



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 8, 2020 – 04:51 AM BST

PDB ID : 1XLT
Title : Crystal structure of Transhydrogenase [(domain I)2:domain III] heterotrimer complex
Authors : Sundaresan, V.; Chartron, J.; Yamaguchi, M.; Stout, C.D.
Deposited on : 2004-09-30
Resolution : 3.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
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) : 2.13.1

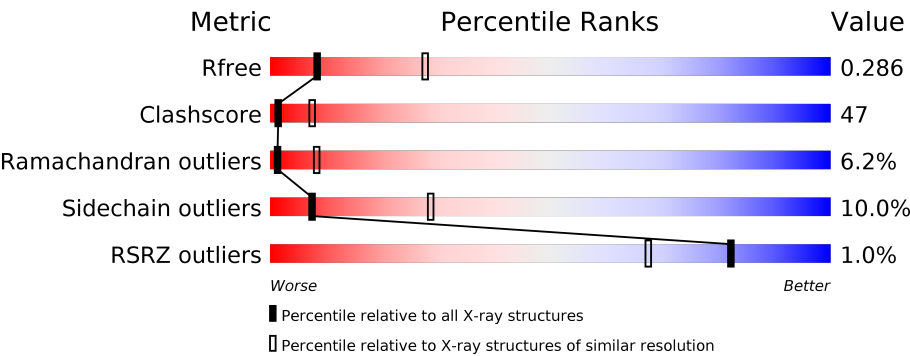
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria 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	384	<div><div>%</div><div><div></div><div>42%</div><div>44%</div><div>8%</div><div>5%</div></div></div>
1	B	384	<div><div></div><div>39%</div><div>43%</div><div>11%</div><div>7%</div></div>
1	D	384	<div><div>2%</div><div><div></div><div>29%</div><div>54%</div><div>13%</div><div></div></div></div>
1	E	384	<div><div>%</div><div><div></div><div>33%</div><div>51%</div><div>8%</div><div>7%</div></div></div>
1	G	384	<div><div></div><div>38%</div><div>49%</div><div>8%</div><div>5%</div></div>
1	H	384	<div><div>3%</div><div><div></div><div>26%</div><div>54%</div><div>12%</div><div>7%</div></div></div>

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Mol	Chain	Length	Quality of chain
2	C	174	
2	F	174	
2	I	174	
3	J	2	
3	K	2	
3	L	2	
3	M	2	
3	N	2	
3	O	2	

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	GLC	N	1	-	-	-	X

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 20480 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 NAD(P) transhydrogenase subunit alpha part 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	363	Total	C	N	O	S	0	0	0
			2670	1688	462	504	16			
1	B	359	Total	C	N	O	S	0	0	0
			2643	1673	458	496	16			
1	D	378	Total	C	N	O	S	0	0	0
			2779	1753	479	529	18			
1	E	359	Total	C	N	O	S	0	0	0
			2644	1673	458	497	16			
1	G	364	Total	C	N	O	S	0	0	0
			2675	1691	463	505	16			
1	H	357	Total	C	N	O	S	0	0	0
			2632	1665	456	495	16			

- Molecule 2 is a protein called NAD(P) transhydrogenase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	174	Total	C	N	O	S	0	0	0
			1318	833	221	252	12			
2	F	173	Total	C	N	O	S	0	0	0
			1307	827	217	251	12			
2	I	173	Total	C	N	O	S	0	0	0
			1307	827	217	251	12			

There are 9 discrepancies between the modelled and reference sequences:

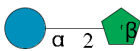
Chain	Residue	Modelled	Actual	Comment	Reference
C	291	ARG	-	cloning artifact	UNP Q59765
C	292	HIS	-	cloning artifact	UNP Q59765
C	293	MET	-	cloning artifact	UNP Q59765
F	291	ARG	-	cloning artifact	UNP Q59765
F	292	HIS	-	cloning artifact	UNP Q59765
F	293	MET	-	cloning artifact	UNP Q59765

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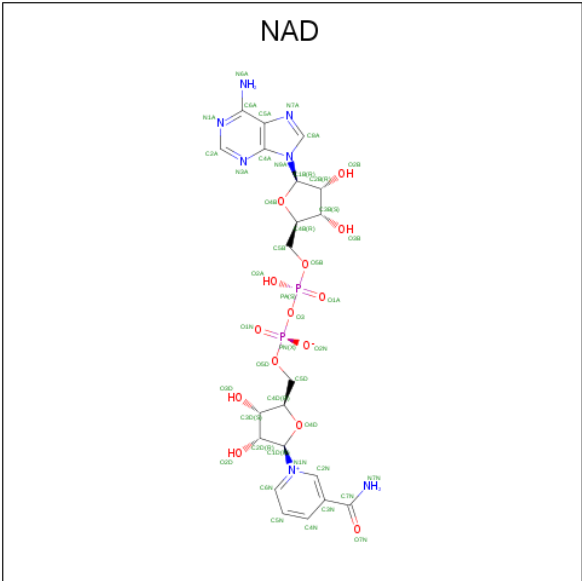
Chain	Residue	Modelled	Actual	Comment	Reference
I	291	ARG	-	cloning artifact	UNP Q59765
I	292	HIS	-	cloning artifact	UNP Q59765
I	293	MET	-	cloning artifact	UNP Q59765

- Molecule 3 is an oligosaccharide called beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	J	2	Total	C	O	0	0	0
			23	12	11			
3	K	2	Total	C	O	0	0	0
			23	12	11			
3	L	2	Total	C	O	0	0	0
			23	12	11			
3	M	2	Total	C	O	0	0	0
			23	12	11			
3	N	2	Total	C	O	0	0	0
			23	12	11			
3	O	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 4 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).

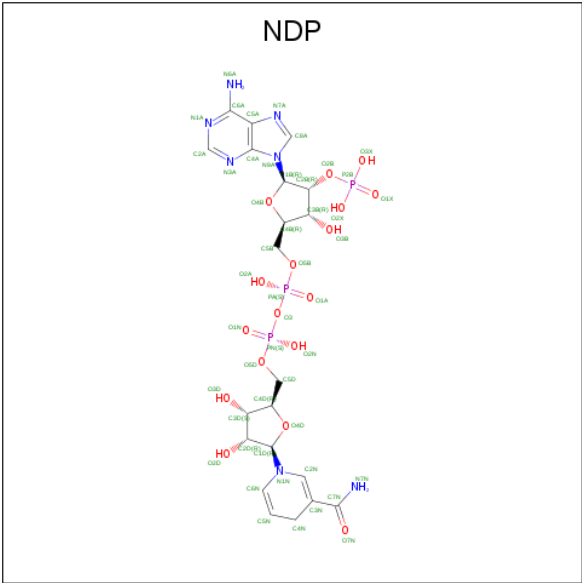


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
4	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
4	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
4	G	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
4	H	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	G	1	Total	Na	0	0
			1	1		
5	A	1	Total	Na	0	0
			1	1		
5	D	1	Total	Na	0	0
			1	1		

- Molecule 6 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

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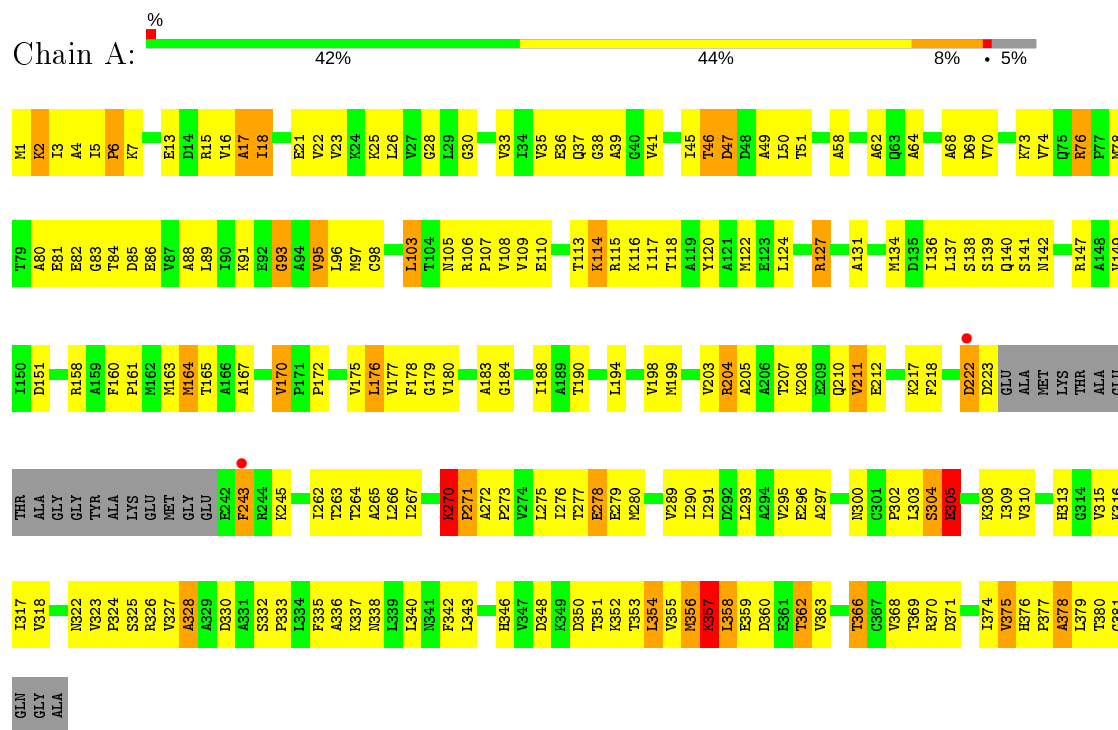
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	F	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
6	I	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

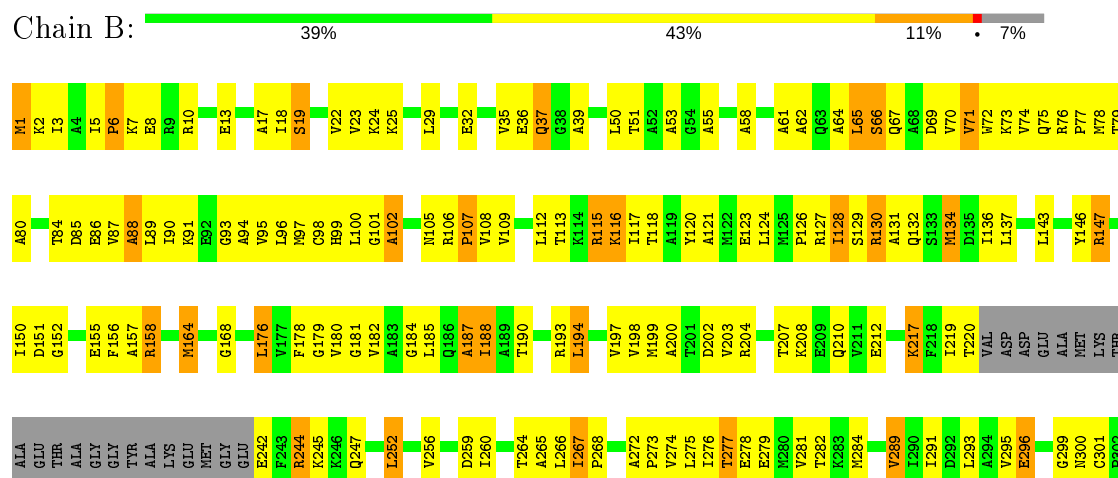
3 Residue-property plots

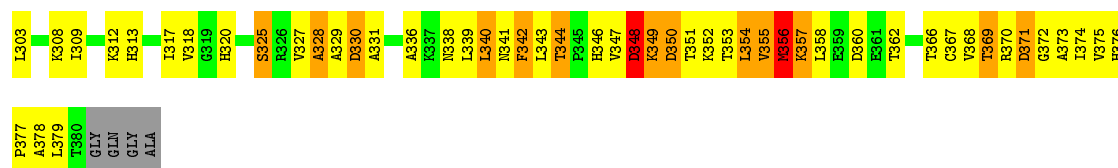
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: NAD(P) transhydrogenase subunit alpha part 1

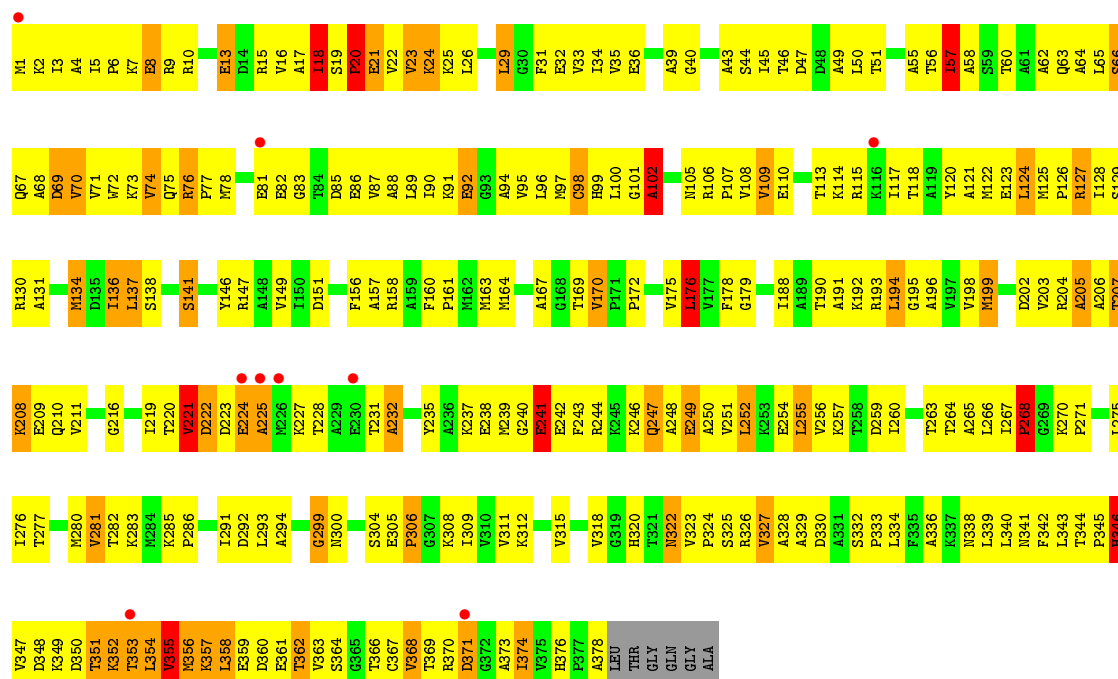


- Molecule 1: NAD(P) transhydrogenase subunit alpha part 1

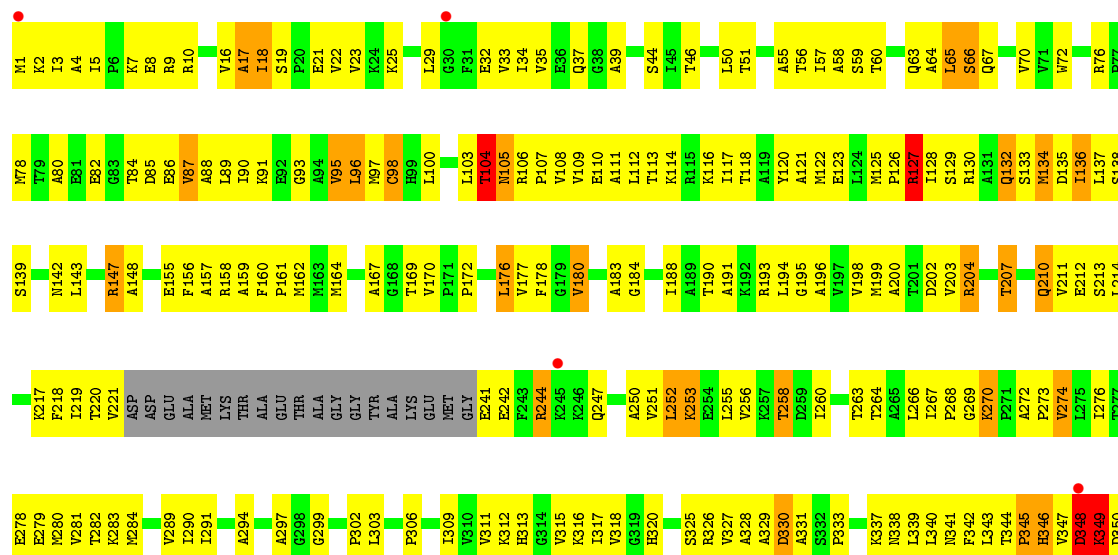




• Molecule 1: NAD(P) transhydrogenase subunit alpha part 1




• Molecule 1: NAD(P) transhydrogenase subunit alpha part 1







- Molecule 3: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain L:  100%



- Molecule 3: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain M:  100%



- Molecule 3: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain N:  100%



- Molecule 3: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain O:  50% 50%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	95.37Å 171.08Å 203.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.68 – 3.10 43.68 – 3.00	Depositor EDS
% Data completeness (in resolution range)	96.5 (43.68-3.10) 95.9 (43.68-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.66 (at 3.01Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.232 , 0.310 0.220 , 0.286	Depositor DCC
R_{free} test set	2977 reflections (4.61%)	wwPDB-VP
Wilson B-factor (Å ²)	78.5	Xtriage
Anisotropy	0.114	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 47.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	20480	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.38% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NDP, GLC, FRU, NAD, NA

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	0.52	1/2705 (0.0%)	0.82	4/3668 (0.1%)
1	B	0.48	0/2678	0.79	2/3631 (0.1%)
1	D	0.54	0/2816	1.02	10/3816 (0.3%)
1	E	0.50	1/2679 (0.0%)	0.87	7/3632 (0.2%)
1	G	0.46	0/2710	0.81	5/3674 (0.1%)
1	H	0.54	1/2667 (0.0%)	0.99	14/3615 (0.4%)
2	C	0.46	0/1342	0.66	0/1813
2	F	0.46	0/1331	0.65	0/1799
2	I	0.51	0/1331	0.85	3/1799 (0.2%)
All	All	0.50	3/20259 (0.0%)	0.86	45/27447 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	D	0	5
1	E	0	1
1	H	1	2
2	I	0	1
All	All	1	11

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	204	ARG	N-CA	-8.40	1.29	1.46
1	H	343	LEU	C-N	-6.48	1.19	1.34
1	E	349	LYS	C-O	6.47	1.35	1.23

The worst 5 of 45 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	125	MET	C-N-CD	9.48	148.30	128.40
1	D	371	ASP	CB-CG-OD2	8.76	126.18	118.30
1	A	47	ASP	CB-CG-OD1	8.75	126.18	118.30
1	D	221	VAL	O-C-N	8.62	136.49	122.70
1	G	350	ASP	CB-CG-OD2	8.56	126.01	118.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	H	366	THR	CA

5 of 11 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	18	ILE	Mainchain
1	B	356	MET	Mainchain
1	D	102	ALA	Mainchain
1	D	247	GLN	Mainchain
1	D	57	ILE	Mainchain

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	2670	0	2804	200	0
1	B	2643	0	2784	248	0
1	D	2779	0	2904	367	0
1	E	2644	0	2781	268	0
1	G	2675	0	2808	241	0
1	H	2632	0	2766	391	0
2	C	1318	0	1305	109	0
2	F	1307	0	1292	92	0
2	I	1307	0	1292	123	0
3	J	23	0	21	0	0
3	K	23	0	21	1	0
3	L	23	0	21	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	M	23	0	21	0	0
3	N	23	0	21	0	0
3	O	23	0	21	1	0
4	A	44	0	26	2	0
4	B	44	0	25	9	0
4	D	44	0	24	3	0
4	G	44	0	24	6	0
4	H	44	0	26	8	0
5	A	1	0	0	0	0
5	D	1	0	0	0	0
5	G	1	0	0	0	0
6	C	48	0	26	4	0
6	F	48	0	26	10	0
6	I	48	0	26	3	0
All	All	20480	0	21065	1966	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 47.

The worst 5 of 1966 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:120:TYR:CD2	1:H:366:THR:HG22	1.64	1.31
1:H:120:TYR:HD2	1:H:366:THR:CG2	1.47	1.27
2:I:401:THR:O	2:I:403:PRO:HD3	1.32	1.25
1:B:70:VAL:HG23	1:B:95:VAL:HB	1.21	1.17
1:H:120:TYR:CD2	1:H:366:THR:CG2	2.26	1.15

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	359/384 (94%)	289 (80%)	51 (14%)	19 (5%)	2	12
1	B	355/384 (92%)	273 (77%)	57 (16%)	25 (7%)	1	7
1	D	376/384 (98%)	277 (74%)	66 (18%)	33 (9%)	1	4
1	E	355/384 (92%)	265 (75%)	66 (19%)	24 (7%)	1	7
1	G	360/384 (94%)	292 (81%)	50 (14%)	18 (5%)	2	13
1	H	353/384 (92%)	258 (73%)	77 (22%)	18 (5%)	2	13
2	C	172/174 (99%)	133 (77%)	35 (20%)	4 (2%)	6	28
2	F	171/174 (98%)	141 (82%)	21 (12%)	9 (5%)	2	12
2	I	171/174 (98%)	125 (73%)	29 (17%)	17 (10%)	0	3
All	All	2672/2826 (95%)	2053 (77%)	452 (17%)	167 (6%)	1	8

5 of 167 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	270	LYS
1	A	357	LYS
1	A	358	LEU
1	A	378	ALA
1	B	371	ASP

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	284/296 (96%)	254 (89%)	30 (11%)	6	26
1	B	281/296 (95%)	253 (90%)	28 (10%)	7	28
1	D	293/296 (99%)	255 (87%)	38 (13%)	4	18
1	E	281/296 (95%)	257 (92%)	24 (8%)	10	37
1	G	284/296 (96%)	260 (92%)	24 (8%)	10	37
1	H	280/296 (95%)	243 (87%)	37 (13%)	4	17
2	C	138/138 (100%)	125 (91%)	13 (9%)	8	32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	F	137/138 (99%)	128 (93%)	9 (7%)	16	47
2	I	137/138 (99%)	128 (93%)	9 (7%)	16	47
All	All	2115/2190 (97%)	1903 (90%)	212 (10%)	7	28

5 of 212 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	249	GLU
1	E	176	LEU
1	H	330	ASP
1	D	268	PRO
1	D	368	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 57 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	300	ASN
1	E	63	GLN
1	H	376	HIS
1	D	320	HIS
1	D	338	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 ⓘ

12 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	GLC	J	1	3	11,11,12	1.25	1 (9%)	15,15,17	0.77	1 (6%)
3	FRU	J	2	3	11,12,12	1.46	2 (18%)	10,18,18	0.59	0
3	GLC	K	1	3	11,11,12	1.17	1 (9%)	15,15,17	0.91	1 (6%)
3	FRU	K	2	3	11,12,12	1.53	2 (18%)	10,18,18	0.65	0
3	GLC	L	1	3	11,11,12	1.29	1 (9%)	15,15,17	0.85	1 (6%)
3	FRU	L	2	3	11,12,12	1.53	2 (18%)	10,18,18	0.64	0
3	GLC	M	1	3	11,11,12	1.03	1 (9%)	15,15,17	0.84	1 (6%)
3	FRU	M	2	3	11,12,12	1.63	2 (18%)	10,18,18	0.71	0
3	GLC	N	1	3	11,11,12	1.37	1 (9%)	15,15,17	0.92	1 (6%)
3	FRU	N	2	3	11,12,12	1.67	3 (27%)	10,18,18	0.62	0
3	GLC	O	1	3	11,11,12	1.34	1 (9%)	15,15,17	0.84	1 (6%)
3	FRU	O	2	3	11,12,12	1.54	2 (18%)	10,18,18	0.68	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GLC	J	1	3	-	2/2/19/22	0/1/1/1
3	FRU	J	2	3	-	0/5/24/24	0/1/1/1
3	GLC	K	1	3	-	1/2/19/22	0/1/1/1
3	FRU	K	2	3	-	2/5/24/24	0/1/1/1
3	GLC	L	1	3	-	2/2/19/22	0/1/1/1
3	FRU	L	2	3	-	0/5/24/24	0/1/1/1
3	GLC	M	1	3	-	0/2/19/22	0/1/1/1
3	FRU	M	2	3	-	0/5/24/24	0/1/1/1
3	GLC	N	1	3	-	2/2/19/22	0/1/1/1
3	FRU	N	2	3	-	2/5/24/24	0/1/1/1
3	GLC	O	1	3	-	2/2/19/22	0/1/1/1
3	FRU	O	2	3	-	2/5/24/24	0/1/1/1

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	2	FRU	C4-C5	-4.13	1.42	1.53
3	J	2	FRU	C4-C5	-3.91	1.43	1.53
3	L	2	FRU	C4-C5	-3.83	1.43	1.53
3	N	2	FRU	O2-C2	3.62	1.46	1.40
3	O	2	FRU	C4-C5	-3.54	1.44	1.53

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	1	GLC	C2-C3-C4	-2.46	106.64	110.89
3	O	1	GLC	C2-C3-C4	-2.39	106.76	110.89
3	L	1	GLC	C2-C3-C4	-2.39	106.76	110.89
3	N	1	GLC	C2-C3-C4	-2.38	106.77	110.89
3	J	1	GLC	C2-C3-C4	-2.37	106.80	110.89

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

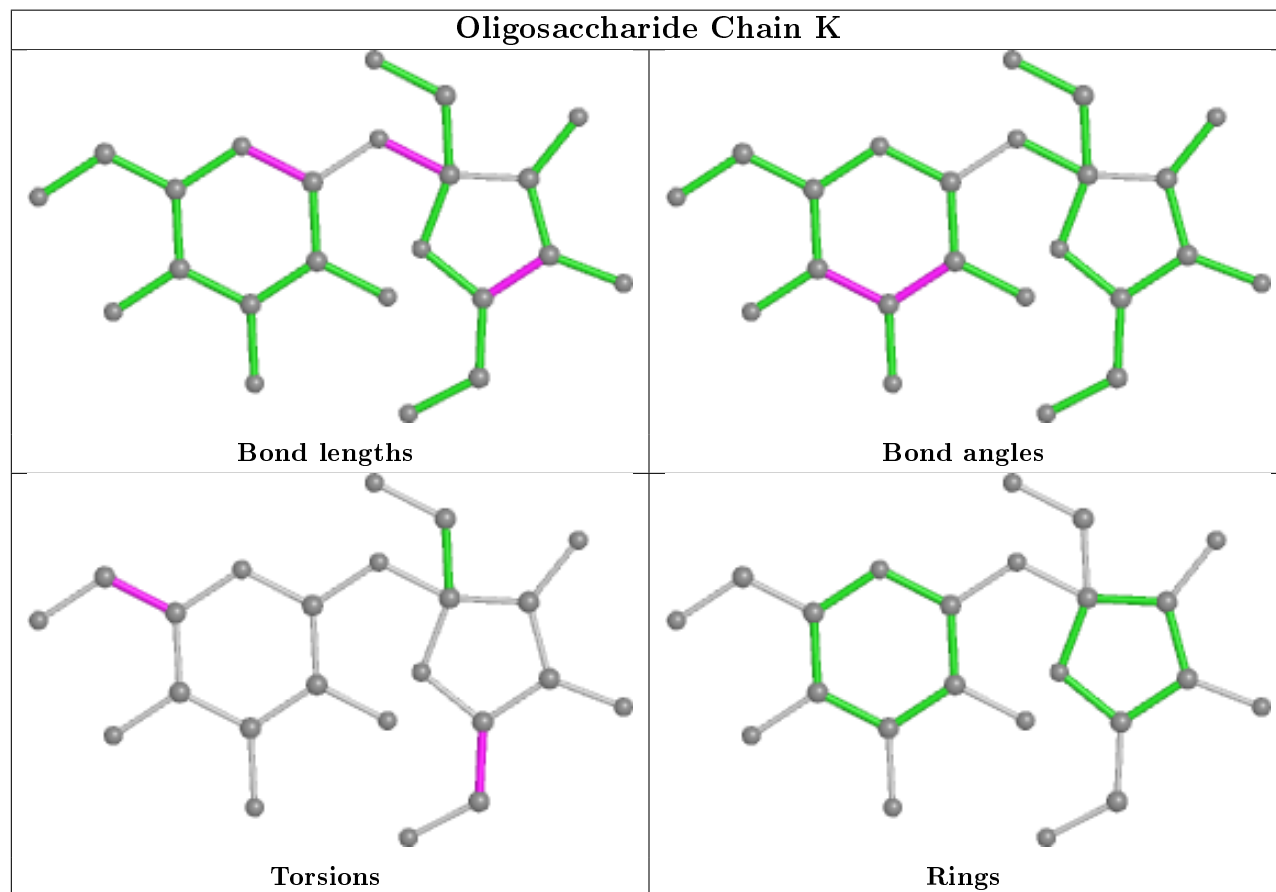
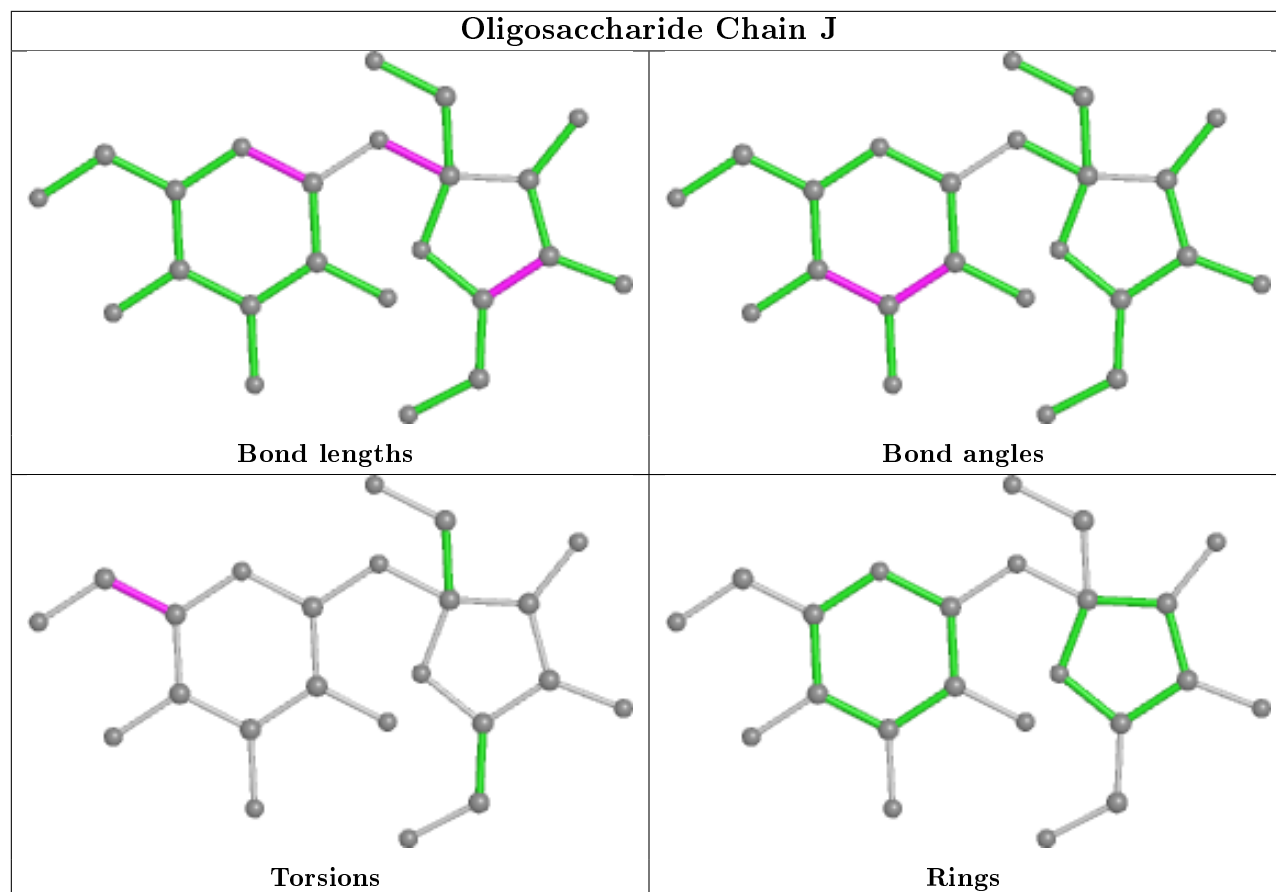
Mol	Chain	Res	Type	Atoms
3	K	2	FRU	C4-C5-C6-O6
3	K	2	FRU	O5-C5-C6-O6
3	N	1	GLC	O5-C5-C6-O6
3	N	2	FRU	C4-C5-C6-O6
3	N	2	FRU	O5-C5-C6-O6

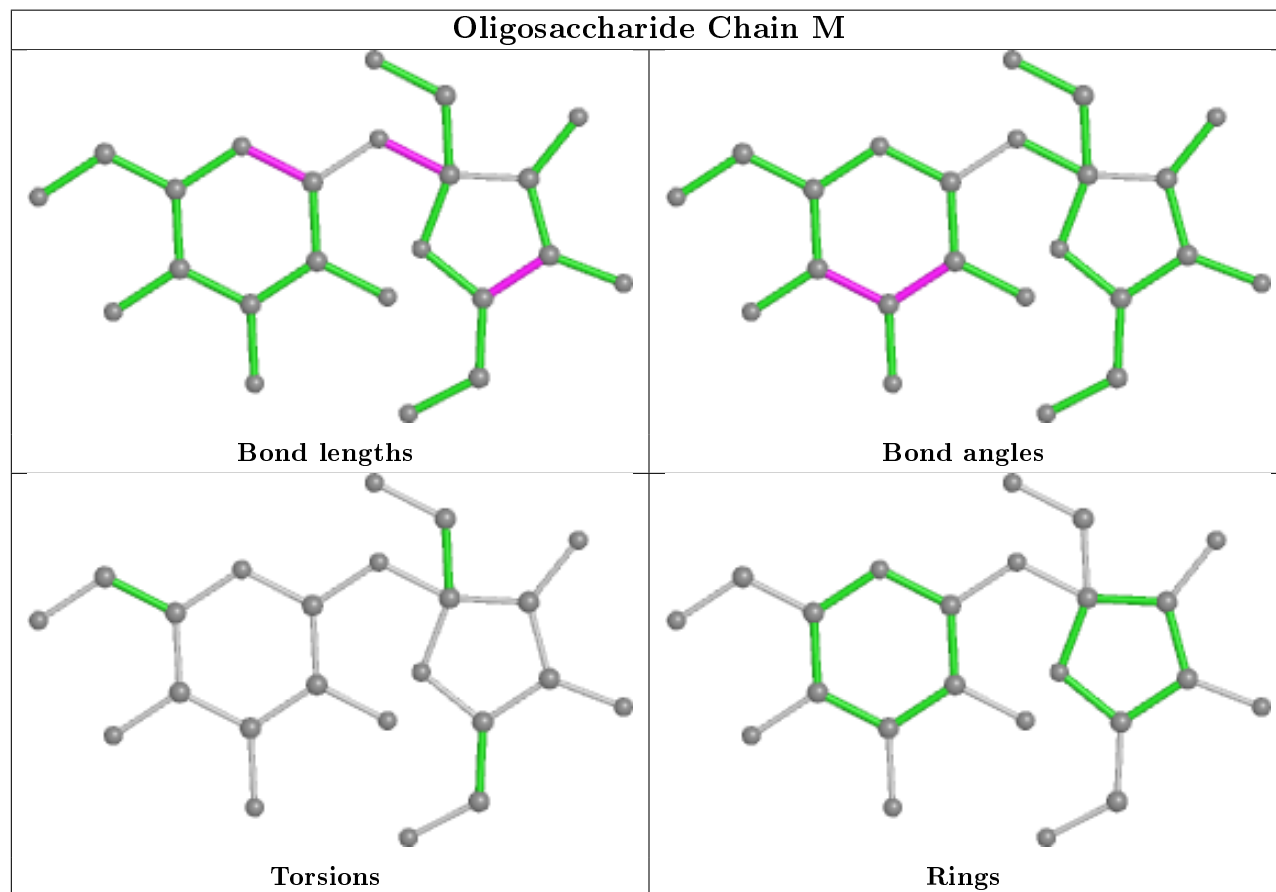
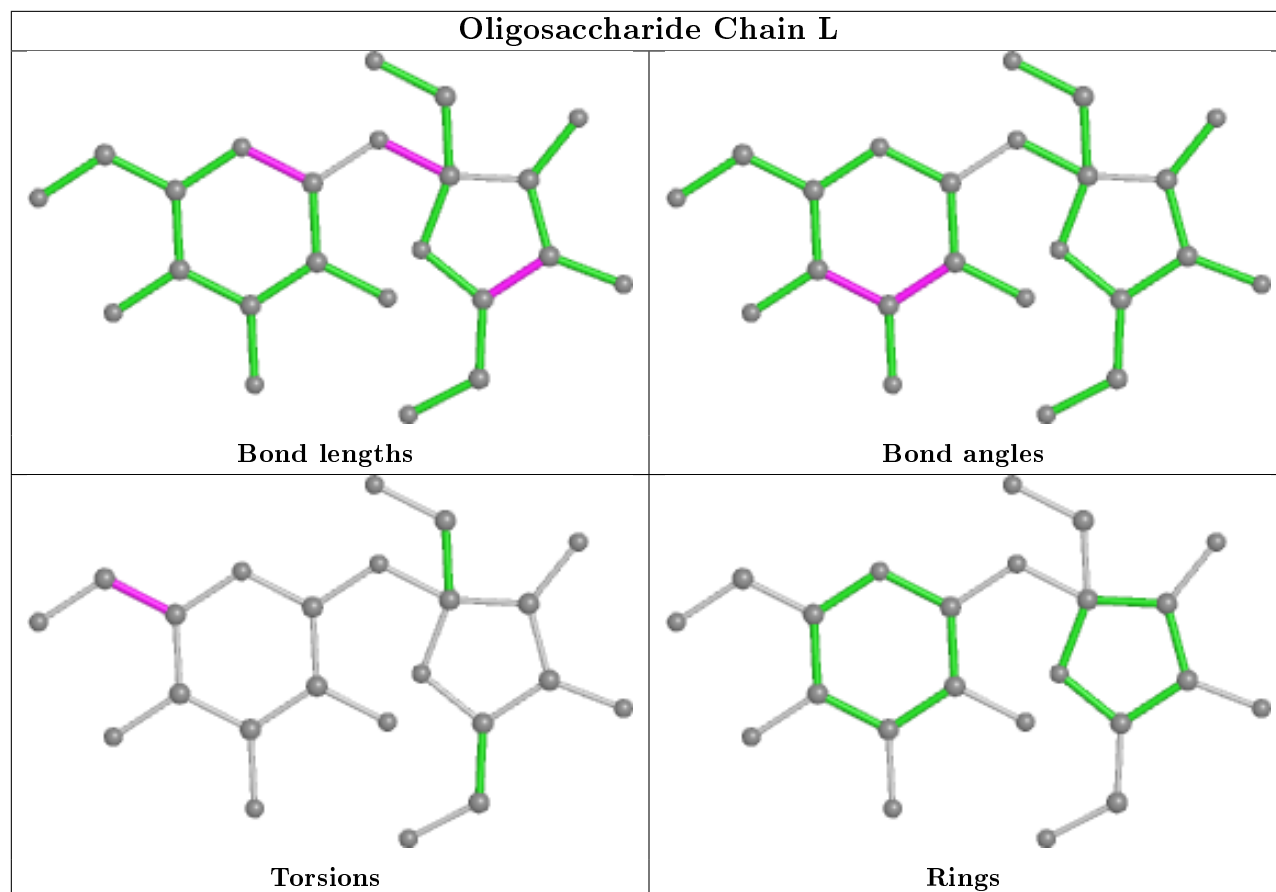
There are no ring outliers.

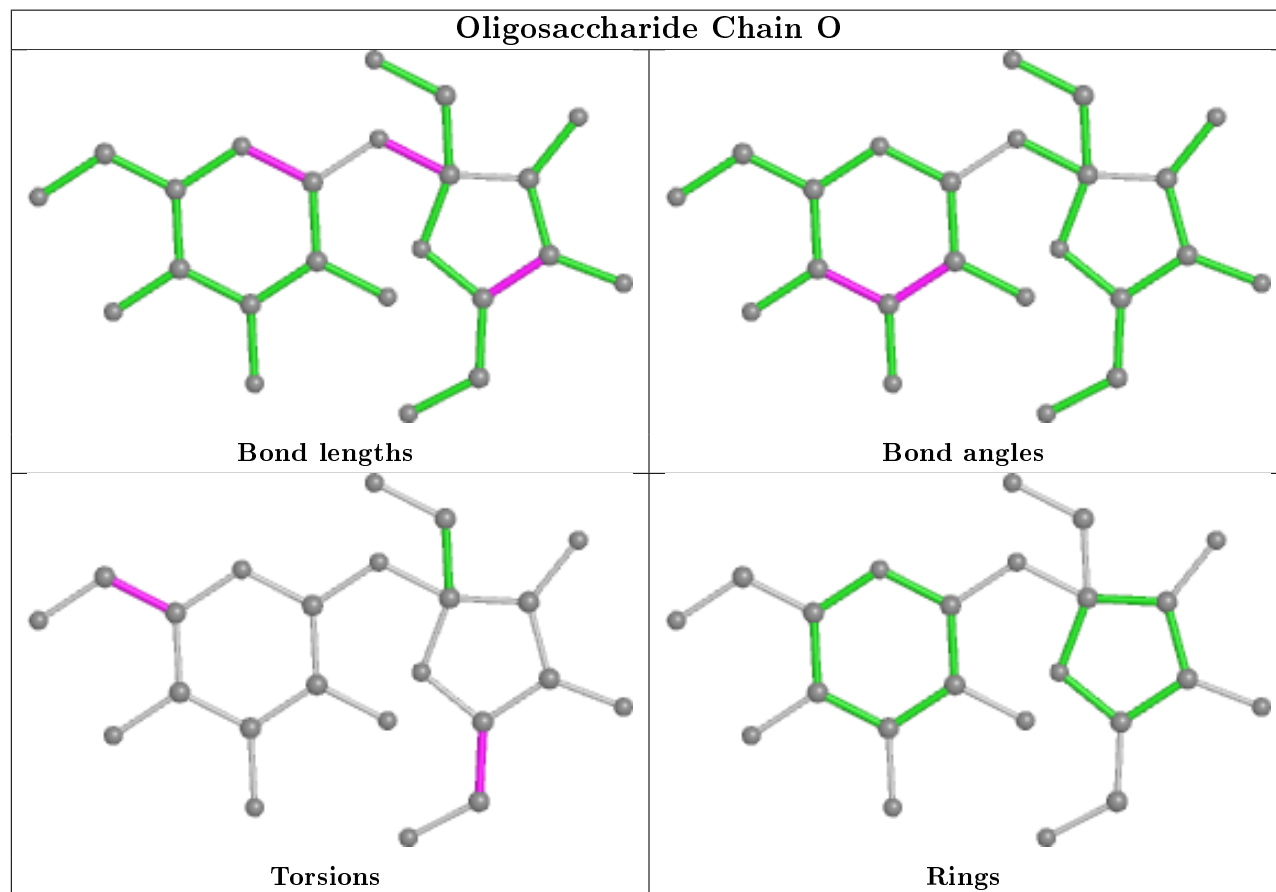
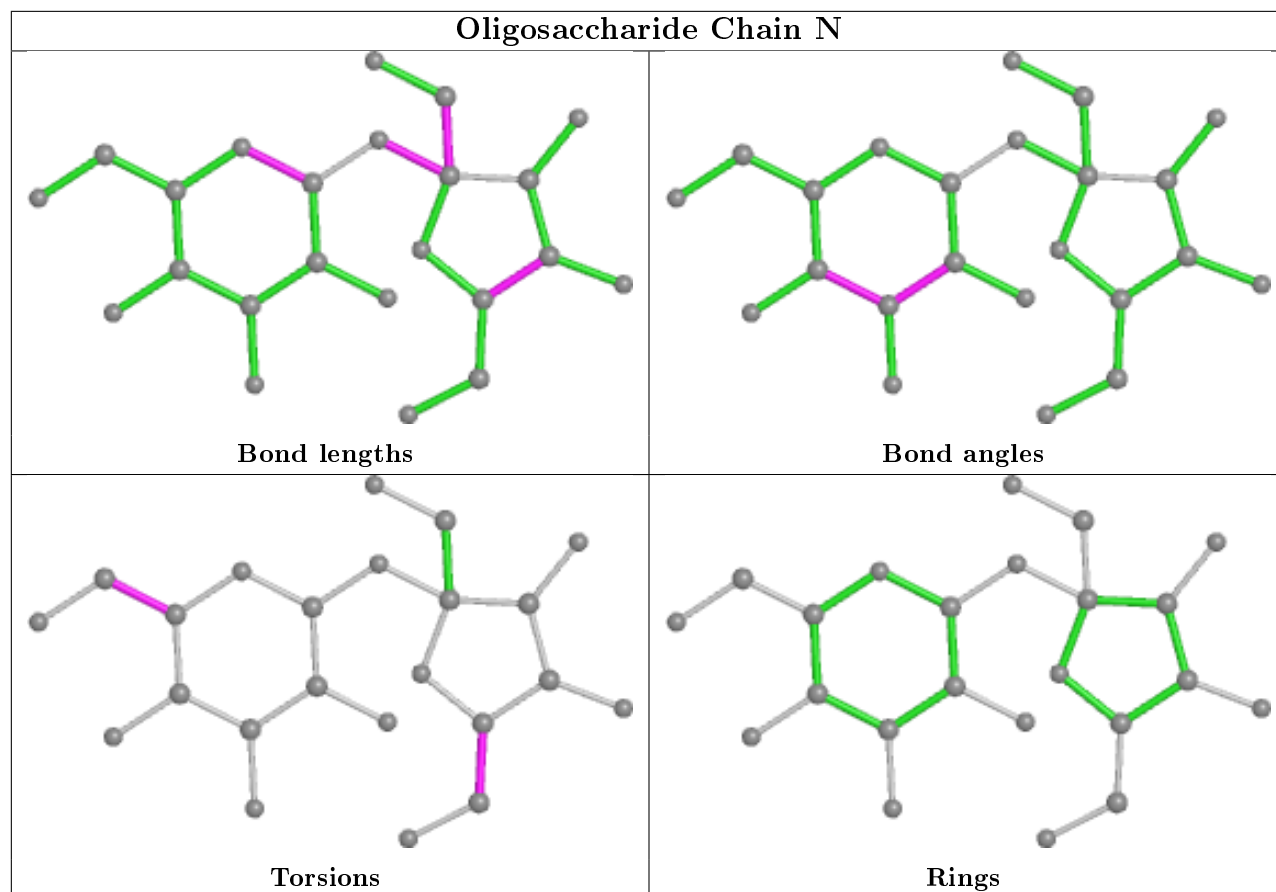
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	O	2	FRU	1	0
3	K	2	FRU	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.







5.6 Ligand geometry

Of 11 ligands modelled in this entry, 3 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAD	H	400	-	42,48,48	2.47	15 (35%)	50,73,73	2.27	17 (34%)
6	NDP	I	500	-	45,52,52	2.39	16 (35%)	53,80,80	2.04	18 (33%)
4	NAD	A	400	-	42,48,48	2.58	18 (42%)	50,73,73	2.49	21 (42%)
4	NAD	B	400	-	42,48,48	2.75	19 (45%)	50,73,73	2.64	17 (34%)
4	NAD	G	400	-	42,48,48	2.55	14 (33%)	50,73,73	2.82	21 (42%)
6	NDP	F	500	-	45,52,52	2.05	13 (28%)	53,80,80	1.95	17 (32%)
6	NDP	C	500	-	45,52,52	2.02	15 (33%)	53,80,80	2.02	20 (37%)
4	NAD	D	400	-	42,48,48	2.47	14 (33%)	50,73,73	2.26	20 (40%)

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
4	NAD	H	400	-	-	11/26/62/62	0/5/5/5
6	NDP	I	500	-	-	13/30/77/77	0/5/5/5
4	NAD	A	400	-	-	15/26/62/62	0/5/5/5
4	NAD	B	400	-	-	16/26/62/62	0/5/5/5
4	NAD	G	400	-	-	8/26/62/62	0/5/5/5
6	NDP	F	500	-	-	14/30/77/77	0/5/5/5
6	NDP	C	500	-	-	12/30/77/77	0/5/5/5
4	NAD	D	400	-	-	9/26/62/62	0/5/5/5

The worst 5 of 124 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	I	500	NDP	O4D-C1D	8.19	1.61	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	400	NAD	O4B-C1B	7.74	1.51	1.41
4	H	400	NAD	O4B-C1B	7.44	1.51	1.41
4	A	400	NAD	O4B-C1B	7.32	1.51	1.41
4	D	400	NAD	O4B-C1B	7.20	1.51	1.41

The worst 5 of 151 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	400	NAD	O5D-C5D-C4D	9.82	142.78	108.99
4	B	400	NAD	O4B-C4B-C5B	8.58	137.60	109.37
4	B	400	NAD	C6N-N1N-C2N	-8.28	114.42	121.97
4	G	400	NAD	C6N-N1N-C2N	-7.62	115.02	121.97
4	A	400	NAD	C6N-N1N-C2N	-7.47	115.17	121.97

There are no chirality outliers.

5 of 98 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	400	NAD	C5B-O5B-PA-O1A
4	H	400	NAD	C5B-O5B-PA-O2A
4	H	400	NAD	C5D-O5D-PN-O3
4	H	400	NAD	C5D-O5D-PN-O1N
4	H	400	NAD	O4D-C1D-N1N-C2N

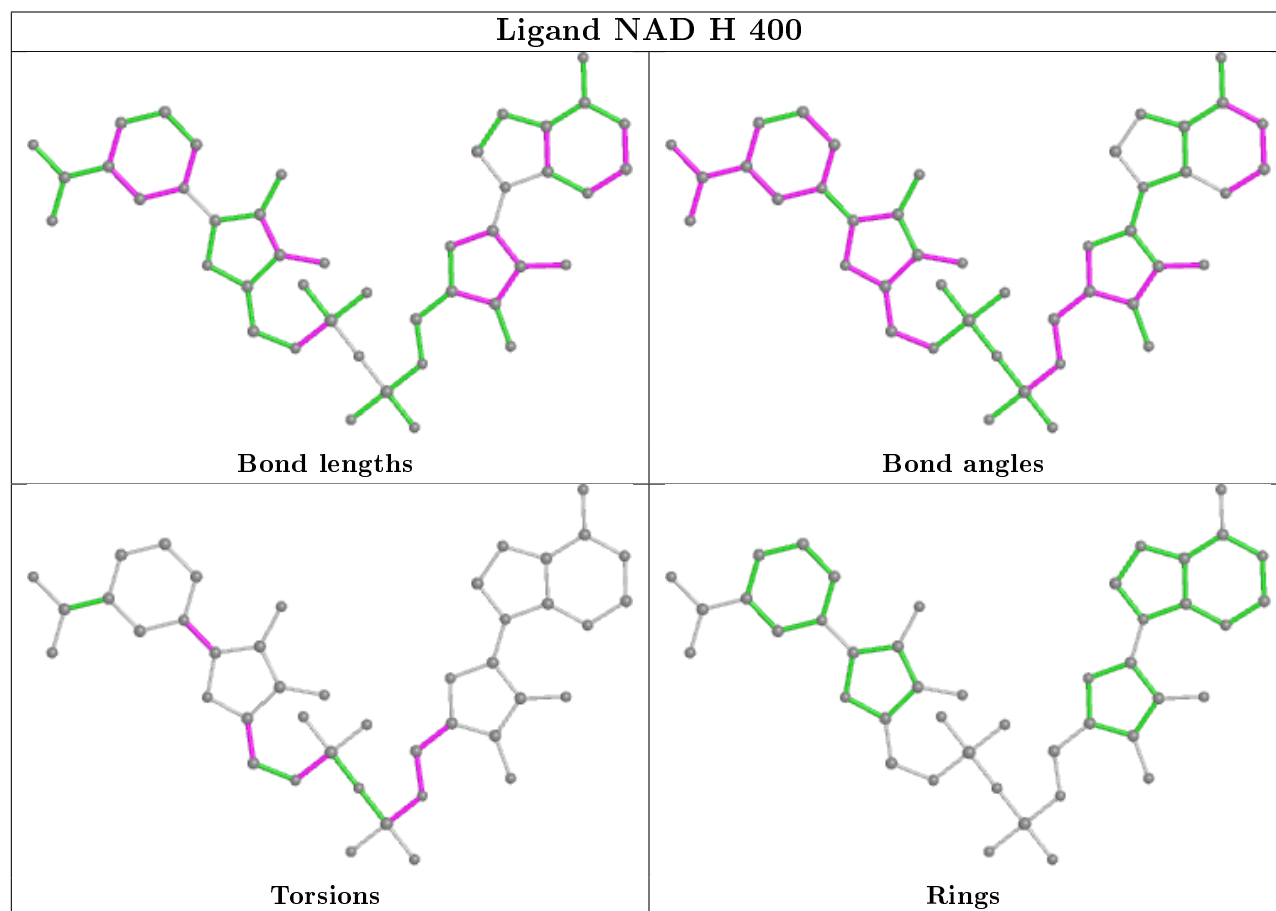
There are no ring outliers.

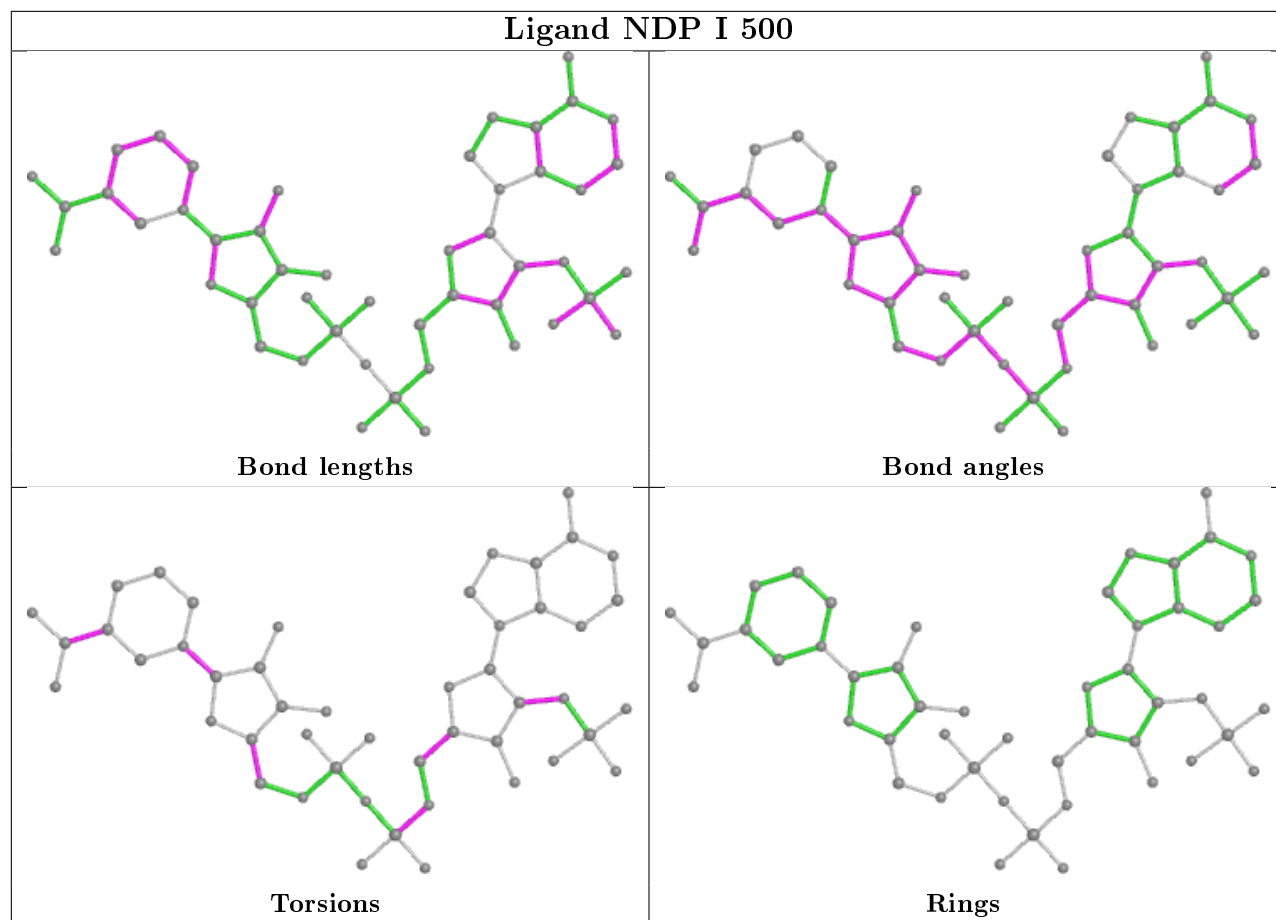
8 monomers are involved in 45 short contacts:

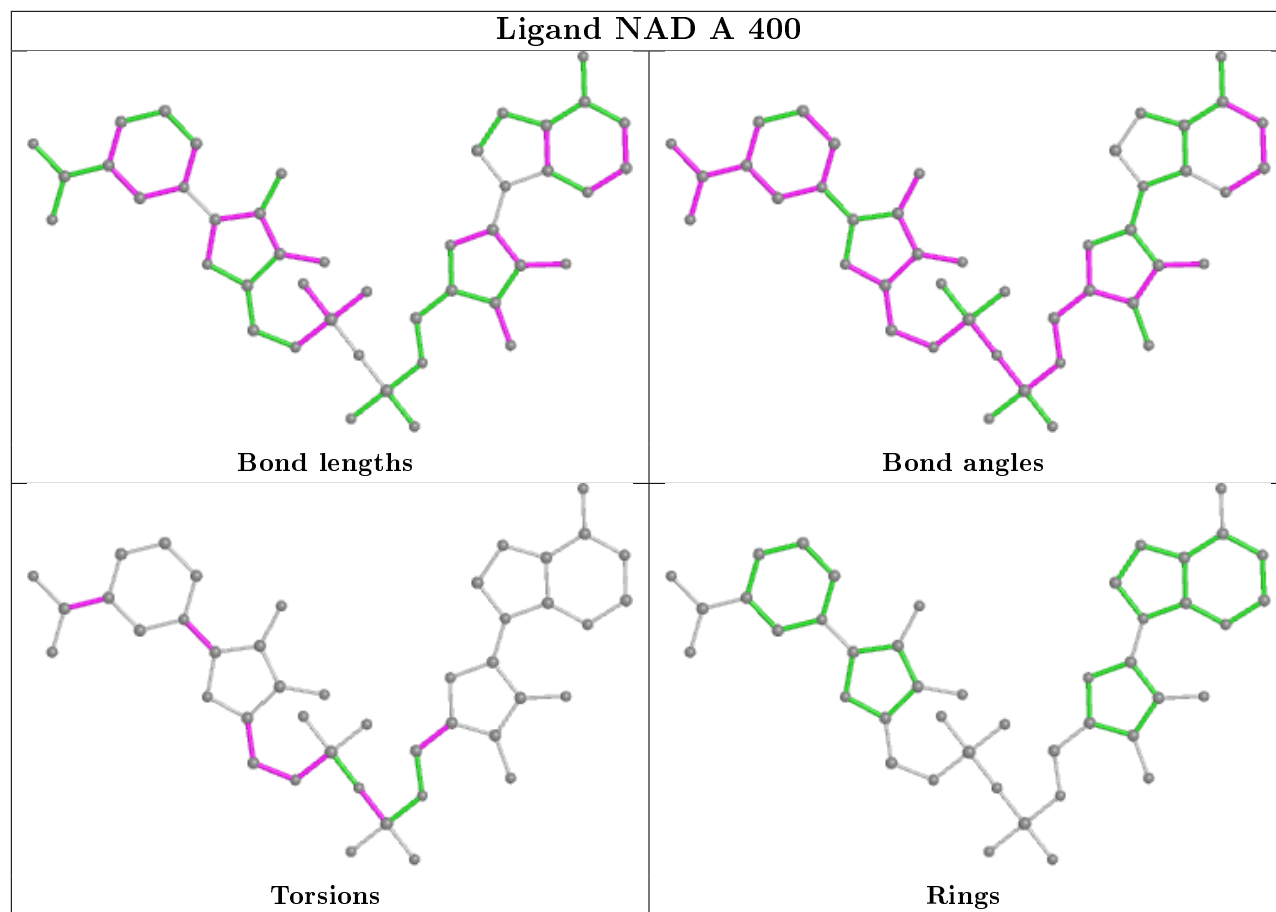
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	400	NAD	8	0
6	I	500	NDP	3	0
4	A	400	NAD	2	0
4	B	400	NAD	9	0
4	G	400	NAD	6	0
6	F	500	NDP	10	0
6	C	500	NDP	4	0
4	D	400	NAD	3	0

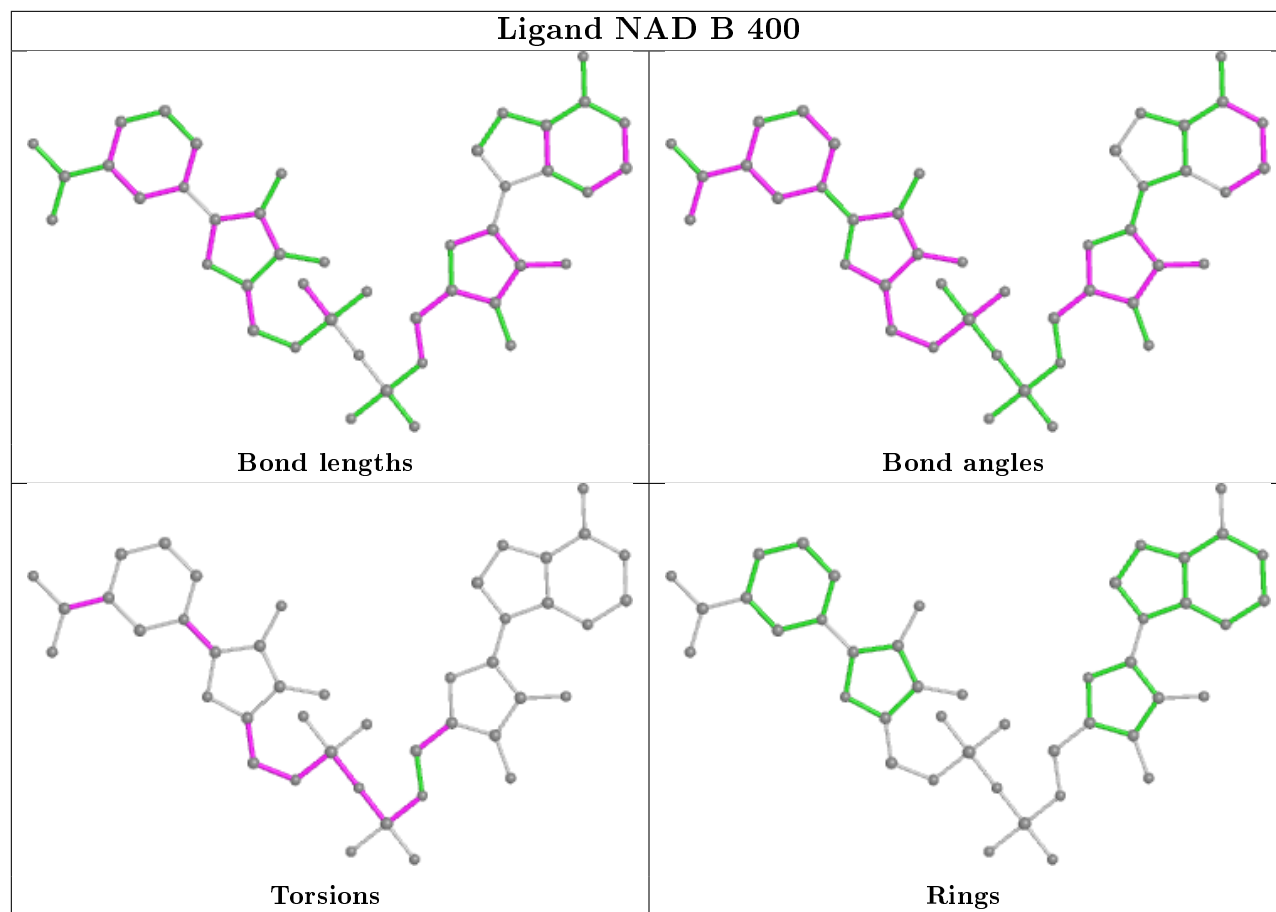
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

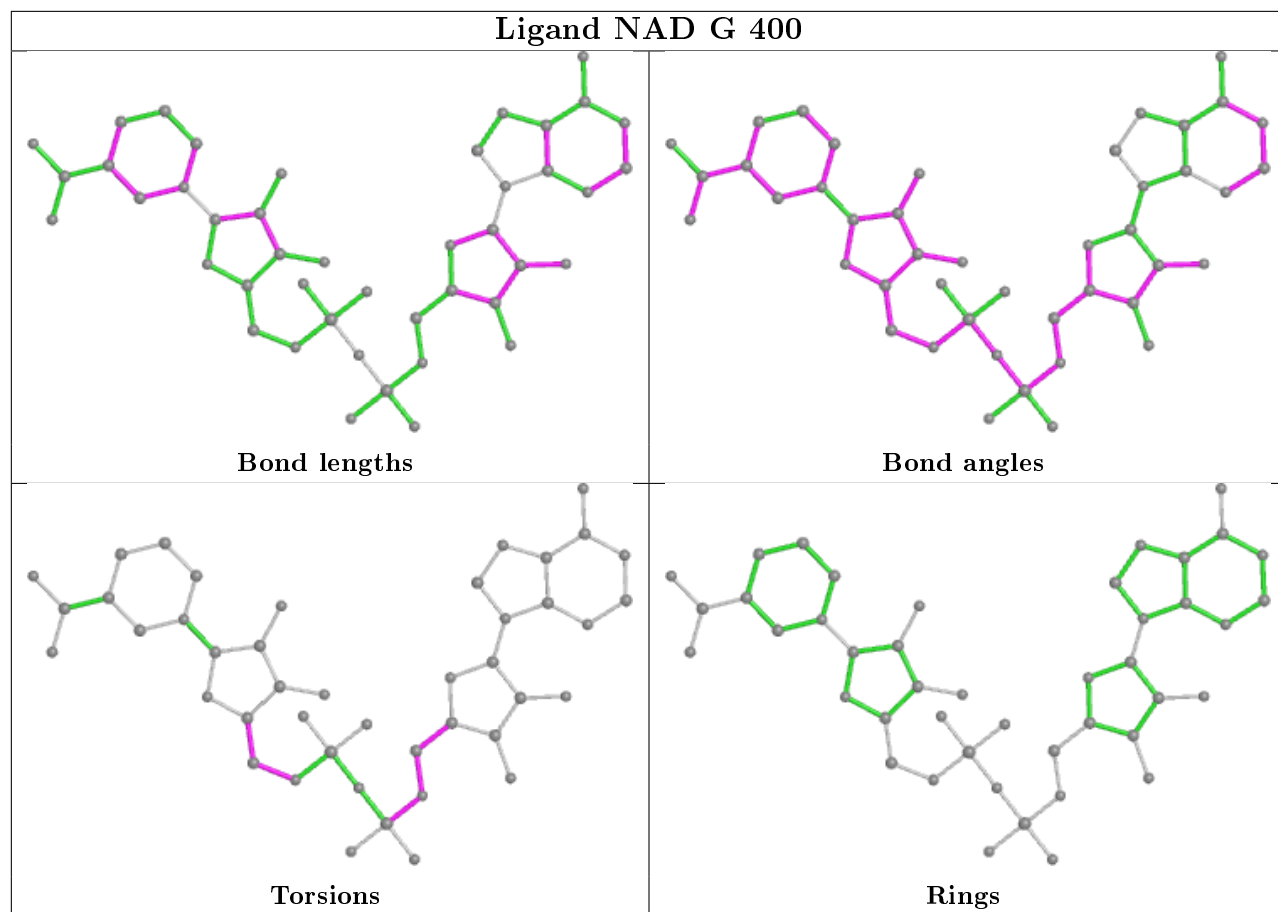
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

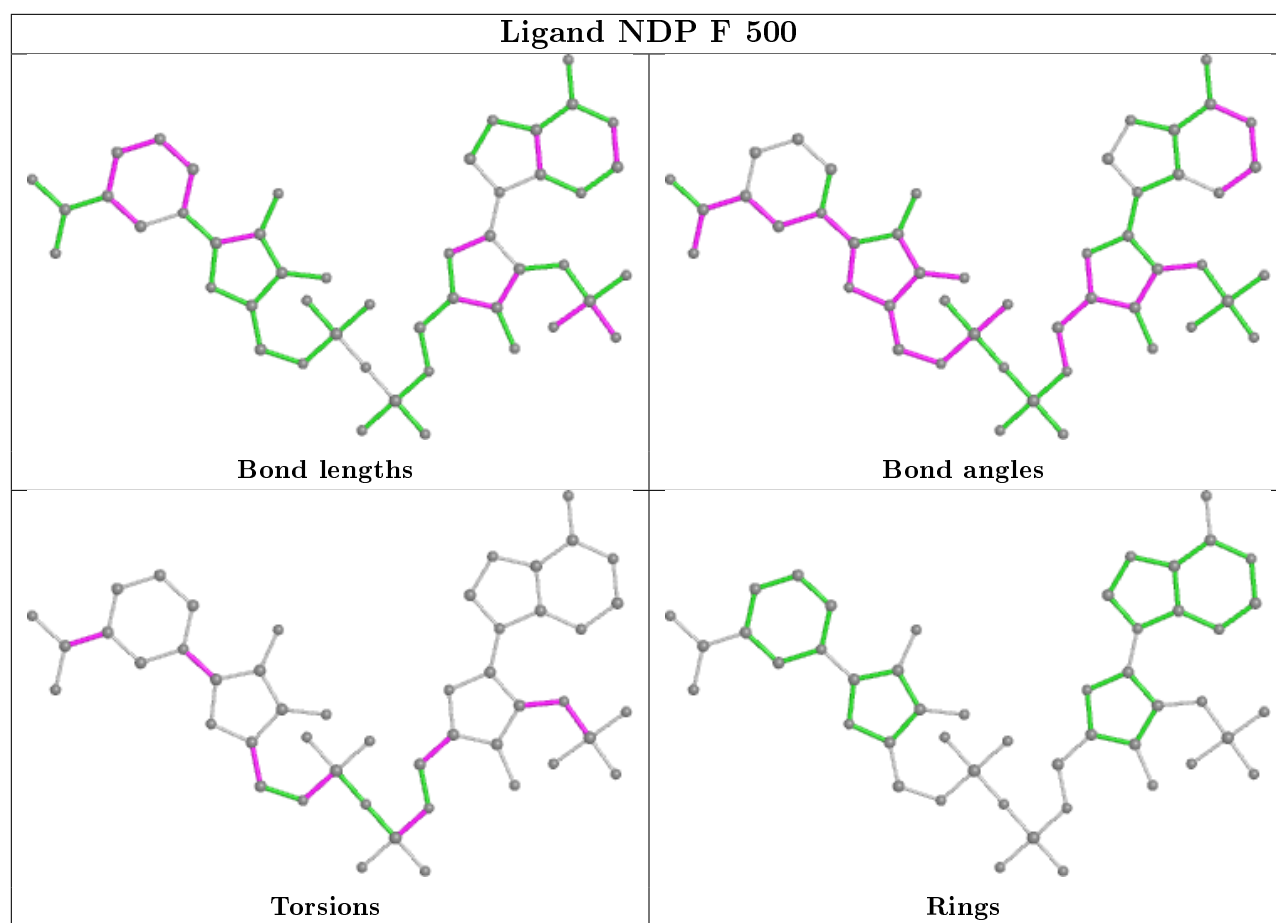


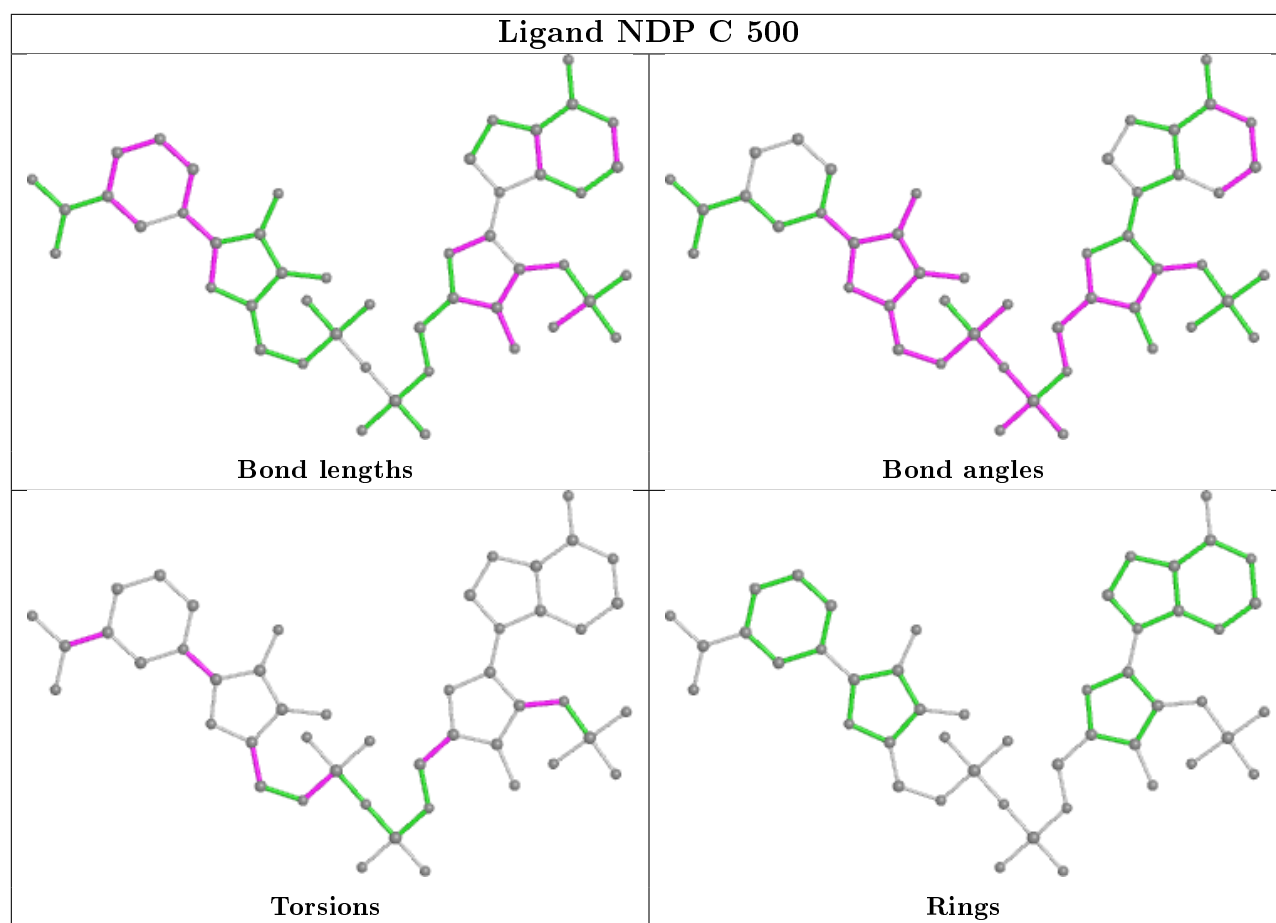


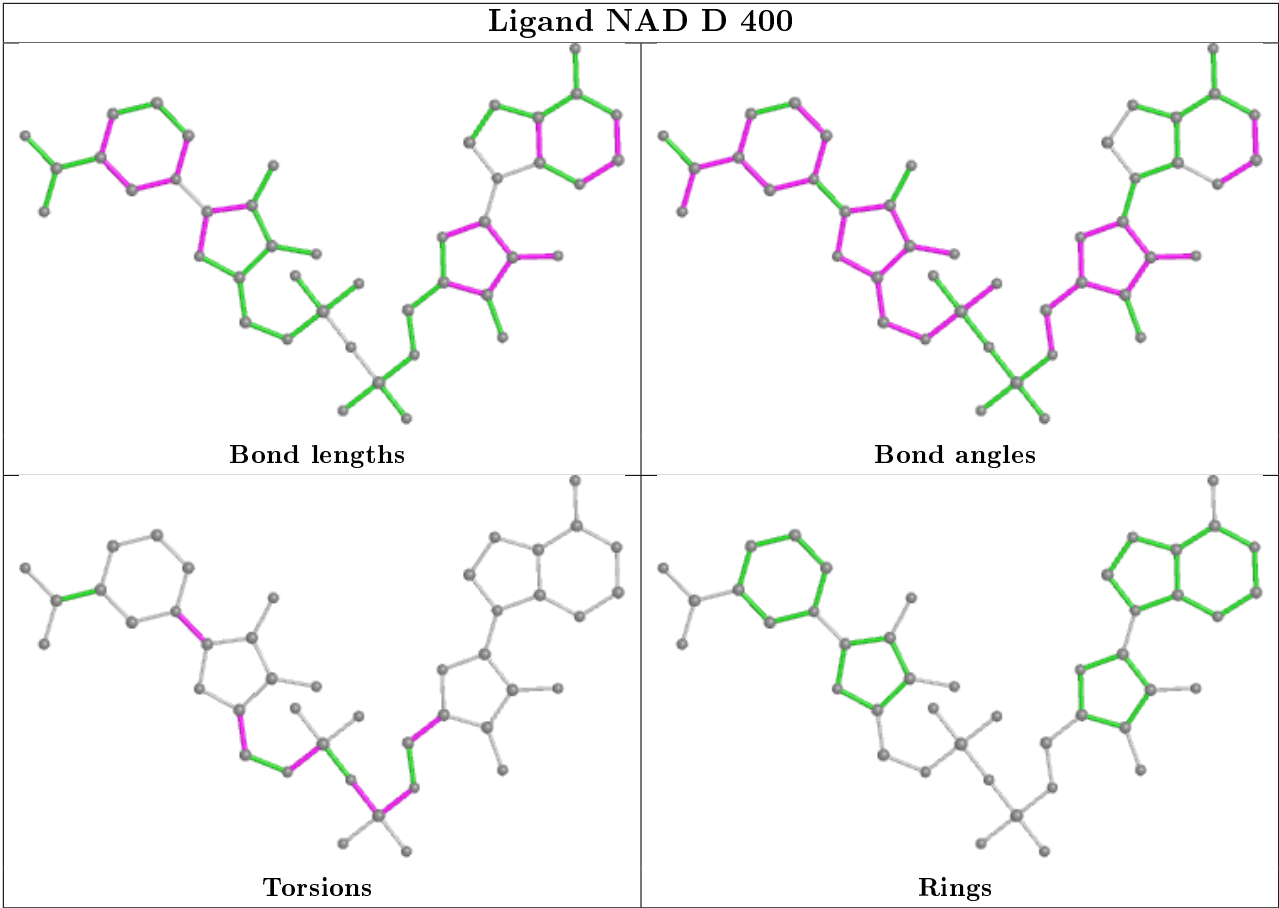












5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	H	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	H	343:LEU	C	344:THR	N	1.19

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	363/384 (94%)	-0.20	2 (0%) 89 78	30, 51, 77, 102	0
1	B	359/384 (93%)	-0.23	0 100 100	28, 52, 72, 98	0
1	D	378/384 (98%)	0.01	9 (2%) 59 37	36, 68, 94, 104	0
1	E	359/384 (93%)	-0.18	4 (1%) 80 64	33, 60, 79, 91	0
1	G	364/384 (94%)	-0.21	1 (0%) 94 88	35, 59, 84, 102	0
1	H	357/384 (92%)	0.06	10 (2%) 53 30	39, 72, 96, 104	0
2	C	174/174 (100%)	-0.39	0 100 100	32, 47, 61, 68	0
2	F	173/174 (99%)	-0.36	0 100 100	40, 52, 63, 75	0
2	I	173/174 (99%)	-0.27	0 100 100	42, 58, 73, 79	0
All	All	2700/2826 (95%)	-0.17	26 (0%) 82 67	28, 57, 90, 104	0

The worst 5 of 26 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1	MET	3.8
1	H	96	LEU	3.3
1	D	225	ALA	3.3
1	H	64	ALA	3.2
1	D	371	ASP	3.0

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

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

6.3 Carbohydrates ⓘ

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,

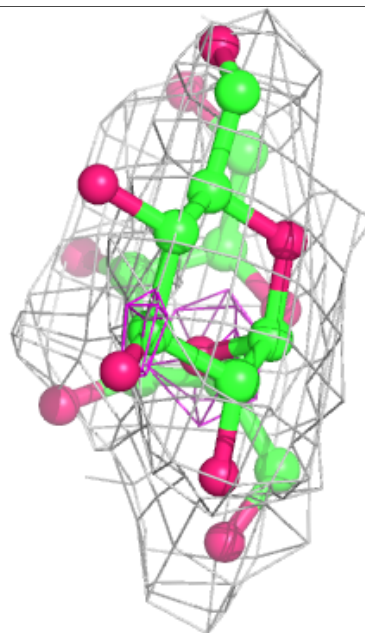
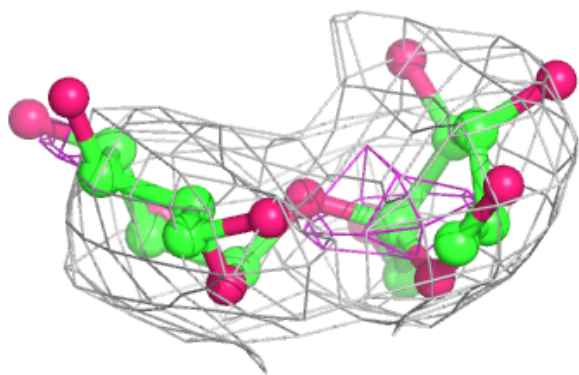
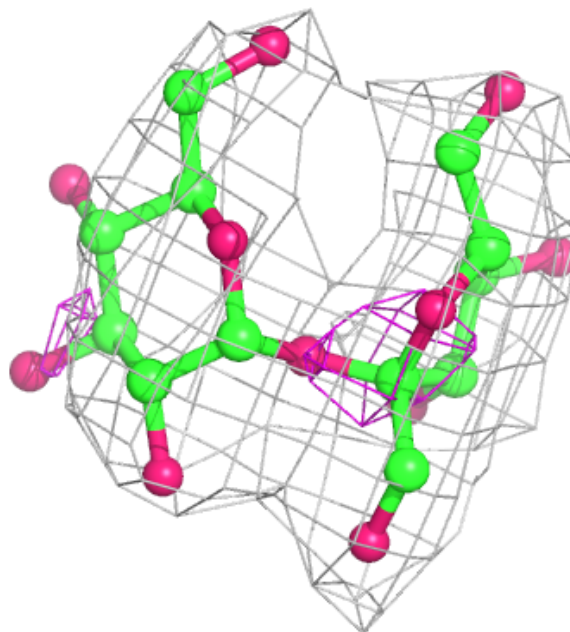
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	GLC	N	1	11/12	0.71	0.47	97,99,99,99	0
3	FRU	K	2	12/12	0.71	0.32	84,88,89,89	0
3	FRU	N	2	12/12	0.79	0.36	98,99,99,99	0
3	GLC	O	1	11/12	0.83	0.36	82,83,83,84	0
3	FRU	L	2	12/12	0.85	0.26	81,82,83,83	0
3	FRU	M	2	12/12	0.87	0.27	70,74,75,76	0
3	GLC	M	1	11/12	0.88	0.21	76,76,77,77	0
3	GLC	J	1	11/12	0.88	0.23	76,77,79,79	0
3	FRU	O	2	12/12	0.89	0.40	84,85,85,87	0
3	GLC	K	1	11/12	0.89	0.26	86,88,88,88	0
3	FRU	J	2	12/12	0.90	0.20	70,73,75,76	0
3	GLC	L	1	11/12	0.90	0.29	79,82,82,83	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

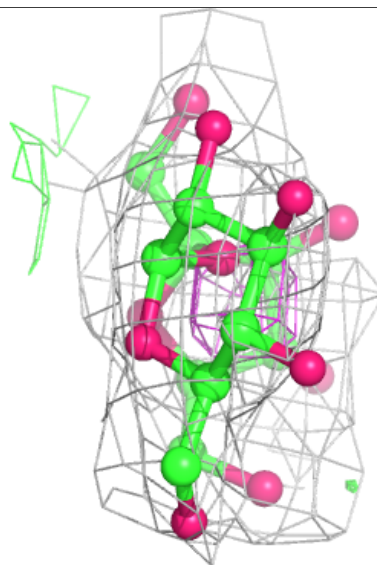
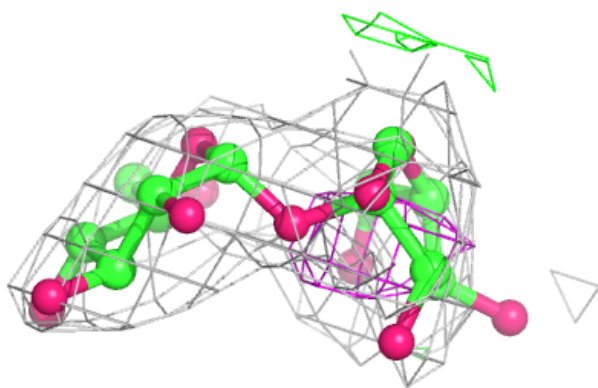
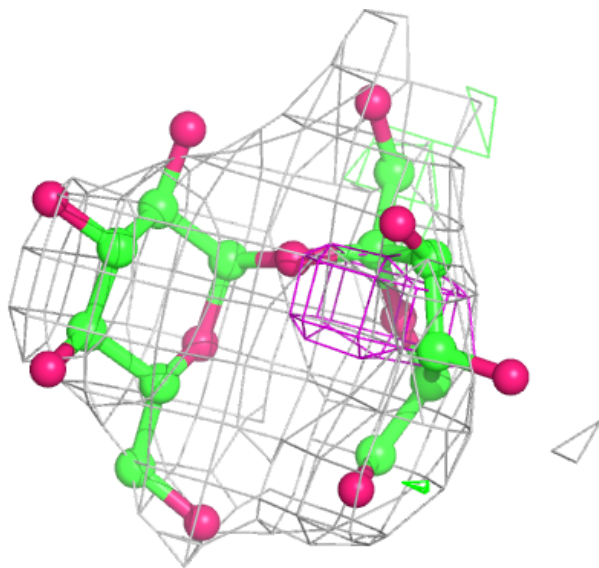
Electron density around Chain J:

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



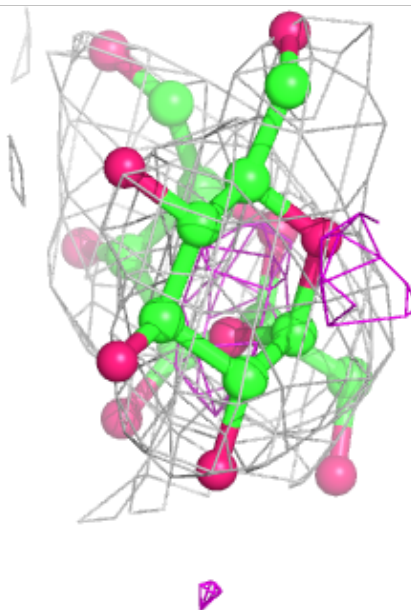
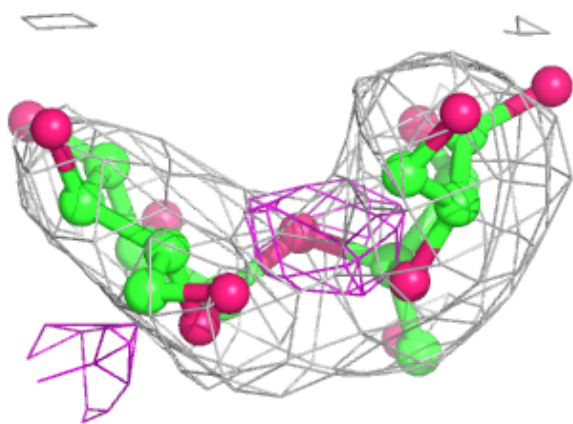
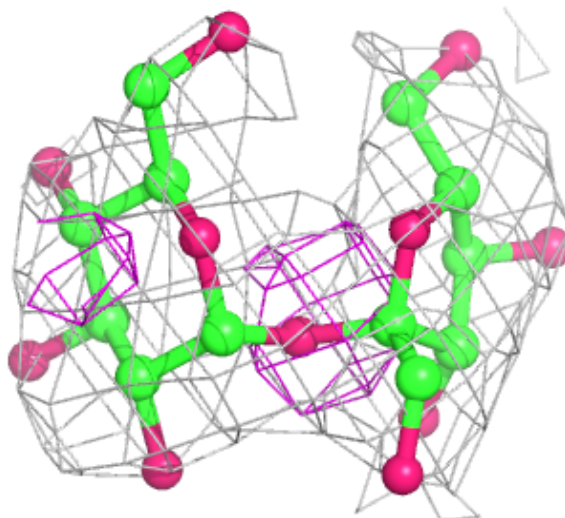
Electron density around Chain K:

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



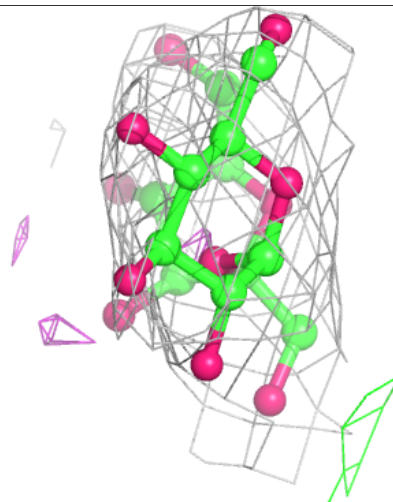
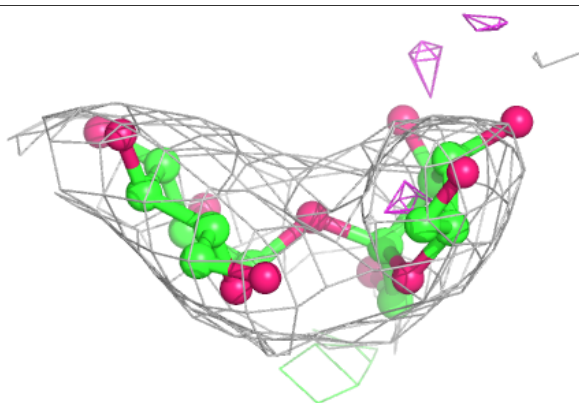
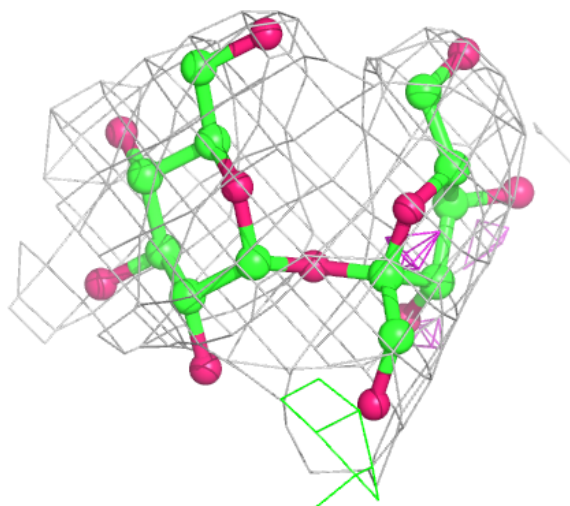
Electron density around Chain L:

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



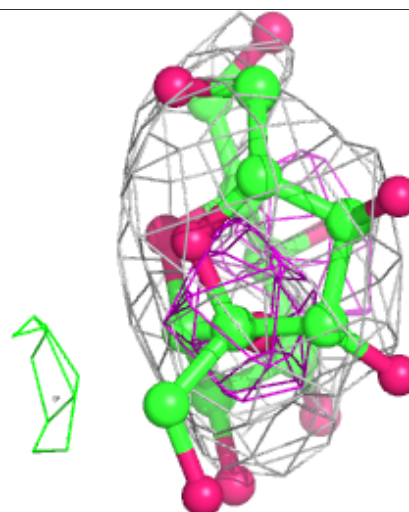
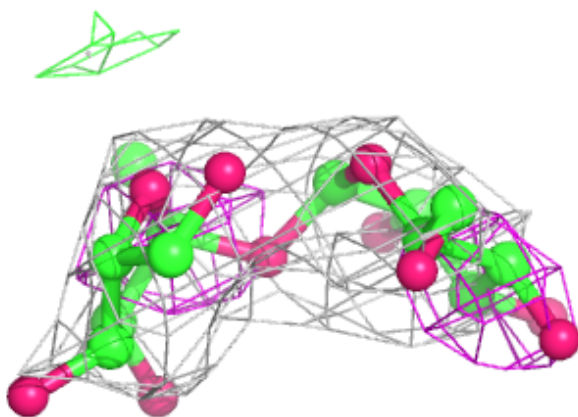
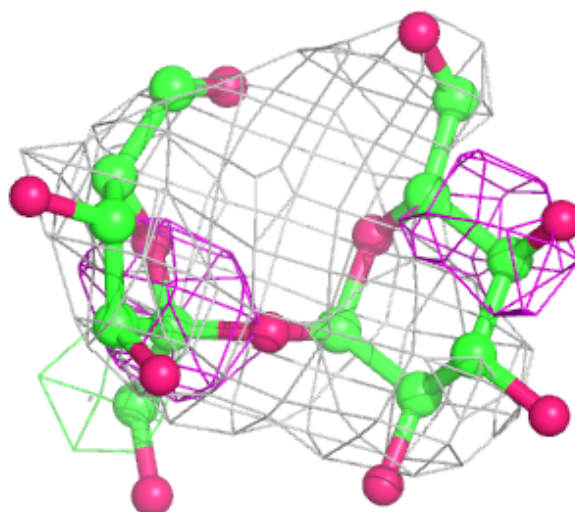
Electron density around Chain M:

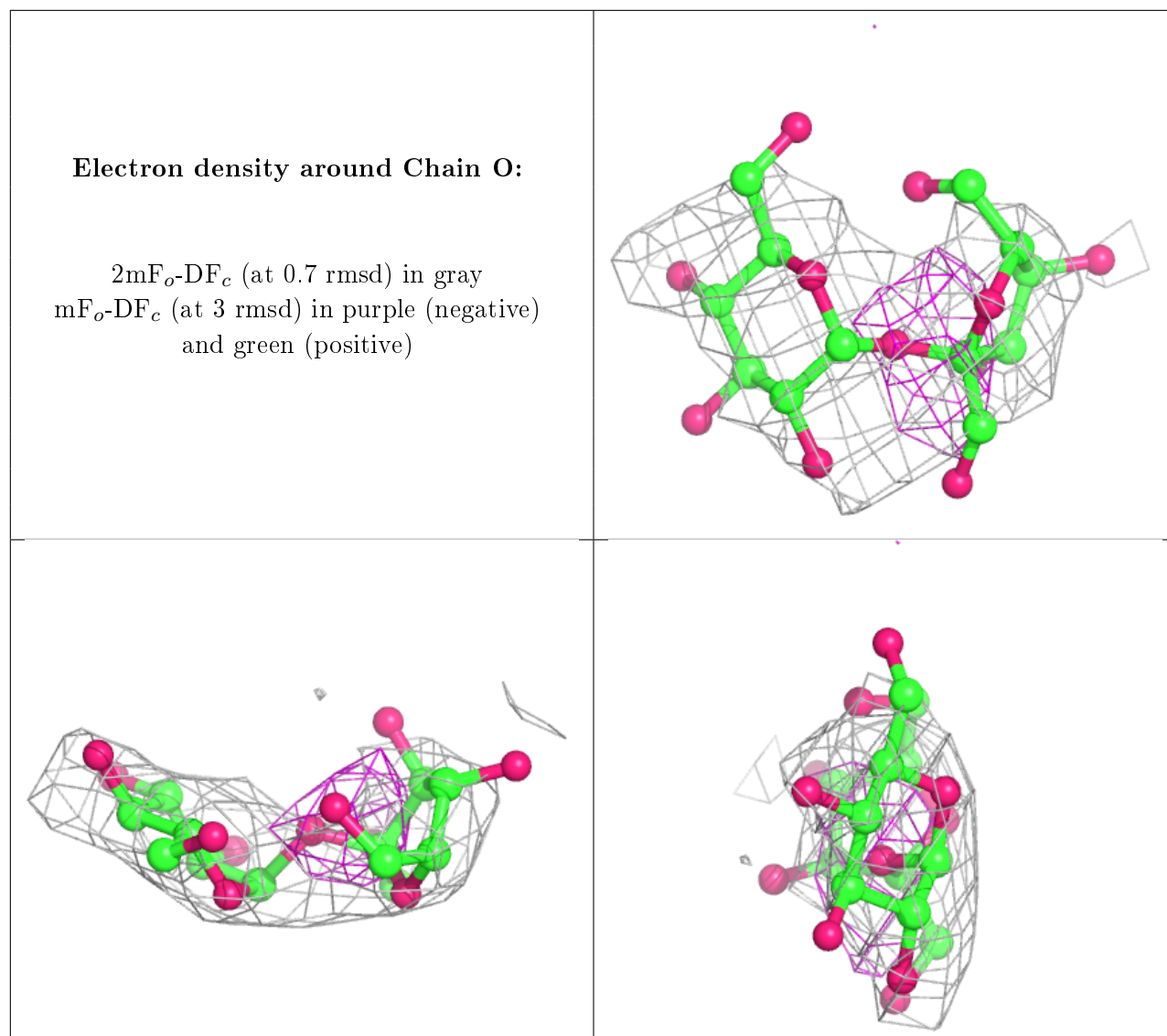
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain N:

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





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.

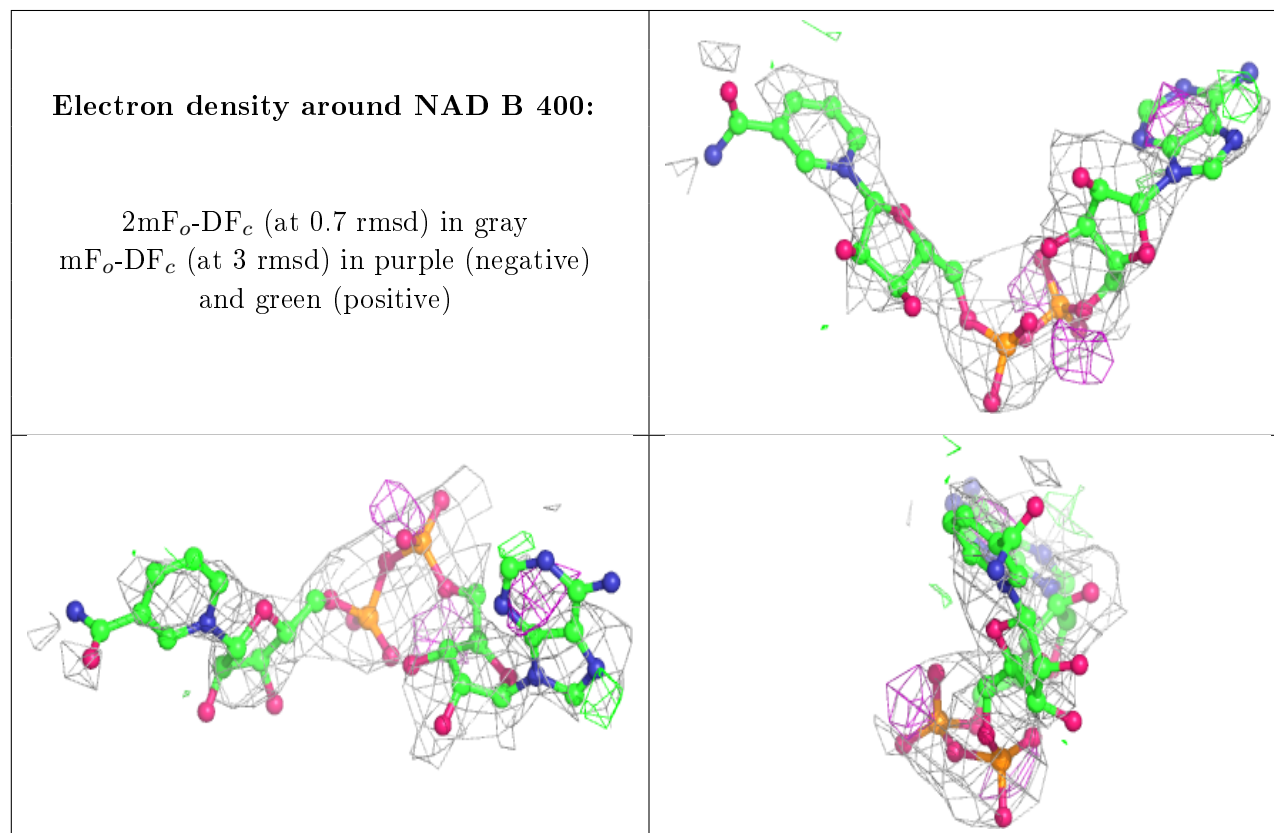
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAD	B	400	44/44	0.75	0.36	104,104,105,105	0
4	NAD	H	400	44/44	0.85	0.28	88,90,99,101	0
5	NA	A	601	1/1	0.87	0.24	50,50,50,50	0
4	NAD	G	400	44/44	0.90	0.24	65,72,87,87	0
4	NAD	A	400	44/44	0.91	0.21	65,71,75,75	0
6	NDP	I	500	48/48	0.92	0.17	56,58,64,64	0
5	NA	D	602	1/1	0.92	0.18	69,69,69,69	0

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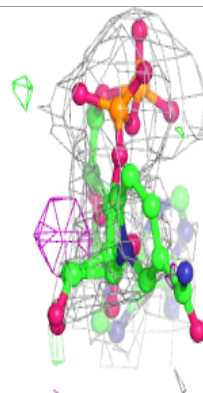
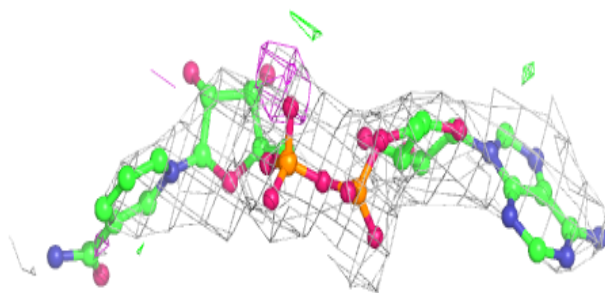
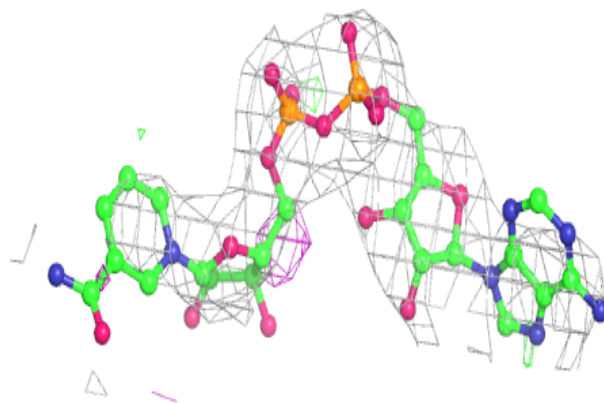
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	NAD	D	400	44/44	0.93	0.20	54,60,64,65	0
6	NDP	F	500	48/48	0.94	0.18	48,52,56,58	0
5	NA	G	603	1/1	0.95	0.10	48,48,48,48	0
6	NDP	C	500	48/48	0.95	0.17	38,40,44,46	0

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.

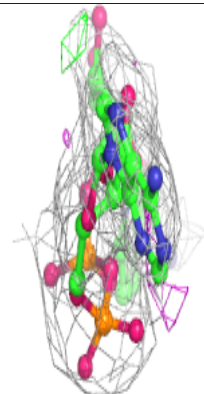
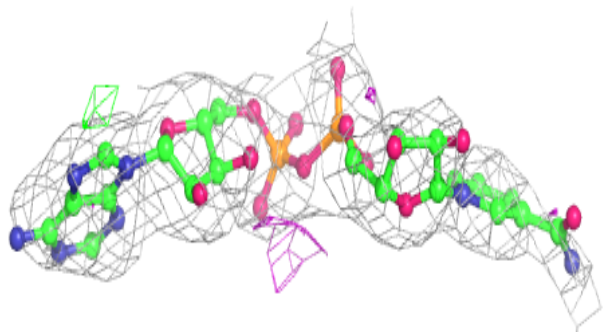
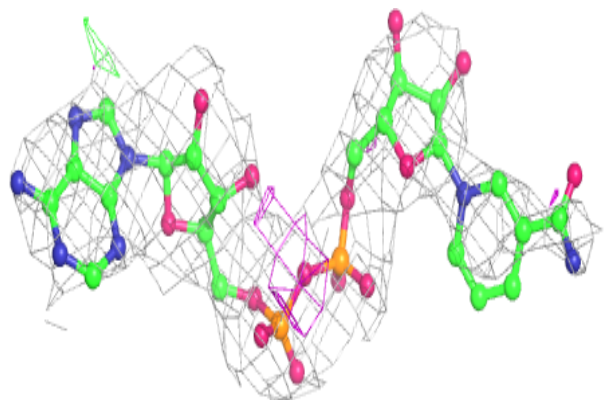


Electron density around NAD H 400:

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

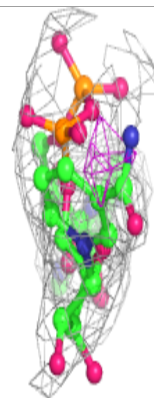
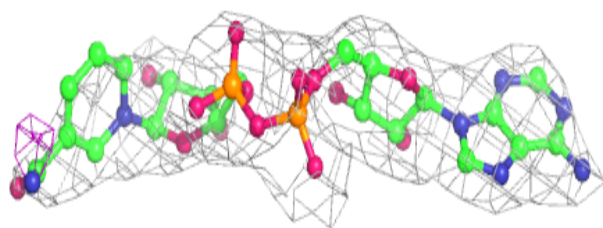
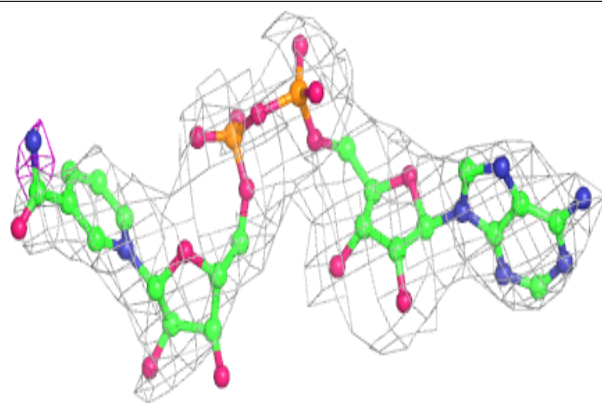
**Electron density around NAD G 400:**

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

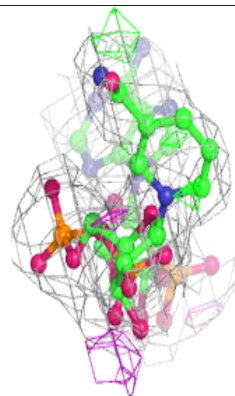
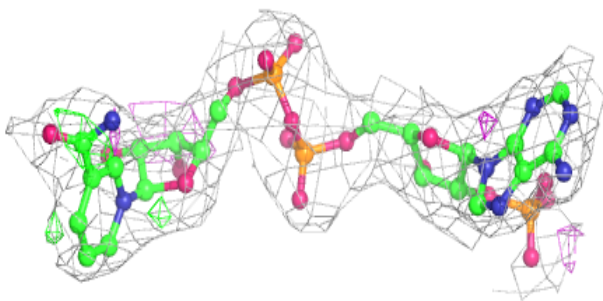
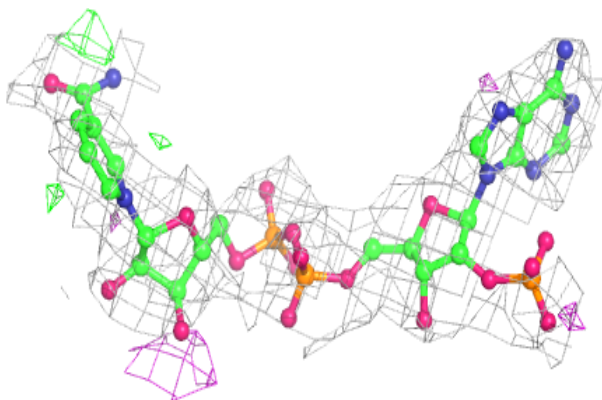


Electron density around NAD A 400:

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

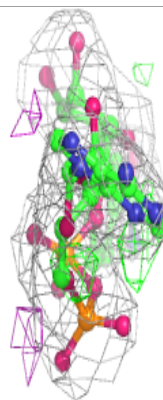
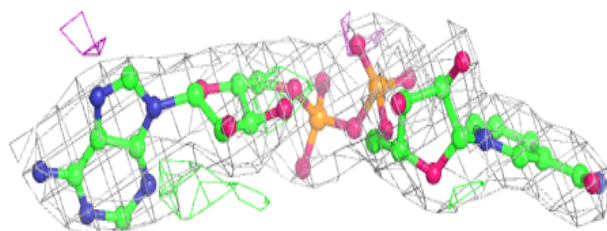
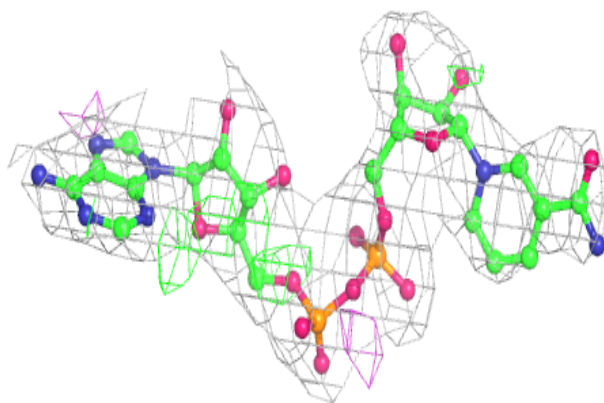
**Electron density around NDP I 500:**

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

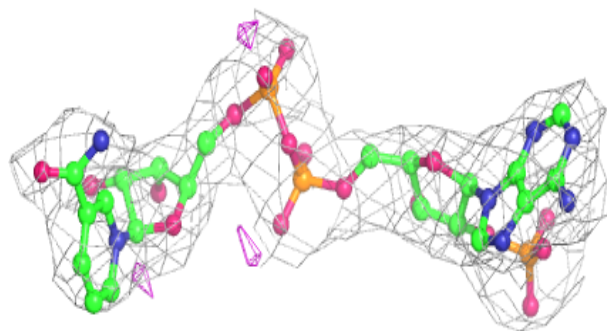
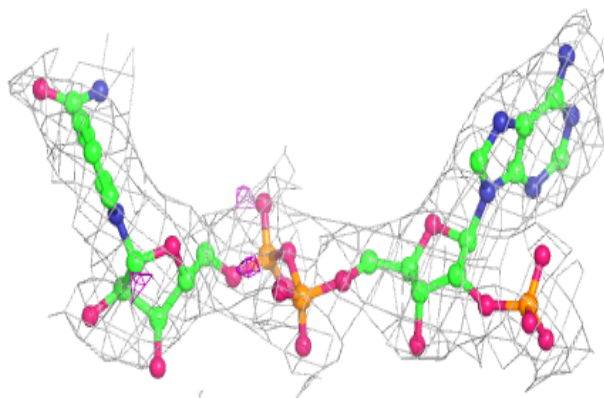


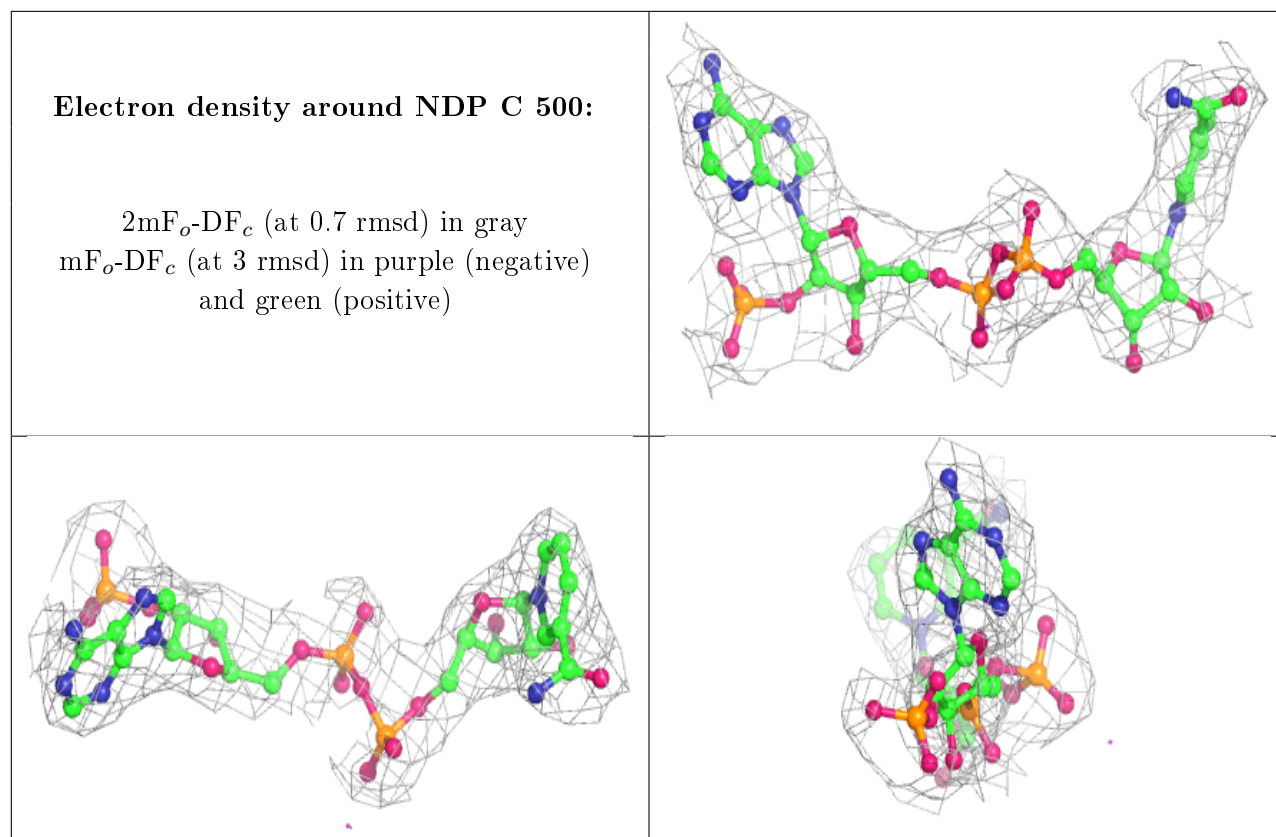
Electron density around NAD D 400:

$2mF_o-DF_c$ (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)





6.5 Other polymers [i](#)

There are no such residues in this entry.