



Full wwPDB X-ray Structure Validation Report i

Apr 4, 2024 – 12:17 PM JST

PDB ID : 8JWM
Title : Crystal structure of AKRtyl-NADP-tylosin complex
Authors : Lin, S.; Dai, S.; Xiao, Z.
Deposited on : 2023-06-29
Resolution : 1.93 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
A user guide is available at
<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>
with specific help available everywhere you see the i symbol.

The types of validation reports are described at
<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references](#) ①) 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 : 2.36
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

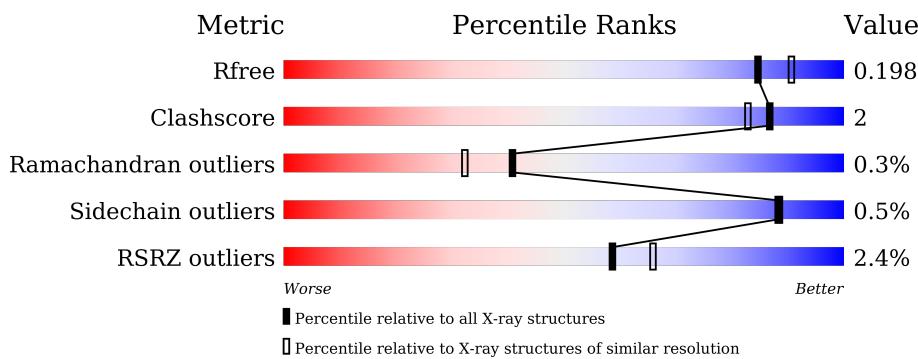
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.93 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	4310 (1.96-1.92)
Clashscore	141614	1023 (1.94-1.94)
Ramachandran outliers	138981	1007 (1.94-1.94)
Sidechain outliers	138945	1007 (1.94-1.94)
RSRZ outliers	127900	4250 (1.96-1.92)

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



Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain			
1	G	351	%	90%	5%	6%
1	H	351	?%	90%	•	6%

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	TYK	B	403	-	-	-	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 23779 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 Aldo/keto reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	330	Total 2552	C 1600	N 462	O 482	S 8	0	0	0
1	B	331	Total 2556	C 1602	N 463	O 483	S 8	0	0	0
1	C	331	Total 2556	C 1602	N 463	O 483	S 8	0	0	0
1	D	331	Total 2556	C 1602	N 463	O 483	S 8	0	0	0
1	E	331	Total 2556	C 1602	N 463	O 483	S 8	0	0	0
1	F	331	Total 2556	C 1602	N 463	O 483	S 8	0	0	0
1	G	331	Total 2556	C 1602	N 463	O 483	S 8	0	0	0
1	H	331	Total 2556	C 1602	N 463	O 483	S 8	0	0	0

There are 160 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP A0A3R7J519
A	-18	GLY	-	expression tag	UNP A0A3R7J519
A	-17	SER	-	expression tag	UNP A0A3R7J519
A	-16	SER	-	expression tag	UNP A0A3R7J519
A	-15	HIS	-	expression tag	UNP A0A3R7J519
A	-14	HIS	-	expression tag	UNP A0A3R7J519
A	-13	HIS	-	expression tag	UNP A0A3R7J519
A	-12	HIS	-	expression tag	UNP A0A3R7J519
A	-11	HIS	-	expression tag	UNP A0A3R7J519
A	-10	HIS	-	expression tag	UNP A0A3R7J519
A	-9	SER	-	expression tag	UNP A0A3R7J519
A	-8	SER	-	expression tag	UNP A0A3R7J519
A	-7	GLY	-	expression tag	UNP A0A3R7J519

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	LEU	-	expression tag	UNP A0A3R7J519
A	-5	VAL	-	expression tag	UNP A0A3R7J519
A	-4	PRO	-	expression tag	UNP A0A3R7J519
A	-3	ARG	-	expression tag	UNP A0A3R7J519
A	-2	GLY	-	expression tag	UNP A0A3R7J519
A	-1	SER	-	expression tag	UNP A0A3R7J519
A	0	HIS	-	expression tag	UNP A0A3R7J519
B	-19	MET	-	initiating methionine	UNP A0A3R7J519
B	-18	GLY	-	expression tag	UNP A0A3R7J519
B	-17	SER	-	expression tag	UNP A0A3R7J519
B	-16	SER	-	expression tag	UNP A0A3R7J519
B	-15	HIS	-	expression tag	UNP A0A3R7J519
B	-14	HIS	-	expression tag	UNP A0A3R7J519
B	-13	HIS	-	expression tag	UNP A0A3R7J519
B	-12	HIS	-	expression tag	UNP A0A3R7J519
B	-11	HIS	-	expression tag	UNP A0A3R7J519
B	-10	HIS	-	expression tag	UNP A0A3R7J519
B	-9	SER	-	expression tag	UNP A0A3R7J519
B	-8	SER	-	expression tag	UNP A0A3R7J519
B	-7	GLY	-	expression tag	UNP A0A3R7J519
B	-6	LEU	-	expression tag	UNP A0A3R7J519
B	-5	VAL	-	expression tag	UNP A0A3R7J519
B	-4	PRO	-	expression tag	UNP A0A3R7J519
B	-3	ARG	-	expression tag	UNP A0A3R7J519
B	-2	GLY	-	expression tag	UNP A0A3R7J519
B	-1	SER	-	expression tag	UNP A0A3R7J519
B	0	HIS	-	expression tag	UNP A0A3R7J519
C	-19	MET	-	initiating methionine	UNP A0A3R7J519
C	-18	GLY	-	expression tag	UNP A0A3R7J519
C	-17	SER	-	expression tag	UNP A0A3R7J519
C	-16	SER	-	expression tag	UNP A0A3R7J519
C	-15	HIS	-	expression tag	UNP A0A3R7J519
C	-14	HIS	-	expression tag	UNP A0A3R7J519
C	-13	HIS	-	expression tag	UNP A0A3R7J519
C	-12	HIS	-	expression tag	UNP A0A3R7J519
C	-11	HIS	-	expression tag	UNP A0A3R7J519
C	-10	HIS	-	expression tag	UNP A0A3R7J519
C	-9	SER	-	expression tag	UNP A0A3R7J519
C	-8	SER	-	expression tag	UNP A0A3R7J519
C	-7	GLY	-	expression tag	UNP A0A3R7J519
C	-6	LEU	-	expression tag	UNP A0A3R7J519
C	-5	VAL	-	expression tag	UNP A0A3R7J519

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	PRO	-	expression tag	UNP A0A3R7J519
C	-3	ARG	-	expression tag	UNP A0A3R7J519
C	-2	GLY	-	expression tag	UNP A0A3R7J519
C	-1	SER	-	expression tag	UNP A0A3R7J519
C	0	HIS	-	expression tag	UNP A0A3R7J519
D	-19	MET	-	initiating methionine	UNP A0A3R7J519
D	-18	GLY	-	expression tag	UNP A0A3R7J519
D	-17	SER	-	expression tag	UNP A0A3R7J519
D	-16	SER	-	expression tag	UNP A0A3R7J519
D	-15	HIS	-	expression tag	UNP A0A3R7J519
D	-14	HIS	-	expression tag	UNP A0A3R7J519
D	-13	HIS	-	expression tag	UNP A0A3R7J519
D	-12	HIS	-	expression tag	UNP A0A3R7J519
D	-11	HIS	-	expression tag	UNP A0A3R7J519
D	-10	HIS	-	expression tag	UNP A0A3R7J519
D	-9	SER	-	expression tag	UNP A0A3R7J519
D	-8	SER	-	expression tag	UNP A0A3R7J519
D	-7	GLY	-	expression tag	UNP A0A3R7J519
D	-6	LEU	-	expression tag	UNP A0A3R7J519
D	-5	VAL	-	expression tag	UNP A0A3R7J519
D	-4	PRO	-	expression tag	UNP A0A3R7J519
D	-3	ARG	-	expression tag	UNP A0A3R7J519
D	-2	GLY	-	expression tag	UNP A0A3R7J519
D	-1	SER	-	expression tag	UNP A0A3R7J519
D	0	HIS	-	expression tag	UNP A0A3R7J519
E	-19	MET	-	initiating methionine	UNP A0A3R7J519
E	-18	GLY	-	expression tag	UNP A0A3R7J519
E	-17	SER	-	expression tag	UNP A0A3R7J519
E	-16	SER	-	expression tag	UNP A0A3R7J519
E	-15	HIS	-	expression tag	UNP A0A3R7J519
E	-14	HIS	-	expression tag	UNP A0A3R7J519
E	-13	HIS	-	expression tag	UNP A0A3R7J519
E	-12	HIS	-	expression tag	UNP A0A3R7J519
E	-11	HIS	-	expression tag	UNP A0A3R7J519
E	-10	HIS	-	expression tag	UNP A0A3R7J519
E	-9	SER	-	expression tag	UNP A0A3R7J519
E	-8	SER	-	expression tag	UNP A0A3R7J519
E	-7	GLY	-	expression tag	UNP A0A3R7J519
E	-6	LEU	-	expression tag	UNP A0A3R7J519
E	-5	VAL	-	expression tag	UNP A0A3R7J519
E	-4	PRO	-	expression tag	UNP A0A3R7J519
E	-3	ARG	-	expression tag	UNP A0A3R7J519

Continued on next page...

Continued from previous page...

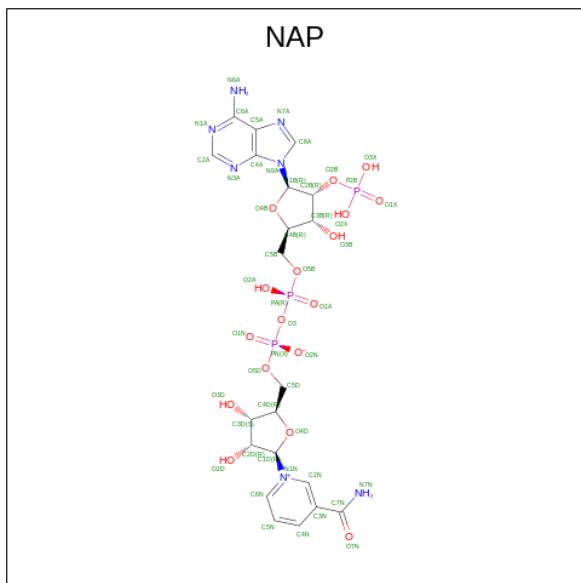
Chain	Residue	Modelled	Actual	Comment	Reference
E	-2	GLY	-	expression tag	UNP A0A3R7J519
E	-1	SER	-	expression tag	UNP A0A3R7J519
E	0	HIS	-	expression tag	UNP A0A3R7J519
F	-19	MET	-	initiating methionine	UNP A0A3R7J519
F	-18	GLY	-	expression tag	UNP A0A3R7J519
F	-17	SER	-	expression tag	UNP A0A3R7J519
F	-16	SER	-	expression tag	UNP A0A3R7J519
F	-15	HIS	-	expression tag	UNP A0A3R7J519
F	-14	HIS	-	expression tag	UNP A0A3R7J519
F	-13	HIS	-	expression tag	UNP A0A3R7J519
F	-12	HIS	-	expression tag	UNP A0A3R7J519
F	-11	HIS	-	expression tag	UNP A0A3R7J519
F	-10	HIS	-	expression tag	UNP A0A3R7J519
F	-9	SER	-	expression tag	UNP A0A3R7J519
F	-8	SER	-	expression tag	UNP A0A3R7J519
F	-7	GLY	-	expression tag	UNP A0A3R7J519
F	-6	LEU	-	expression tag	UNP A0A3R7J519
F	-5	VAL	-	expression tag	UNP A0A3R7J519
F	-4	PRO	-	expression tag	UNP A0A3R7J519
F	-3	ARG	-	expression tag	UNP A0A3R7J519
F	-2	GLY	-	expression tag	UNP A0A3R7J519
F	-1	SER	-	expression tag	UNP A0A3R7J519
F	0	HIS	-	expression tag	UNP A0A3R7J519
G	-19	MET	-	initiating methionine	UNP A0A3R7J519
G	-18	GLY	-	expression tag	UNP A0A3R7J519
G	-17	SER	-	expression tag	UNP A0A3R7J519
G	-16	SER	-	expression tag	UNP A0A3R7J519
G	-15	HIS	-	expression tag	UNP A0A3R7J519
G	-14	HIS	-	expression tag	UNP A0A3R7J519
G	-13	HIS	-	expression tag	UNP A0A3R7J519
G	-12	HIS	-	expression tag	UNP A0A3R7J519
G	-11	HIS	-	expression tag	UNP A0A3R7J519
G	-10	HIS	-	expression tag	UNP A0A3R7J519
G	-9	SER	-	expression tag	UNP A0A3R7J519
G	-8	SER	-	expression tag	UNP A0A3R7J519
G	-7	GLY	-	expression tag	UNP A0A3R7J519
G	-6	LEU	-	expression tag	UNP A0A3R7J519
G	-5	VAL	-	expression tag	UNP A0A3R7J519
G	-4	PRO	-	expression tag	UNP A0A3R7J519
G	-3	ARG	-	expression tag	UNP A0A3R7J519
G	-2	GLY	-	expression tag	UNP A0A3R7J519
G	-1	SER	-	expression tag	UNP A0A3R7J519

Continued on next page...

Continued from previous page...

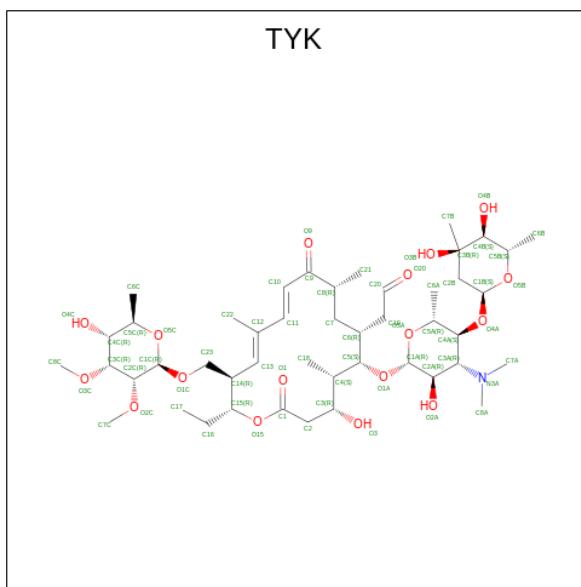
Chain	Residue	Modelled	Actual	Comment	Reference
G	0	HIS	-	expression tag	UNP A0A3R7J519
H	-19	MET	-	initiating methionine	UNP A0A3R7J519
H	-18	GLY	-	expression tag	UNP A0A3R7J519
H	-17	SER	-	expression tag	UNP A0A3R7J519
H	-16	SER	-	expression tag	UNP A0A3R7J519
H	-15	HIS	-	expression tag	UNP A0A3R7J519
H	-14	HIS	-	expression tag	UNP A0A3R7J519
H	-13	HIS	-	expression tag	UNP A0A3R7J519
H	-12	HIS	-	expression tag	UNP A0A3R7J519
H	-11	HIS	-	expression tag	UNP A0A3R7J519
H	-10	HIS	-	expression tag	UNP A0A3R7J519
H	-9	SER	-	expression tag	UNP A0A3R7J519
H	-8	SER	-	expression tag	UNP A0A3R7J519
H	-7	GLY	-	expression tag	UNP A0A3R7J519
H	-6	LEU	-	expression tag	UNP A0A3R7J519
H	-5	VAL	-	expression tag	UNP A0A3R7J519
H	-4	PRO	-	expression tag	UNP A0A3R7J519
H	-3	ARG	-	expression tag	UNP A0A3R7J519
H	-2	GLY	-	expression tag	UNP A0A3R7J519
H	-1	SER	-	expression tag	UNP A0A3R7J519
H	0	HIS	-	expression tag	UNP A0A3R7J519

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 3 is TYLOSIN (three-letter code: TYK) (formula: C₄₆H₇₇NO₁₇) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total C N O					0	0
3	B	1	64 46 1 17					0	0
3	B	1	Total C N O					0	0
3	B	1	64 46 1 17					0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total C N O 64 46 1 17	0	0
3	E	1	Total C N O 64 46 1 17	0	0
3	F	1	Total C N O 64 46 1 17	0	0
3	G	1	Total C N O 64 46 1 17	0	0

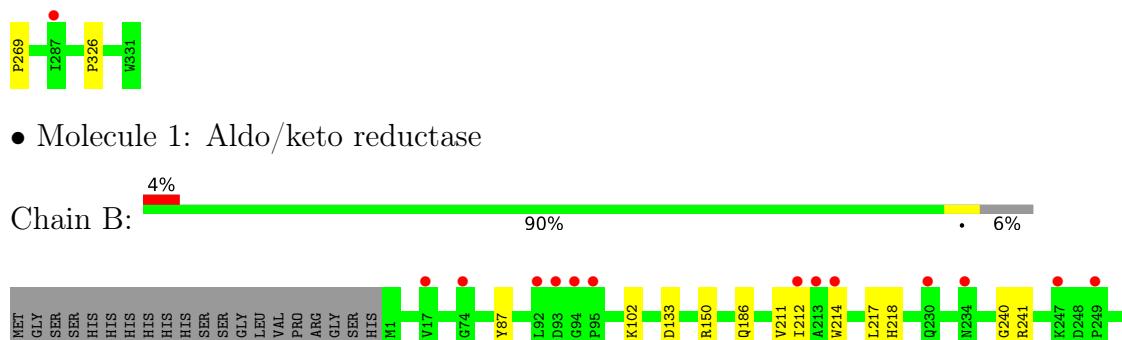
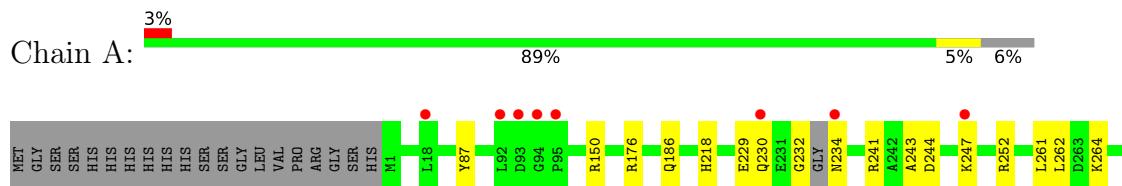
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	301	Total O 301 301	0	0
4	B	280	Total O 280 280	0	0
4	C	322	Total O 322 322	0	0
4	D	327	Total O 327 327	0	0
4	E	322	Total O 322 322	0	0
4	F	325	Total O 325 325	0	0
4	G	307	Total O 307 307	0	0
4	H	319	Total O 319 319	0	0

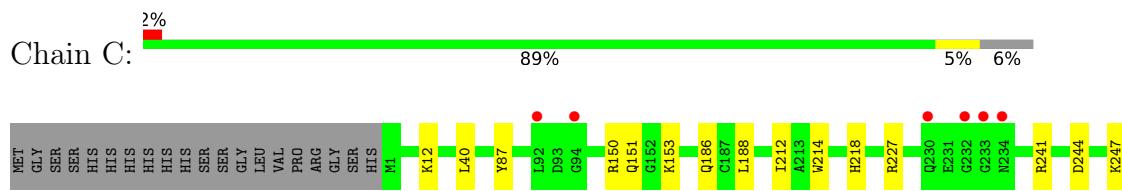
3 Residue-property plots

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.

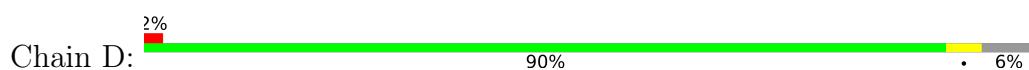
- Molecule 1: Aldo/keto reductase



- Molecule 1: Aldo/keto reductase

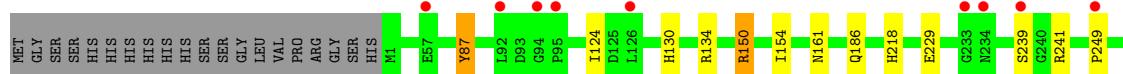
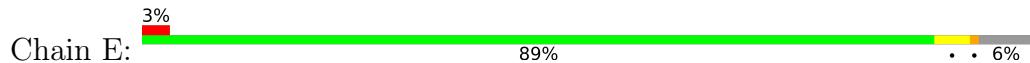


- Molecule 1: Aldo/keto reductase





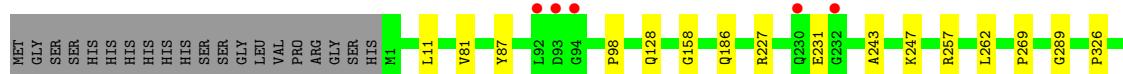
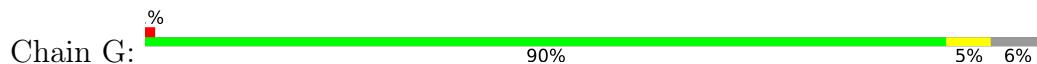
- Molecule 1: Aldo/keto reductase



- Molecule 1: Aldo/keto reductase



- Molecule 1: Aldo/keto reductase



- Molecule 1: Aldo/keto reductase



4 Data and refinement statistics i

Property	Value	Source
Space group	P 2 1 21	Depositor
Cell constants a, b, c, α , β , γ	83.01 Å 198.31 Å 199.99 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.15 – 1.93 35.15 – 1.93	Depositor EDS
% Data completeness (in resolution range)	98.7 (35.15-1.93) 98.7 (35.15-1.93)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle^1$	1.66 (at 1.92 Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R , R_{free}	0.164 , 0.198 0.164 , 0.198	Depositor DCC
R_{free} test set	11929 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	19.3	Xtriage
Anisotropy	0.015	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 48.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.013 for -h,l,k	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	23779	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.22% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality i

5.1 Standard geometry i

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

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	0.43	0/2607	0.57	0/3538
1	B	0.43	0/2612	0.58	0/3546
1	C	0.43	0/2612	0.58	0/3546
1	D	0.46	0/2612	0.57	0/3546
1	E	0.41	0/2612	0.56	0/3546
1	F	0.45	0/2612	0.58	0/3546
1	G	0.44	0/2612	0.58	0/3546
1	H	0.43	0/2612	0.56	0/3546
All	All	0.43	0/20891	0.57	0/28360

There are no bond length outliers.

There are no bond angle outliers.

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	2552	0	2490	14	0
1	B	2556	0	2494	8	0
1	C	2556	0	2494	13	0
1	D	2556	0	2494	9	0
1	E	2556	0	2494	15	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2556	0	2494	6	0
1	G	2556	0	2494	11	0
1	H	2556	0	2494	11	0
2	A	48	0	25	1	0
2	B	48	0	25	1	0
2	C	48	0	25	1	0
2	D	48	0	25	1	0
2	E	48	0	25	1	0
2	F	48	0	25	1	0
2	G	48	0	25	2	0
2	H	48	0	25	1	0
3	A	64	0	77	3	0
3	B	128	0	154	6	0
3	C	64	0	77	2	0
3	E	64	0	77	1	0
3	F	64	0	77	2	0
3	G	64	0	77	3	0
4	A	301	0	0	2	0
4	B	280	0	0	0	0
4	C	322	0	0	1	0
4	D	327	0	0	1	0
4	E	322	0	0	2	0
4	F	325	0	0	0	0
4	G	307	0	0	0	0
4	H	319	0	0	0	0
All	All	23779	0	20687	87	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 2.

All (87) 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:E:150:ARG:NH2	1:H:150:ARG:HD3	2.03	0.72
1:E:150:ARG:HH22	1:H:150:ARG:HD3	1.56	0.70
1:A:176:ARG:HD3	1:H:176:ARG:HG3	1.74	0.68
1:B:241:ARG:H	3:B:403:TYK:H6A2	1.63	0.62
1:C:186:GLN:HG2	1:C:214:TRP:HD1	1.65	0.62
1:D:150:ARG:HE	1:E:150:ARG:NH1	2.00	0.60
1:A:229:GLU:OE1	1:A:252:ARG:NH2	2.29	0.59
4:A:511:HOH:O	1:H:176:ARG:HD2	2.02	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:218:HIS:CE1	1:D:241:ARG:HD3	2.37	0.58
1:F:113:ASP:O	1:F:117:LYS:HG3	2.03	0.58
1:A:218:HIS:CE1	1:A:241:ARG:HD3	2.39	0.57
1:B:186:GLN:HG2	1:B:214:TRP:HD1	1.70	0.56
1:A:264:LYS:N	1:A:264:LYS:HD2	2.22	0.55
1:D:186:GLN:OE1	2:D:401:NAP:H2N	2.06	0.54
1:B:218:HIS:CE1	1:B:241:ARG:HD3	2.43	0.53
1:A:186:GLN:OE1	2:A:401:NAP:H2N	2.08	0.52
1:E:229:GLU:OE1	1:E:252:ARG:NH2	2.39	0.52
1:G:186:GLN:OE1	2:G:401:NAP:H2N	2.10	0.51
1:B:186:GLN:OE1	2:B:401:NAP:H2N	2.10	0.51
1:A:232:GLY:C	1:A:234:ASN:OD1	2.49	0.51
1:G:227:ARG:NH1	1:G:231:GLU:OE1	2.42	0.51
1:C:218:HIS:CE1	1:C:241:ARG:HD3	2.45	0.51
1:E:150:ARG:HH22	1:H:150:ARG:NH1	2.10	0.50
1:D:150:ARG:NE	1:E:150:ARG:NH1	2.60	0.50
1:B:240:GLY:HA2	3:B:403:TYK:H8A3	1.94	0.50
1:H:186:GLN:OE1	2:H:401:NAP:H2N	2.12	0.50
1:F:186:GLN:OE1	2:F:401:NAP:H2N	2.13	0.49
1:C:186:GLN:OE1	2:C:401:NAP:H2N	2.13	0.48
3:B:403:TYK:H222	3:B:403:TYK:HC3A	1.96	0.48
1:E:134:ARG:HG2	4:E:692:HOH:O	2.14	0.47
1:E:218:HIS:CE1	1:E:241:ARG:HD3	2.50	0.47
1:E:249:PRO:O	1:E:253:GLU:HG3	2.15	0.47
1:H:218:HIS:CE1	1:H:241:ARG:HD3	2.50	0.46
1:C:257:ARG:HD3	3:C:402:TYK:HC1C	1.97	0.46
1:H:228:LYS:O	1:H:231:GLU:HG3	2.16	0.46
1:E:186:GLN:OE1	2:E:401:NAP:H2N	2.15	0.46
3:A:402:TYK:H71	3:A:402:TYK:H4	1.79	0.45
1:E:257:ARG:HD2	4:E:609:HOH:O	2.16	0.45
1:A:261:LEU:HD13	3:A:402:TYK:H6C3	1.98	0.45
1:E:313:THR:O	1:E:317:GLU:HG3	2.16	0.45
1:G:243:ALA:O	1:G:247:LYS:HG2	2.17	0.45
3:B:403:TYK:H7A3	3:B:403:TYK:HC2A	1.68	0.45
1:D:92:LEU:HD12	1:D:93:ASP:N	2.32	0.44
1:F:260:ASP:O	1:F:264:LYS:HG2	2.16	0.44
3:C:402:TYK:H71	3:C:402:TYK:H4	1.81	0.44
1:F:92:LEU:HD23	1:F:92:LEU:HA	1.83	0.44
1:G:257:ARG:HD3	3:G:402:TYK:HC1C	1.99	0.44
1:C:326:PRO:HG3	1:D:161:ASN:O	2.18	0.43
1:A:230:GLN:OE1	4:A:501:HOH:O	2.21	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:326:PRO:HG3	1:H:161:ASN:O	2.17	0.43
1:C:151:GLN:OE1	1:C:153:LYS:HE3	2.18	0.43
1:C:244:ASP:O	1:C:247:LYS:HG2	2.19	0.43
1:C:12:LYS:HD2	1:G:98:PRO:HB3	2.01	0.42
1:D:57:GLU:HG2	4:D:704:HOH:O	2.19	0.42
1:H:239:SER:OG	1:H:240:GLY:N	2.52	0.42
1:A:262:LEU:CD1	1:A:269:PRO:HA	2.50	0.42
1:E:87:TYR:HB3	1:E:130:HIS:HB3	2.01	0.42
1:F:11:LEU:HD21	1:F:81:VAL:HG11	2.00	0.42
3:F:402:TYK:H71	3:F:402:TYK:H4	1.75	0.42
1:G:247:LYS:N	1:G:247:LYS:HD3	2.35	0.42
3:G:402:TYK:H22	3:G:402:TYK:H182	1.72	0.42
1:B:102:LYS:HB3	1:B:133:ASP:OD2	2.18	0.42
1:B:211:VAL:HB	1:B:283:VAL:HA	2.02	0.42
1:D:262:LEU:HD12	1:D:269:PRO:HA	2.02	0.42
3:B:403:TYK:H8	3:B:403:TYK:H21	2.01	0.42
1:E:124:ILE:O	1:E:154:ILE:HA	2.19	0.41
3:A:402:TYK:H22	3:A:402:TYK:H182	1.78	0.41
1:C:40:LEU:HD12	1:C:40:LEU:HA	1.93	0.41
1:G:11:LEU:HD21	1:G:81:VAL:HG11	2.01	0.41
1:A:243:ALA:O	1:A:247:LYS:HG3	2.19	0.41
1:A:150:ARG:NH1	1:C:150:ARG:HD2	2.36	0.41
1:A:176:ARG:HD3	1:H:176:ARG:CG	2.46	0.41
1:C:188:LEU:HB2	1:C:214:TRP:CZ2	2.56	0.41
1:G:128:GLN:HA	1:G:158:GLY:O	2.20	0.41
1:G:262:LEU:HD12	1:G:269:PRO:HA	2.02	0.41
1:F:102:LYS:HB3	1:F:133:ASP:OD2	2.19	0.41
3:F:402:TYK:H3	3:F:402:TYK:H6	1.92	0.41
1:G:289:GLY:O	2:G:401:NAP:H3B	2.21	0.40
1:A:244:ASP:HA	1:A:247:LYS:HE2	2.04	0.40
1:C:227:ARG:HD3	4:C:601:HOH:O	2.21	0.40
3:E:402:TYK:H14	3:E:402:TYK:H221	1.86	0.40
3:G:402:TYK:H4	3:G:402:TYK:H71	1.85	0.40
3:B:402:TYK:H71	3:B:402:TYK:H4	1.79	0.40
1:B:217:LEU:HD22	1:B:273:ALA:HB3	2.03	0.40
1:C:313:THR:O	1:C:317:GLU:HG3	2.22	0.40
1:D:97:TRP:CD2	1:D:98:PRO:HD2	2.57	0.40
1:E:161:ASN:O	1:G:326:PRO:HG3	2.21	0.40

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	326/351 (93%)	317 (97%)	8 (2%)	1 (0%)	41 32
1	B	329/351 (94%)	319 (97%)	9 (3%)	1 (0%)	41 32
1	C	329/351 (94%)	321 (98%)	7 (2%)	1 (0%)	41 32
1	D	329/351 (94%)	320 (97%)	8 (2%)	1 (0%)	41 32
1	E	329/351 (94%)	318 (97%)	10 (3%)	1 (0%)	41 32
1	F	329/351 (94%)	319 (97%)	9 (3%)	1 (0%)	41 32
1	G	329/351 (94%)	318 (97%)	10 (3%)	1 (0%)	41 32
1	H	329/351 (94%)	318 (97%)	10 (3%)	1 (0%)	41 32
All	All	2629/2808 (94%)	2550 (97%)	71 (3%)	8 (0%)	41 32

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	87	TYR
1	B	87	TYR
1	C	87	TYR
1	D	87	TYR
1	E	87	TYR
1	F	87	TYR
1	G	87	TYR
1	H	87	TYR

5.3.2 Protein sidechains [\(i\)](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	258/275 (94%)	258 (100%)	0	100	100
1	B	258/275 (94%)	256 (99%)	2 (1%)	81	78
1	C	258/275 (94%)	257 (100%)	1 (0%)	91	91
1	D	258/275 (94%)	257 (100%)	1 (0%)	91	91
1	E	258/275 (94%)	255 (99%)	3 (1%)	71	64
1	F	258/275 (94%)	257 (100%)	1 (0%)	91	91
1	G	258/275 (94%)	258 (100%)	0	100	100
1	H	258/275 (94%)	255 (99%)	3 (1%)	71	64
All	All	2064/2200 (94%)	2053 (100%)	11 (0%)	88	88

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	150	ARG
1	B	212	ILE
1	C	212	ILE
1	D	316	ASP
1	E	150	ARG
1	E	239	SER
1	E	257	ARG
1	F	92	LEU
1	H	250	GLN
1	H	316	ASP
1	H	317	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [\(i\)](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [\(i\)](#)

15 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	TYK	A	402	-	67,67,67	0.78	1 (1%)	83,97,97	1.41	13 (15%)
3	TYK	E	402	-	67,67,67	0.73	1 (1%)	83,97,97	1.27	7 (8%)
2	NAP	A	401	-	45,52,52	2.28	11 (24%)	56,80,80	1.30	5 (8%)
2	NAP	G	401	-	45,52,52	2.20	13 (28%)	56,80,80	1.27	6 (10%)
2	NAP	D	401	-	45,52,52	2.23	10 (22%)	56,80,80	1.25	7 (12%)
2	NAP	B	401	-	45,52,52	2.26	11 (24%)	56,80,80	1.40	6 (10%)
2	NAP	H	401	-	45,52,52	2.26	12 (26%)	56,80,80	1.31	6 (10%)
3	TYK	C	402	-	67,67,67	0.78	2 (2%)	83,97,97	1.37	10 (12%)
2	NAP	F	401	-	45,52,52	2.19	11 (24%)	56,80,80	1.38	7 (12%)
3	TYK	G	402	-	67,67,67	0.84	2 (2%)	83,97,97	1.36	12 (14%)
3	TYK	B	402	-	67,67,67	0.81	3 (4%)	83,97,97	1.45	14 (16%)
2	NAP	E	401	-	45,52,52	2.27	11 (24%)	56,80,80	1.29	6 (10%)
3	TYK	B	403	-	67,67,67	0.77	1 (1%)	83,97,97	2.04	22 (26%)
2	NAP	C	401	-	45,52,52	2.17	12 (26%)	56,80,80	1.35	7 (12%)
3	TYK	F	402	-	67,67,67	0.87	3 (4%)	83,97,97	1.66	13 (15%)

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	TYK	A	402	-	-	7/67/126/126	0/3/4/4

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	TYK	E	402	-	-	6/67/126/126	0/3/4/4
2	NAP	A	401	-	-	2/31/67/67	0/5/5/5
2	NAP	G	401	-	-	2/31/67/67	0/5/5/5
2	NAP	D	401	-	-	1/31/67/67	0/5/5/5
2	NAP	B	401	-	-	3/31/67/67	0/5/5/5
2	NAP	H	401	-	-	2/31/67/67	0/5/5/5
3	TYK	C	402	-	-	12/67/126/126	0/3/4/4
2	NAP	F	401	-	-	2/31/67/67	0/5/5/5
3	TYK	G	402	-	-	7/67/126/126	0/3/4/4
3	TYK	B	402	-	-	10/67/126/126	0/3/4/4
2	NAP	E	401	-	-	2/31/67/67	0/5/5/5
3	TYK	B	403	-	-	34/67/126/126	0/3/4/4
2	NAP	C	401	-	-	2/31/67/67	0/5/5/5
3	TYK	F	402	-	-	15/67/126/126	0/3/4/4

All (104) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	NAP	O4D-C1D	7.41	1.51	1.41
2	C	401	NAP	O4B-C1B	7.09	1.51	1.41
2	H	401	NAP	O4D-C1D	7.04	1.50	1.41
2	D	401	NAP	O4D-C1D	6.94	1.50	1.41
2	G	401	NAP	O4B-C1B	6.94	1.50	1.41
2	A	401	NAP	O4D-C1D	6.88	1.50	1.41
2	D	401	NAP	O4B-C1B	6.87	1.50	1.41
2	F	401	NAP	O4D-C1D	6.86	1.50	1.41
2	A	401	NAP	O4B-C1B	6.75	1.50	1.41
2	E	401	NAP	O4B-C1B	6.74	1.50	1.41
2	E	401	NAP	O4D-C1D	6.64	1.50	1.41
2	H	401	NAP	C7N-N7N	6.54	1.45	1.33
2	A	401	NAP	C7N-N7N	6.49	1.45	1.33
2	B	401	NAP	O4B-C1B	6.45	1.50	1.41
2	C	401	NAP	O4D-C1D	6.37	1.50	1.41
2	G	401	NAP	O4D-C1D	6.36	1.50	1.41
2	F	401	NAP	O4B-C1B	6.32	1.49	1.41
2	E	401	NAP	C7N-N7N	6.26	1.44	1.33
2	H	401	NAP	O4B-C1B	6.20	1.49	1.41
2	B	401	NAP	C7N-N7N	6.14	1.44	1.33
2	G	401	NAP	C7N-N7N	6.13	1.44	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	401	NAP	C7N-N7N	5.98	1.44	1.33
2	D	401	NAP	C7N-N7N	5.86	1.44	1.33
2	C	401	NAP	C7N-N7N	5.74	1.43	1.33
3	B	403	TYK	O15-C1	4.17	1.46	1.34
3	E	402	TYK	O15-C1	3.93	1.45	1.34
2	E	401	NAP	P2B-O2B	3.86	1.66	1.59
3	A	402	TYK	O15-C1	3.81	1.45	1.34
3	B	402	TYK	O15-C1	3.75	1.44	1.34
3	G	402	TYK	O15-C1	3.73	1.44	1.34
3	C	402	TYK	O15-C1	3.66	1.44	1.34
2	H	401	NAP	P2B-O2B	3.61	1.66	1.59
2	D	401	NAP	P2B-O2B	3.53	1.66	1.59
3	F	402	TYK	O15-C1	3.43	1.44	1.34
2	B	401	NAP	P2B-O2B	3.39	1.65	1.59
2	F	401	NAP	P2B-O2B	3.31	1.65	1.59
2	A	401	NAP	P2B-O2B	3.29	1.65	1.59
2	E	401	NAP	O4D-C4D	3.28	1.52	1.45
2	A	401	NAP	C2D-C1D	-3.18	1.48	1.53
2	B	401	NAP	C2D-C1D	-3.17	1.48	1.53
2	G	401	NAP	C6A-N6A	3.12	1.45	1.34
2	A	401	NAP	C6A-N6A	3.07	1.45	1.34
2	C	401	NAP	C6A-N6A	3.03	1.45	1.34
2	B	401	NAP	C3B-C2B	-2.99	1.46	1.52
2	E	401	NAP	C6A-N6A	2.99	1.44	1.34
3	F	402	TYK	O15-C15	-2.98	1.41	1.46
2	H	401	NAP	C6A-N6A	2.98	1.44	1.34
2	B	401	NAP	C6A-N6A	2.94	1.44	1.34
2	F	401	NAP	C6A-N6A	2.93	1.44	1.34
2	D	401	NAP	C6A-N6A	2.93	1.44	1.34
2	H	401	NAP	O4D-C4D	2.90	1.51	1.45
2	E	401	NAP	C2D-C1D	-2.90	1.49	1.53
2	E	401	NAP	C3B-C2B	-2.87	1.46	1.52
2	G	401	NAP	C2D-C1D	-2.87	1.49	1.53
2	F	401	NAP	C2D-C1D	-2.77	1.49	1.53
2	A	401	NAP	C3B-C2B	-2.73	1.46	1.52
2	D	401	NAP	O7N-C7N	-2.73	1.18	1.24
2	B	401	NAP	O4D-C4D	2.70	1.51	1.45
2	A	401	NAP	O4D-C4D	2.70	1.51	1.45
2	C	401	NAP	O4B-C4B	2.69	1.51	1.45
2	F	401	NAP	O4D-C4D	2.65	1.50	1.45
2	G	401	NAP	O4D-C4D	2.65	1.50	1.45
2	D	401	NAP	C2D-C1D	-2.63	1.49	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	401	NAP	O4D-C4D	2.63	1.50	1.45
2	H	401	NAP	C2D-C1D	-2.62	1.49	1.53
2	C	401	NAP	O7N-C7N	-2.59	1.19	1.24
2	G	401	NAP	C3B-C2B	-2.58	1.47	1.52
2	D	401	NAP	C3B-C2B	-2.55	1.47	1.52
2	C	401	NAP	P2B-O2B	2.54	1.64	1.59
2	H	401	NAP	C3B-C2B	-2.52	1.47	1.52
2	A	401	NAP	O4B-C4B	2.52	1.50	1.45
3	G	402	TYK	O1C-C1C	2.51	1.44	1.40
3	F	402	TYK	O1C-C1C	2.49	1.44	1.40
2	B	401	NAP	O4B-C4B	2.48	1.50	1.45
2	A	401	NAP	C2D-C3D	-2.48	1.46	1.53
2	G	401	NAP	C2D-C3D	-2.45	1.46	1.53
2	E	401	NAP	C2D-C3D	-2.44	1.46	1.53
2	F	401	NAP	C3B-C2B	-2.44	1.47	1.52
3	B	402	TYK	O1C-C1C	2.42	1.44	1.40
2	C	401	NAP	C2D-C3D	-2.42	1.46	1.53
2	E	401	NAP	O7N-C7N	-2.42	1.19	1.24
2	F	401	NAP	C2D-C3D	-2.39	1.46	1.53
2	C	401	NAP	C3B-C2B	-2.39	1.47	1.52
2	B	401	NAP	C2D-C3D	-2.37	1.46	1.53
3	B	402	TYK	O15-C15	-2.36	1.42	1.46
3	C	402	TYK	O15-C15	-2.35	1.42	1.46
2	H	401	NAP	O4B-C4B	2.34	1.50	1.45
2	H	401	NAP	C3N-C7N	2.32	1.54	1.50
2	E	401	NAP	O4B-C4B	2.31	1.50	1.45
2	G	401	NAP	P2B-O2B	2.31	1.63	1.59
2	C	401	NAP	C2D-C1D	-2.31	1.50	1.53
2	D	401	NAP	C2D-C3D	-2.30	1.47	1.53
2	C	401	NAP	O4D-C4D	2.23	1.50	1.45
2	G	401	NAP	O4B-C4B	2.19	1.49	1.45
2	G	401	NAP	O7N-C7N	-2.17	1.20	1.24
2	G	401	NAP	C3D-C4D	-2.12	1.47	1.53
2	F	401	NAP	O4B-C4B	2.10	1.49	1.45
2	F	401	NAP	C4A-N3A	-2.10	1.32	1.35
2	C	401	NAP	C4A-N3A	-2.08	1.32	1.35
2	H	401	NAP	O7N-C7N	-2.08	1.20	1.24
2	B	401	NAP	C4A-N3A	-2.07	1.32	1.35
2	A	401	NAP	O7N-C7N	-2.06	1.20	1.24
2	G	401	NAP	C3N-C7N	2.05	1.53	1.50
2	H	401	NAP	C2D-C3D	-2.04	1.47	1.53

All (141) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	402	TYK	C10-C11-C12	-8.08	114.02	126.23
3	B	403	TYK	C10-C11-C12	6.55	136.13	126.23
3	B	403	TYK	O15-C1-C2	5.43	121.44	111.46
3	A	402	TYK	O15-C1-C2	5.00	120.64	111.46
3	F	402	TYK	C15-O15-C1	-4.84	108.42	117.83
3	E	402	TYK	C10-C11-C12	-4.73	119.08	126.23
3	B	403	TYK	C11-C12-C13	4.46	134.07	119.42
2	F	401	NAP	C6N-N1N-C2N	-4.45	117.91	121.97
2	B	401	NAP	C4A-C5A-N7A	-4.32	104.89	109.40
3	G	402	TYK	O15-C1-C2	4.24	119.26	111.46
2	C	401	NAP	C4A-C5A-N7A	-4.24	104.98	109.40
2	A	401	NAP	C4A-C5A-N7A	-4.24	104.98	109.40
3	B	402	TYK	O1C-C1C-C2C	4.14	116.20	108.22
3	G	402	TYK	O1C-C1C-C2C	4.01	115.95	108.22
2	F	401	NAP	C4A-C5A-N7A	-4.00	105.23	109.40
3	E	402	TYK	O15-C1-C2	3.99	118.79	111.46
3	B	403	TYK	O5A-C1A-C2A	-3.96	101.96	110.35
3	B	403	TYK	C21-C8-C9	-3.91	103.43	110.20
3	C	402	TYK	O15-C1-C2	3.91	118.64	111.46
2	H	401	NAP	C4A-C5A-N7A	-3.91	105.33	109.40
3	C	402	TYK	C6-C5-C4	-3.89	104.89	114.14
2	A	401	NAP	C6N-N1N-C2N	-3.88	118.44	121.97
2	E	401	NAP	N3A-C2A-N1A	-3.85	122.66	128.68
3	C	402	TYK	C10-C11-C12	-3.80	120.49	126.23
3	F	402	TYK	O15-C1-C2	3.73	118.31	111.46
2	C	401	NAP	N3A-C2A-N1A	-3.73	122.86	128.68
3	B	403	TYK	C1A-O5A-C5A	-3.71	107.30	113.67
2	B	401	NAP	C6N-N1N-C2N	-3.70	118.60	121.97
2	E	401	NAP	C6N-N1N-C2N	-3.70	118.60	121.97
2	B	401	NAP	N3A-C2A-N1A	-3.68	122.93	128.68
2	B	401	NAP	C3D-C2D-C1D	3.67	106.51	100.98
2	D	401	NAP	C4A-C5A-N7A	-3.67	105.57	109.40
2	E	401	NAP	C4A-C5A-N7A	-3.64	105.61	109.40
2	D	401	NAP	N3A-C2A-N1A	-3.62	123.02	128.68
2	G	401	NAP	C4A-C5A-N7A	-3.59	105.65	109.40
3	B	403	TYK	C8-C9-C10	3.57	127.27	118.29
2	F	401	NAP	N3A-C2A-N1A	-3.57	123.10	128.68
3	B	403	TYK	C3-C2-C1	-3.57	106.27	114.07
3	B	403	TYK	C3-C4-C5	3.56	121.53	111.19
2	G	401	NAP	N3A-C2A-N1A	-3.55	123.13	128.68
2	H	401	NAP	N3A-C2A-N1A	-3.54	123.14	128.68
2	G	401	NAP	C1B-N9A-C4A	-3.54	120.42	126.64
3	E	402	TYK	O1A-C5-C4	3.54	112.49	108.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	402	TYK	C6-C5-C4	-3.50	105.80	114.14
2	H	401	NAP	C3D-C2D-C1D	3.49	106.23	100.98
2	E	401	NAP	C3D-C2D-C1D	3.47	106.21	100.98
3	B	403	TYK	C22-C12-C13	-3.44	112.33	123.07
2	D	401	NAP	C6N-N1N-C2N	-3.44	118.83	121.97
3	B	403	TYK	O1A-C5-C4	3.42	112.34	108.22
2	H	401	NAP	C6N-N1N-C2N	-3.41	118.86	121.97
2	A	401	NAP	N3A-C2A-N1A	-3.41	123.35	128.68
2	F	401	NAP	C1B-N9A-C4A	-3.39	120.68	126.64
3	F	402	TYK	O1C-C1C-C2C	3.39	114.76	108.22
2	H	401	NAP	C1B-N9A-C4A	-3.35	120.75	126.64
2	C	401	NAP	C3D-C2D-C1D	3.34	106.01	100.98
2	G	401	NAP	C6N-N1N-C2N	-3.34	118.93	121.97
3	B	402	TYK	C3C-C4C-C5C	3.27	117.21	110.12
3	B	402	TYK	C10-C11-C12	-3.25	121.32	126.23
2	A	401	NAP	C3D-C2D-C1D	3.24	105.86	100.98
2	B	401	NAP	C1B-N9A-C4A	-3.21	121.00	126.64
3	F	402	TYK	C18-C4-C5	3.16	117.08	111.40
3	B	402	TYK	C18-C4-C3	-3.15	106.23	111.17
3	A	402	TYK	C10-C11-C12	-3.14	121.49	126.23
3	F	402	TYK	C11-C12-C13	3.13	129.70	119.42
3	B	402	TYK	O15-C1-C2	3.13	117.20	111.46
3	G	402	TYK	C18-C4-C3	-3.12	106.29	111.17
2	E	401	NAP	C1B-N9A-C4A	-3.11	121.17	126.64
3	G	402	TYK	C10-C11-C12	-3.09	121.57	126.23
2	C	401	NAP	C6N-N1N-C2N	-3.07	119.18	121.97
2	D	401	NAP	C1B-N9A-C4A	-3.05	121.28	126.64
2	F	401	NAP	C3D-C2D-C1D	3.05	105.57	100.98
3	B	403	TYK	O5A-C5A-C4A	3.03	114.78	109.13
3	A	402	TYK	C6-C5-C4	-3.00	107.00	114.14
2	G	401	NAP	C3D-C2D-C1D	2.97	105.45	100.98
3	B	403	TYK	O1A-C1A-C2A	2.96	115.77	108.10
3	B	402	TYK	C18-C4-C5	2.92	116.64	111.40
2	C	401	NAP	C1B-N9A-C4A	-2.91	121.53	126.64
3	E	402	TYK	C6-C5-C4	-2.91	107.22	114.14
3	A	402	TYK	O1A-C5-C4	2.88	111.69	108.22
3	G	402	TYK	C1C-O5C-C5C	-2.87	108.73	113.67
3	B	403	TYK	C22-C12-C11	-2.87	113.55	118.08
3	A	402	TYK	C4C-C3C-C2C	2.82	118.11	111.66
2	D	401	NAP	C3D-C2D-C1D	2.80	105.20	100.98
3	A	402	TYK	C18-C4-C3	-2.80	106.79	111.17
3	B	402	TYK	C1C-O5C-C5C	-2.79	108.88	113.67

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	402	TYK	C18-C4-C3	-2.75	106.86	111.17
3	G	402	TYK	C18-C4-C5	2.75	116.33	111.40
3	B	402	TYK	C6-C5-C4	-2.73	107.64	114.14
2	G	401	NAP	O2B-C2B-C1B	-2.71	100.34	110.10
3	C	402	TYK	C18-C4-C3	-2.70	106.94	111.17
3	B	403	TYK	O3-C3-C2	-2.69	103.08	109.56
3	A	402	TYK	C18-C4-C5	2.69	116.22	111.40
2	H	401	NAP	O2B-C2B-C1B	-2.67	100.50	110.10
3	B	403	TYK	C15-O15-C1	-2.67	112.64	117.83
3	B	402	TYK	O5C-C1C-C2C	-2.64	104.27	109.51
3	C	402	TYK	C1A-O5A-C5A	-2.64	109.14	113.67
3	B	402	TYK	O1A-C5-C4	2.62	111.38	108.22
3	A	402	TYK	C1A-O5A-C5A	-2.61	109.17	113.67
3	G	402	TYK	C1A-O5A-C5A	-2.60	109.20	113.67
3	E	402	TYK	C18-C4-C5	2.52	115.92	111.40
3	A	402	TYK	C15-O15-C1	-2.51	112.94	117.83
3	A	402	TYK	O15-C15-C14	2.51	112.93	107.42
3	E	402	TYK	C18-C4-C3	-2.51	107.25	111.17
3	G	402	TYK	C6-C5-C4	-2.49	108.20	114.14
3	C	402	TYK	C18-C4-C5	2.48	115.85	111.40
3	B	402	TYK	C1A-O5A-C5A	-2.45	109.46	113.67
3	B	403	TYK	C18-C4-C5	-2.44	107.02	111.40
3	C	402	TYK	O15-C15-C14	2.43	112.74	107.42
3	E	402	TYK	C1A-O5A-C5A	-2.41	109.53	113.67
3	A	402	TYK	O15-C1-O1	-2.41	117.89	123.70
3	C	402	TYK	C15-O15-C1	-2.40	113.15	117.83
2	C	401	NAP	O7N-C7N-C3N	2.40	122.51	119.63
3	B	403	TYK	O1-C1-C2	-2.40	119.44	124.73
3	F	402	TYK	C22-C12-C13	-2.39	115.61	123.07
3	C	402	TYK	O15-C15-C16	-2.38	103.12	106.92
2	A	401	NAP	C1B-N9A-C4A	-2.36	122.50	126.64
3	G	402	TYK	O15-C15-C14	2.36	112.59	107.42
2	C	401	NAP	O2B-C2B-C1B	-2.34	101.68	110.10
3	B	403	TYK	O9-C9-C8	-2.32	116.93	121.25
2	D	401	NAP	C3N-C7N-N7N	2.30	120.52	117.75
2	D	401	NAP	O7N-C7N-N7N	-2.30	119.31	122.58
2	F	401	NAP	C2N-C3N-C4N	2.28	120.85	118.26
3	B	403	TYK	O4A-C1B-C2B	2.24	112.88	109.01
2	E	401	NAP	O2B-C2B-C1B	-2.24	102.05	110.10
3	B	403	TYK	C1A-C2A-C3A	-2.24	105.57	109.24
3	B	402	TYK	C15-O15-C1	-2.20	113.54	117.83
3	A	402	TYK	O1C-C1C-C2C	2.18	112.42	108.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	402	TYK	O5C-C5C-C4C	-2.17	105.63	109.52
3	F	402	TYK	C22-C12-C11	-2.15	114.69	118.08
3	F	402	TYK	C3-C2-C1	-2.13	109.41	114.07
3	B	402	TYK	C4C-C3C-C2C	2.12	116.50	111.66
3	G	402	TYK	C3C-C4C-C5C	2.07	114.62	110.12
3	B	402	TYK	O5C-C5C-C6C	2.07	111.17	106.70
3	F	402	TYK	C1A-O1A-C5	-2.06	112.86	117.96
3	A	402	TYK	O20-C20-C19	-2.06	119.44	125.43
3	G	402	TYK	O15-C1-O1	-2.04	118.76	123.70
3	F	402	TYK	C1A-O5A-C5A	-2.04	110.16	113.67
3	G	402	TYK	O1A-C5-C4	2.04	110.68	108.22
2	B	401	NAP	C2N-C3N-C4N	2.03	120.56	118.26
2	F	401	NAP	O2B-C2B-C1B	-2.03	102.80	110.10
3	B	403	TYK	O15-C15-C16	2.01	110.13	106.92

There are no chirality outliers.

All (107) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	NAP	O4D-C1D-N1N-C6N
2	B	401	NAP	O4D-C1D-N1N-C6N
2	C	401	NAP	O4D-C1D-N1N-C6N
2	E	401	NAP	O4D-C1D-N1N-C6N
2	F	401	NAP	O4D-C1D-N1N-C6N
2	G	401	NAP	O4D-C1D-N1N-C6N
2	H	401	NAP	O4D-C1D-N1N-C6N
3	A	402	TYK	C10-C11-C12-C13
3	A	402	TYK	C10-C11-C12-C22
3	A	402	TYK	C14-C15-C16-C17
3	A	402	TYK	O15-C15-C16-C17
3	A	402	TYK	C2C-C1C-O1C-C23
3	A	402	TYK	O5C-C1C-O1C-C23
3	B	402	TYK	C10-C11-C12-C13
3	B	402	TYK	C10-C11-C12-C22
3	B	402	TYK	C14-C15-C16-C17
3	B	402	TYK	O15-C15-C16-C17
3	B	402	TYK	C2C-C1C-O1C-C23
3	B	402	TYK	O5C-C1C-O1C-C23
3	B	403	TYK	C20-C19-C6-C7
3	B	403	TYK	C2-C1-O15-C15
3	B	403	TYK	C2-C3-C4-C5
3	B	403	TYK	C2-C3-C4-C18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	B	403	TYK	C3-C4-C5-C6
3	B	403	TYK	C3-C4-C5-O1A
3	B	403	TYK	C18-C4-C5-C6
3	B	403	TYK	C18-C4-C5-O1A
3	B	403	TYK	C4-C5-C6-C19
3	B	403	TYK	C4-C5-C6-C7
3	B	403	TYK	O1A-C5-C6-C19
3	B	403	TYK	O1A-C5-C6-C7
3	B	403	TYK	C4-C5-O1A-C1A
3	B	403	TYK	C11-C10-C9-C8
3	B	403	TYK	C11-C10-C9-O9
3	B	403	TYK	C12-C13-C14-C23
3	B	403	TYK	C14-C15-C16-C17
3	B	403	TYK	O15-C15-C16-C17
3	B	403	TYK	C2B-C1B-O4A-C4A
3	B	403	TYK	O5B-C1B-O4A-C4A
3	C	402	TYK	C10-C11-C12-C13
3	C	402	TYK	C10-C11-C12-C22
3	C	402	TYK	C15-C14-C23-O1C
3	C	402	TYK	C14-C15-C16-C17
3	C	402	TYK	O15-C15-C16-C17
3	C	402	TYK	C2C-C1C-O1C-C23
3	C	402	TYK	O5C-C1C-O1C-C23
3	F	402	TYK	C12-C13-C14-C23
3	F	402	TYK	C13-C14-C15-C16
3	F	402	TYK	C13-C14-C15-O15
3	F	402	TYK	C23-C14-C15-C16
3	F	402	TYK	C23-C14-C15-O15
3	F	402	TYK	C13-C14-C23-O1C
3	F	402	TYK	C15-C14-C23-O1C
3	F	402	TYK	C14-C15-C16-C17
3	F	402	TYK	O15-C15-C16-C17
3	F	402	TYK	C14-C23-O1C-C1C
3	F	402	TYK	C2C-C1C-O1C-C23
3	F	402	TYK	O5C-C1C-O1C-C23
3	G	402	TYK	O15-C15-C16-C17
3	G	402	TYK	C2C-C1C-O1C-C23
3	G	402	TYK	O5C-C1C-O1C-C23
3	B	403	TYK	O1-C1-O15-C15
3	E	402	TYK	C2C-C1C-O1C-C23
3	B	403	TYK	O3-C3-C4-C18
3	B	403	TYK	C5-C6-C7-C8

Continued on next page...

Continued from previous page...

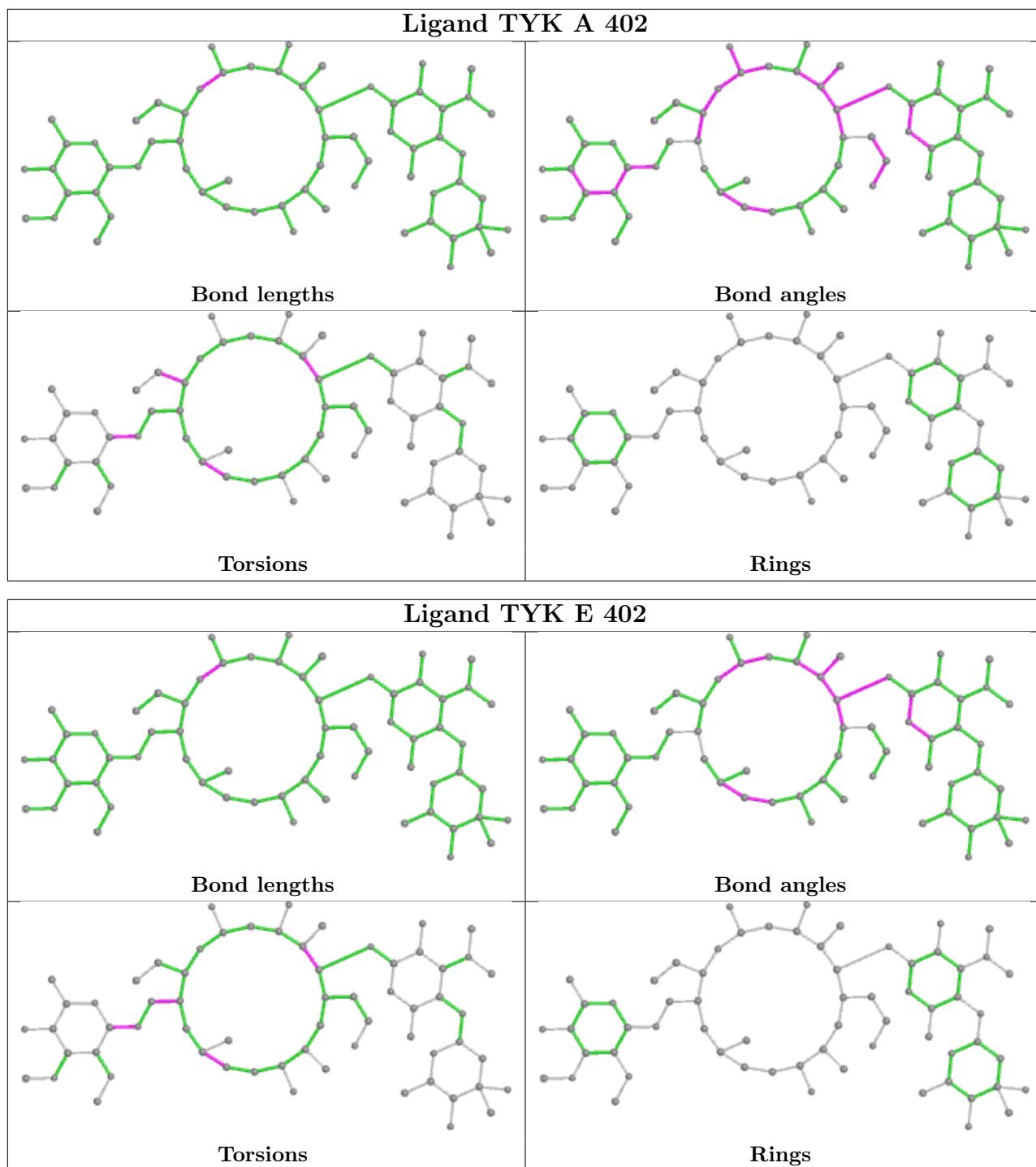
Mol	Chain	Res	Type	Atoms
3	B	403	TYK	C10-C11-C12-C22
3	B	403	TYK	C10-C11-C12-C13
3	B	403	TYK	C1-C2-C3-C4
3	B	403	TYK	C6-C19-C20-O20
3	E	402	TYK	C15-C14-C23-O1C
2	A	401	NAP	PN-O3-PA-O5B
2	B	401	NAP	PN-O3-PA-O5B
2	C	401	NAP	PN-O3-PA-O5B
2	D	401	NAP	PN-O3-PA-O5B
2	E	401	NAP	PN-O3-PA-O5B
2	F	401	NAP	PN-O3-PA-O5B
2	G	401	NAP	PN-O3-PA-O5B
2	H	401	NAP	PN-O3-PA-O5B
3	B	402	TYK	C20-C19-C6-C7
3	F	402	TYK	C20-C19-C6-C7
3	C	402	TYK	C18-C4-C5-C6
3	B	403	TYK	C19-C6-C7-C8
3	G	402	TYK	C14-C15-C16-C17
3	B	403	TYK	C13-C14-C15-C16
3	E	402	TYK	C13-C14-C23-O1C
3	B	402	TYK	C14-C23-O1C-C1C
3	C	402	TYK	C14-C23-O1C-C1C
3	G	402	TYK	C14-C23-O1C-C1C
3	E	402	TYK	C18-C4-C5-C6
3	B	403	TYK	O3-C3-C4-C5
3	B	403	TYK	C13-C14-C15-O15
3	E	402	TYK	C10-C11-C12-C13
3	A	402	TYK	C18-C4-C5-C6
3	E	402	TYK	C10-C11-C12-C22
3	C	402	TYK	C6-C19-C20-O20
3	G	402	TYK	C15-C14-C23-O1C
3	B	402	TYK	C18-C4-C5-C6
3	G	402	TYK	C18-C4-C5-C6
3	F	402	TYK	C18-C4-C5-C6
3	B	402	TYK	C20-C19-C6-C5
3	B	403	TYK	C20-C19-C6-C5
2	B	401	NAP	C2B-O2B-P2B-O2X
3	B	403	TYK	C1-C2-C3-O3
3	B	403	TYK	C22-C12-C13-C14
3	F	402	TYK	C22-C12-C13-C14
3	C	402	TYK	C2C-C3C-O3C-C8C
3	C	402	TYK	C13-C14-C23-O1C

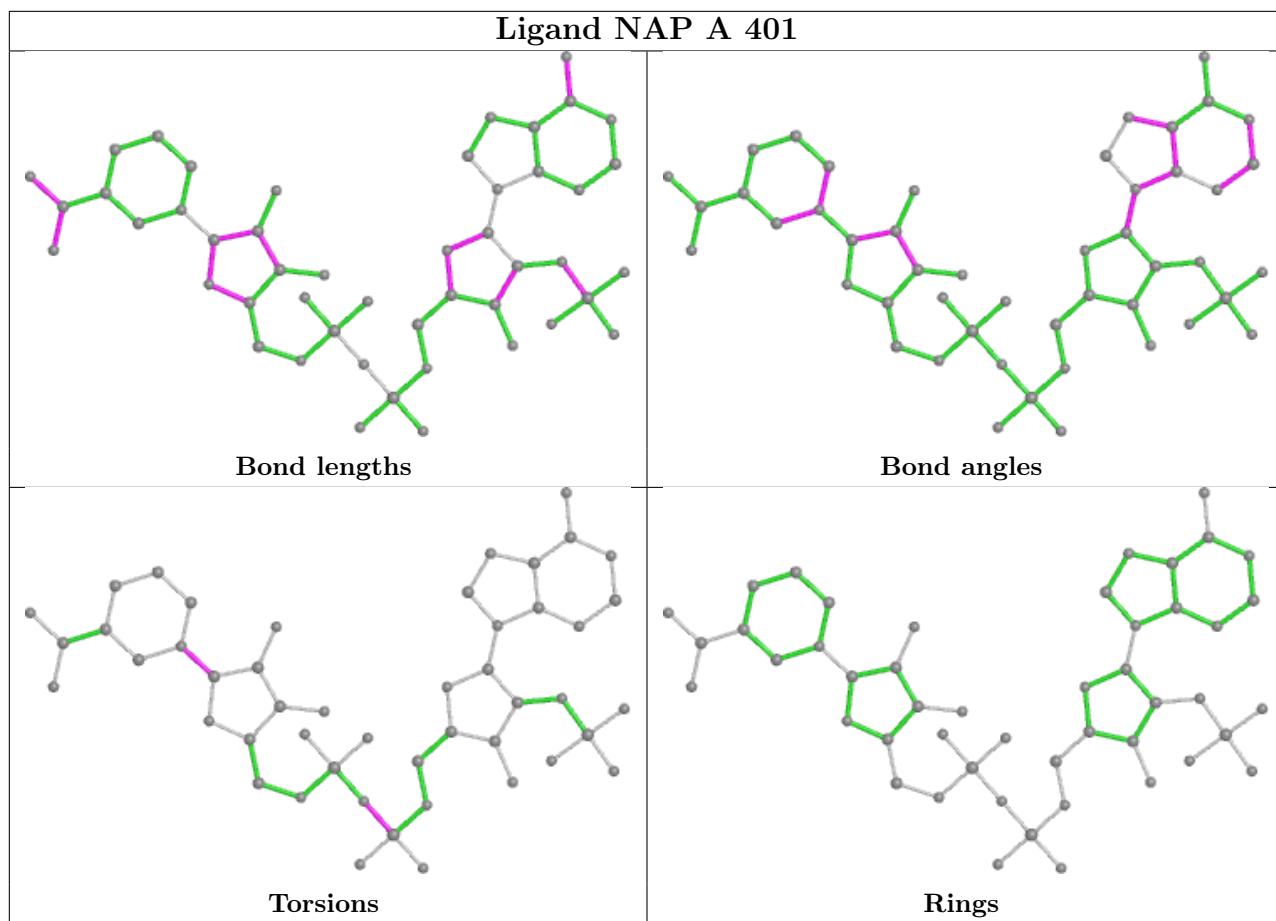
There are no ring outliers.

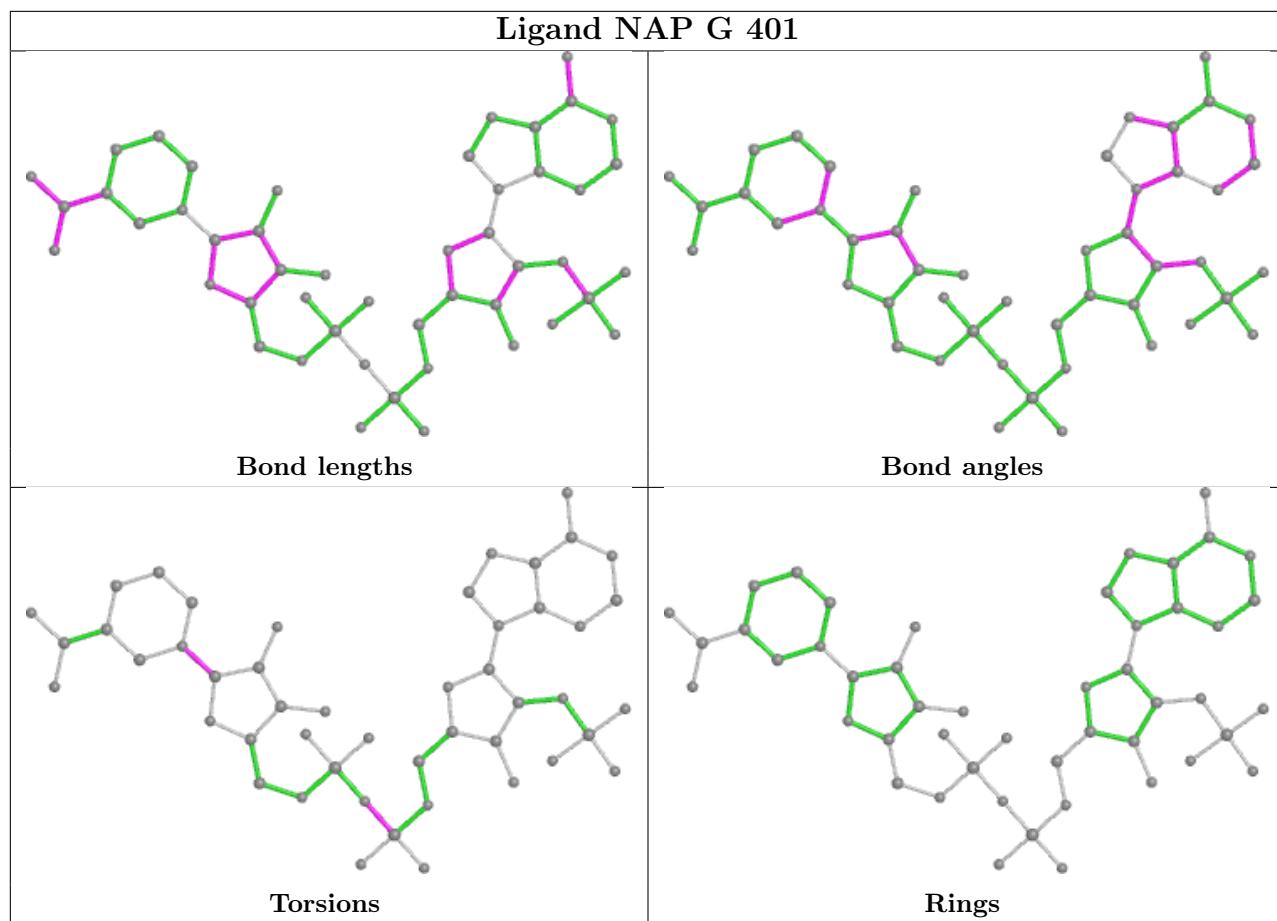
15 monomers are involved in 26 short contacts:

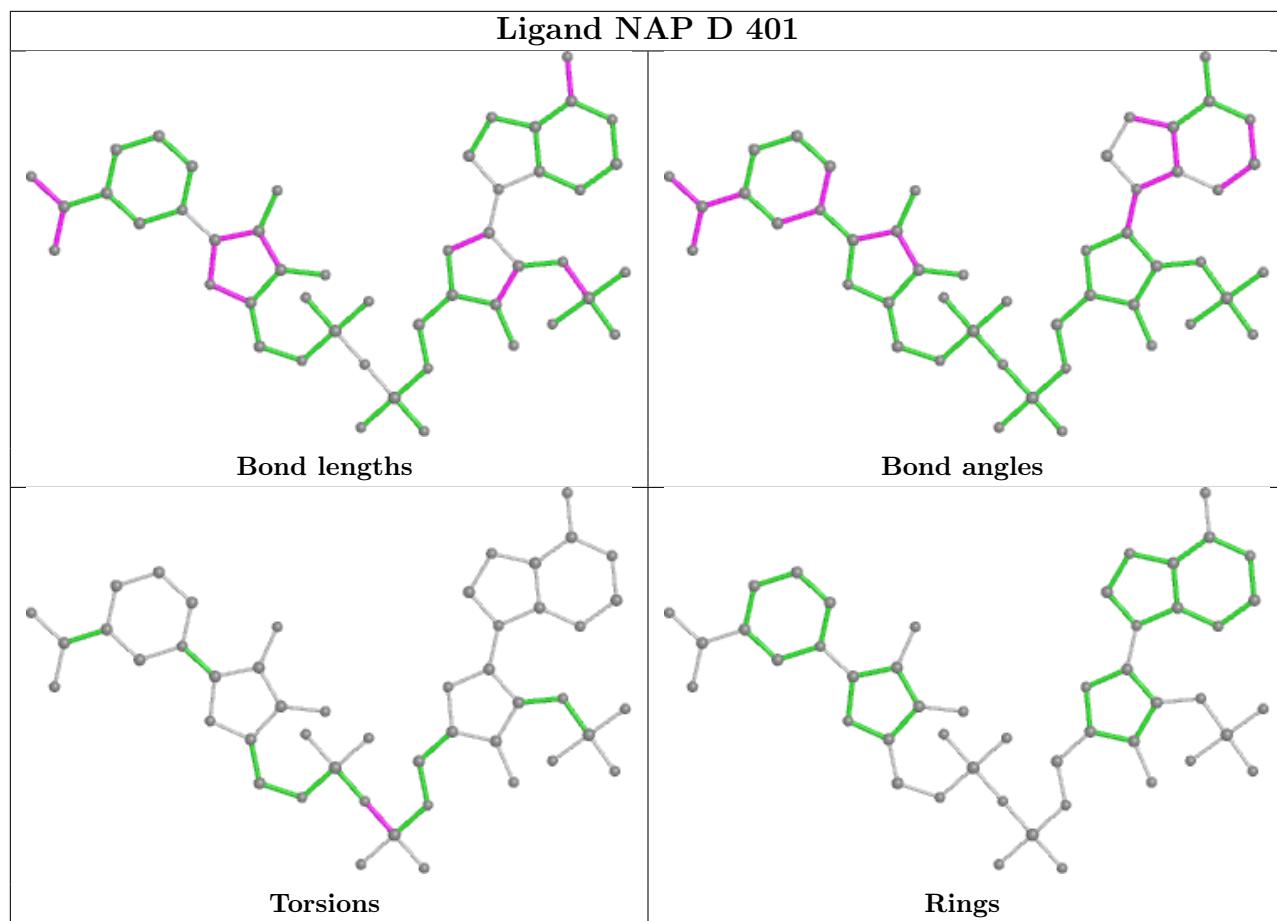
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	402	TYK	3	0
3	E	402	TYK	1	0
2	A	401	NAP	1	0
2	G	401	NAP	2	0
2	D	401	NAP	1	0
2	B	401	NAP	1	0
2	H	401	NAP	1	0
3	C	402	TYK	2	0
2	F	401	NAP	1	0
3	G	402	TYK	3	0
3	B	402	TYK	1	0
2	E	401	NAP	1	0
3	B	403	TYK	5	0
2	C	401	NAP	1	0
3	F	402	TYK	2	0

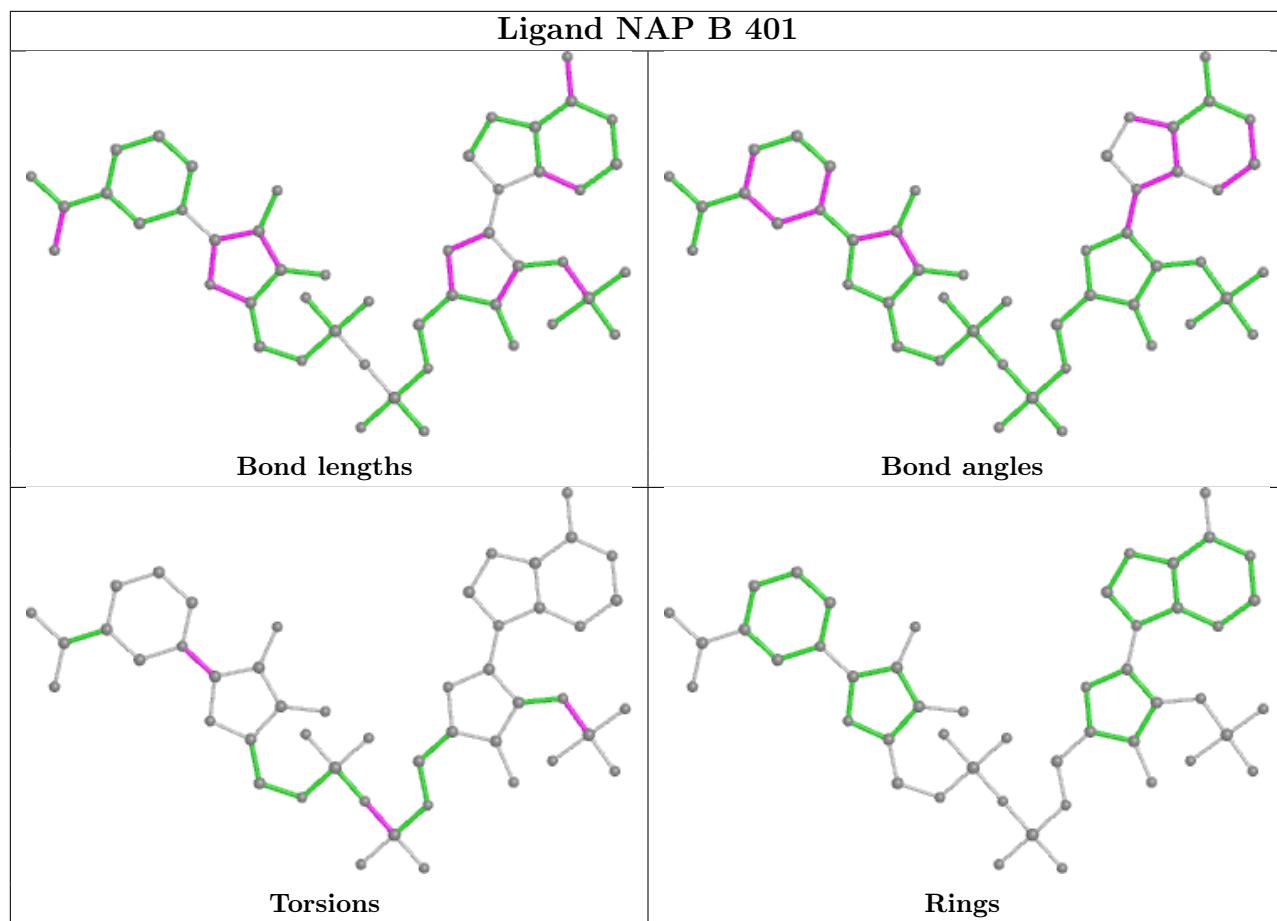
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

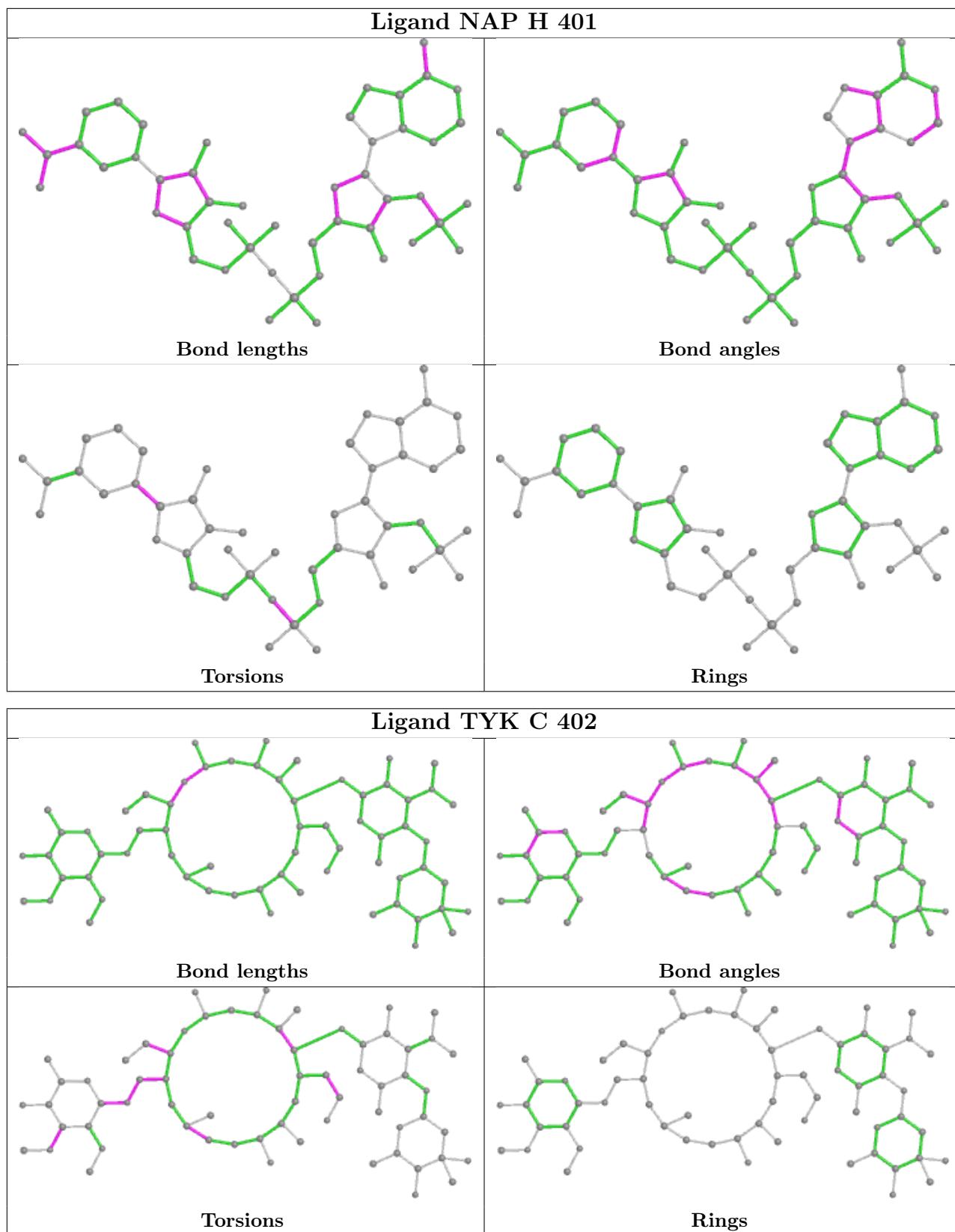


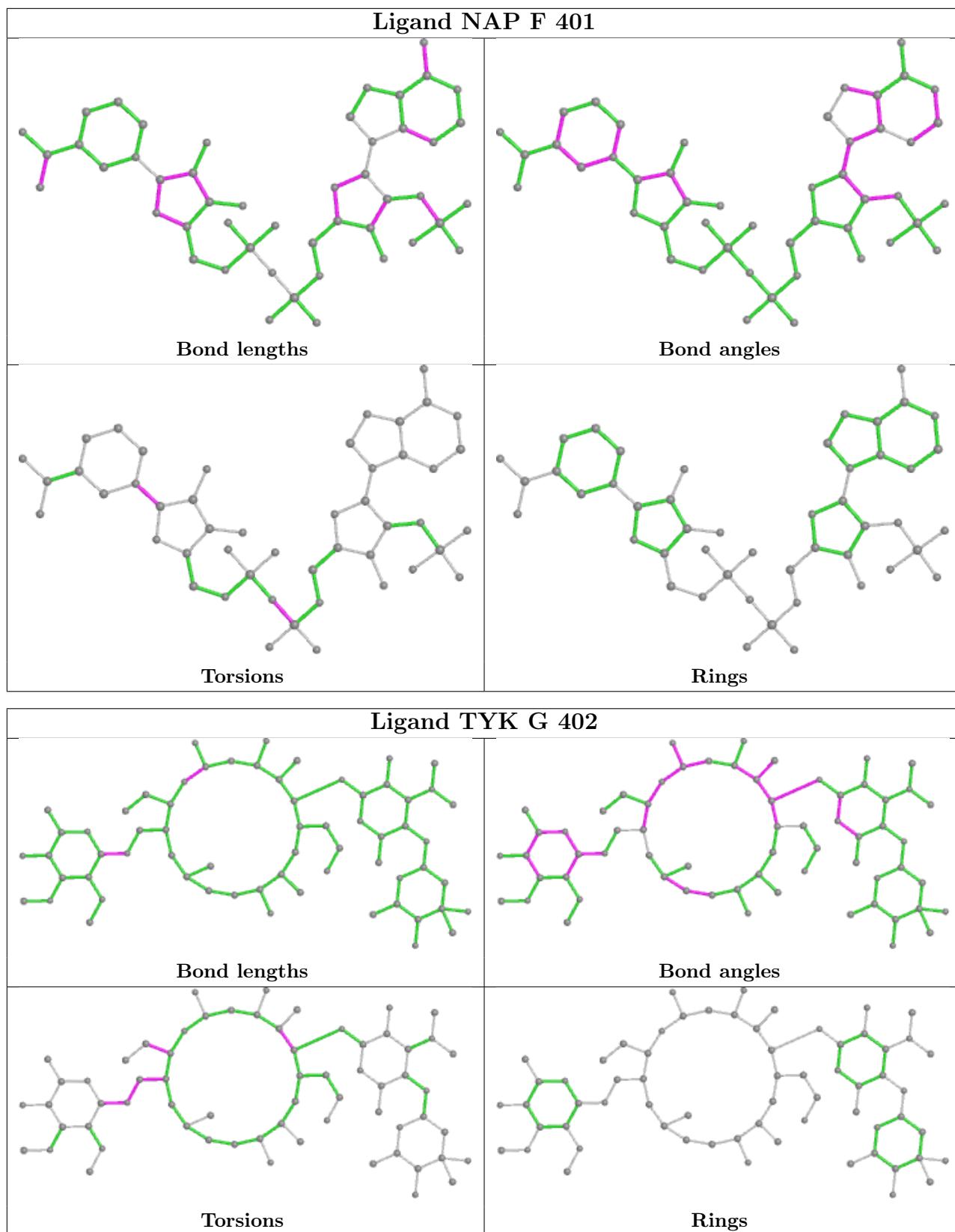


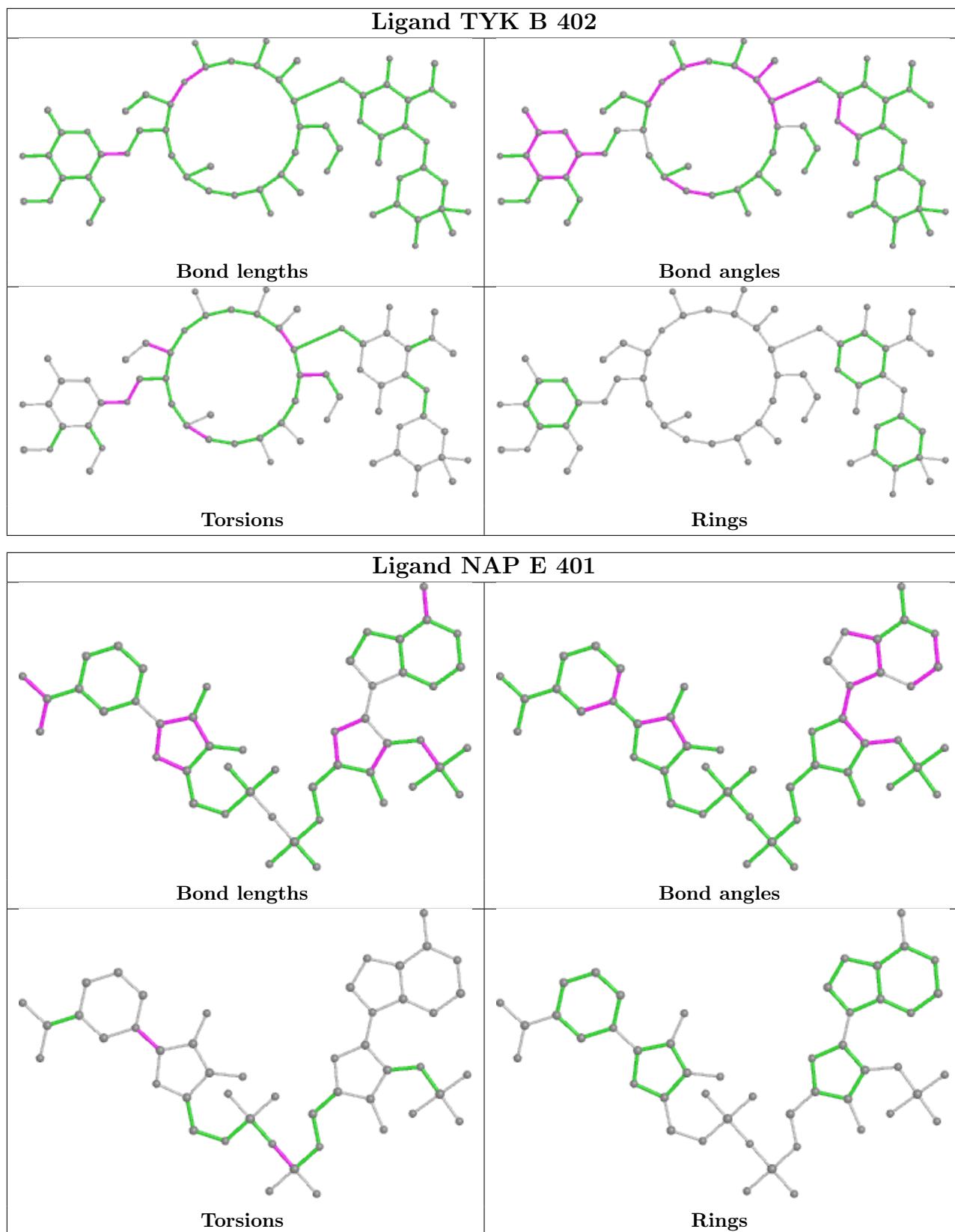


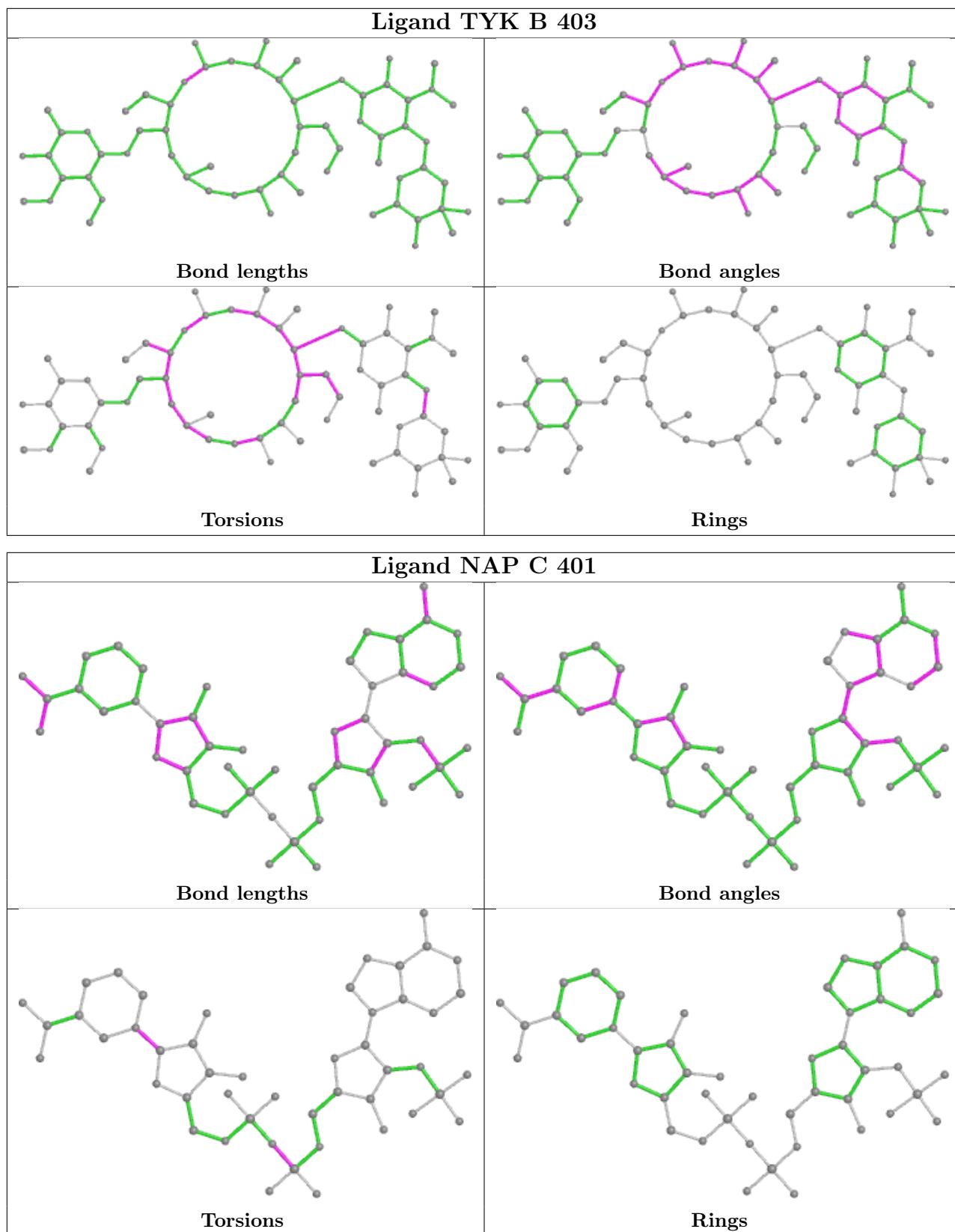


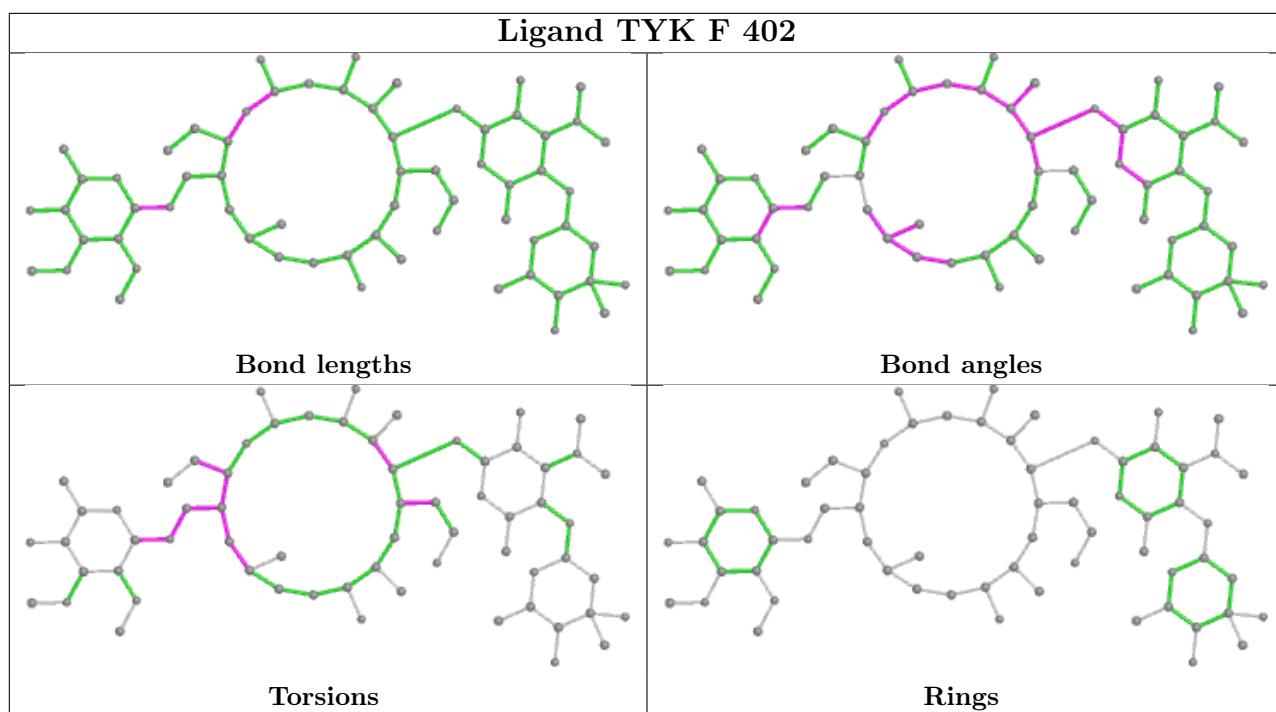












5.7 Other polymers [\(i\)](#)

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 i

6.1 Protein, DNA and RNA chains i

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	330/351 (94%)	-0.05	9 (2%) 54 61	11, 19, 37, 51	0
1	B	331/351 (94%)	0.04	13 (3%) 39 47	11, 20, 37, 45	0
1	C	331/351 (94%)	-0.17	6 (1%) 68 74	10, 18, 34, 50	0
1	D	331/351 (94%)	-0.09	7 (2%) 63 70	11, 19, 32, 40	0
1	E	331/351 (94%)	-0.01	11 (3%) 46 54	11, 21, 38, 48	0
1	F	331/351 (94%)	-0.24	5 (1%) 73 79	10, 17, 31, 55	0
1	G	331/351 (94%)	-0.12	5 (1%) 73 79	10, 18, 35, 50	0
1	H	331/351 (94%)	-0.05	7 (2%) 63 70	12, 20, 35, 50	0
All	All	2647/2808 (94%)	-0.08	63 (2%) 59 66	10, 19, 36, 55	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	92	LEU	4.6
1	B	92	LEU	4.5
1	C	233	GLY	4.4
1	A	234	ASN	4.3
1	B	94	GLY	4.3
1	A	92	LEU	4.2
1	H	232	GLY	4.2
1	A	230	GLN	4.1
1	C	230	GLN	4.0
1	D	92	LEU	3.9
1	G	93	ASP	3.9
1	C	232	GLY	3.7
1	H	234	ASN	3.6
1	E	234	ASN	3.6
1	H	92	LEU	3.5
1	B	212	ILE	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	92	LEU	3.5
1	F	92	LEU	3.5
1	F	94	GLY	3.4
1	B	74	GLY	3.4
1	G	232	GLY	3.4
1	E	94	GLY	3.4
1	F	93	ASP	3.3
1	A	95	PRO	3.3
1	B	234	ASN	3.3
1	E	287	ILE	3.2
1	C	92	LEU	3.1
1	B	93	ASP	3.1
1	D	247	LYS	3.0
1	C	94	GLY	3.0
1	A	94	GLY	2.9
1	B	230	GLN	2.9
1	C	234	ASN	2.8
1	E	239	SER	2.7
1	G	230	GLN	2.6
1	F	95	PRO	2.6
1	E	264	LYS	2.6
1	H	230	GLN	2.6
1	H	94	GLY	2.5
1	B	213	ALA	2.5
1	E	249	PRO	2.4
1	D	309	ASP	2.4
1	B	95	PRO	2.4
1	A	247	LYS	2.4
1	B	249	PRO	2.4
1	D	94	GLY	2.4
1	A	18	LEU	2.3
1	H	233	GLY	2.3
1	E	95	PRO	2.3
1	A	287	ILE	2.2
1	D	230	GLN	2.2
1	D	234	ASN	2.2
1	G	94	GLY	2.2
1	B	214	TRP	2.2
1	A	93	ASP	2.2
1	H	239	SER	2.1
1	E	233	GLY	2.1
1	F	55	TRP	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	17	VAL	2.1
1	B	247	LYS	2.1
1	D	126	LEU	2.1
1	E	57	GLU	2.0
1	E	126	LEU	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 monosaccharides in this entry.

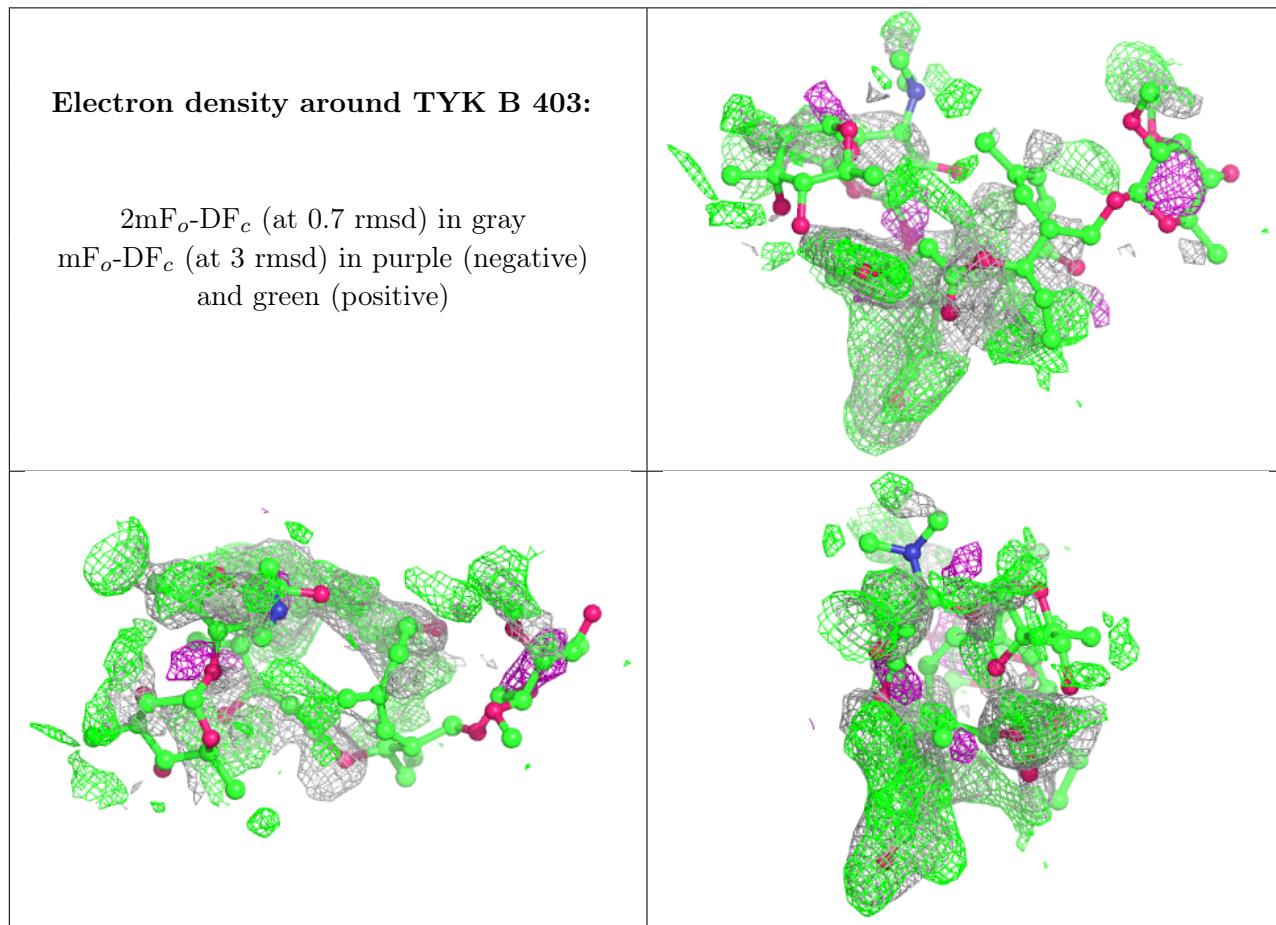
6.4 Ligands [\(i\)](#)

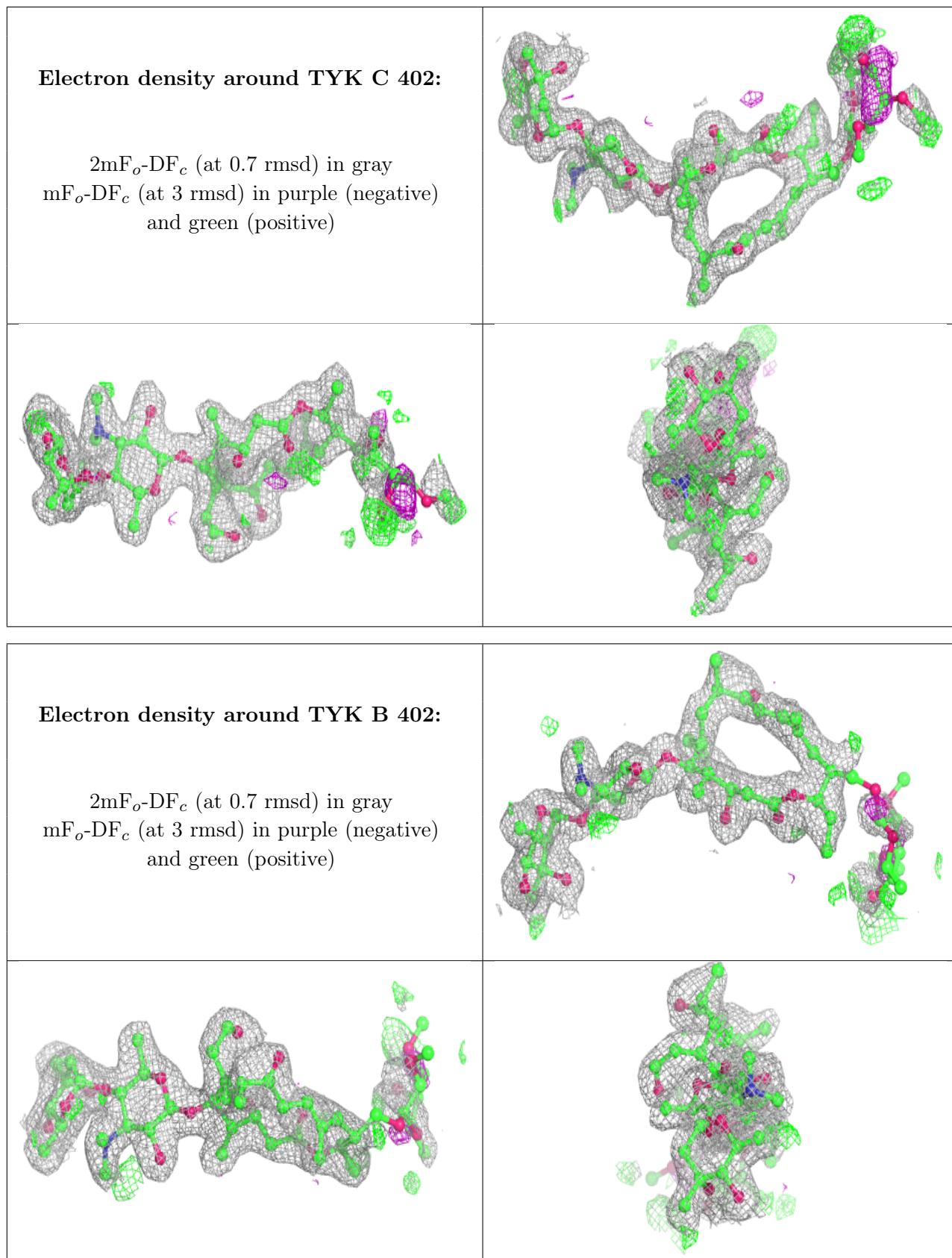
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

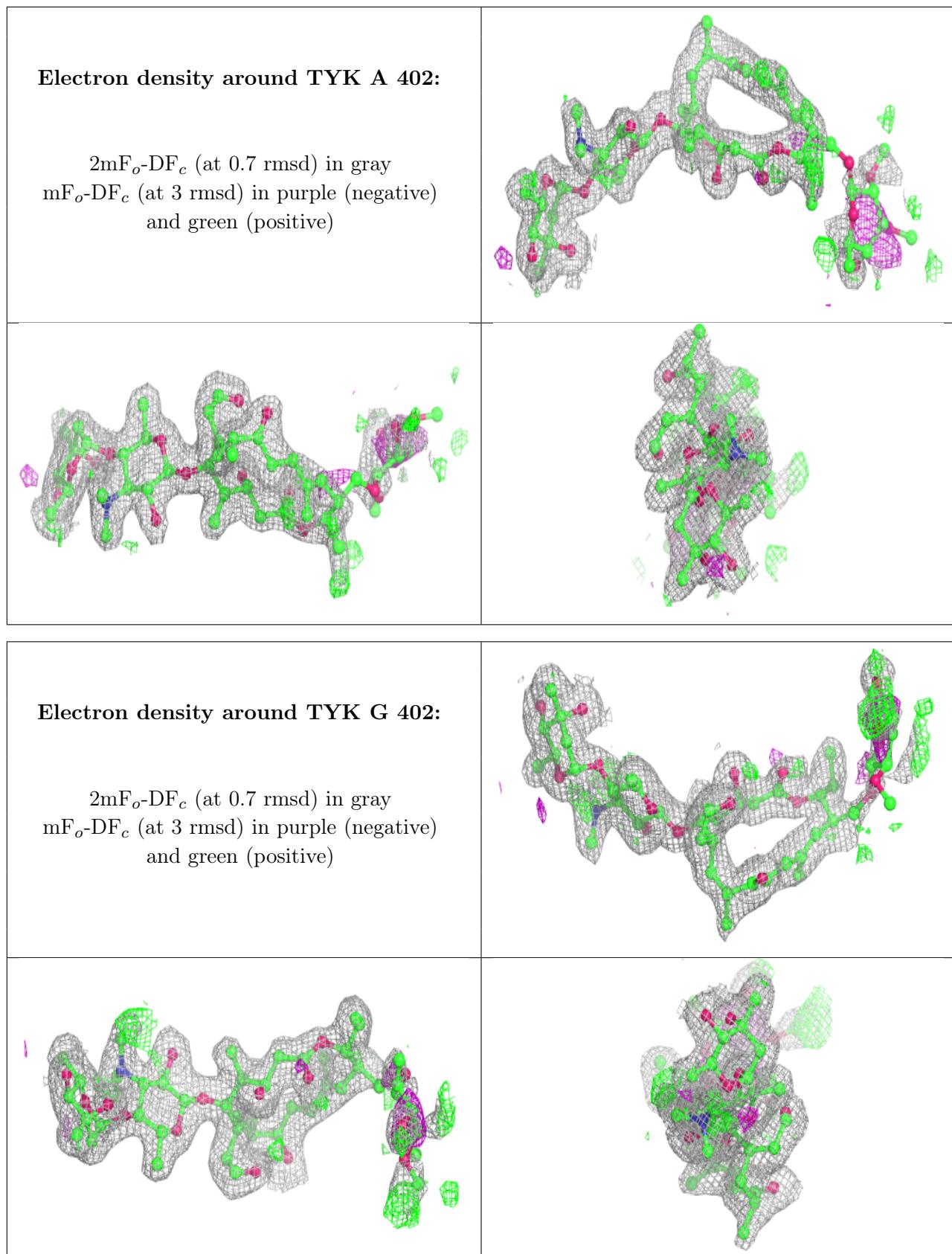
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	TYK	B	403	64/64	0.25	0.60	16,69,87,89	64
3	TYK	C	402	64/64	0.78	0.21	18,35,69,73	0
3	TYK	B	402	64/64	0.79	0.25	20,37,84,90	0
3	TYK	A	402	64/64	0.80	0.24	21,36,74,81	64
3	TYK	G	402	64/64	0.80	0.20	17,30,71,73	0
3	TYK	F	402	64/64	0.83	0.21	18,38,85,89	0
3	TYK	E	402	64/64	0.83	0.24	21,36,102,105	0
2	NAP	E	401	48/48	0.96	0.09	13,20,25,30	0
2	NAP	H	401	48/48	0.96	0.10	13,19,25,26	0
2	NAP	A	401	48/48	0.96	0.10	13,18,25,27	0
2	NAP	D	401	48/48	0.97	0.09	13,17,20,21	0
2	NAP	B	401	48/48	0.97	0.10	13,18,22,24	0
2	NAP	G	401	48/48	0.98	0.10	10,16,21,22	0
2	NAP	C	401	48/48	0.98	0.09	11,16,23,24	0
2	NAP	F	401	48/48	0.98	0.09	9,14,19,20	0

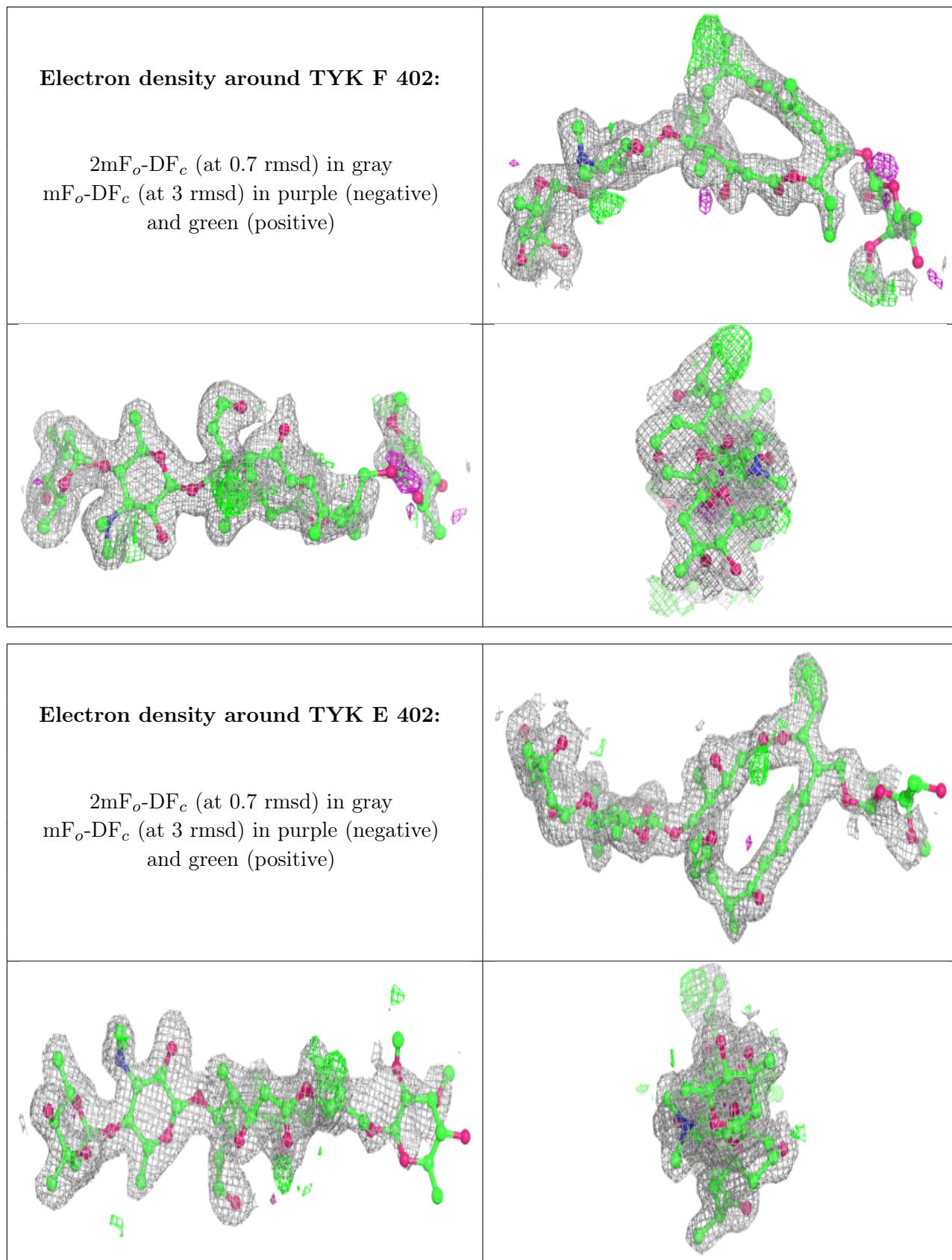
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

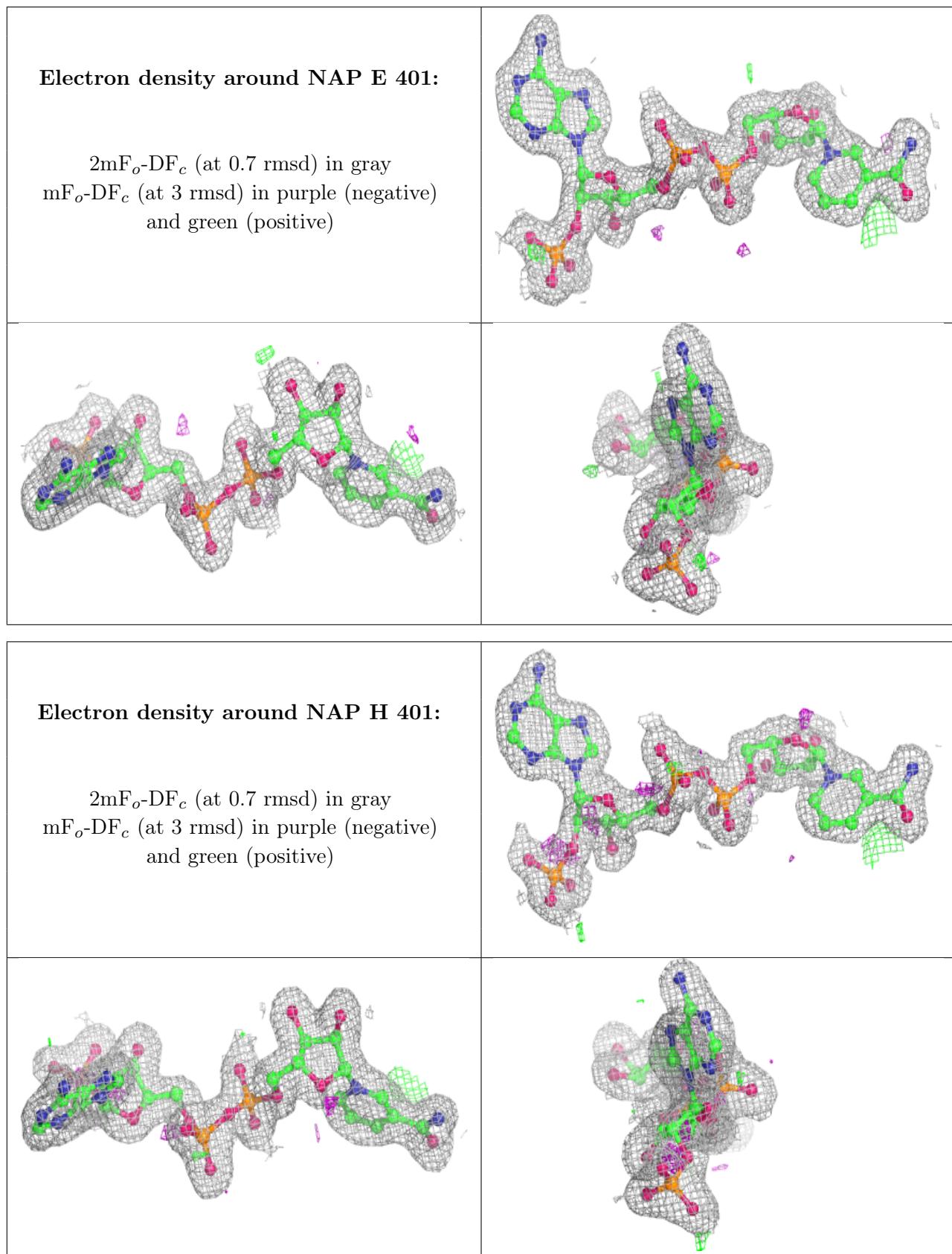
as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

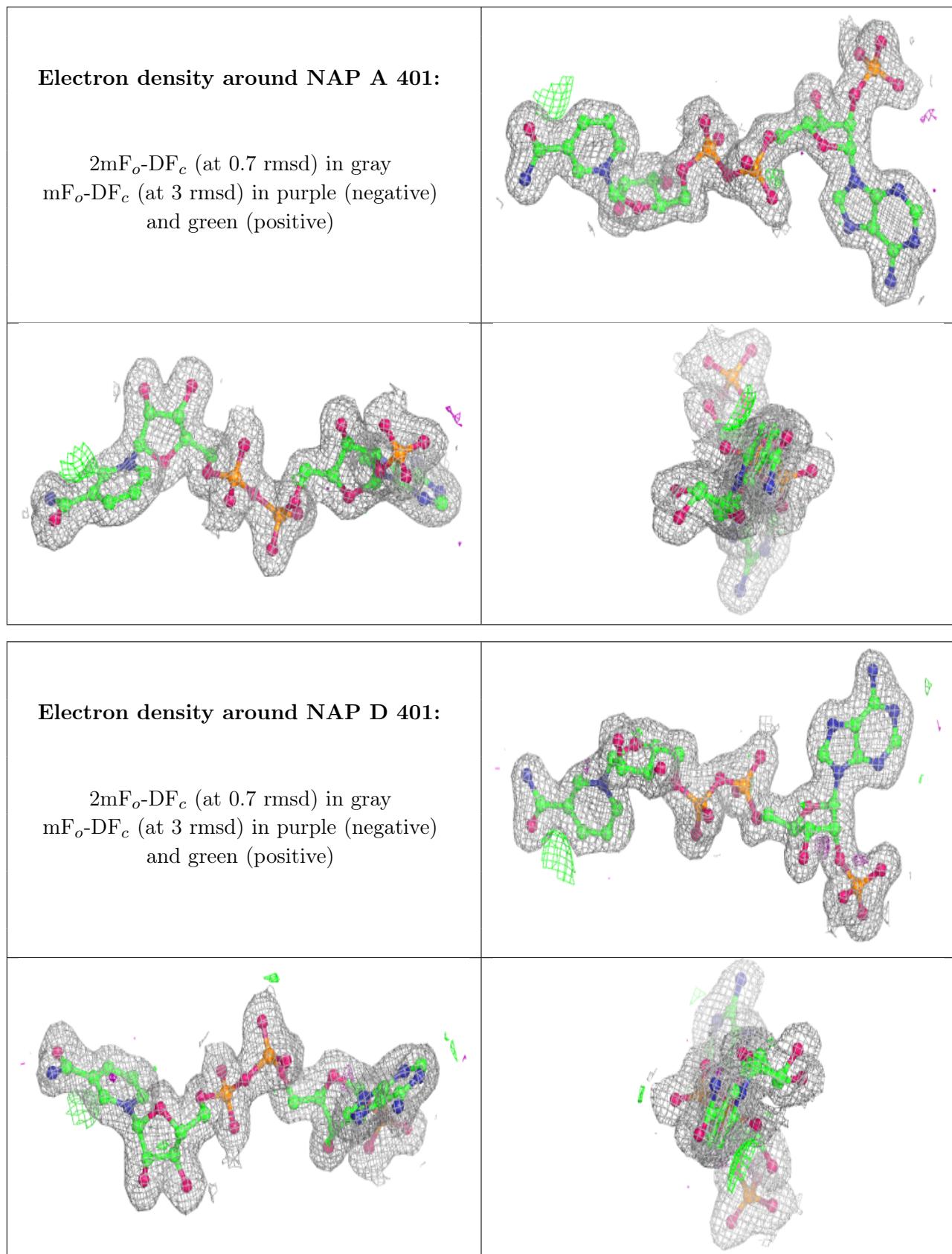


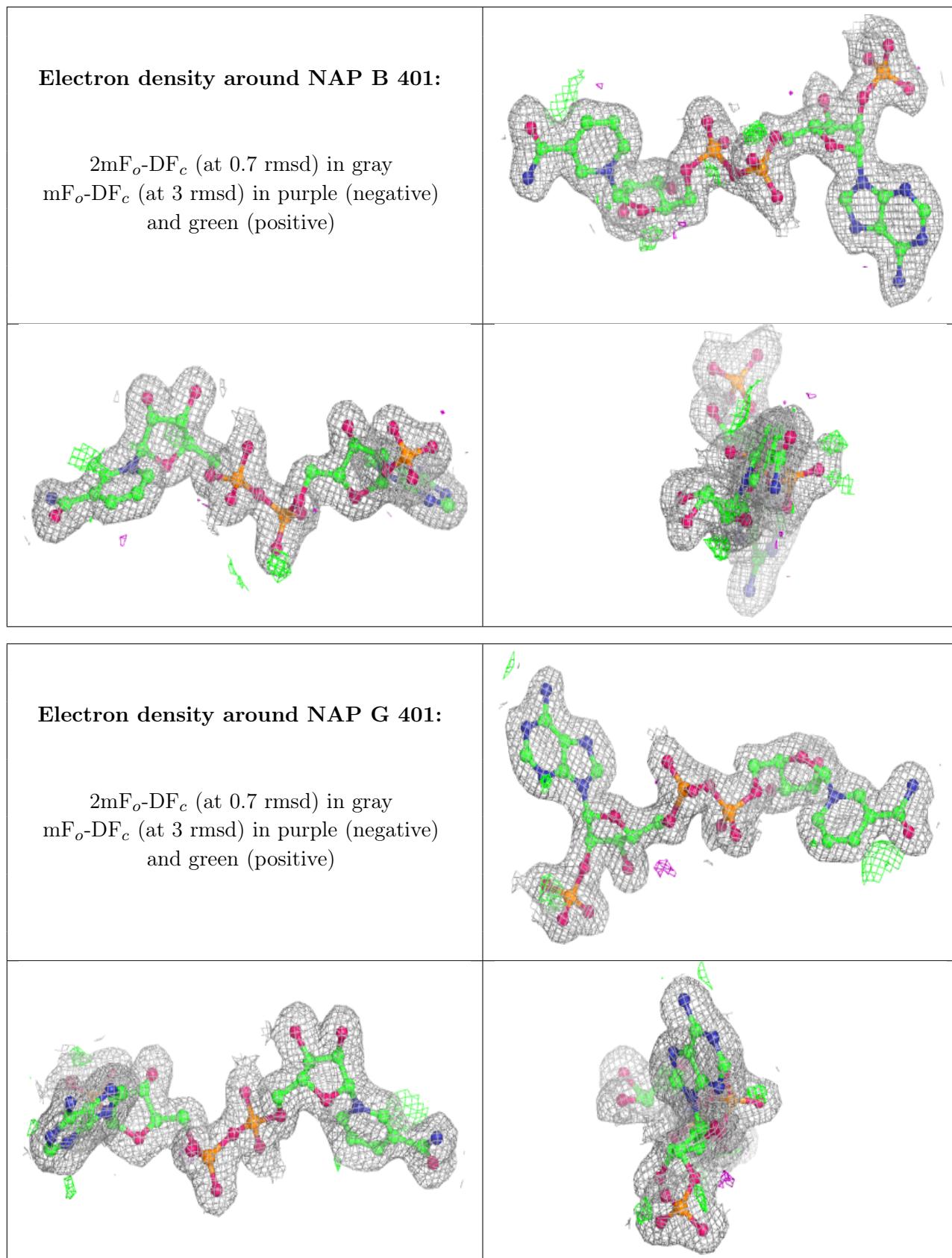


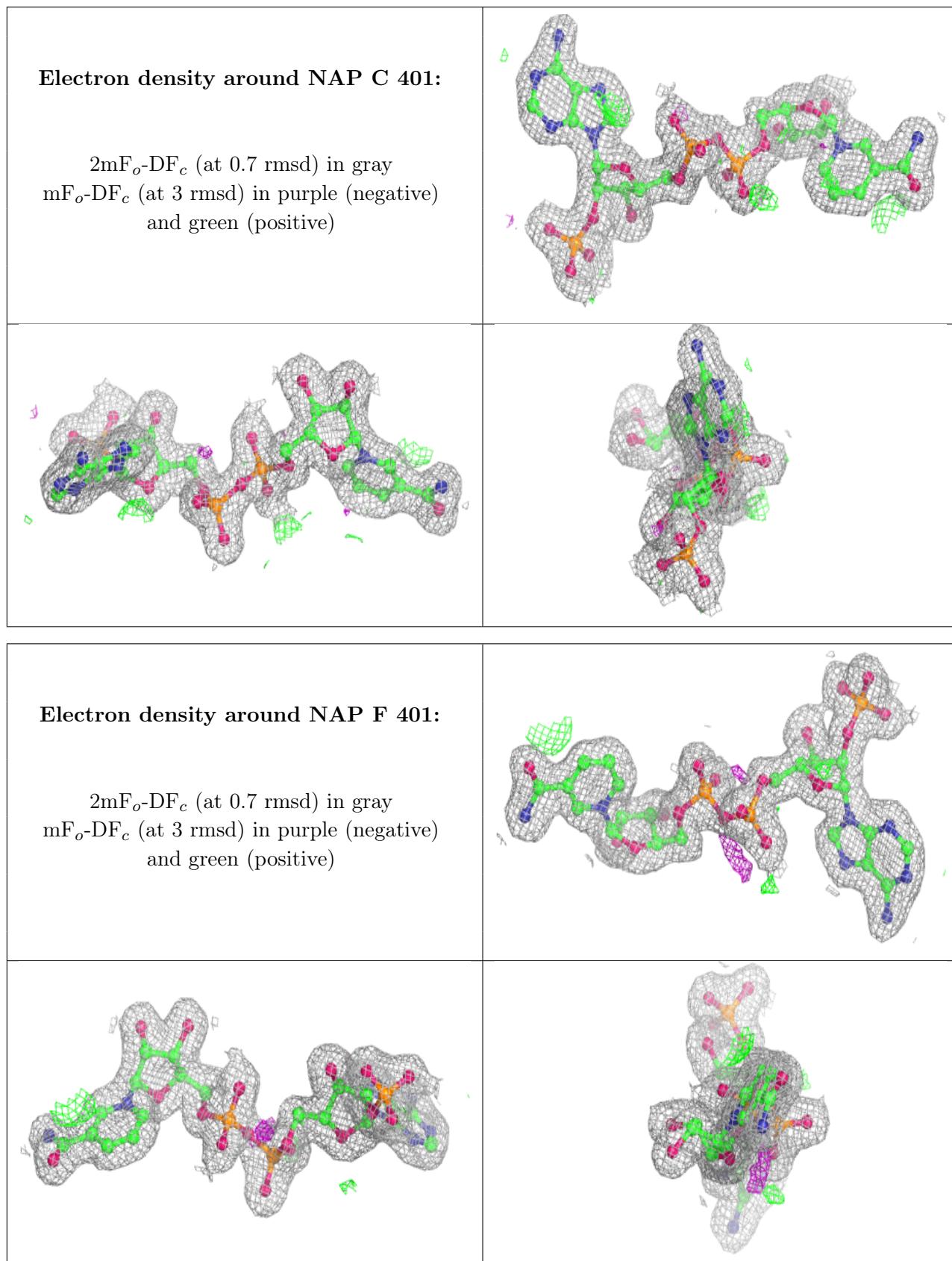












6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.