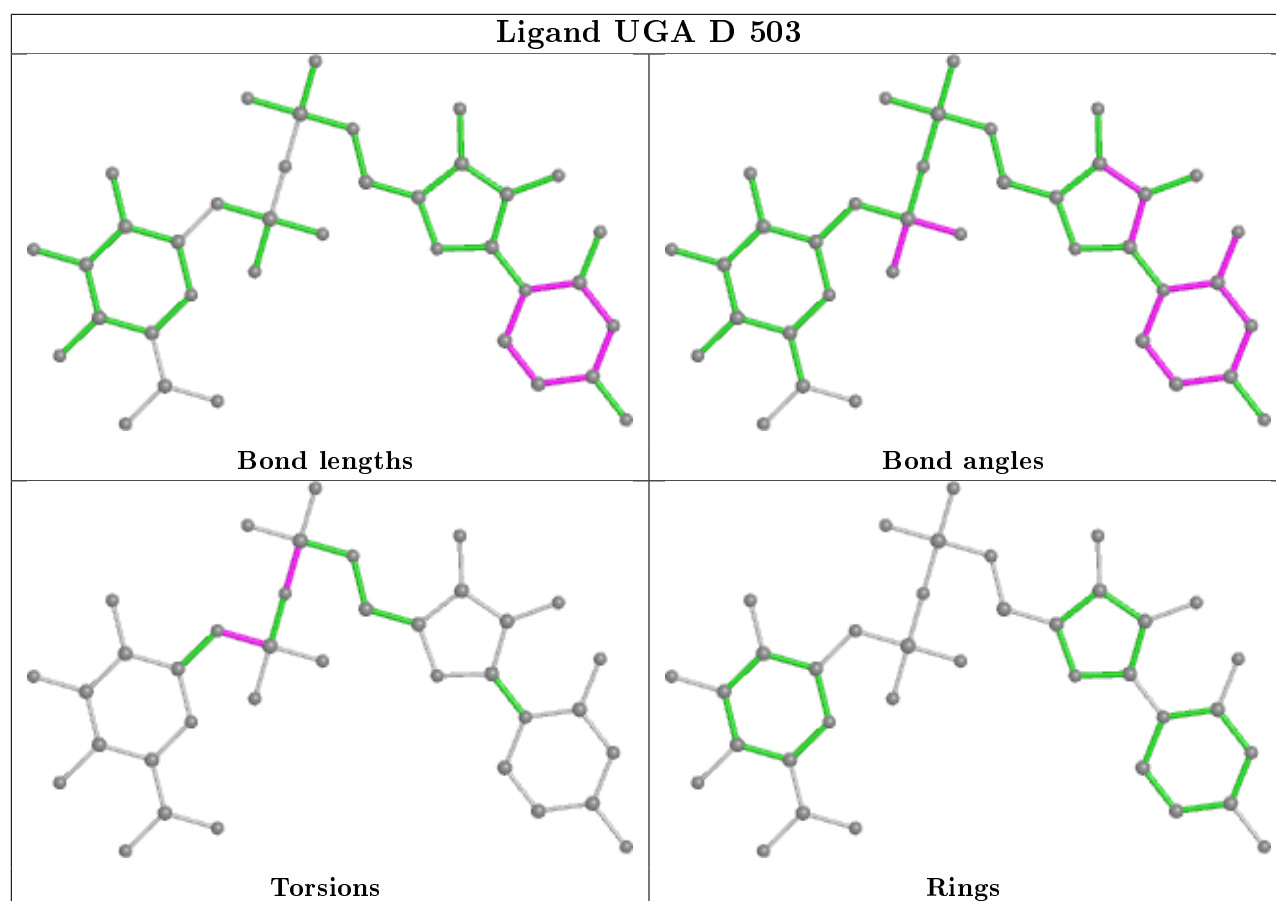


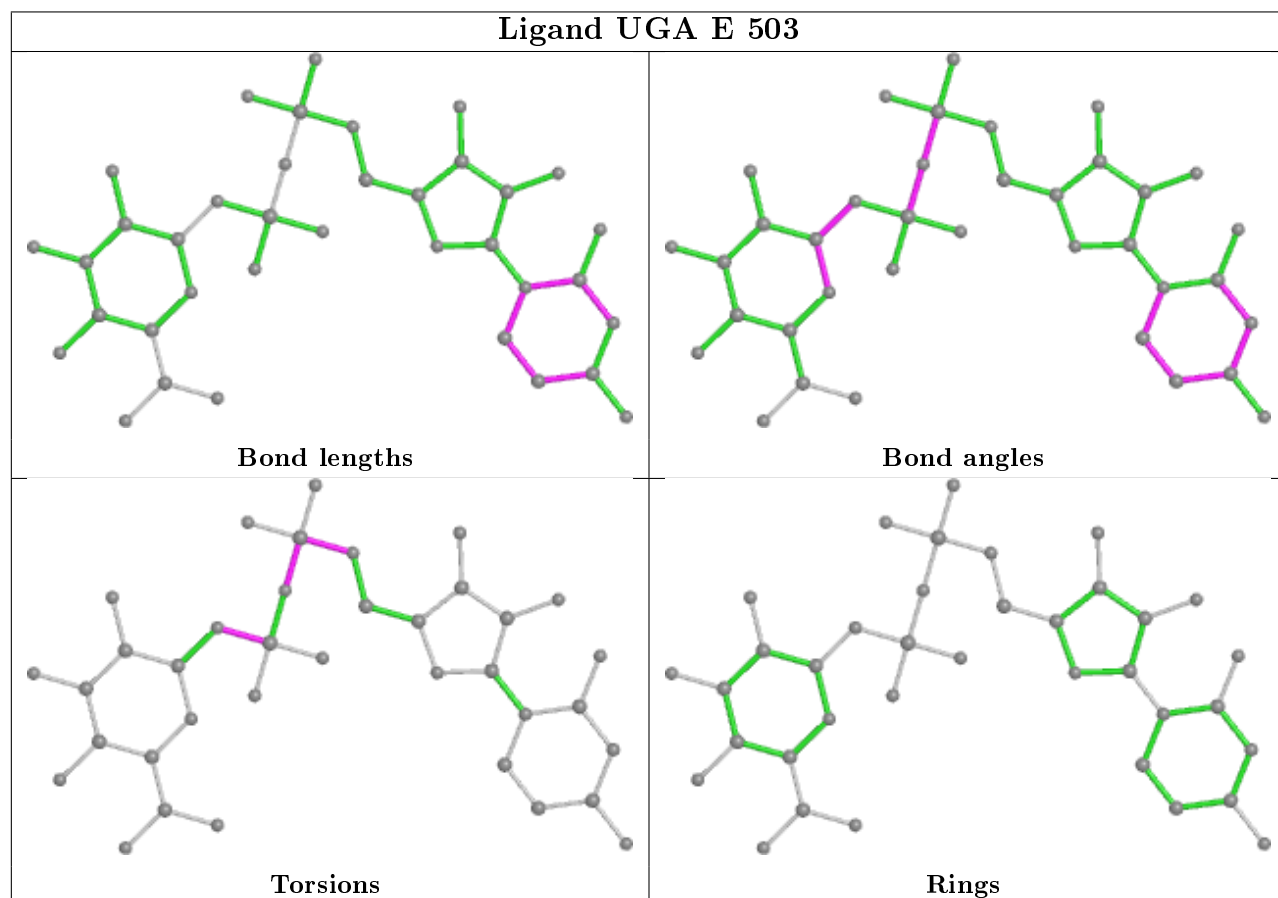
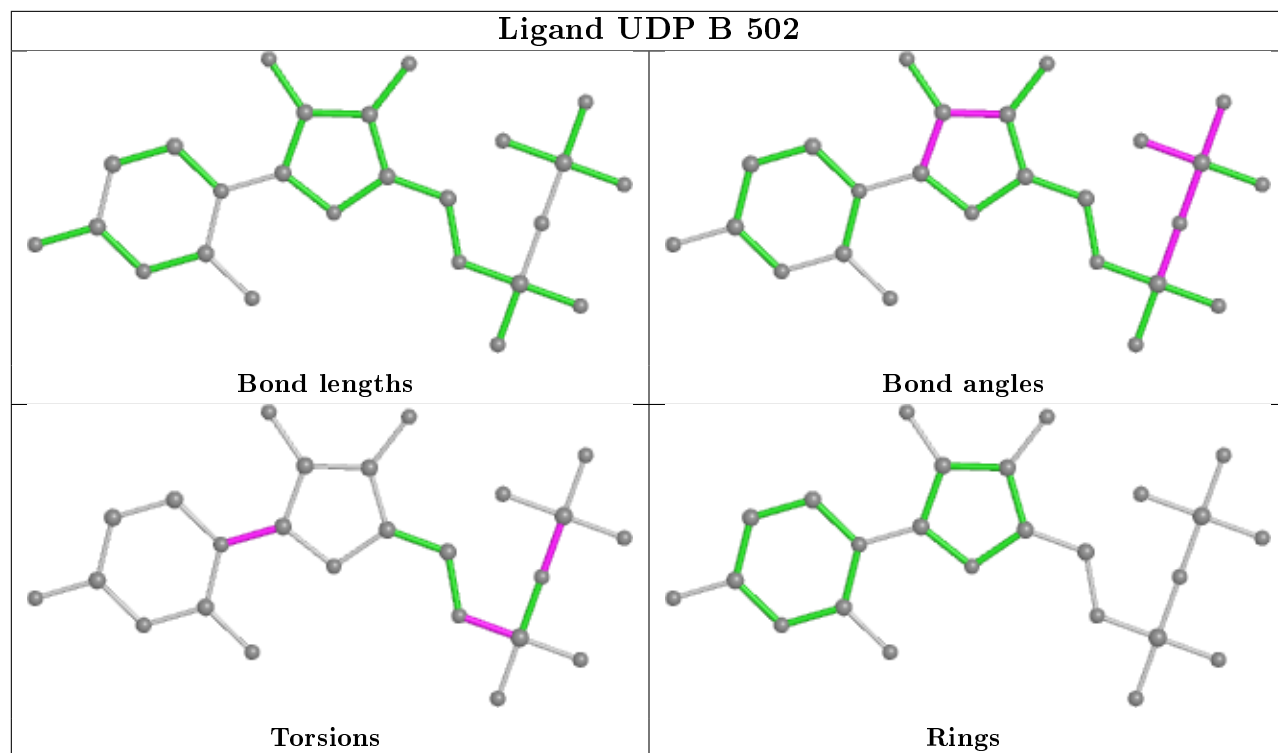




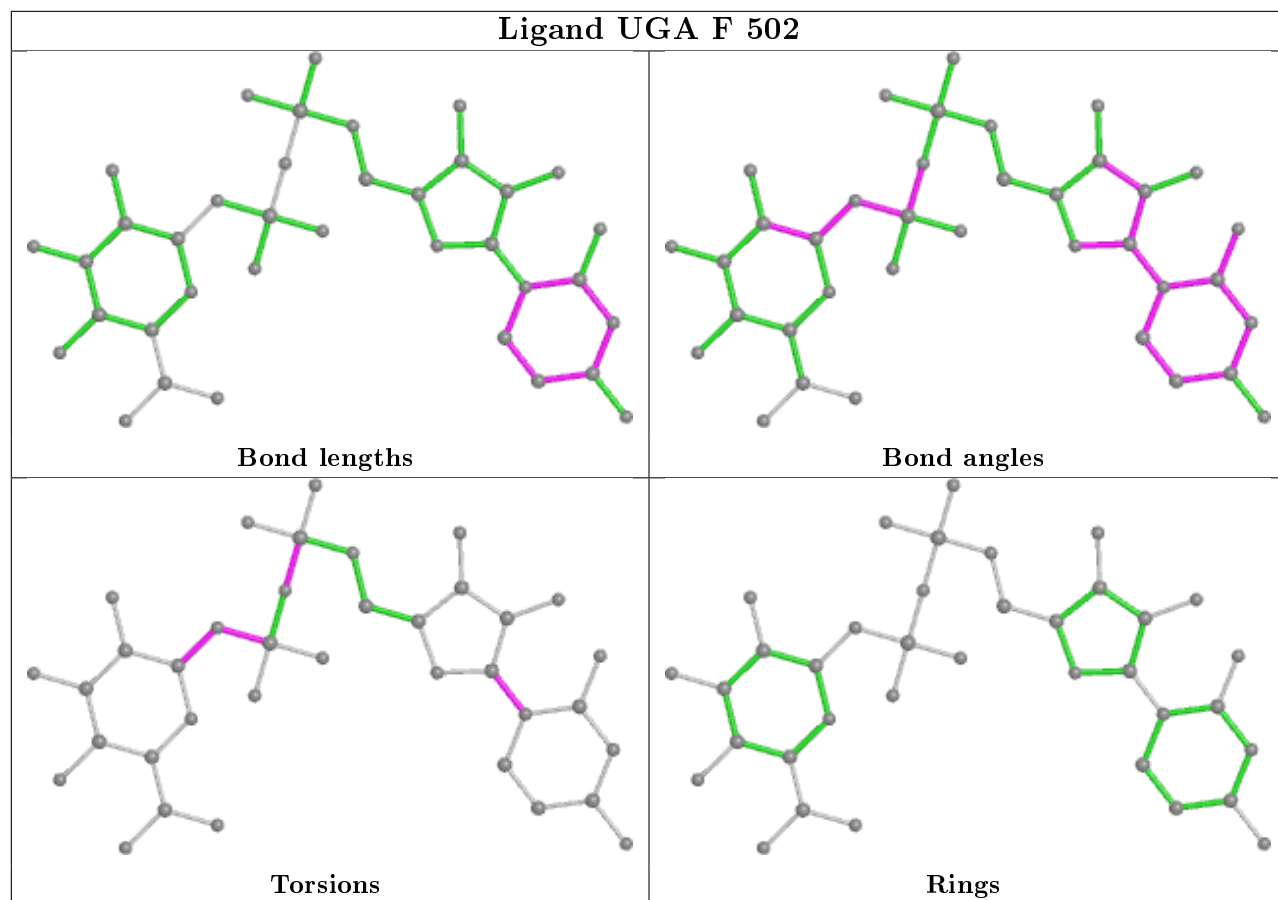


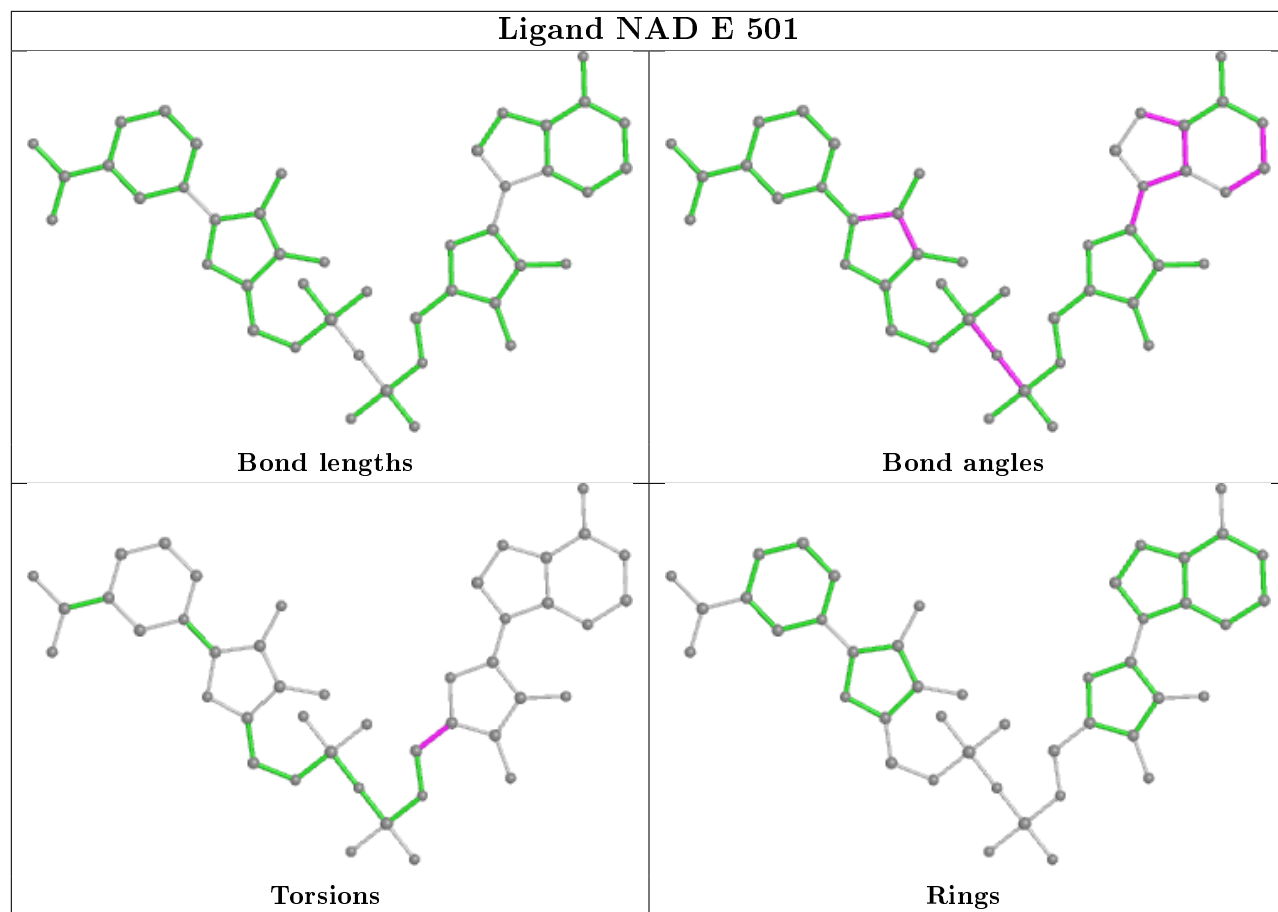


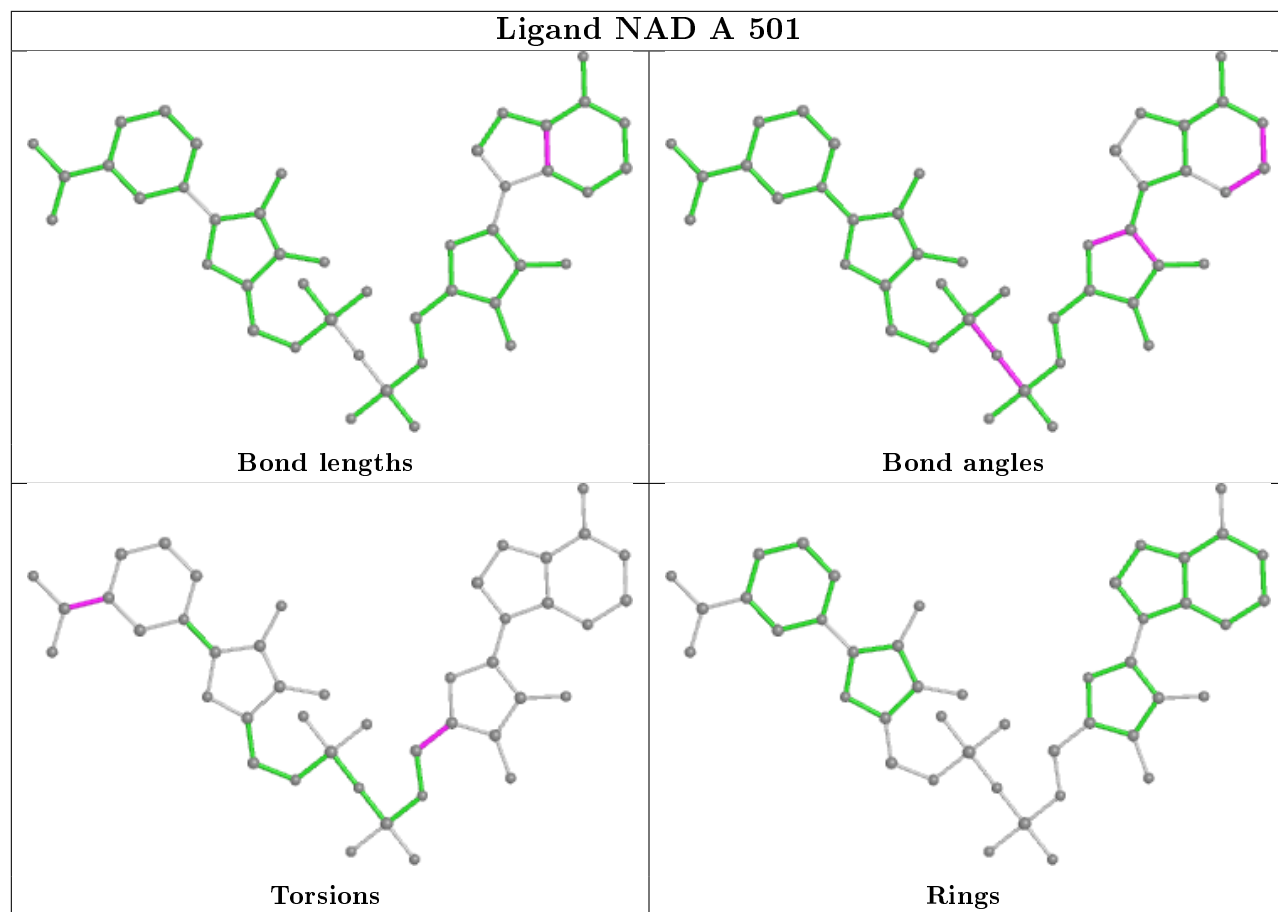


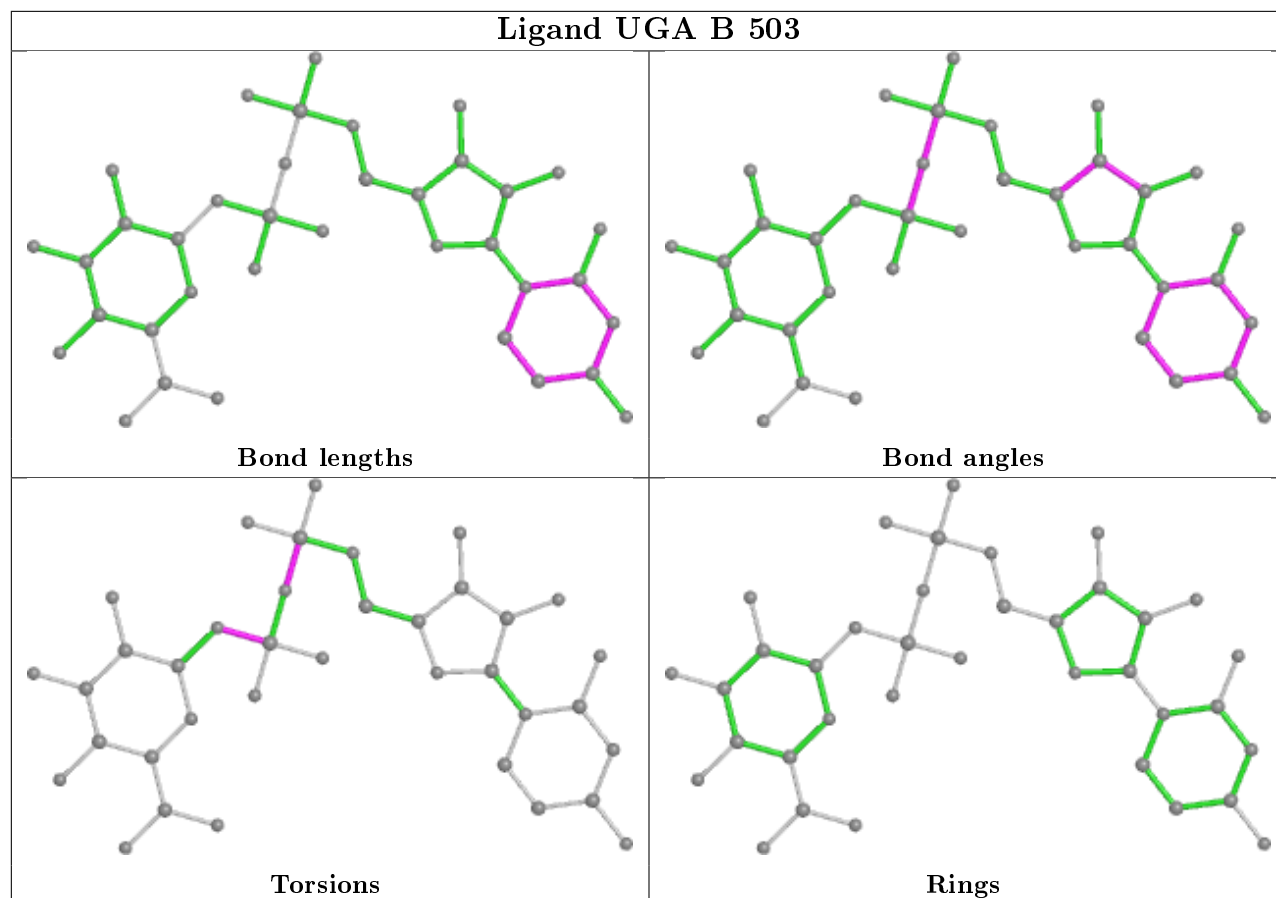












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	267/336 (79%)	0.54	38 (14%) 2 1	45, 83, 138, 167	0
1	B	274/336 (81%)	0.16	11 (4%) 38 35	33, 54, 104, 131	0
1	C	271/336 (80%)	-0.21	2 (0%) 87 86	38, 59, 95, 130	0
1	D	273/336 (81%)	-0.00	3 (1%) 80 78	40, 65, 111, 126	0
1	E	269/336 (80%)	0.45	23 (8%) 10 8	57, 89, 127, 152	0
1	F	261/336 (77%)	0.55	27 (10%) 6 4	63, 105, 136, 168	0
All	All	1615/2016 (80%)	0.24	104 (6%) 19 16	33, 75, 126, 168	0

All (104) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	282	LEU	6.2
1	B	290	TYR	5.7
1	F	131	HIS	5.6
1	A	338	ILE	5.3
1	A	395	LEU	5.3
1	F	332	LEU	5.2
1	D	170	TYR	4.7
1	E	282	LEU	4.7
1	A	279	LEU	4.4
1	B	351	LEU	4.2
1	E	361	ARG	4.0
1	B	279	LEU	4.0
1	F	343	GLY	3.7
1	A	350	PHE	3.7
1	F	299	PHE	3.7
1	F	132	TRP	3.6
1	E	297	ARG	3.6
1	E	392	ARG	3.6
1	A	283	GLN	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	273	VAL	3.6
1	E	279	LEU	3.5
1	A	334	PHE	3.5
1	A	332	LEU	3.4
1	E	288	THR	3.4
1	A	339	LYS	3.4
1	F	381	GLU	3.4
1	F	338	ILE	3.3
1	F	335	ALA	3.3
1	A	342	VAL	3.2
1	A	392	ARG	3.2
1	B	348	ILE	3.1
1	A	277	PHE	3.1
1	A	287	LEU	3.1
1	A	286	PRO	3.1
1	F	388	ILE	3.1
1	E	273	VAL	3.1
1	A	282	LEU	3.0
1	E	90	ARG	3.0
1	B	331	ILE	3.0
1	F	345	GLY	3.0
1	B	282	LEU	2.9
1	E	151	ILE	2.9
1	A	398	GLN	2.9
1	E	331	ILE	2.9
1	B	286	PRO	2.9
1	C	164	SER	2.8
1	A	284	GLY	2.8
1	A	164	SER	2.8
1	F	392	ARG	2.7
1	B	293	GLY	2.7
1	A	343	GLY	2.7
1	F	344	SER	2.6
1	E	347	GLU	2.6
1	A	391	PHE	2.6
1	C	290	TYR	2.6
1	F	317	VAL	2.6
1	E	290	TYR	2.5
1	A	348	ILE	2.5
1	A	272	ARG	2.5
1	A	288	THR	2.5
1	E	343	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	253	VAL	2.5
1	F	170	TYR	2.5
1	E	272	ARG	2.5
1	A	281	ALA	2.5
1	F	331	ILE	2.5
1	E	345	GLY	2.4
1	E	287	LEU	2.4
1	E	397	TYR	2.4
1	B	287	LEU	2.4
1	E	396	GLU	2.4
1	A	396	GLU	2.4
1	D	88	ARG	2.4
1	E	289	VAL	2.4
1	F	285	GLU	2.4
1	F	393	LYS	2.4
1	E	153	VAL	2.3
1	E	344	SER	2.3
1	B	288	THR	2.3
1	A	170	TYR	2.3
1	A	285	GLU	2.3
1	F	370	LEU	2.3
1	A	274	VAL	2.2
1	D	342	VAL	2.2
1	F	205	VAL	2.2
1	A	289	VAL	2.2
1	E	281	ALA	2.2
1	A	347	GLU	2.2
1	E	340	ASN	2.2
1	A	98	GLY	2.2
1	F	340	ASN	2.1
1	F	135	HIS	2.1
1	F	384	LEU	2.1
1	F	251	VAL	2.1
1	F	342	VAL	2.1
1	A	280	GLN	2.1
1	F	396	GLU	2.1
1	A	362	LYS	2.1
1	F	284	GLY	2.1
1	B	349	GLN	2.1
1	A	233	GLU	2.1
1	A	278	ILE	2.0
1	A	290	TYR	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	344	SER	2.0

## 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 carbohydrates 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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	UDP	D	502	25/25	0.82	0.23	84,100,120,147	0
3	UDP	A	502	25/25	0.82	0.24	100,124,141,142	0
3	UDP	B	502	25/25	0.82	0.35	81,108,119,173	0
5	SO4	F	504	5/5	0.84	0.18	121,123,127,128	0
6	POP	F	503	9/9	0.85	0.26	86,91,184,186	3
6	POP	E	502	9/9	0.85	0.14	71,81,135,148	3
5	SO4	E	504	5/5	0.86	0.24	109,118,119,123	0
5	SO4	A	504	5/5	0.86	0.14	132,135,137,140	0
6	POP	C	503	9/9	0.87	0.17	64,95,130,200	1
5	SO4	D	505	5/5	0.92	0.23	88,96,98,107	0
5	SO4	C	504	5/5	0.92	0.23	79,90,95,100	0
4	UGA	F	502	37/37	0.93	0.17	90,98,139,142	0
5	SO4	B	504	5/5	0.94	0.16	77,78,85,97	0
4	UGA	A	503	37/37	0.94	0.18	70,87,112,114	0
4	UGA	E	503	37/37	0.95	0.19	60,81,112,120	0
5	SO4	A	505	5/5	0.95	0.17	95,96,100,102	0
5	SO4	D	504	5/5	0.96	0.33	75,83,84,87	0
2	NAD	F	501	44/44	0.96	0.19	54,76,103,105	0
2	NAD	E	501	44/44	0.96	0.19	51,67,89,94	0
4	UGA	B	503	37/37	0.96	0.16	36,69,115,120	0
4	UGA	D	503	37/37	0.96	0.13	40,59,90,93	0
2	NAD	A	501	44/44	0.97	0.22	47,67,76,84	0

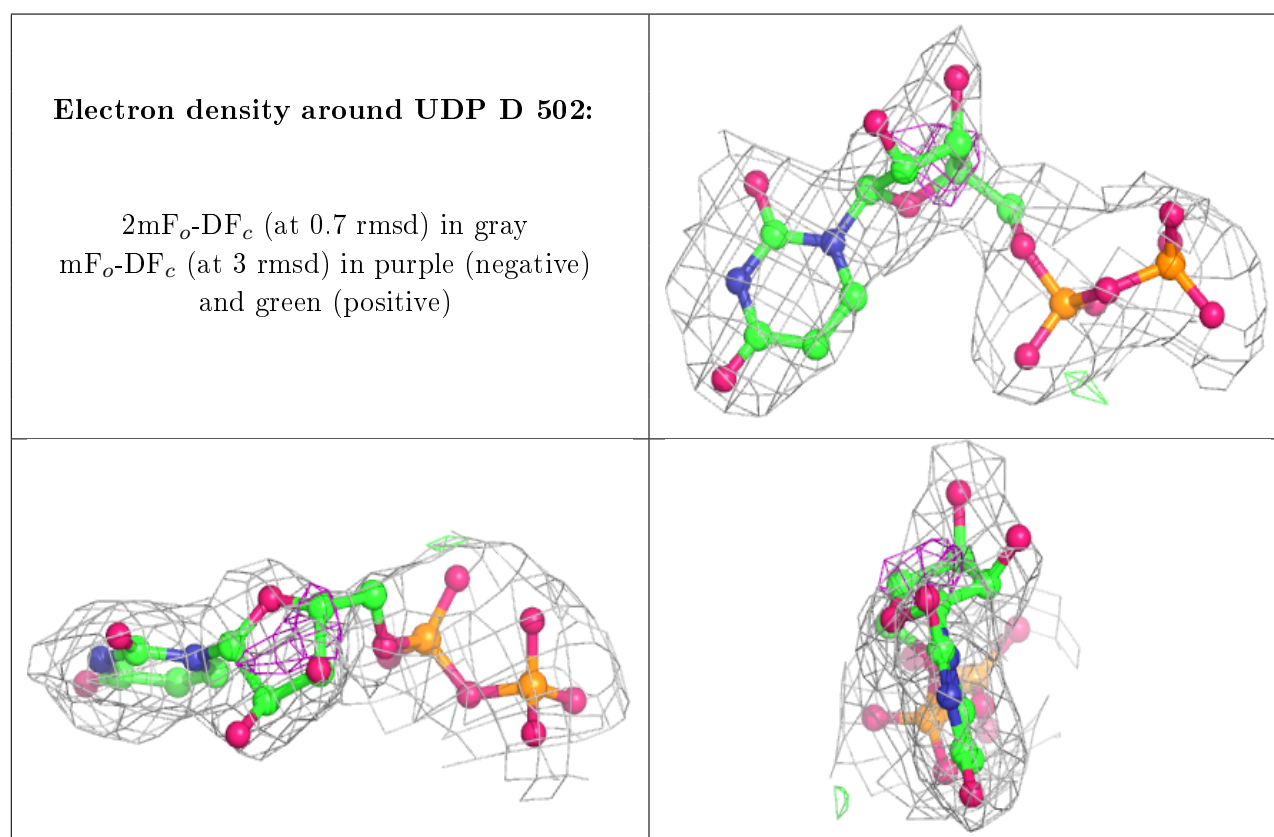
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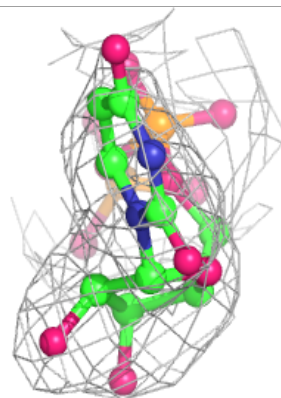
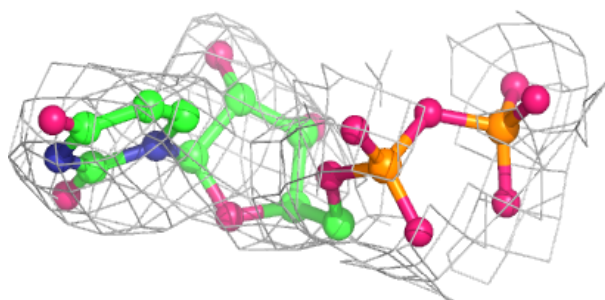
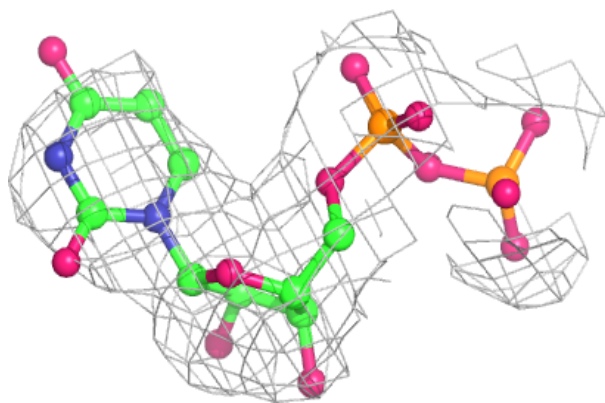
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	UGA	C	502	37/37	0.97	0.15	45,63,114,118	0
2	NAD	D	501	44/44	0.97	0.19	36,51,71,88	0
2	NAD	B	501	44/44	0.98	0.18	23,40,51,63	0
2	NAD	C	501	44/44	0.98	0.18	25,42,58,77	0
5	SO4	B	505	5/5	0.98	0.16	56,62,73,75	0

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.

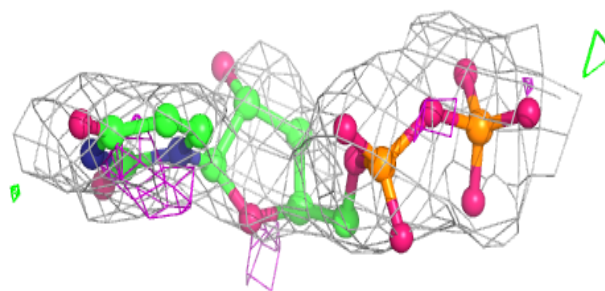
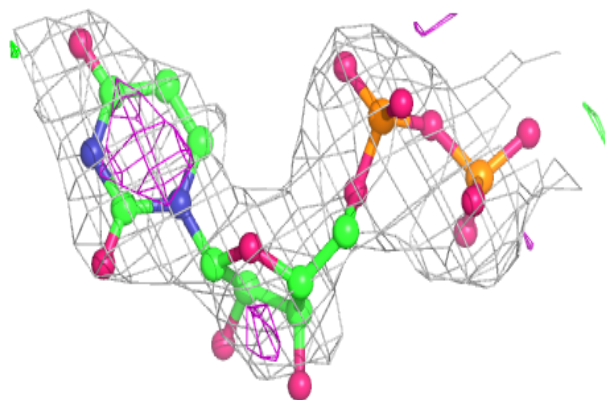


**Electron density around UDP A 502:**

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

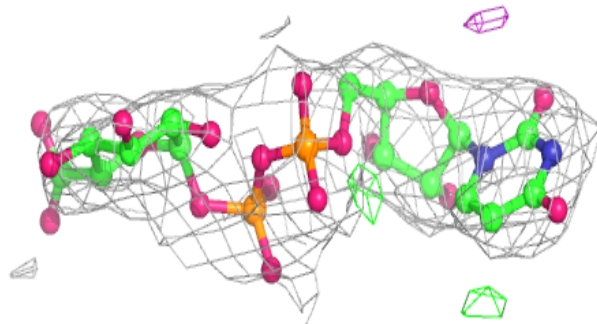
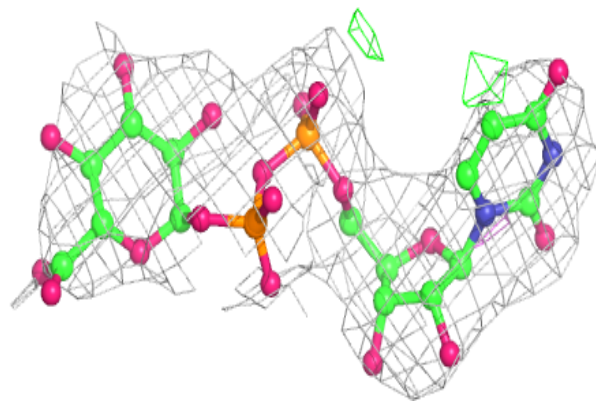
**Electron density around UDP B 502:**

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

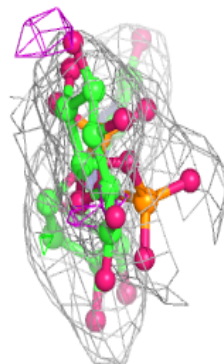
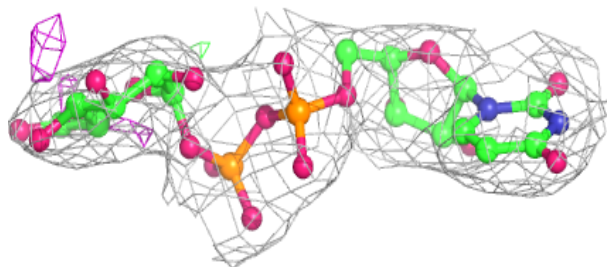
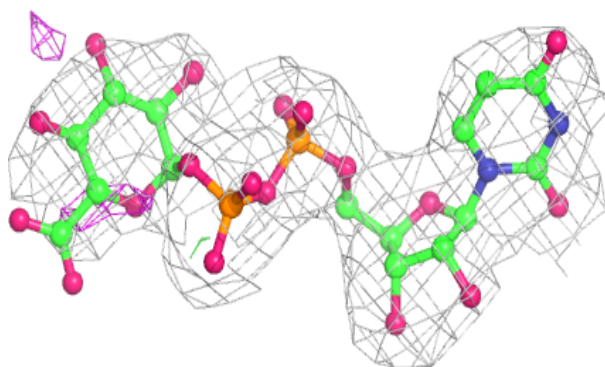


**Electron density around UGA F 502:**

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

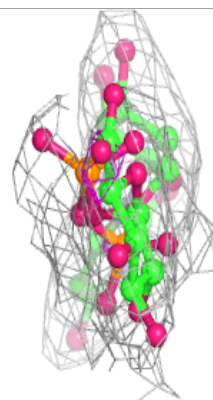
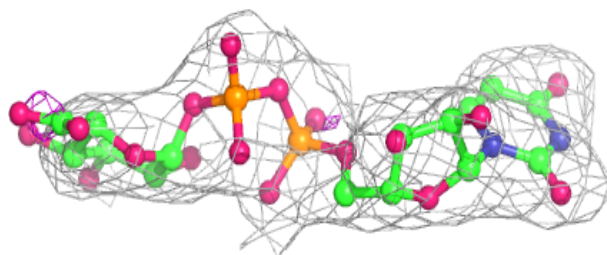
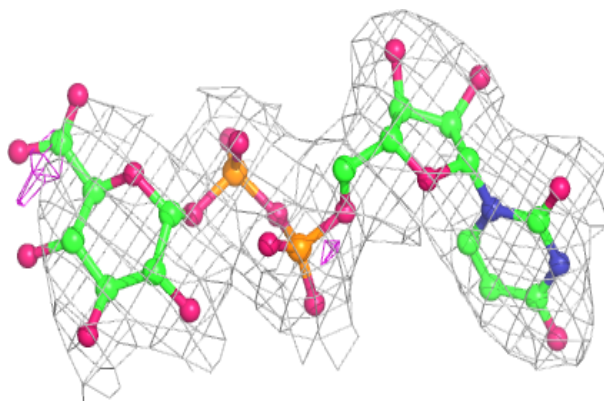
**Electron density around UGA A 503:**

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

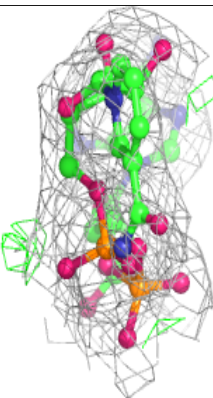
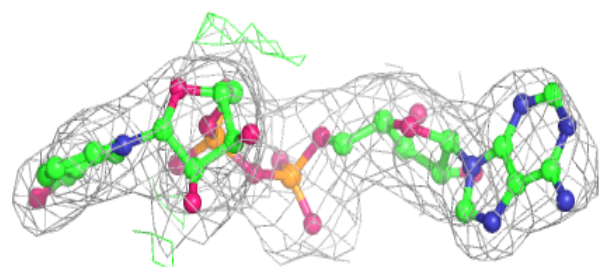
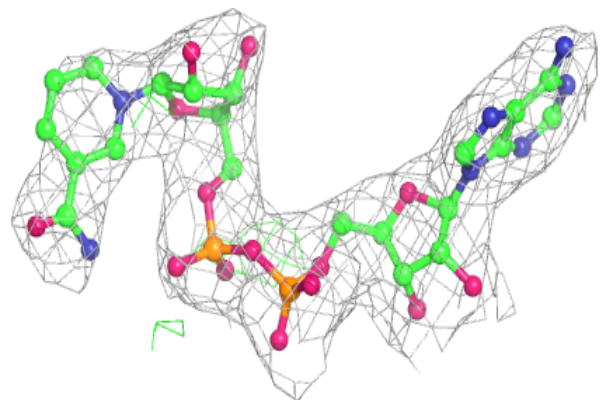


**Electron density around UGA E 503:**

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

**Electron density around NAD F 501:**

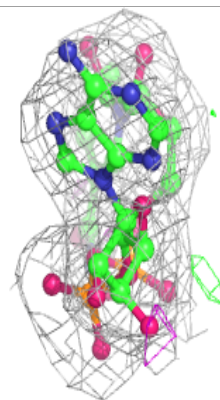
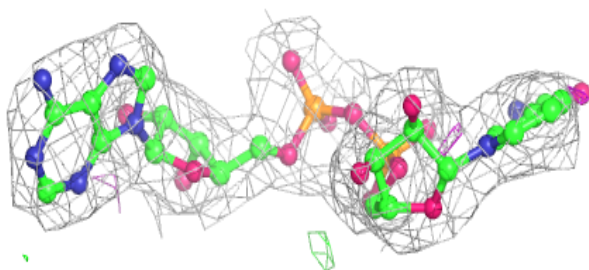
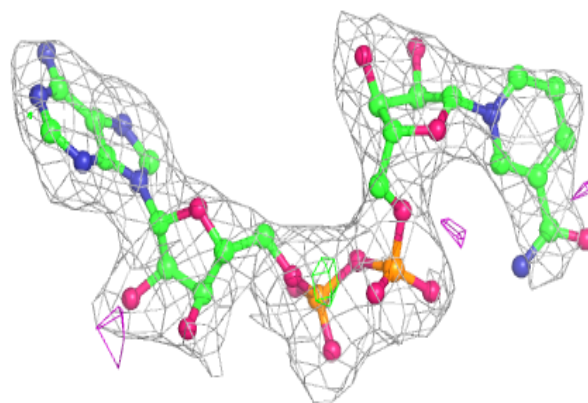
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



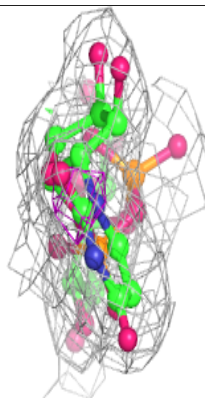
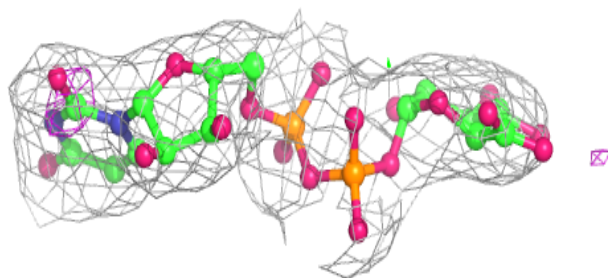
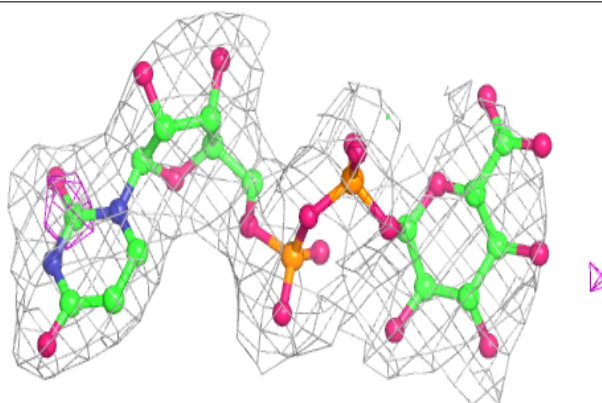


**Electron density around NAD E 501:**

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

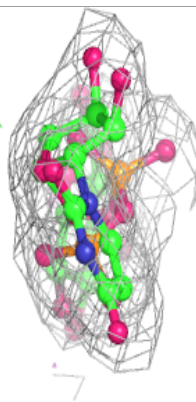
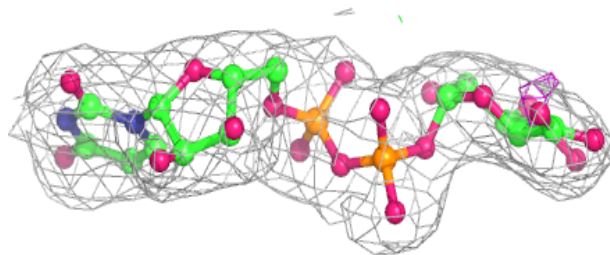
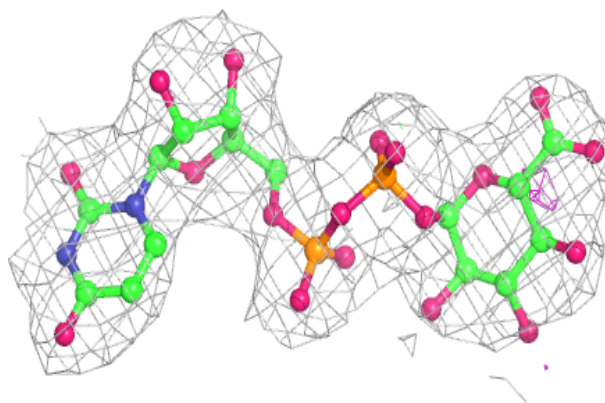
**Electron density around UGA B 503:**

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

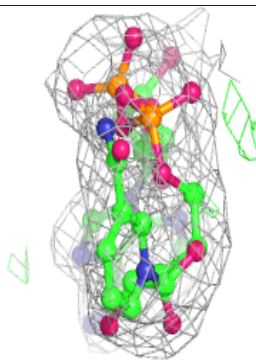
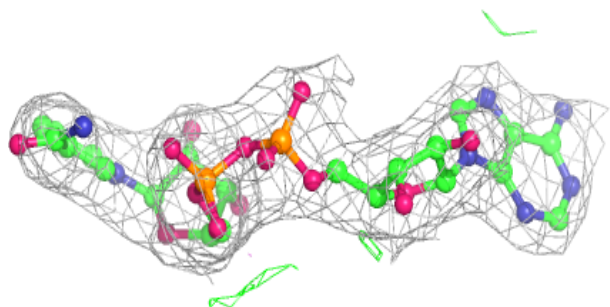
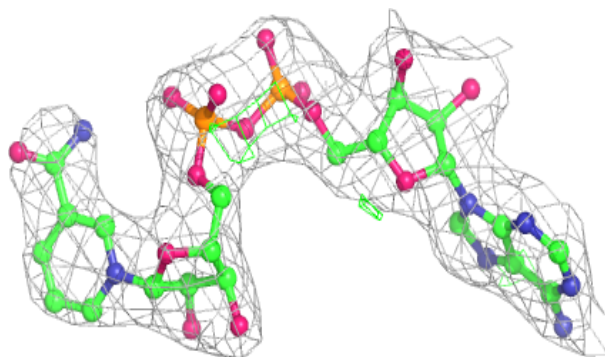


**Electron density around UGA D 503:**

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

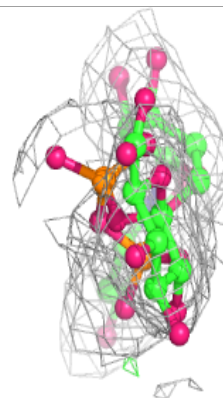
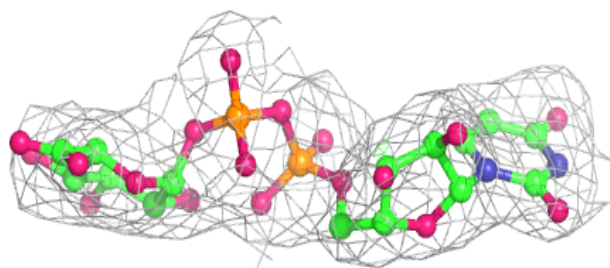
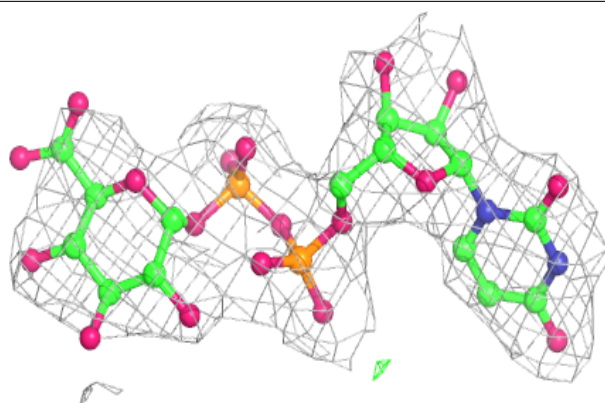
**Electron density around NAD A 501:**

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

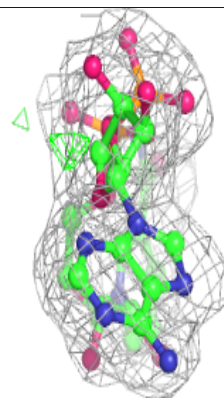
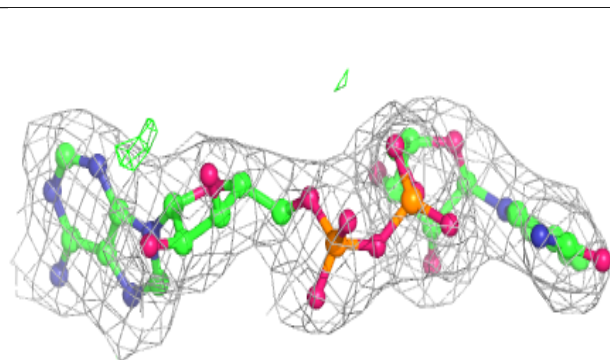
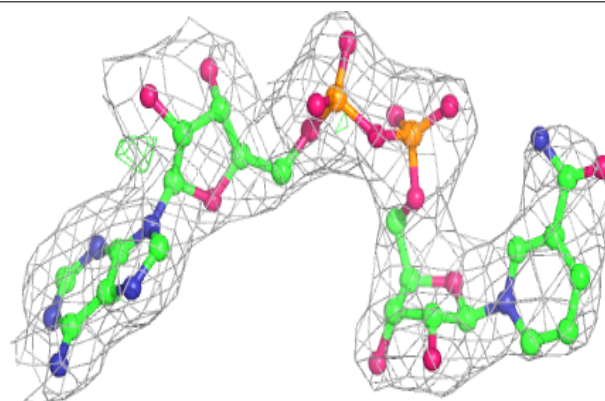


**Electron density around UGA C 502:**

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

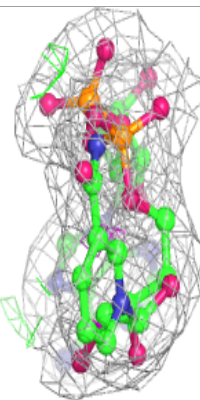
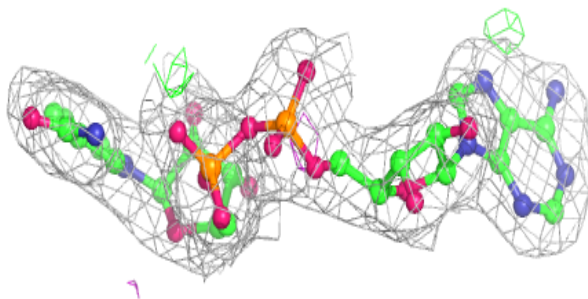
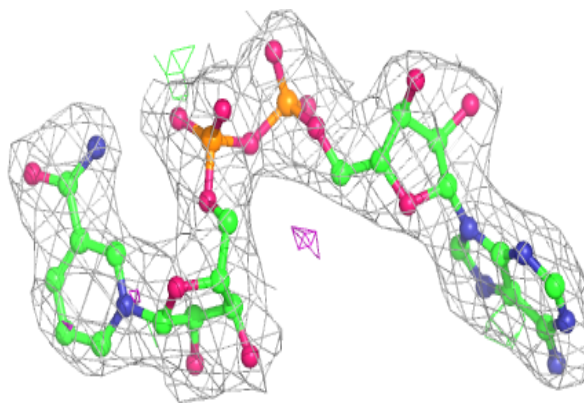
**Electron density around NAD D 501:**

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

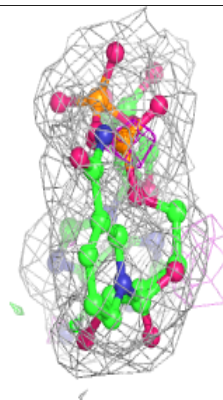
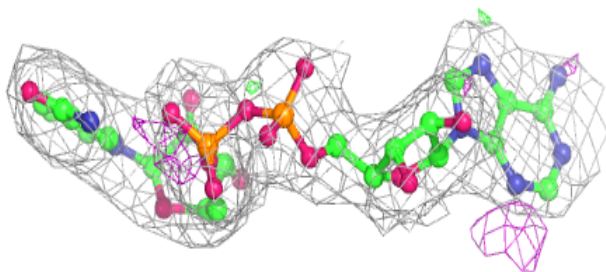
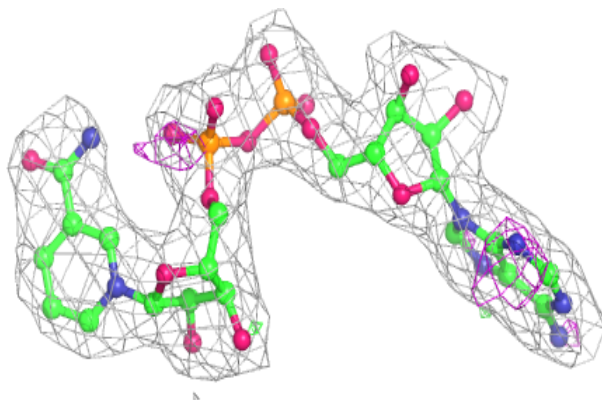


**Electron density around NAD B 501:**

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

**Electron density around NAD C 501:**

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





## 6.5 Other polymers

There are no such residues in this entry.