



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 09:34 PM UTC

PDB ID : 4TM1 / pdb_00004tm1
Title : Kutzneria sp. 744 ornithine N-hydroxylase, KtzI-FADred-NADP+-Br
Authors : Setser, J.W.; Drennan, C.L.
Deposited on : 2014-05-30
Resolution : 2.39 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 ⓘ symbol.

The types of validation reports are described at

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

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

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

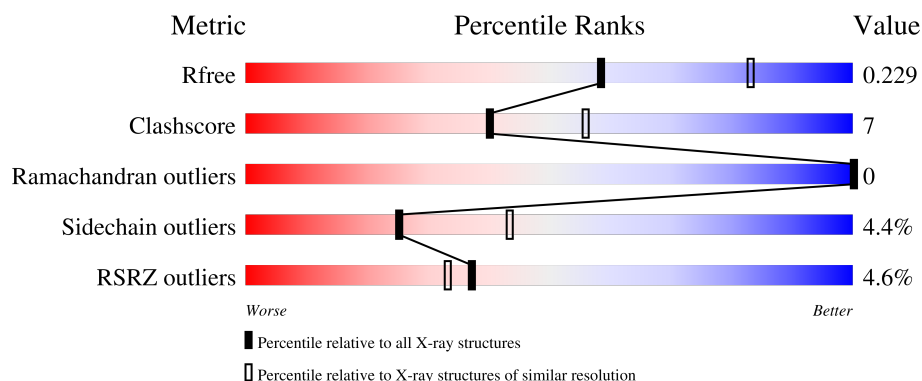
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.39 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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

Mol	Chain	Length	Quality of chain
1	A	443	 3% 76% 15% • 7%
1	B	443	 4% 82% 11% 7%
1	C	443	 5% 80% 12% • 7%
1	D	443	 5% 81% 11% • 7%

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
4	BR	A	510	-	-	X	-
4	BR	C	508	-	-	X	-
4	BR	D	507	-	-	X	-
4	BR	D	512	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13618 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 KtzI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	414	Total	C	N	O	S	0	0	0
			3211	2018	574	609	10			
1	B	414	Total	C	N	O	S	0	0	0
			3177	2001	564	602	10			
1	C	414	Total	C	N	O	S	0	0	0
			3174	1999	566	599	10			
1	D	414	Total	C	N	O	S	0	0	0
			3190	2007	571	602	10			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	MET	-	initiating methionine	UNP A8CF85
A	-17	GLY	-	expression tag	UNP A8CF85
A	-16	SER	-	expression tag	UNP A8CF85
A	-15	SER	-	expression tag	UNP A8CF85
A	-14	HIS	-	expression tag	UNP A8CF85
A	-13	HIS	-	expression tag	UNP A8CF85
A	-12	HIS	-	expression tag	UNP A8CF85
A	-11	HIS	-	expression tag	UNP A8CF85
A	-10	HIS	-	expression tag	UNP A8CF85
A	-9	HIS	-	expression tag	UNP A8CF85
A	-8	SER	-	expression tag	UNP A8CF85
A	-7	SER	-	expression tag	UNP A8CF85
A	-6	GLY	-	expression tag	UNP A8CF85
A	-5	LEU	-	expression tag	UNP A8CF85
A	-4	VAL	-	expression tag	UNP A8CF85
A	-3	PRO	-	expression tag	UNP A8CF85
A	-2	ARG	-	expression tag	UNP A8CF85
A	-1	GLY	-	expression tag	UNP A8CF85
A	0	SER	-	expression tag	UNP A8CF85
A	1	HIS	-	expression tag	UNP A8CF85
A	2	MET	-	expression tag	UNP A8CF85

Continued on next page...

Continued from previous page...

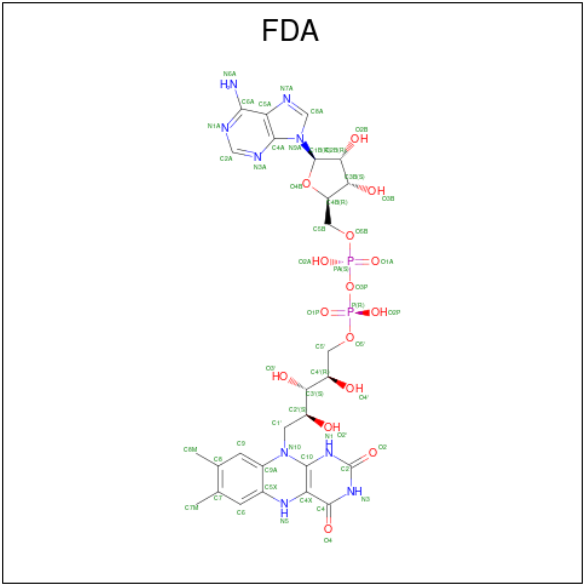
Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	MET	-	initiating methionine	UNP A8CF85
B	-17	GLY	-	expression tag	UNP A8CF85
B	-16	SER	-	expression tag	UNP A8CF85
B	-15	SER	-	expression tag	UNP A8CF85
B	-14	HIS	-	expression tag	UNP A8CF85
B	-13	HIS	-	expression tag	UNP A8CF85
B	-12	HIS	-	expression tag	UNP A8CF85
B	-11	HIS	-	expression tag	UNP A8CF85
B	-10	HIS	-	expression tag	UNP A8CF85
B	-9	HIS	-	expression tag	UNP A8CF85
B	-8	SER	-	expression tag	UNP A8CF85
B	-7	SER	-	expression tag	UNP A8CF85
B	-6	GLY	-	expression tag	UNP A8CF85
B	-5	LEU	-	expression tag	UNP A8CF85
B	-4	VAL	-	expression tag	UNP A8CF85
B	-3	PRO	-	expression tag	UNP A8CF85
B	-2	ARG	-	expression tag	UNP A8CF85
B	-1	GLY	-	expression tag	UNP A8CF85
B	0	SER	-	expression tag	UNP A8CF85
B	1	HIS	-	expression tag	UNP A8CF85
B	2	MET	-	expression tag	UNP A8CF85
C	-18	MET	-	initiating methionine	UNP A8CF85
C	-17	GLY	-	expression tag	UNP A8CF85
C	-16	SER	-	expression tag	UNP A8CF85
C	-15	SER	-	expression tag	UNP A8CF85
C	-14	HIS	-	expression tag	UNP A8CF85
C	-13	HIS	-	expression tag	UNP A8CF85
C	-12	HIS	-	expression tag	UNP A8CF85
C	-11	HIS	-	expression tag	UNP A8CF85
C	-10	HIS	-	expression tag	UNP A8CF85
C	-9	HIS	-	expression tag	UNP A8CF85
C	-8	SER	-	expression tag	UNP A8CF85
C	-7	SER	-	expression tag	UNP A8CF85
C	-6	GLY	-	expression tag	UNP A8CF85
C	-5	LEU	-	expression tag	UNP A8CF85
C	-4	VAL	-	expression tag	UNP A8CF85
C	-3	PRO	-	expression tag	UNP A8CF85
C	-2	ARG	-	expression tag	UNP A8CF85
C	-1	GLY	-	expression tag	UNP A8CF85
C	0	SER	-	expression tag	UNP A8CF85
C	1	HIS	-	expression tag	UNP A8CF85
C	2	MET	-	expression tag	UNP A8CF85

Continued on next page...

Continued from previous page...

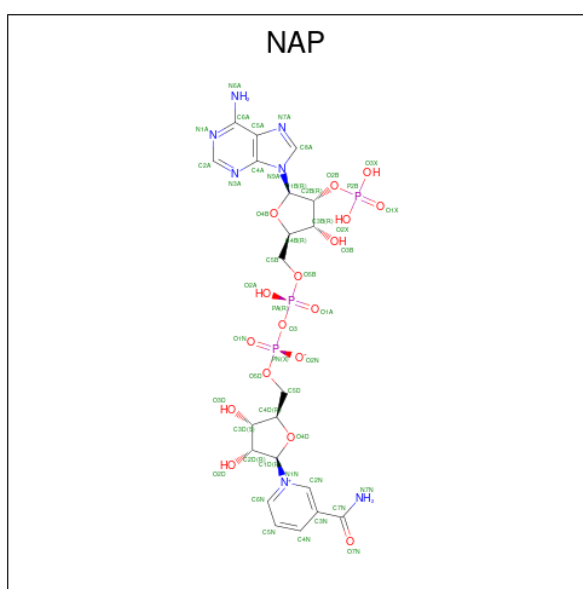
Chain	Residue	Modelled	Actual	Comment	Reference
D	-18	MET	-	initiating methionine	UNP A8CF85
D	-17	GLY	-	expression tag	UNP A8CF85
D	-16	SER	-	expression tag	UNP A8CF85
D	-15	SER	-	expression tag	UNP A8CF85
D	-14	HIS	-	expression tag	UNP A8CF85
D	-13	HIS	-	expression tag	UNP A8CF85
D	-12	HIS	-	expression tag	UNP A8CF85
D	-11	HIS	-	expression tag	UNP A8CF85
D	-10	HIS	-	expression tag	UNP A8CF85
D	-9	HIS	-	expression tag	UNP A8CF85
D	-8	SER	-	expression tag	UNP A8CF85
D	-7	SER	-	expression tag	UNP A8CF85
D	-6	GLY	-	expression tag	UNP A8CF85
D	-5	LEU	-	expression tag	UNP A8CF85
D	-4	VAL	-	expression tag	UNP A8CF85
D	-3	PRO	-	expression tag	UNP A8CF85
D	-2	ARG	-	expression tag	UNP A8CF85
D	-1	GLY	-	expression tag	UNP A8CF85
D	0	SER	-	expression tag	UNP A8CF85
D	1	HIS	-	expression tag	UNP A8CF85
D	2	MET	-	expression tag	UNP A8CF85

- Molecule 2 is DIHYDROFLAVINE-ADENINE DINUCLEOTIDE (CCD ID: FDA) (formula: $C_{27}H_{35}N_9O_{15}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



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

- Molecule 4 is BROMIDE ION (CCD ID: BR) (formula: Br).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	9	Total	Br	0	0
			9	9		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	7	Total 7	Br 7	0	0
4	C	7	Total 7	Br 7	0	0
4	D	12	Total 12	Br 12	0	0

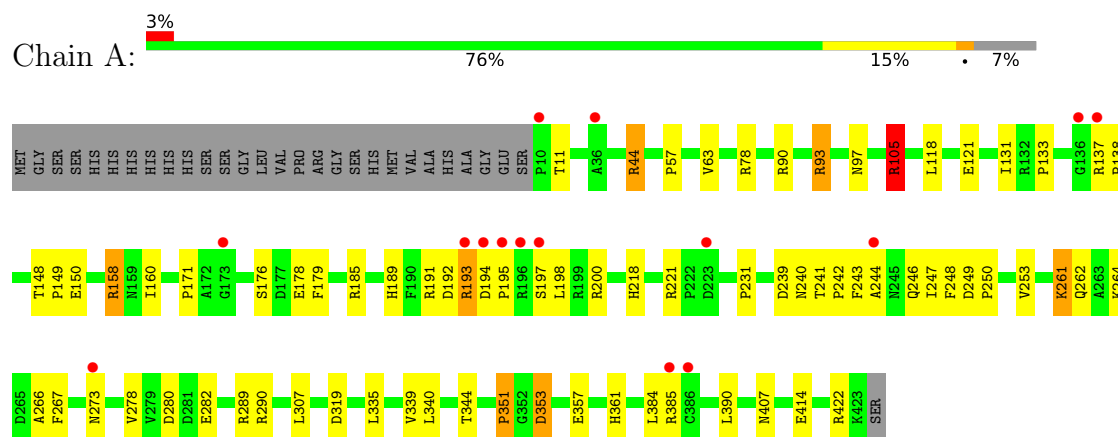
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	135	Total 135	O 135	0	0
5	B	96	Total 96	O 96	0	0
5	C	101	Total 101	O 101	0	0
5	D	95	Total 95	O 95	0	0

3 Residue-property plots [i](#)

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

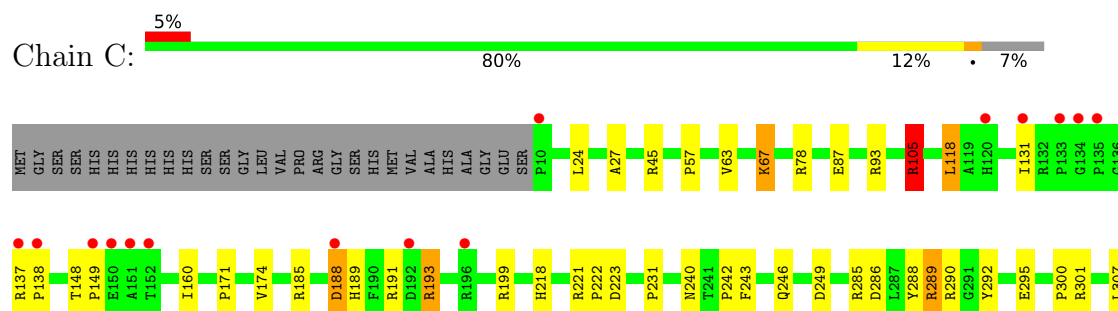
• Molecule 1: KtzI

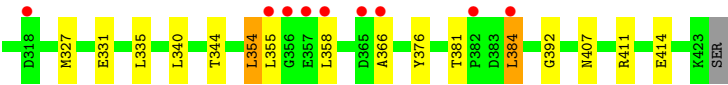


• Molecule 1: KtzI

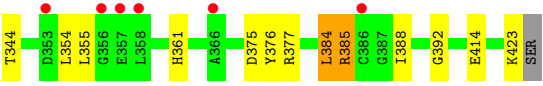
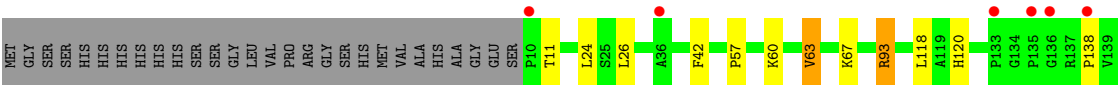
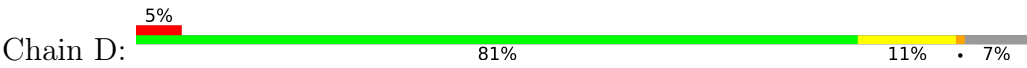


• Molecule 1: KtzI





● Molecule 1: KtzI



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	81.89Å 151.71Å 162.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.90 – 2.39 45.90 – 2.39	Depositor EDS
% Data completeness (in resolution range)	96.7 (45.90-2.39) 96.7 (45.90-2.39)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.89 (at 2.39Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.199 , 0.222 0.209 , 0.229	Depositor DCC
R_{free} test set	3955 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	36.4	Xtriage
Anisotropy	0.597	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 30.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13618	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.42% 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: BR, NAP, FDA

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	0.73	8/3290 (0.2%)	0.90	4/4482 (0.1%)
1	B	0.51	2/3256 (0.1%)	0.85	4/4441 (0.1%)
1	C	0.69	3/3253 (0.1%)	0.87	5/4437 (0.1%)
1	D	0.65	1/3269 (0.0%)	0.88	6/4456 (0.1%)
All	All	0.65	14/13068 (0.1%)	0.87	19/17816 (0.1%)

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	105	ARG	C-O	-6.62	1.16	1.24
1	B	24	LEU	C-O	-6.13	1.17	1.24
1	A	282	GLU	C-O	-5.47	1.17	1.24
1	A	353	ASP	C-O	-5.45	1.17	1.24
1	A	351	PRO	N-CD	5.44	1.55	1.47
1	C	105	ARG	C-O	-5.34	1.17	1.24
1	D	247	ILE	C-O	-5.34	1.17	1.24
1	A	253	VAL	C-O	-5.27	1.17	1.24
1	B	44	ARG	C-O	-5.26	1.17	1.24
1	A	266	ALA	C-O	-5.25	1.18	1.24
1	A	63	VAL	C-O	-5.17	1.18	1.24
1	C	331	GLU	C-O	-5.17	1.17	1.23
1	A	414	GLU	C-O	-5.15	1.18	1.24
1	C	174	VAL	C-O	-5.08	1.19	1.24

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	221	ARG	CA-C-N	7.16	127.32	119.87
1	B	221	ARG	C-N-CA	7.16	127.32	119.87
1	D	221	ARG	CA-C-N	6.92	127.07	119.87

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	221	ARG	C-N-CA	6.92	127.07	119.87
1	A	221	ARG	CA-C-N	6.67	126.80	119.87
1	A	221	ARG	C-N-CA	6.67	126.80	119.87
1	C	366	ALA	N-CA-C	6.55	118.97	111.11
1	D	120	HIS	N-CA-C	6.02	119.39	110.48
1	C	355	LEU	N-CA-C	6.02	118.80	111.82
1	B	392	GLY	N-CA-C	-5.78	106.46	111.95
1	D	11	THR	N-CA-C	5.56	117.79	108.73
1	A	192	ASP	CB-CA-C	-5.55	102.09	110.92
1	A	253	VAL	N-CA-C	-5.48	105.19	110.72
1	C	392	GLY	N-CA-C	-5.34	106.87	111.95
1	B	355	LEU	N-CA-C	5.30	118.90	112.23
1	C	381	THR	CA-C-N	-5.18	114.74	119.82
1	C	381	THR	C-N-CA	-5.18	114.74	119.82
1	D	392	GLY	N-CA-C	-5.18	107.02	111.95
1	D	355	LEU	N-CA-C	5.15	117.80	111.82

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3211	0	3044	67	0
1	B	3177	0	2993	32	0
1	C	3174	0	2992	46	0
1	D	3190	0	3016	44	0
2	A	53	0	30	2	0
2	B	53	0	29	0	0
2	C	53	0	30	0	0
2	D	53	0	29	0	0
3	A	48	0	25	0	0
3	B	48	0	25	0	0
3	C	48	0	25	0	0
3	D	48	0	25	0	0
4	A	9	0	0	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	7	0	0	1	0
4	C	7	0	0	4	0
4	D	12	0	0	7	0
5	A	135	0	0	9	0
5	B	96	0	0	4	0
5	C	101	0	0	6	0
5	D	95	0	0	2	0
All	All	13618	0	12263	167	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 7.

All (167) 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:A:249:ASP:OD2	1:A:250:PRO:HD2	1.38	1.23
1:C:57:PRO:HA	1:C:105:ARG:HH12	1.07	1.11
1:B:329:ARG:HG2	1:B:329:ARG:HH11	1.18	1.07
1:A:262:GLN:HE21	1:D:327:MET:HG2	1.20	1.03
1:A:249:ASP:OD2	1:A:250:PRO:CD	2.08	1.00
1:A:57:PRO:HA	1:A:105:ARG:HH12	1.28	0.97
1:A:57:PRO:HA	1:A:105:ARG:NH1	1.81	0.94
1:C:57:PRO:HA	1:C:105:ARG:NH1	1.81	0.94
1:D:193:ARG:HH11	1:D:193:ARG:HG2	1.34	0.92
1:D:414:GLU:OE1	4:D:513:BR:BR	2.57	0.78
1:A:244:ALA:HA	5:A:731:HOH:O	1.83	0.77
1:C:193:ARG:HH11	1:C:193:ARG:HG2	1.50	0.76
1:D:179:PHE:HD2	4:D:512:BR:BR	2.23	0.76
1:A:262:GLN:NE2	1:D:327:MET:HG2	1.98	0.75
1:B:262:GLN:NE2	1:C:327:MET:HG2	2.02	0.74
1:D:361:HIS:CB	1:D:384:LEU:HD12	2.17	0.74
1:A:262:GLN:HE21	1:D:327:MET:CG	1.99	0.73
1:A:244:ALA:O	1:A:247:ILE:HD12	1.88	0.72
1:A:200:ARG:NH1	1:A:319:ASP:OD1	2.23	0.72
1:C:240:ASN:ND2	5:C:696:HOH:O	2.21	0.72
1:A:273:ASN:HB2	5:A:730:HOH:O	1.89	0.72
1:D:193:ARG:HG2	1:D:193:ARG:NH1	2.01	0.72
1:D:361:HIS:HB2	1:D:384:LEU:HD12	1.72	0.72
1:B:414:GLU:OE1	4:B:509:BR:BR	2.63	0.72
1:B:295:GLU:OE2	1:D:93:ARG:NE	2.22	0.71
1:A:93:ARG:HG2	1:C:292:TYR:CD2	2.25	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:240:ASN:ND2	5:D:684:HOH:O	2.23	0.71
1:D:309:HIS:NE2	1:D:327:MET:HE3	2.06	0.70
1:D:307:LEU:HD12	4:D:503:BR:BR	2.46	0.70
1:A:93:ARG:HG2	1:C:292:TYR:HD2	1.55	0.70
1:B:329:ARG:HB3	1:B:331:GLU:HG2	1.74	0.69
1:C:191:ARG:NH2	5:C:691:HOH:O	2.24	0.69
1:C:414:GLU:OE1	4:C:508:BR:BR	2.66	0.68
1:B:240:ASN:ND2	5:B:690:HOH:O	2.27	0.68
1:A:240:ASN:ND2	5:A:720:HOH:O	2.28	0.66
1:A:93:ARG:NH2	1:C:295:GLU:OE2	2.28	0.66
1:A:249:ASP:OD2	1:A:250:PRO:N	2.30	0.65
1:A:351:PRO:HG3	1:A:390:LEU:HD13	1.78	0.64
1:B:329:ARG:HG2	1:B:329:ARG:NH1	1.97	0.64
1:A:191:ARG:CG	1:A:191:ARG:HH21	2.13	0.62
1:D:375:ASP:O	1:D:376:TYR:HB2	1.99	0.62
1:C:45:ARG:NH2	5:C:690:HOH:O	2.32	0.61
1:B:148:THR:HB	1:B:149:PRO:HD2	1.82	0.61
1:A:243:PHE:HD2	1:D:284:ILE:HG23	1.65	0.61
1:C:286:ASP:OD1	1:C:289:ARG:NH1	2.34	0.61
4:D:507:BR:BR	5:D:673:HOH:O	2.71	0.61
1:C:358:LEU:HD22	1:C:384:LEU:HD11	1.82	0.60
1:A:44:ARG:HG2	2:A:501:FDA:C4A	2.31	0.60
1:D:148:THR:HB	1:D:149:PRO:HD2	1.83	0.60
1:A:361:HIS:ND1	5:A:601:HOH:O	2.28	0.59
1:C:185:ARG:HA	1:C:188:ASP:OD2	2.01	0.59
1:A:90:ARG:HG2	1:C:295:GLU:OE1	2.03	0.59
1:C:301:ARG:NH1	5:C:673:HOH:O	2.30	0.59
1:C:148:THR:HB	1:C:149:PRO:HD2	1.83	0.58
1:A:148:THR:HB	1:A:149:PRO:HD2	1.84	0.58
1:A:133:PRO:HG2	1:A:357:GLU:CD	2.29	0.58
1:C:171:PRO:HG3	1:C:344:THR:HG21	1.85	0.58
1:D:93:ARG:NH2	1:D:93:ARG:HG2	2.18	0.58
1:A:218:HIS:CE1	1:A:290:ARG:HB3	2.39	0.57
1:B:218:HIS:CE1	1:B:290:ARG:HG2	2.39	0.57
1:D:63:VAL:HG22	1:D:67:LYS:HD2	1.86	0.57
1:A:93:ARG:NE	1:C:295:GLU:OE2	2.37	0.57
1:D:179:PHE:CD2	4:D:512:BR:BR	3.11	0.57
1:A:171:PRO:HG3	1:A:344:THR:HG21	1.86	0.56
1:A:262:GLN:HG2	1:D:327:MET:SD	2.45	0.56
1:D:160:ILE:HD11	1:D:388:ILE:HG12	1.87	0.56
1:A:244:ALA:O	1:A:247:ILE:CD1	2.52	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:137:ARG:HA	1:B:138:PRO:C	2.31	0.56
1:A:191:ARG:HH21	1:A:191:ARG:HG2	1.72	0.55
1:A:179:PHE:HB2	4:A:510:BR:BR	2.62	0.55
1:C:67:LYS:HE2	4:C:504:BR:BR	2.62	0.55
1:A:361:HIS:HB2	1:A:384:LEU:HD12	1.88	0.54
1:D:179:PHE:HB2	4:D:512:BR:BR	2.61	0.54
1:D:361:HIS:HB3	1:D:384:LEU:HD12	1.89	0.54
1:A:93:ARG:CG	1:C:292:TYR:HD2	2.20	0.54
1:C:131:ILE:HD13	1:C:160:ILE:HD13	1.90	0.54
1:B:361:HIS:HB2	1:B:384:LEU:HD12	1.89	0.54
1:D:171:PRO:HG3	1:D:344:THR:HG21	1.89	0.54
1:D:231:PRO:HB3	1:D:309:HIS:CE1	2.44	0.53
1:A:93:ARG:HH21	1:C:295:GLU:CD	2.16	0.53
1:B:131:ILE:HD13	1:B:160:ILE:HD13	1.91	0.53
1:D:93:ARG:HG2	1:D:93:ARG:HH21	1.73	0.53
1:B:171:PRO:HG3	1:B:344:THR:HG21	1.89	0.52
1:A:185:ARG:O	1:A:189:HIS:HD2	1.92	0.52
1:B:269:ARG:NH1	5:B:647:HOH:O	2.42	0.51
1:C:193:ARG:HG2	1:C:193:ARG:NH1	2.22	0.51
1:C:243:PHE:O	1:C:246:GLN:HB2	2.11	0.51
1:C:193:ARG:HH11	1:C:193:ARG:CG	2.19	0.51
1:D:93:ARG:HH21	1:D:93:ARG:CG	2.23	0.51
1:B:242:PRO:HB2	1:C:288:TYR:CD1	2.46	0.51
1:A:179:PHE:HD2	4:A:510:BR:BR	2.49	0.51
1:B:231:PRO:HB3	1:B:309:HIS:CE1	2.46	0.51
1:A:131:ILE:HD13	1:A:160:ILE:HD13	1.93	0.50
1:A:243:PHE:O	1:A:246:GLN:HB2	2.12	0.50
1:A:273:ASN:O	1:A:278:VAL:HG21	2.11	0.50
1:A:264:LYS:O	1:A:267:PHE:HB2	2.12	0.49
1:D:42:PHE:HE1	1:D:153:ARG:HH21	1.59	0.49
1:B:285:ARG:HH11	1:B:285:ARG:HG2	1.77	0.49
1:C:193:ARG:NH1	1:C:193:ARG:CG	2.75	0.48
1:C:185:ARG:O	1:C:189:HIS:HD2	1.95	0.48
1:B:243:PHE:HB2	5:B:693:HOH:O	2.13	0.48
1:D:377:ARG:NH1	1:D:377:ARG:HG2	2.28	0.48
1:A:137:ARG:HA	1:A:138:PRO:C	2.39	0.47
1:A:239:ASP:CG	1:D:237:VAL:HG12	2.39	0.47
1:B:288:TYR:CD1	1:C:242:PRO:HB2	2.49	0.47
1:D:26:LEU:HD21	1:D:161:VAL:HG21	1.95	0.47
1:A:97:ASN:OD1	5:A:673:HOH:O	2.20	0.47
1:C:376:TYR:CE1	1:C:411:ARG:HG3	2.50	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:218:HIS:CE1	1:C:290:ARG:HG2	2.49	0.47
1:A:244:ALA:CA	5:A:731:HOH:O	2.55	0.46
1:C:223:ASP:HB2	5:C:668:HOH:O	2.15	0.46
1:D:286:ASP:OD1	1:D:289:ARG:NH2	2.42	0.46
1:B:231:PRO:O	1:B:307:LEU:HA	2.16	0.46
1:D:63:VAL:CG2	1:D:67:LYS:HD2	2.46	0.46
1:A:191:ARG:CG	1:A:191:ARG:NH2	2.72	0.46
1:B:377:ARG:NH1	5:B:619:HOH:O	2.43	0.45
1:A:246:GLN:C	1:A:248:PHE:N	2.73	0.45
1:A:240:ASN:ND2	5:A:721:HOH:O	2.49	0.45
1:C:300:PRO:HD3	4:C:509:BR:BR	2.72	0.45
1:D:193:ARG:NH1	1:D:193:ARG:CG	2.73	0.45
1:A:261:LYS:HD3	1:A:261:LYS:HA	1.57	0.45
1:B:189:HIS:O	1:B:193:ARG:HG2	2.17	0.45
1:B:329:ARG:NH1	1:B:329:ARG:CG	2.73	0.45
1:D:160:ILE:CD1	1:D:388:ILE:HG23	2.47	0.44
1:A:78:ARG:NH1	5:A:659:HOH:O	2.51	0.44
1:B:329:ARG:HH11	1:B:329:ARG:CG	2.06	0.44
1:D:377:ARG:HG2	1:D:377:ARG:HH11	1.82	0.44
1:B:288:TYR:CG	1:C:242:PRO:HB2	2.53	0.44
1:A:351:PRO:CG	1:A:390:LEU:HD13	2.46	0.43
1:C:78:ARG:NH1	5:C:644:HOH:O	2.51	0.43
1:D:60:LYS:HB3	1:D:60:LYS:HE2	1.74	0.43
1:C:231:PRO:O	1:C:307:LEU:HA	2.19	0.43
1:C:137:ARG:HA	1:C:138:PRO:C	2.44	0.43
1:C:354:LEU:HD12	1:C:354:LEU:HA	1.88	0.43
1:D:57:PRO:HB2	4:D:507:BR:BR	2.74	0.43
1:D:231:PRO:O	1:D:307:LEU:HA	2.19	0.43
1:B:197:SER:O	1:B:198:LEU:HD23	2.19	0.43
1:A:231:PRO:O	1:A:307:LEU:HA	2.20	0.42
1:C:221:ARG:HA	1:C:222:PRO:HD2	1.94	0.42
1:C:407:ASN:ND2	4:C:508:BR:BR	3.07	0.42
1:A:11:THR:O	1:A:158:ARG:NH2	2.53	0.42
1:A:247:ILE:HD12	1:A:247:ILE:H	1.84	0.42
1:A:93:ARG:CZ	1:C:295:GLU:OE2	2.66	0.42
1:A:194:ASP:HA	1:A:195:PRO:HD3	1.96	0.42
1:D:268:TRP:O	1:D:272:ARG:HB2	2.20	0.42
1:A:242:PRO:HB2	1:D:288:TYR:CG	2.55	0.42
1:A:407:ASN:ND2	4:A:504:BR:BR	3.07	0.42
1:D:138:PRO:HB2	1:D:385:ARG:HG3	2.01	0.42
1:D:375:ASP:O	1:D:376:TYR:CB	2.64	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:ARG:CG	1:C:295:GLU:OE1	2.68	0.41
1:A:241:THR:O	1:A:244:ALA:HB3	2.20	0.41
1:A:249:ASP:O	1:A:250:PRO:C	2.62	0.41
1:A:422:ARG:CD	5:A:735:HOH:O	2.68	0.41
1:C:246:GLN:HG2	1:C:249:ASP:OD2	2.20	0.41
1:A:246:GLN:C	1:A:248:PHE:H	2.28	0.41
1:B:150:GLU:CD	1:B:150:GLU:H	2.28	0.41
1:B:248:PHE:HB3	1:B:406:SER:HB2	2.03	0.41
1:D:198:LEU:HD22	1:D:339:VAL:HG23	2.02	0.41
1:A:197:SER:O	1:A:198:LEU:HD23	2.20	0.41
1:B:169:ARG:NH1	1:B:346:TYR:O	2.54	0.41
1:A:44:ARG:HG2	2:A:501:FDA:N3A	2.36	0.41
1:A:198:LEU:HD22	1:A:339:VAL:HG23	2.03	0.41
1:A:178:GLU:HG3	1:A:193:ARG:HH22	1.86	0.40
1:B:285:ARG:HH11	1:B:285:ARG:CG	2.32	0.40
1:A:249:ASP:CG	1:B:92:VAL:HG11	2.46	0.40
1:B:242:PRO:HB2	1:C:288:TYR:CG	2.57	0.40
1:C:27:ALA:HB1	1:C:118:LEU:HD21	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	412/443 (93%)	396 (96%)	16 (4%)	0	100	100
1	B	412/443 (93%)	401 (97%)	11 (3%)	0	100	100
1	C	412/443 (93%)	396 (96%)	16 (4%)	0	100	100
1	D	412/443 (93%)	395 (96%)	17 (4%)	0	100	100
All	All	1648/1772 (93%)	1588 (96%)	60 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	336/372 (90%)	320 (95%)	16 (5%)	23	40
1	B	329/372 (88%)	318 (97%)	11 (3%)	33	55
1	C	328/372 (88%)	312 (95%)	16 (5%)	22	39
1	D	331/372 (89%)	316 (96%)	15 (4%)	24	42
All	All	1324/1488 (89%)	1266 (96%)	58 (4%)	25	43

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	ARG
1	A	93	ARG
1	A	105	ARG
1	A	118	LEU
1	A	121	GLU
1	A	150	GLU
1	A	158	ARG
1	A	176	SER
1	A	193	ARG
1	A	261	LYS
1	A	280	ASP
1	A	289	ARG
1	A	335	LEU
1	A	340	LEU
1	A	353	ASP
1	A	385	ARG
1	B	63	VAL
1	B	105	ARG
1	B	118	LEU
1	B	150	GLU
1	B	155	VAL
1	B	176	SER
1	B	185	ARG
1	B	329	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	335	LEU
1	B	340	LEU
1	B	354	LEU
1	C	24	LEU
1	C	63	VAL
1	C	67	LYS
1	C	87	GLU
1	C	93	ARG
1	C	105	ARG
1	C	118	LEU
1	C	188	ASP
1	C	193	ARG
1	C	199	ARG
1	C	285	ARG
1	C	289	ARG
1	C	335	LEU
1	C	340	LEU
1	C	354	LEU
1	C	384	LEU
1	D	24	LEU
1	D	63	VAL
1	D	93	ARG
1	D	118	LEU
1	D	160	ILE
1	D	176	SER
1	D	193	ARG
1	D	269	ARG
1	D	329	ARG
1	D	335	LEU
1	D	340	LEU
1	D	354	LEU
1	D	384	LEU
1	D	385	ARG
1	D	423	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	HIS
1	A	86	HIS
1	A	175	GLN
1	A	189	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	220	ASN
1	A	240	ASN
1	A	262	GLN
1	A	273	ASN
1	A	306	ASN
1	B	86	HIS
1	B	175	GLN
1	B	220	ASN
1	B	227	HIS
1	B	306	ASN
1	B	309	HIS
1	C	86	HIS
1	C	189	HIS
1	C	240	ASN
1	C	306	ASN
1	D	62	GLN
1	D	227	HIS
1	D	361	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 43 ligands modelled in this entry, 35 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	$\# Z > 2$
2	FDA	A	501	-	57,58,58	2.27	21 (36%)	78,89,89	1.65	15 (19%)
2	FDA	D	501	-	57,58,58	2.27	20 (35%)	78,89,89	1.67	14 (17%)
3	NAP	C	502	-	50,52,52	1.68	7 (14%)	71,80,80	1.54	12 (16%)
3	NAP	B	502	-	50,52,52	1.66	7 (14%)	71,80,80	1.60	13 (18%)
2	FDA	C	501	-	57,58,58	2.26	20 (35%)	78,89,89	2.57	23 (29%)
3	NAP	D	502	-	50,52,52	2.02	16 (32%)	71,80,80	1.60	13 (18%)
2	FDA	B	501	-	57,58,58	2.26	20 (35%)	78,89,89	2.56	25 (32%)
3	NAP	A	502	-	50,52,52	1.66	7 (14%)	71,80,80	1.58	12 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FDA	A	501	-	-	6/34/50/50	0/6/6/6
2	FDA	D	501	-	-	6/34/50/50	0/6/6/6
3	NAP	C	502	-	-	4/35/67/67	0/5/5/5
3	NAP	B	502	-	-	3/35/67/67	0/5/5/5
2	FDA	C	501	-	-	8/34/50/50	0/6/6/6
3	NAP	D	502	-	-	2/35/67/67	0/5/5/5
2	FDA	B	501	-	-	10/34/50/50	0/6/6/6
3	NAP	A	502	-	-	2/35/67/67	0/5/5/5

All (118) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	FDA	C6A-N6A	5.66	1.48	1.34
2	A	501	FDA	C6A-N6A	5.65	1.48	1.34
2	C	501	FDA	C6A-N6A	5.61	1.48	1.34
2	B	501	FDA	C6A-N6A	5.54	1.48	1.34
2	B	501	FDA	O2B-C2B	-5.43	1.29	1.43
2	D	501	FDA	O2B-C2B	-5.42	1.29	1.43
2	C	501	FDA	O2B-C2B	-5.41	1.29	1.43
2	A	501	FDA	O2B-C2B	-5.37	1.29	1.43
3	D	502	NAP	C6A-N6A	4.92	1.46	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	502	NAP	C6A-N6A	4.87	1.46	1.34
3	A	502	NAP	PN-O3	-4.80	1.54	1.59
3	C	502	NAP	C6A-N6A	4.79	1.46	1.34
3	A	502	NAP	C6A-N6A	4.71	1.46	1.34
3	C	502	NAP	PN-O3	-4.70	1.54	1.59
2	D	501	FDA	PA-O3P	-4.52	1.54	1.59
3	B	502	NAP	PN-O3	-4.50	1.54	1.59
2	A	501	FDA	C10-N1	4.37	1.44	1.37
2	A	501	FDA	C2-N1	4.34	1.44	1.37
3	B	502	NAP	C3B-C2B	-4.32	1.43	1.53
3	C	502	NAP	C3B-C2B	-4.32	1.43	1.53
3	A	502	NAP	C3B-C2B	-4.30	1.43	1.53
2	D	501	FDA	C10-N1	4.29	1.44	1.37
2	B	501	FDA	C2-N3	4.27	1.44	1.37
2	A	501	FDA	C2B-C3B	-4.25	1.41	1.53
2	C	501	FDA	C10-N1	4.20	1.44	1.37
2	C	501	FDA	C2-N1	4.17	1.44	1.37
2	B	501	FDA	C10-N1	4.17	1.44	1.37
2	B	501	FDA	C9A-N10	-4.17	1.33	1.41
2	D	501	FDA	C2-N1	4.14	1.44	1.37
2	A	501	FDA	PA-O3P	-4.14	1.55	1.59
3	B	502	NAP	C2D-C3D	-4.13	1.42	1.53
2	D	501	FDA	C2B-C3B	-4.12	1.42	1.53
3	C	502	NAP	C2D-C3D	-4.07	1.42	1.53
3	D	502	NAP	C2D-C3D	-4.07	1.42	1.53
2	D	501	FDA	C2-N3	4.05	1.44	1.37
3	D	502	NAP	PN-O3	-4.05	1.55	1.59
2	B	501	FDA	C2B-C3B	-4.02	1.42	1.53
2	B	501	FDA	C2-N1	4.01	1.44	1.37
3	D	502	NAP	C3B-C2B	-4.00	1.44	1.53
3	C	502	NAP	C7N-N7N	3.99	1.40	1.33
2	A	501	FDA	C9A-N10	-3.99	1.34	1.41
3	A	502	NAP	C2D-C3D	-3.97	1.42	1.53
2	D	501	FDA	C9A-N10	-3.96	1.34	1.41
2	C	501	FDA	C2B-C3B	-3.95	1.42	1.53
3	A	502	NAP	C7N-N7N	3.94	1.40	1.33
2	C	501	FDA	C2-N3	3.93	1.44	1.37
2	A	501	FDA	C2-N3	3.89	1.43	1.37
2	C	501	FDA	C9A-N10	-3.85	1.34	1.41
2	D	501	FDA	O3'-C3'	-3.85	1.33	1.43
2	A	501	FDA	O3'-C3'	-3.84	1.33	1.43
2	C	501	FDA	O3'-C3'	-3.81	1.33	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	502	NAP	C7N-N7N	3.81	1.40	1.33
3	D	502	NAP	P2B-O3X	-3.69	1.41	1.54
3	B	502	NAP	C7N-N7N	3.66	1.39	1.33
3	D	502	NAP	PN-O2N	-3.47	1.39	1.55
2	B	501	FDA	O3'-C3'	-3.44	1.34	1.43
2	B	501	FDA	O2'-C2'	-3.27	1.36	1.43
2	A	501	FDA	C5X-N5	-3.27	1.34	1.39
2	B	501	FDA	PA-O3P	-3.27	1.56	1.59
2	C	501	FDA	C5X-N5	-3.22	1.34	1.39
3	D	502	NAP	PA-O3	-3.18	1.56	1.59
2	D	501	FDA	O4'-C4'	-3.18	1.36	1.43
2	A	501	FDA	O2'-C2'	-3.15	1.36	1.43
2	C	501	FDA	O4'-C4'	-3.13	1.36	1.43
2	B	501	FDA	O4'-C4'	-3.12	1.36	1.43
2	C	501	FDA	PA-O3P	-3.10	1.56	1.59
2	D	501	FDA	O2'-C2'	-3.10	1.36	1.43
3	D	502	NAP	P2B-O2X	-3.10	1.43	1.54
2	A	501	FDA	O4'-C4'	-3.06	1.36	1.43
2	C	501	FDA	O2'-C2'	-3.03	1.37	1.43
2	D	501	FDA	C5X-N5	-3.03	1.34	1.39
2	B	501	FDA	C5X-N5	-2.99	1.34	1.39
2	C	501	FDA	P-O3P	2.94	1.62	1.59
3	D	502	NAP	PA-O1A	-2.91	1.40	1.50
2	B	501	FDA	PA-O1A	2.89	1.60	1.50
3	D	502	NAP	PN-O1N	-2.89	1.40	1.50
3	D	502	NAP	PA-O2A	-2.78	1.42	1.55
3	D	502	NAP	P2B-O1X	-2.78	1.41	1.50
2	C	501	FDA	PA-O1A	2.74	1.60	1.50
2	A	501	FDA	C5X-C9A	-2.59	1.37	1.40
2	A	501	FDA	PA-O1A	2.56	1.59	1.50
3	B	502	NAP	O4D-C4D	-2.55	1.39	1.45
3	C	502	NAP	O4D-C4D	-2.52	1.39	1.45
2	D	501	FDA	C1'-C2'	-2.51	1.49	1.52
3	D	502	NAP	O4D-C4D	-2.50	1.39	1.45
2	C	501	FDA	C8A-N7A	2.50	1.36	1.31
2	A	501	FDA	O4B-C1B	-2.48	1.36	1.42
2	D	501	FDA	O4B-C1B	-2.48	1.36	1.42
2	D	501	FDA	PA-O1A	2.47	1.59	1.50
2	A	501	FDA	C1'-C2'	-2.45	1.49	1.52
2	B	501	FDA	C1'-N10	2.44	1.53	1.47
2	C	501	FDA	C5X-C9A	-2.43	1.37	1.40
2	C	501	FDA	C1'-N10	2.42	1.53	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	FDA	C1'-C2'	-2.40	1.49	1.52
3	A	502	NAP	O4D-C4D	-2.40	1.39	1.45
2	C	501	FDA	C1'-C2'	-2.39	1.49	1.52
2	B	501	FDA	O4B-C1B	-2.38	1.36	1.42
2	C	501	FDA	O4B-C1B	-2.38	1.36	1.42
2	B	501	FDA	C8A-N7A	2.35	1.36	1.31
2	A	501	FDA	C1'-N10	2.35	1.53	1.47
2	B	501	FDA	P-O3P	2.32	1.62	1.59
2	D	501	FDA	C8A-N7A	2.31	1.36	1.31
2	B	501	FDA	C4X-C4	2.30	1.48	1.41
3	D	502	NAP	C5A-N7A	-2.30	1.34	1.39
2	A	501	FDA	C4X-C4	2.27	1.48	1.41
3	D	502	NAP	PA-O5B	-2.25	1.50	1.59
3	C	502	NAP	C5A-N7A	-2.23	1.35	1.39
2	D	501	FDA	C1'-N10	2.19	1.53	1.47
3	A	502	NAP	C8A-N7A	2.16	1.35	1.31
2	D	501	FDA	C4X-C4	2.14	1.48	1.41
2	A	501	FDA	C8A-N7A	2.13	1.35	1.31
2	D	501	FDA	C1B-N9A	-2.11	1.40	1.46
2	C	501	FDA	C4X-C4	2.11	1.48	1.41
3	B	502	NAP	C5A-N7A	-2.11	1.35	1.39
2	D	501	FDA	C5A-N7A	-2.11	1.35	1.39
2	A	501	FDA	C1B-N9A	-2.05	1.40	1.46
2	A	501	FDA	C5A-N7A	-2.02	1.35	1.39
2	B	501	FDA	C5X-C9A	-2.00	1.38	1.40

All (127) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	FDA	O3P-PA-O1A	-9.57	81.92	110.70
2	C	501	FDA	O3P-PA-O1A	-9.44	82.32	110.70
2	B	501	FDA	O2A-PA-O3P	-8.65	83.90	107.27
2	C	501	FDA	O2A-PA-O3P	-8.57	84.12	107.27
2	B	501	FDA	O5'-P-O1P	-7.13	80.67	108.94
2	C	501	FDA	O5'-P-O1P	-6.94	81.45	108.94
3	D	502	NAP	C5A-C4A-N3A	-5.72	118.84	126.72
2	C	501	FDA	O2P-P-O5'	-5.27	83.70	107.57
3	C	502	NAP	C5A-C4A-N3A	-5.25	119.49	126.72
3	A	502	NAP	N3A-C2A-N1A	-5.23	120.66	128.58
2	B	501	FDA	O2P-P-O5'	-5.03	84.79	107.57
3	A	502	NAP	C5A-C4A-N3A	-5.01	119.81	126.72
3	B	502	NAP	N3A-C2A-N1A	-4.96	121.08	128.58

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	502	NAP	C5A-C4A-N3A	-4.90	119.97	126.72
2	C	501	FDA	O2P-P-O3P	4.82	120.31	107.27
2	D	501	FDA	C4-N3-C2	-4.78	119.78	126.37
3	D	502	NAP	N3A-C2A-N1A	-4.78	121.34	128.58
2	A	501	FDA	N3A-C2A-N1A	-4.65	121.54	128.58
2	C	501	FDA	N3A-C2A-N1A	-4.65	121.54	128.58
2	C	501	FDA	C4-N3-C2	-4.62	120.01	126.37
2	A	501	FDA	C4-N3-C2	-4.60	120.03	126.37
2	B	501	FDA	C4-N3-C2	-4.54	120.12	126.37
3	C	502	NAP	N3A-C2A-N1A	-4.53	121.73	128.58
2	B	501	FDA	O3P-P-O1P	4.45	124.10	110.70
2	A	501	FDA	C5A-C4A-N3A	-4.45	120.59	126.72
2	B	501	FDA	O2P-P-O3P	4.41	119.18	107.27
2	D	501	FDA	N3A-C2A-N1A	-4.37	121.96	128.58
2	B	501	FDA	N3A-C2A-N1A	-4.34	122.01	128.58
2	C	501	FDA	C5A-C4A-N3A	-4.23	120.89	126.72
2	C	501	FDA	O3P-P-O1P	4.14	123.17	110.70
2	B	501	FDA	C5A-C4A-N3A	-4.13	121.03	126.72
2	D	501	FDA	C5A-C4A-N3A	-3.97	121.25	126.72
3	D	502	NAP	N3A-C4A-N9A	3.86	133.73	127.17
2	D	501	FDA	N9A-C8A-N7A	-3.84	108.49	113.94
2	A	501	FDA	N9A-C8A-N7A	-3.65	108.76	113.94
3	D	502	NAP	C2A-N3A-C4A	3.63	120.70	111.83
3	A	502	NAP	C2A-N3A-C4A	3.63	120.69	111.83
3	C	502	NAP	N3A-C4A-N9A	3.58	133.26	127.17
2	C	501	FDA	N9A-C8A-N7A	-3.57	108.86	113.94
3	B	502	NAP	N9A-C8A-N7A	-3.50	108.97	113.94
2	B	501	FDA	N9A-C8A-N7A	-3.45	109.04	113.94
3	B	502	NAP	N3A-C4A-N9A	3.45	133.03	127.17
2	C	501	FDA	O5B-C5B-C4B	3.35	120.41	108.99
3	D	502	NAP	N9A-C8A-N7A	-3.30	109.25	113.94
3	A	502	NAP	N9A-C8A-N7A	-3.30	109.25	113.94
3	B	502	NAP	C2A-N3A-C4A	3.27	119.81	111.83
3	C	502	NAP	C2A-N3A-C4A	3.25	119.78	111.83
2	A	501	FDA	C2A-N3A-C4A	3.25	119.77	111.83
2	D	501	FDA	O4-C4-C4X	-3.21	119.53	127.26
3	C	502	NAP	N9A-C8A-N7A	-3.20	109.40	113.94
2	C	501	FDA	C2A-N3A-C4A	3.19	119.63	111.83
3	A	502	NAP	N3A-C4A-N9A	3.16	132.54	127.17
2	D	501	FDA	O2P-P-O3P	3.11	115.69	107.27
2	C	501	FDA	O4-C4-C4X	-3.09	119.82	127.26
2	D	501	FDA	C4A-N9A-C8A	3.08	108.97	105.74

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	FDA	O5B-PA-O1A	3.06	121.07	108.94
2	A	501	FDA	N3A-C4A-N9A	3.00	132.27	127.17
2	B	501	FDA	C2A-N3A-C4A	3.00	119.15	111.83
2	C	501	FDA	O5B-PA-O1A	3.00	120.81	108.94
2	B	501	FDA	N3-C2-N1	2.96	120.40	115.74
2	B	501	FDA	O5B-C5B-C4B	2.94	119.00	108.99
3	A	502	NAP	C4D-O4D-C1D	-2.93	107.24	109.92
2	D	501	FDA	C4X-C4-N3	2.92	120.15	112.13
2	D	501	FDA	C2A-N3A-C4A	2.90	118.92	111.83
2	A	501	FDA	O4-C4-C4X	-2.88	120.32	127.26
2	D	501	FDA	C5A-N7A-C8A	2.88	107.97	103.45
3	B	502	NAP	C2B-C1B-N9A	2.88	118.49	113.75
2	D	501	FDA	C4A-C5A-N7A	-2.87	107.30	110.58
2	D	501	FDA	N3-C2-N1	2.84	120.20	115.74
2	A	501	FDA	C4X-C4-N3	2.83	119.89	112.13
3	A	502	NAP	O5D-C5D-C4D	2.82	118.58	108.99
2	C	501	FDA	N3-C2-N1	2.82	120.17	115.74
2	C	501	FDA	C4A-C5A-N7A	-2.81	107.37	110.58
2	A	501	FDA	C5A-N7A-C8A	2.81	107.86	103.45
3	C	502	NAP	C3N-C7N-N7N	2.80	121.19	117.74
3	D	502	NAP	C4D-O4D-C1D	-2.79	107.37	109.92
2	B	501	FDA	C4A-N9A-C8A	2.79	108.67	105.74
2	C	501	FDA	C5A-N7A-C8A	2.78	107.82	103.45
2	A	501	FDA	O5'-C5'-C4'	2.78	116.78	109.36
2	B	501	FDA	C4X-C4-N3	2.77	119.74	112.13
3	B	502	NAP	C4D-O4D-C1D	-2.77	107.39	109.92
3	D	502	NAP	C5A-N7A-C8A	2.76	107.79	103.45
2	A	501	FDA	C4A-N9A-C8A	2.76	108.63	105.74
2	C	501	FDA	C4X-C4-N3	2.75	119.69	112.13
2	B	501	FDA	O4-C4-C4X	-2.73	120.67	127.26
3	B	502	NAP	O5D-C5D-C4D	2.71	118.22	108.99
2	A	501	FDA	N3-C2-N1	2.71	119.99	115.74
2	B	501	FDA	N3A-C4A-N9A	2.70	131.76	127.17
3	B	502	NAP	C4A-N9A-C8A	2.67	108.55	105.74
2	A	501	FDA	C4A-C5A-N7A	-2.60	107.61	110.58
2	C	501	FDA	N3A-C4A-N9A	2.60	131.59	127.17
2	B	501	FDA	O5'-C5'-C4'	2.59	116.27	109.36
2	B	501	FDA	C4A-C5A-N7A	-2.59	107.62	110.58
3	C	502	NAP	C5A-N7A-C8A	2.58	107.51	103.45
3	D	502	NAP	C4A-C5A-N7A	-2.57	107.64	110.58
3	B	502	NAP	C5A-N7A-C8A	2.56	107.48	103.45
2	C	501	FDA	C4A-N9A-C8A	2.56	108.42	105.74

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	FDA	C5A-N7A-C8A	2.55	107.46	103.45
2	D	501	FDA	N3A-C4A-N9A	2.54	131.49	127.17
3	C	502	NAP	O5D-C5D-C4D	2.54	117.63	108.99
3	C	502	NAP	C4A-C5A-N7A	-2.52	107.70	110.58
3	A	502	NAP	C2B-C1B-N9A	2.51	117.89	113.75
2	C	501	FDA	C2'-C1'-N10	2.46	121.81	110.20
2	D	501	FDA	O5'-C5'-C4'	2.41	115.80	109.36
3	B	502	NAP	O4B-C4B-C5B	2.39	116.98	109.33
3	A	502	NAP	C4A-C5A-N7A	-2.36	107.88	110.58
3	D	502	NAP	O4B-C4B-C5B	2.35	116.87	109.33
2	C	501	FDA	O3'-C3'-C2'	-2.35	103.58	108.93
3	A	502	NAP	C4A-N9A-C8A	2.32	108.17	105.74
2	C	501	FDA	O2A-PA-O5B	2.30	118.00	107.57
3	C	502	NAP	O4B-C4B-C5B	2.30	116.70	109.33
3	A	502	NAP	C5A-N7A-C8A	2.29	107.05	103.45
3	C	502	NAP	C4A-N9A-C8A	2.28	108.14	105.74
3	B	502	NAP	O2A-PA-O3	2.28	113.43	107.27
3	B	502	NAP	C4A-C5A-N7A	-2.25	108.01	110.58
2	B	501	FDA	C4-C4X-N5	2.25	122.12	116.37
3	D	502	NAP	O4B-C1B-N9A	2.24	112.39	108.09
2	A	501	FDA	O2P-P-O3P	2.18	113.17	107.27
2	A	501	FDA	O4B-C4B-C5B	2.18	116.30	109.33
3	A	502	NAP	C3N-C7N-N7N	2.13	120.37	117.74
2	B	501	FDA	O4B-C4B-C5B	2.12	116.12	109.33
3	D	502	NAP	C2B-C1B-N9A	2.11	117.22	113.75
2	B	501	FDA	O2A-PA-O5B	2.08	116.98	107.57
2	B	501	FDA	C1'-C2'-C3'	2.05	115.22	109.66
3	D	502	NAP	C4A-N9A-C8A	2.04	107.88	105.74
3	C	502	NAP	C4D-O4D-C1D	-2.03	108.06	109.92
3	D	502	NAP	O3-PA-O1A	2.01	116.76	110.70

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	FDA	C5'-O5'-P-O1P
2	B	501	FDA	C5B-O5B-PA-O3P
2	C	501	FDA	C5B-O5B-PA-O3P
2	D	501	FDA	C5'-O5'-P-O1P
2	A	501	FDA	O4B-C4B-C5B-O5B
2	B	501	FDA	O4B-C4B-C5B-O5B
2	C	501	FDA	O4B-C4B-C5B-O5B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	D	501	FDA	O4'-C4'-C5'-O5'
2	A	501	FDA	C3B-C4B-C5B-O5B
2	B	501	FDA	C3B-C4B-C5B-O5B
2	C	501	FDA	C3B-C4B-C5B-O5B
2	B	501	FDA	O3'-C3'-C4'-C5'
2	B	501	FDA	C2'-C3'-C4'-C5'
2	D	501	FDA	O4B-C4B-C5B-O5B
2	A	501	FDA	C3'-C4'-C5'-O5'
2	D	501	FDA	C3'-C4'-C5'-O5'
2	C	501	FDA	C2'-C3'-C4'-C5'
2	D	501	FDA	C2'-C3'-C4'-C5'
2	B	501	FDA	P-O3P-PA-O5B
2	C	501	FDA	P-O3P-PA-O5B
2	C	501	FDA	O3'-C3'-C4'-C5'
2	B	501	FDA	C2'-C3'-C4'-O4'
3	B	502	NAP	PN-O3-PA-O1A
3	D	502	NAP	C2B-O2B-P2B-O1X
2	A	501	FDA	C2'-C3'-C4'-C5'
2	B	501	FDA	O3'-C3'-C4'-O4'
3	C	502	NAP	PN-O3-PA-O1A
2	D	501	FDA	C3B-C4B-C5B-O5B
3	B	502	NAP	C2B-O2B-P2B-O3X
2	C	501	FDA	C3'-C4'-C5'-O5'
2	B	501	FDA	C4B-C5B-O5B-PA
3	A	502	NAP	C2B-O2B-P2B-O1X
2	A	501	FDA	O4'-C4'-C5'-O5'
2	B	501	FDA	C3'-C4'-C5'-O5'
2	C	501	FDA	C4B-C5B-O5B-PA
3	C	502	NAP	C2B-C1B-N9A-C8A
3	C	502	NAP	O4B-C4B-C5B-O5B
3	B	502	NAP	C2B-O2B-P2B-O2X
3	A	502	NAP	O4B-C4B-C5B-O5B
3	C	502	NAP	O4B-C1B-N9A-C8A
3	D	502	NAP	C2B-C1B-N9A-C8A

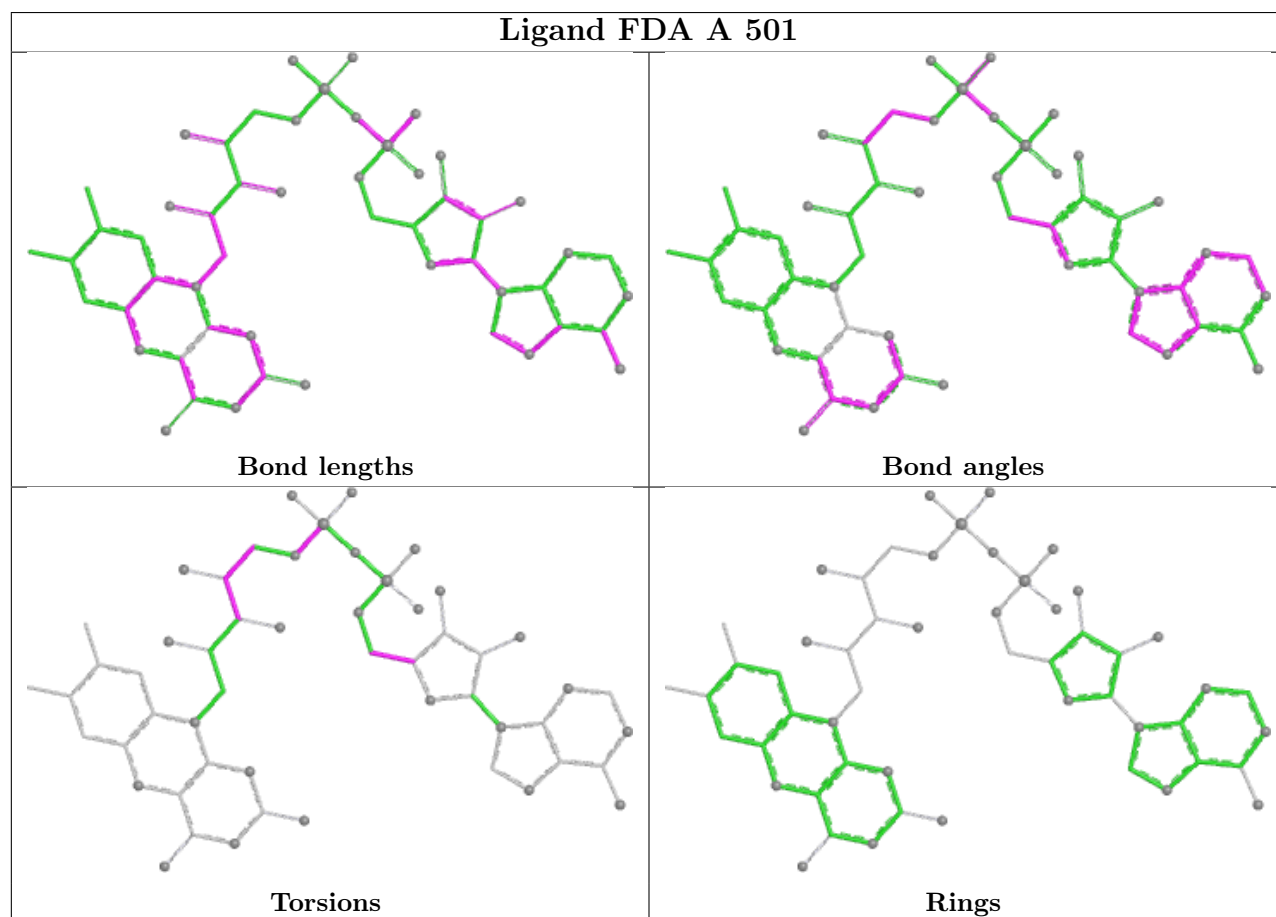
There are no ring outliers.

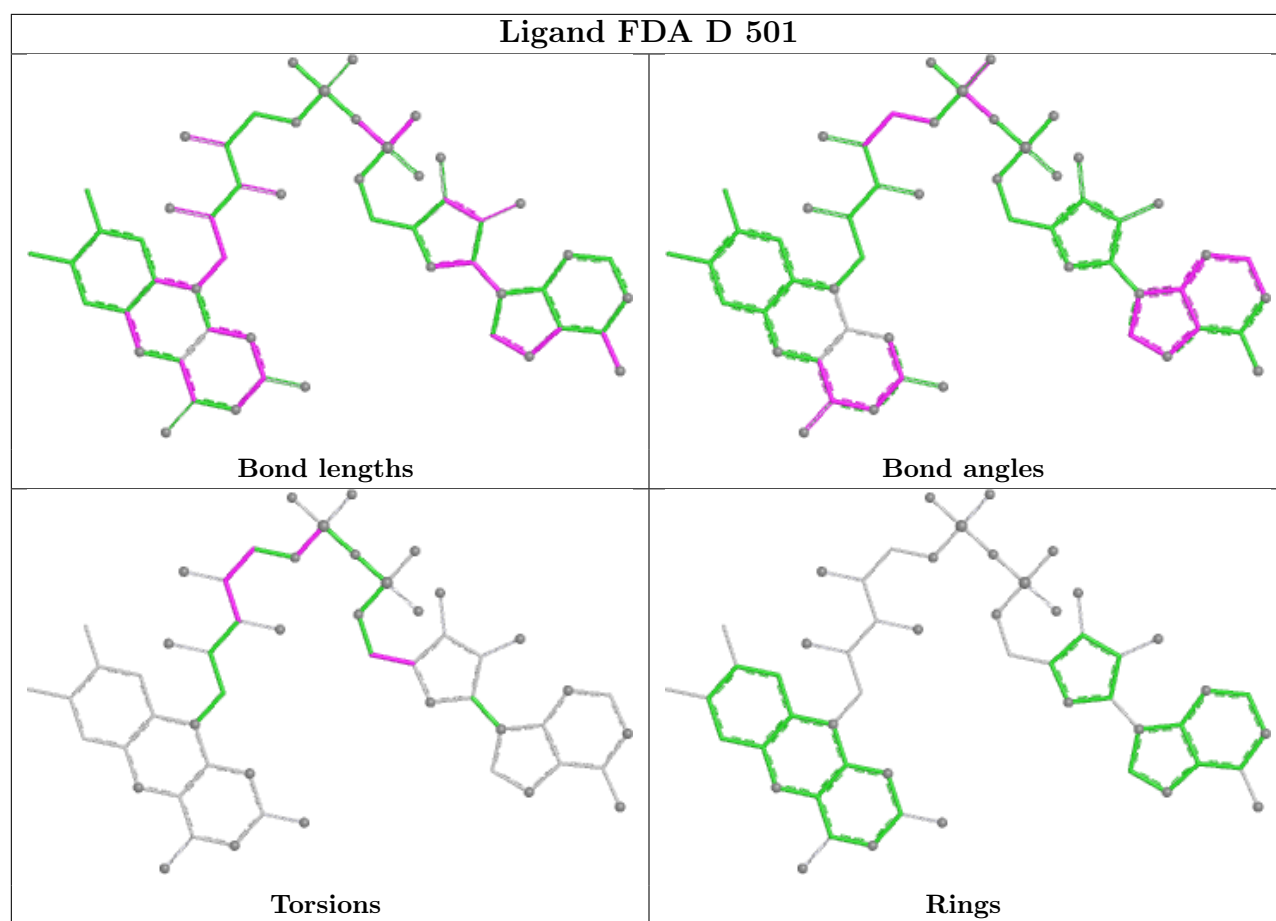
1 monomer is involved in 2 short contacts:

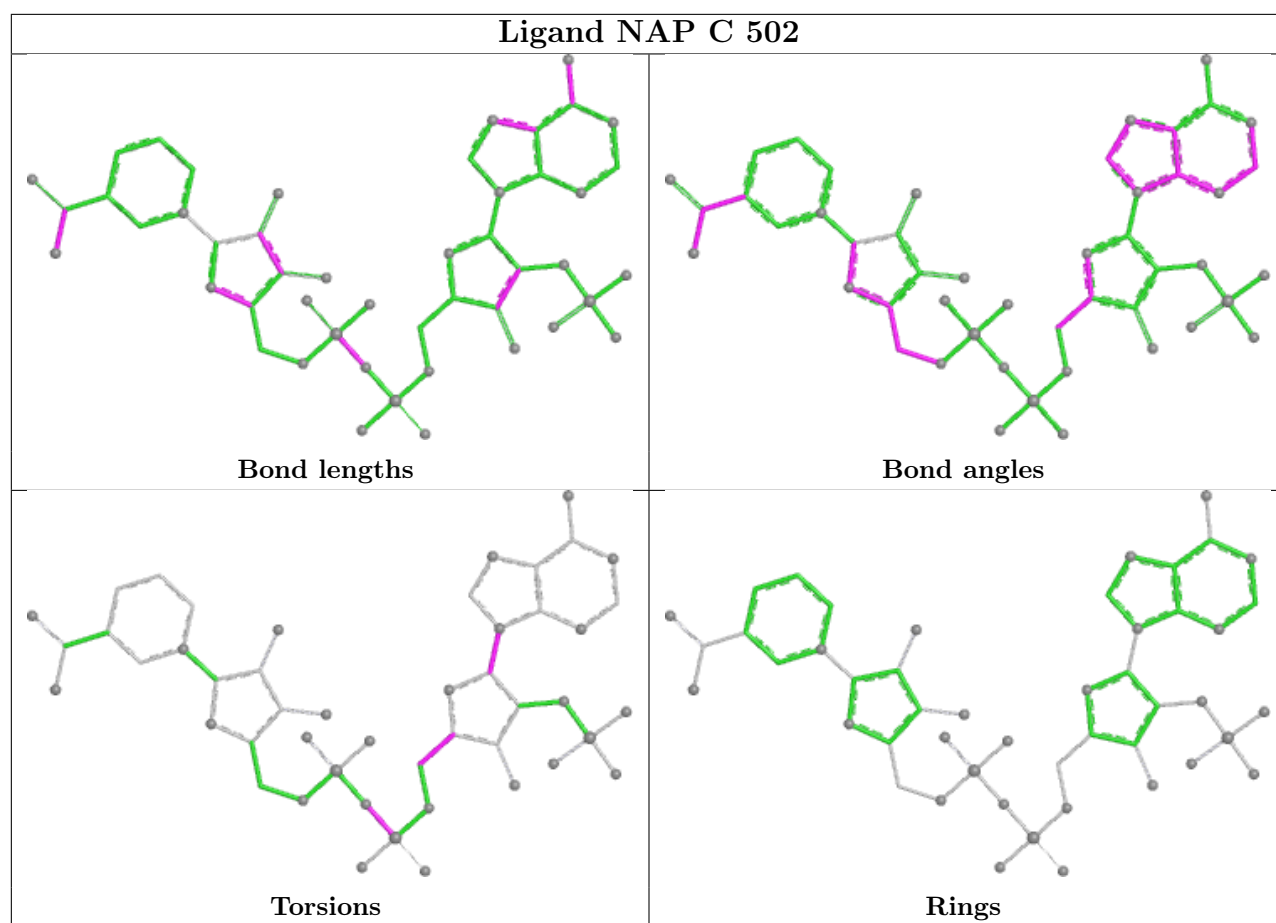
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	FDA	2	0

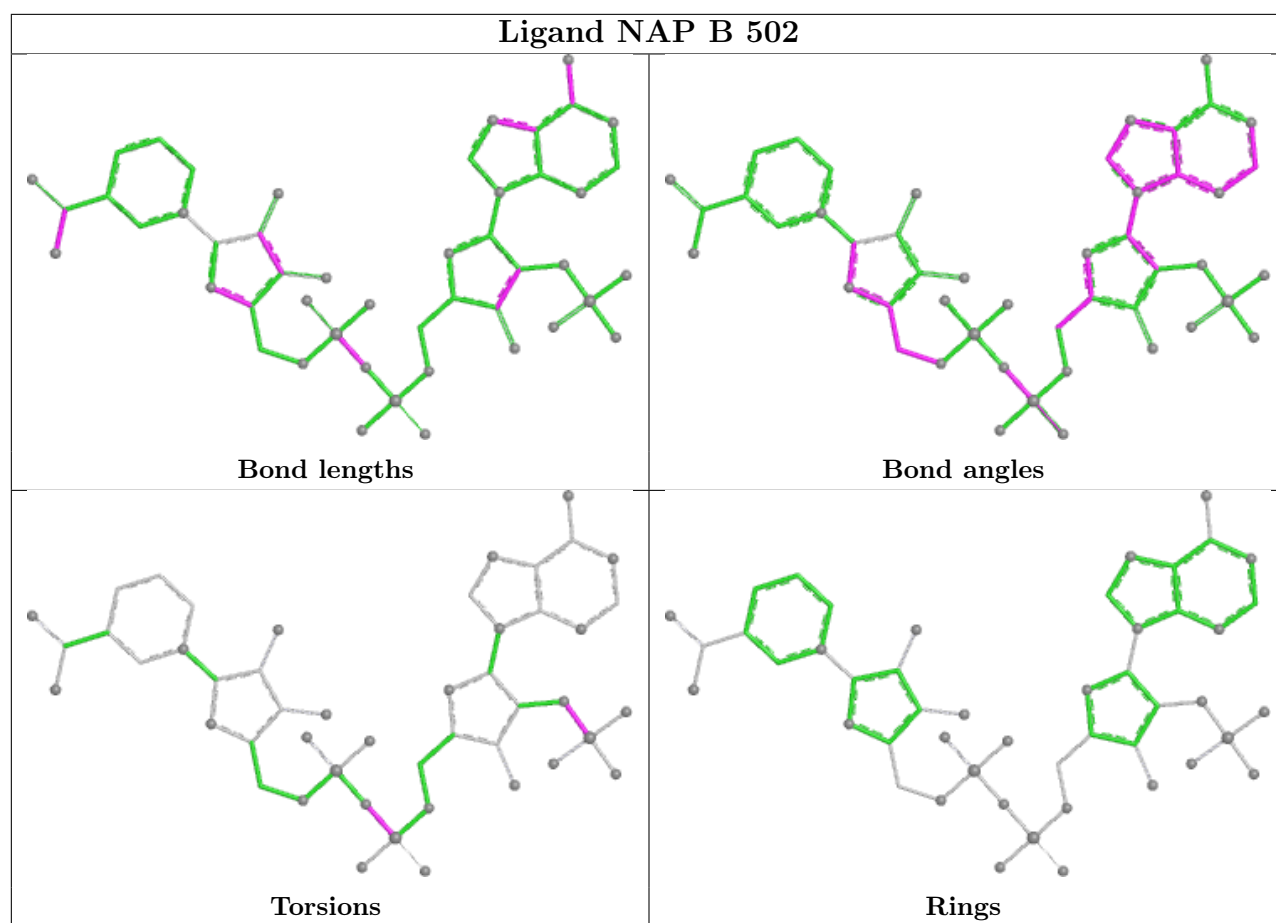
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

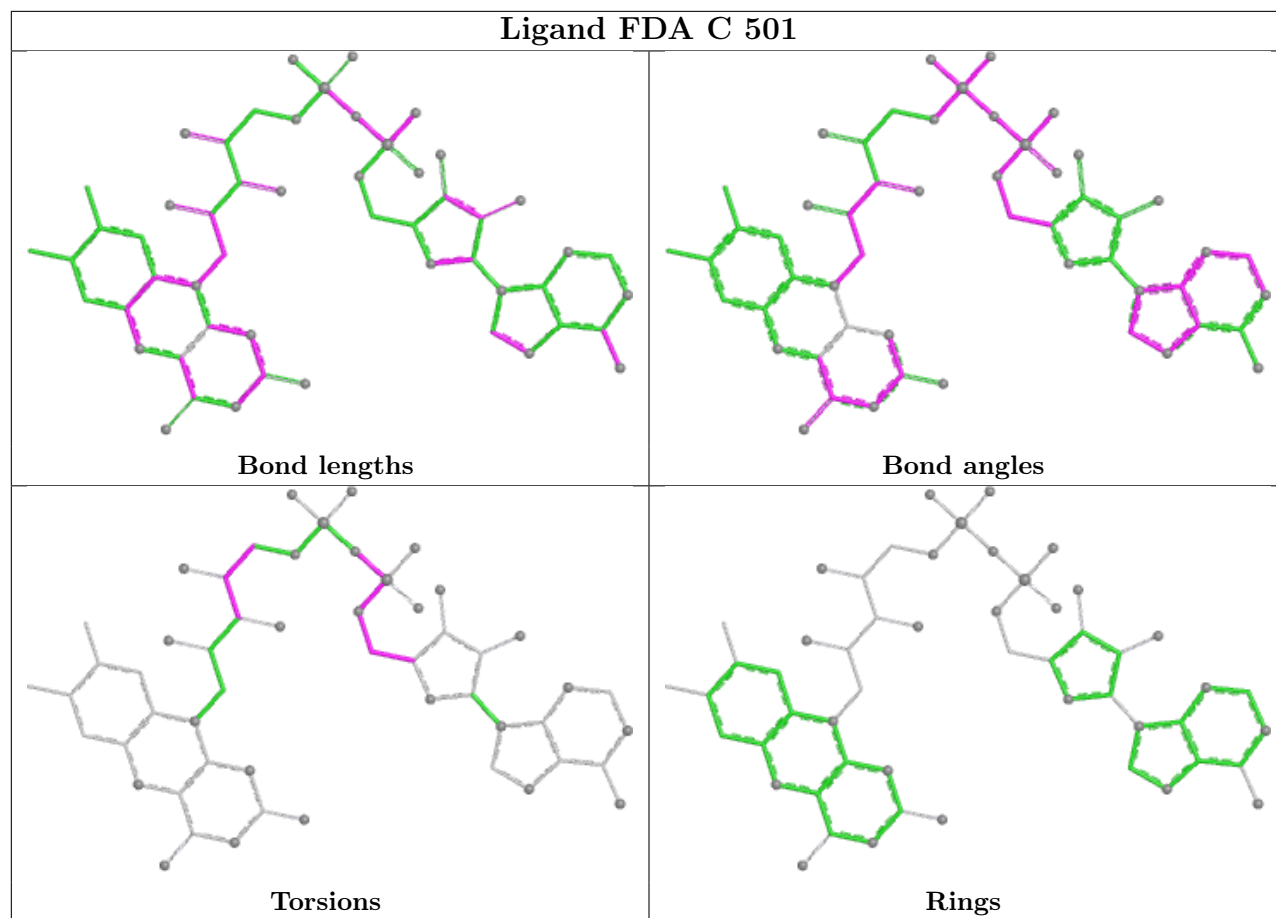
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within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

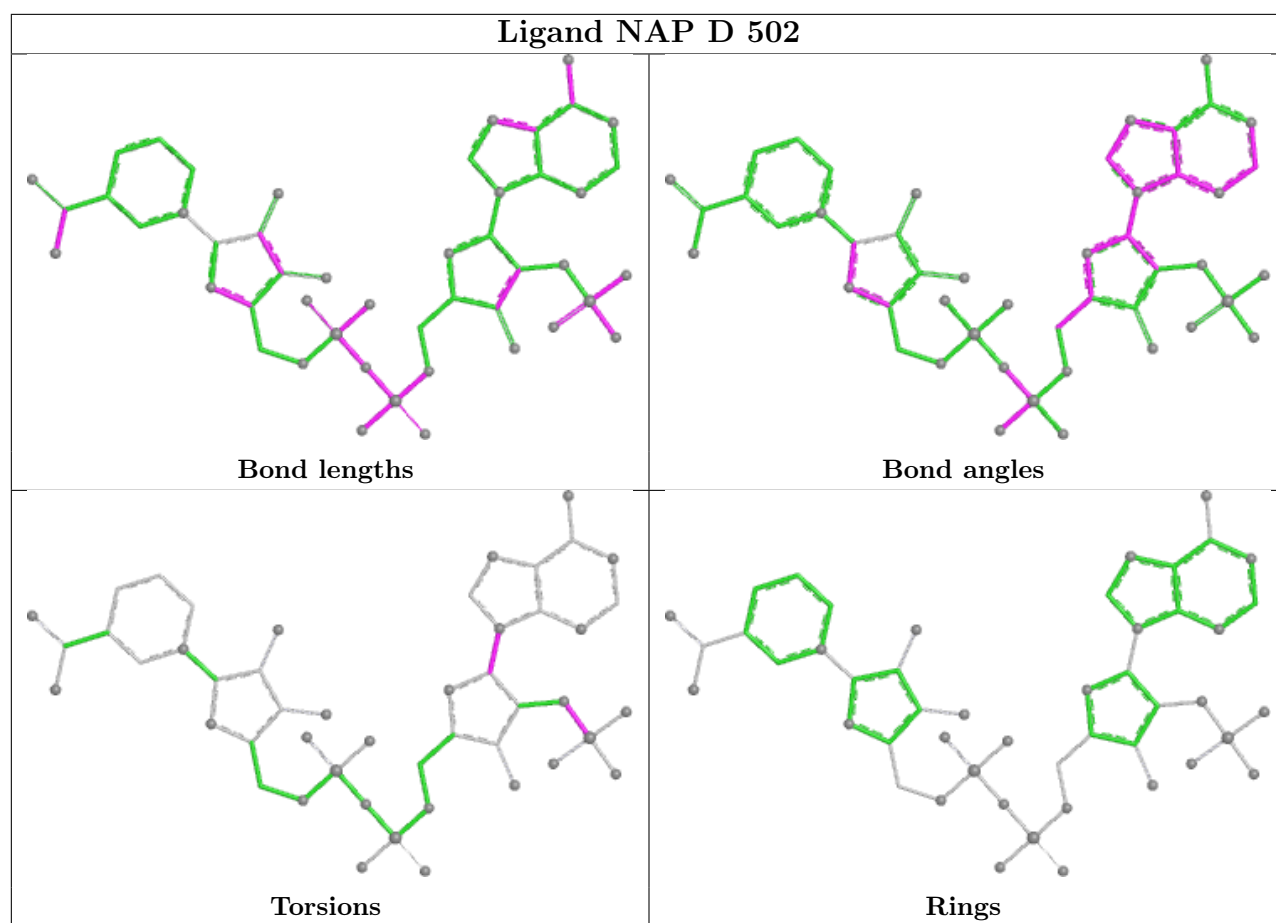


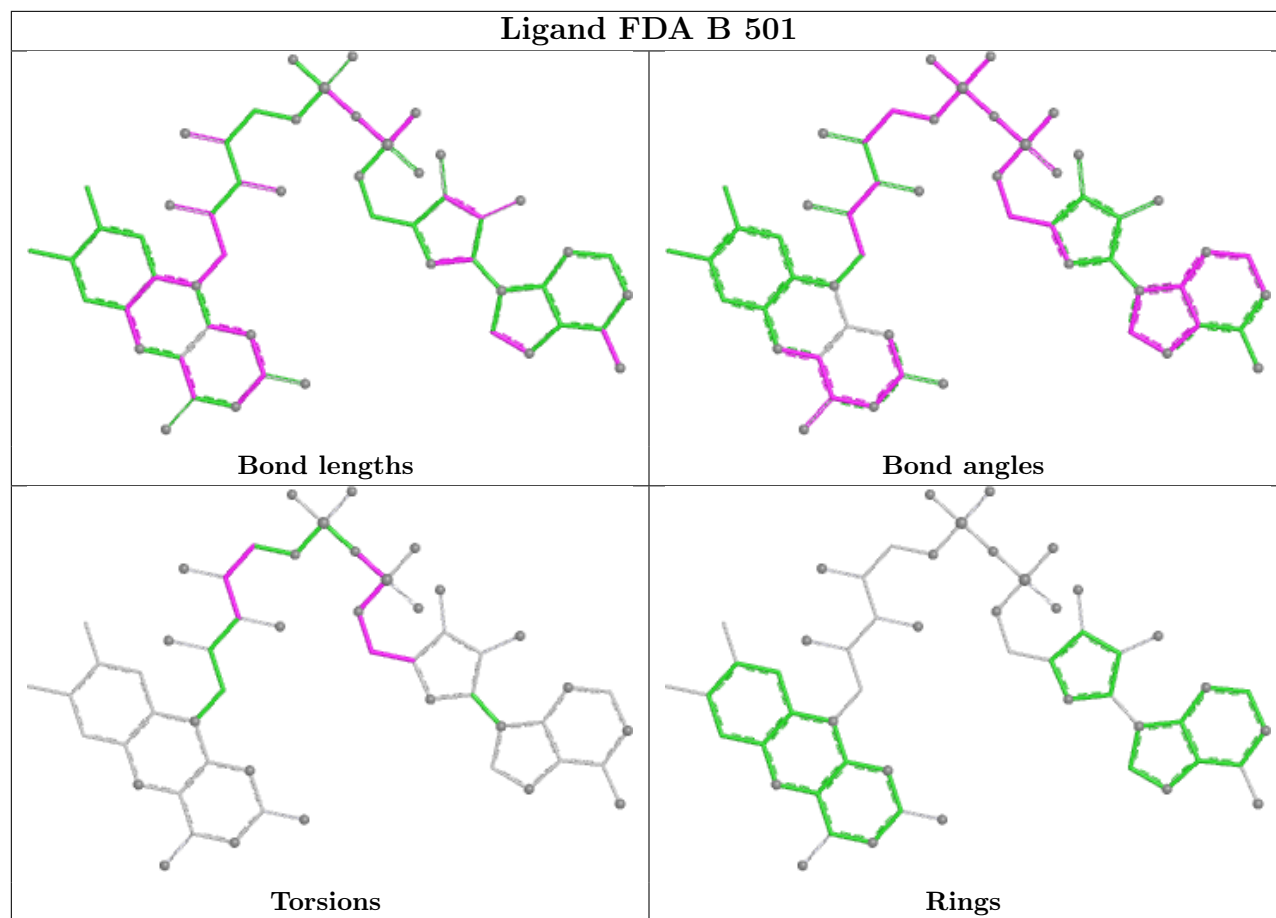


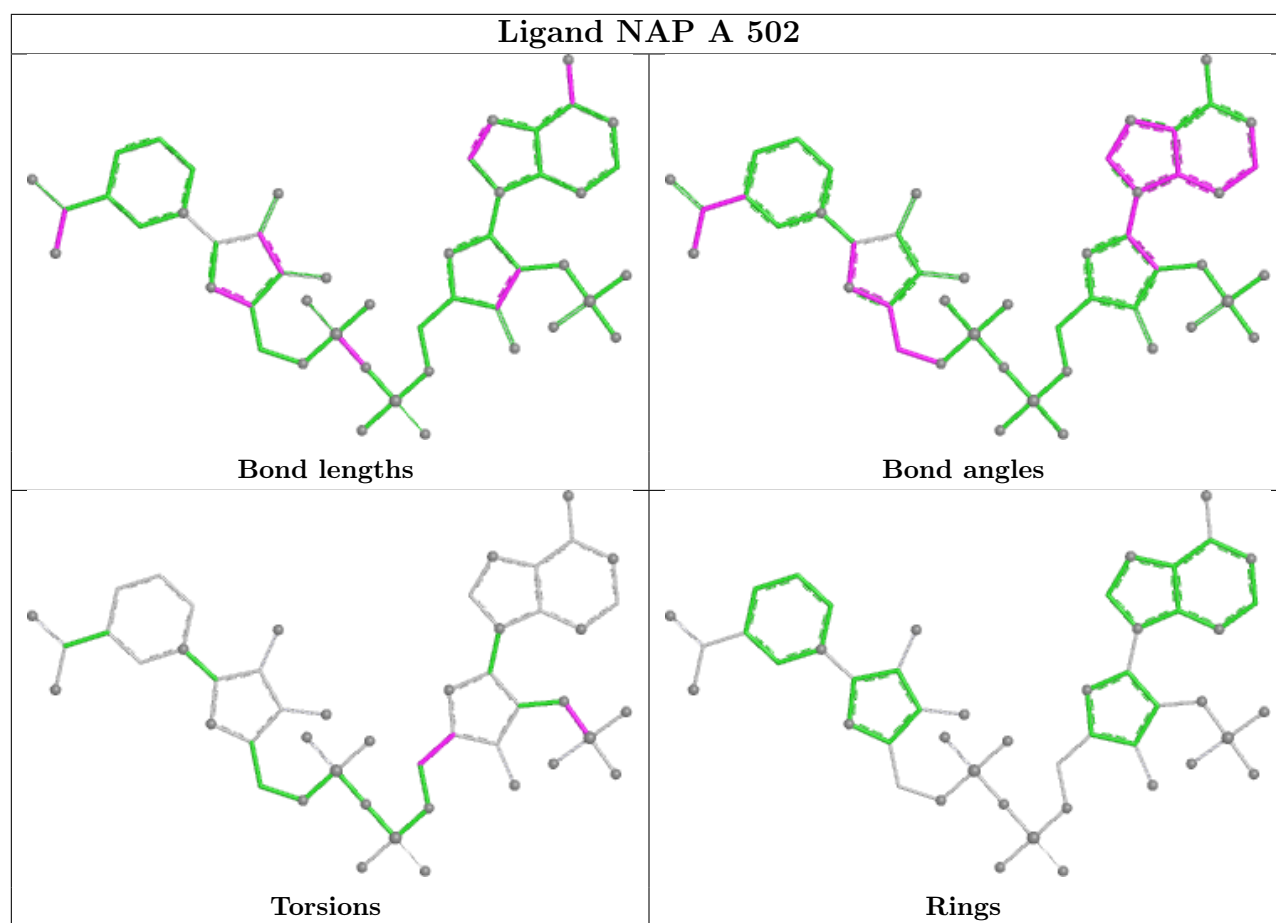












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	414/443 (93%)	0.18	15 (3%) 46 42	17, 28, 51, 81	0
1	B	414/443 (93%)	0.18	16 (3%) 43 39	18, 29, 54, 82	0
1	C	414/443 (93%)	0.23	24 (5%) 29 25	17, 29, 57, 74	0
1	D	414/443 (93%)	0.21	21 (5%) 33 30	19, 29, 54, 82	0
All	All	1656/1772 (93%)	0.20	76 (4%) 37 33	17, 29, 55, 82	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	138	PRO	6.3
1	D	10	PRO	5.2
1	C	10	PRO	4.8
1	B	194	ASP	4.6
1	B	195	PRO	4.4
1	D	135	PRO	4.4
1	D	196	ARG	4.0
1	A	196	ARG	3.8
1	B	192	ASP	3.6
1	A	10	PRO	3.6
1	D	356	GLY	3.5
1	C	366	ALA	3.4
1	B	220	ASN	3.4
1	B	120	HIS	3.4
1	A	194	ASP	3.4
1	A	195	PRO	3.3
1	A	197	SER	3.2
1	B	318	ASP	3.1
1	A	273	ASN	3.1
1	A	136	GLY	3.0
1	D	194	ASP	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	196	ARG	2.9
1	D	357	GLU	2.8
1	C	192	ASP	2.8
1	C	358	LEU	2.8
1	D	197	SER	2.8
1	B	353	ASP	2.7
1	C	356	GLY	2.7
1	D	195	PRO	2.7
1	C	196	ARG	2.7
1	A	193	ARG	2.7
1	A	244	ALA	2.6
1	C	382	PRO	2.6
1	B	151	ALA	2.6
1	C	365	ASP	2.6
1	D	220	ASN	2.6
1	D	353	ASP	2.6
1	D	136	GLY	2.6
1	B	198	LEU	2.5
1	C	150	GLU	2.5
1	C	357	GLU	2.5
1	C	355	LEU	2.5
1	C	151	ALA	2.5
1	D	386	CYS	2.5
1	C	188	ASP	2.5
1	D	133	PRO	2.5
1	B	149	PRO	2.4
1	A	223	ASP	2.4
1	D	36	ALA	2.4
1	D	150	GLU	2.4
1	C	134	GLY	2.3
1	C	135	PRO	2.3
1	C	137	ARG	2.3
1	B	309	HIS	2.3
1	A	385	ARG	2.3
1	C	152	THR	2.2
1	C	120	HIS	2.2
1	A	137	ARG	2.2
1	B	191	ARG	2.2
1	B	10	PRO	2.2
1	C	149	PRO	2.2
1	B	119	ALA	2.2
1	D	140	ASP	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	193	ARG	2.1
1	C	133	PRO	2.1
1	D	366	ALA	2.1
1	C	131	ILE	2.1
1	C	384	LEU	2.1
1	D	160	ILE	2.1
1	D	358	LEU	2.1
1	D	138	PRO	2.1
1	A	36	ALA	2.1
1	C	318	ASP	2.1
1	A	173	GLY	2.1
1	B	148	THR	2.0
1	A	386	CYS	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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
4	BR	C	509	1/1	0.91	0.08	53,53,53,53	1
4	BR	A	508	1/1	0.93	0.10	44,44,44,44	1
4	BR	D	510	1/1	0.94	0.06	47,47,47,47	1
4	BR	D	511	1/1	0.94	0.05	52,52,52,52	1
4	BR	D	512	1/1	0.95	0.08	47,47,47,47	1
4	BR	D	513	1/1	0.95	0.06	34,34,34,34	1
4	BR	C	508	1/1	0.96	0.07	41,41,41,41	1
2	FDA	D	501	53/53	0.96	0.06	16,21,29,30	0
4	BR	B	509	1/1	0.96	0.05	31,31,31,31	1
4	BR	B	505	1/1	0.97	0.06	43,43,43,43	1

Continued on next page...

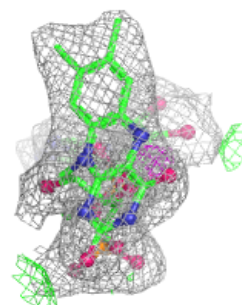
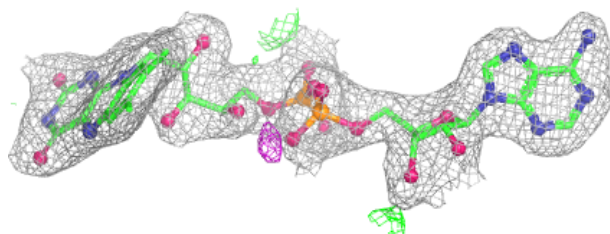
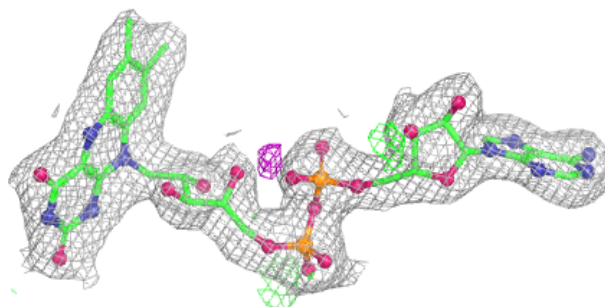
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	BR	B	508	1/1	0.97	0.07	41,41,41,41	1
2	FDA	B	501	53/53	0.97	0.06	16,21,26,27	0
3	NAP	B	502	48/48	0.97	0.06	17,21,27,31	0
3	NAP	C	502	48/48	0.97	0.06	15,19,24,27	0
4	BR	D	507	1/1	0.97	0.05	41,41,41,41	1
3	NAP	D	502	48/48	0.97	0.06	17,21,26,35	0
4	BR	A	503	1/1	0.97	0.04	29,29,29,29	1
2	FDA	C	501	53/53	0.97	0.06	13,22,33,34	0
4	BR	A	510	1/1	0.97	0.07	52,52,52,52	1
3	NAP	A	502	48/48	0.98	0.05	16,20,24,30	0
4	BR	A	505	1/1	0.98	0.07	42,42,42,42	1
4	BR	D	503	1/1	0.98	0.05	48,48,48,48	1
4	BR	D	504	1/1	0.98	0.05	40,40,40,40	1
4	BR	D	506	1/1	0.98	0.09	36,36,36,36	1
4	BR	B	506	1/1	0.98	0.08	32,32,32,32	1
4	BR	A	507	1/1	0.98	0.07	33,33,33,33	1
2	FDA	A	501	53/53	0.98	0.05	14,21,26,28	0
4	BR	C	503	1/1	0.98	0.05	37,37,37,37	1
4	BR	C	505	1/1	0.98	0.05	36,36,36,36	1
4	BR	D	514	1/1	0.98	0.04	29,29,29,29	1
4	BR	A	511	1/1	0.99	0.06	32,32,32,32	1
4	BR	B	503	1/1	0.99	0.11	37,37,37,37	1
4	BR	D	505	1/1	0.99	0.07	36,36,36,36	1
4	BR	B	504	1/1	0.99	0.07	34,34,34,34	1
4	BR	C	504	1/1	0.99	0.05	37,37,37,37	0
4	BR	D	508	1/1	0.99	0.06	29,29,29,29	1
4	BR	D	509	1/1	0.99	0.06	32,32,32,32	1
4	BR	A	509	1/1	0.99	0.07	30,30,30,30	1
4	BR	C	506	1/1	0.99	0.07	31,31,31,31	1
4	BR	C	507	1/1	0.99	0.05	34,34,34,34	1
4	BR	A	504	1/1	0.99	0.05	32,32,32,32	1
4	BR	B	507	1/1	0.99	0.06	38,38,38,38	1
4	BR	A	506	1/1	1.00	0.05	29,29,29,29	1

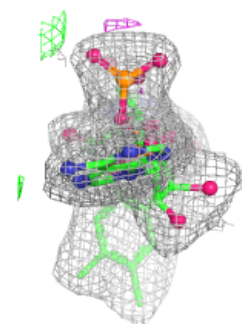
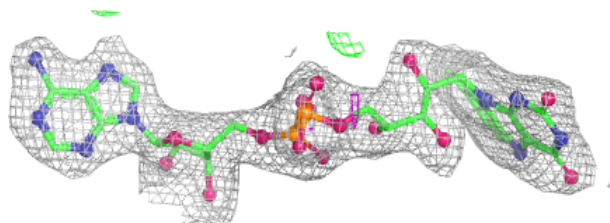
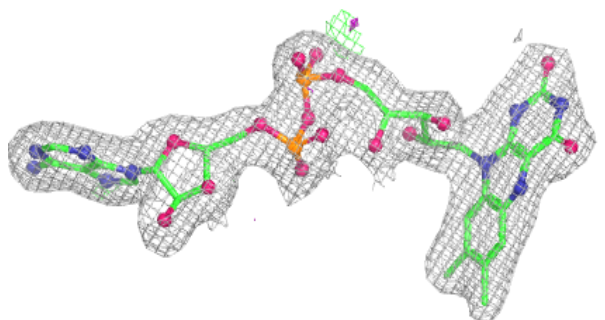
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around FDA D 501:

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

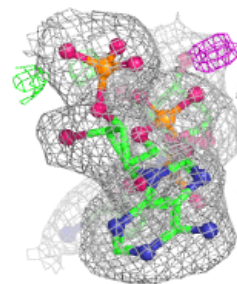
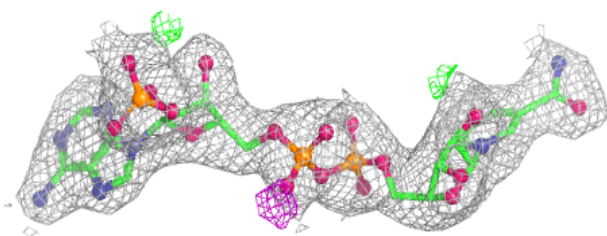
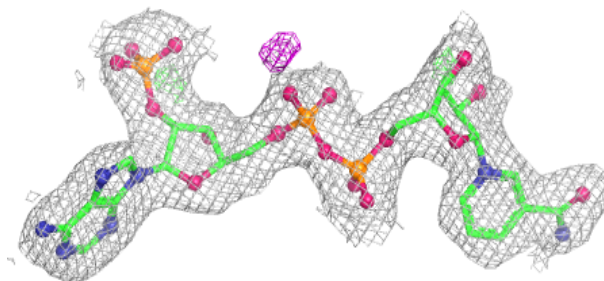
**Electron density around FDA B 501:**

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

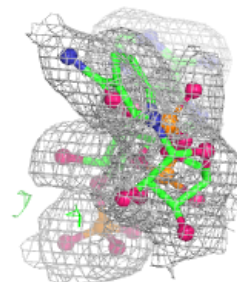
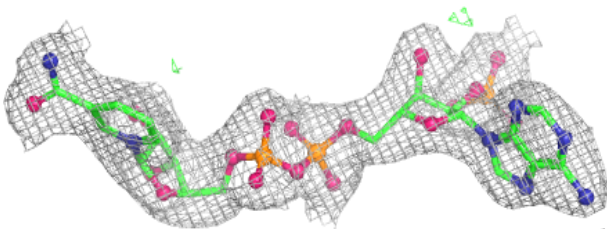
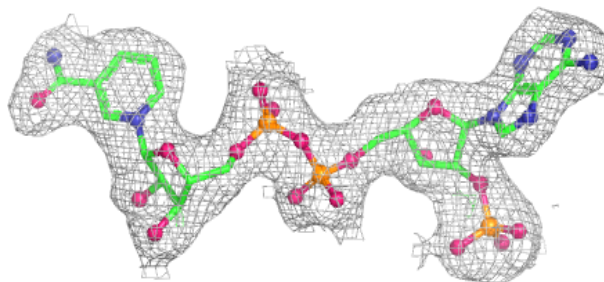


Electron density around NAP B 502:

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

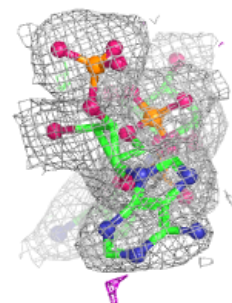
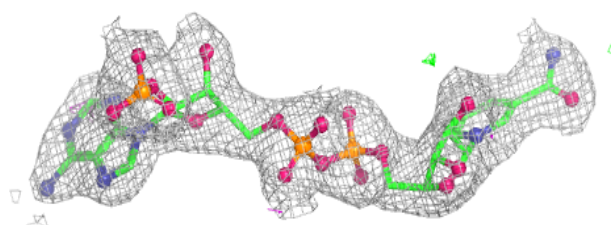
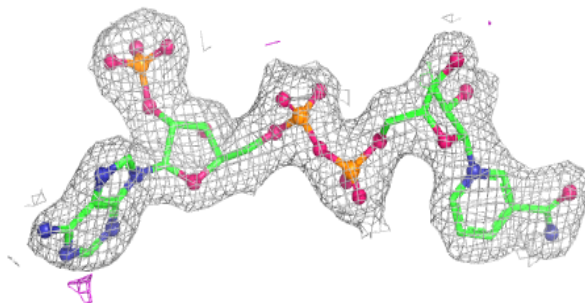
**Electron density around NAP C 502:**

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

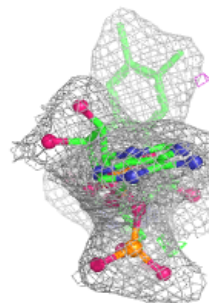
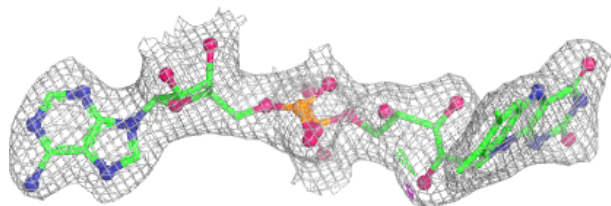
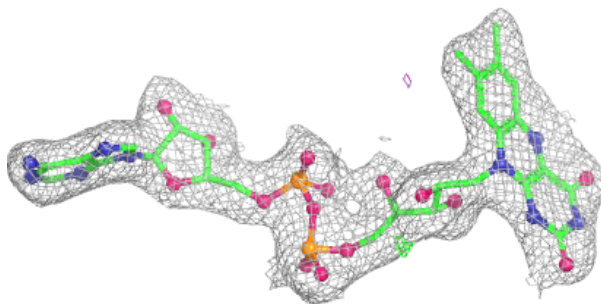


Electron density around NAP D 502:

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

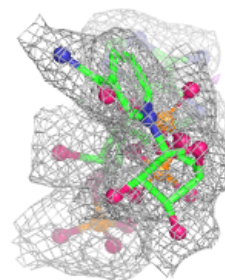
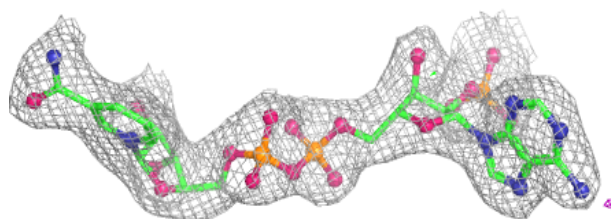
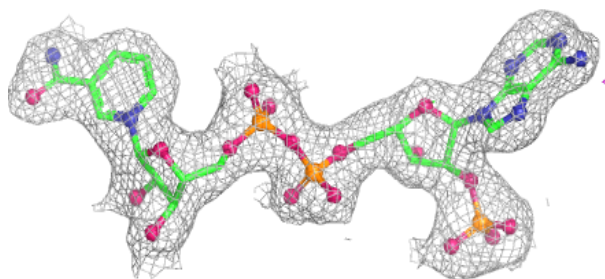
**Electron density around FDA C 501:**

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

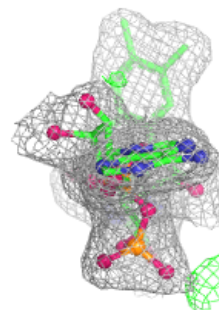
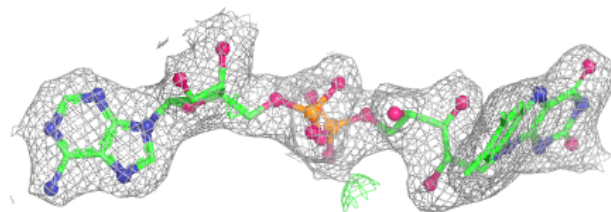
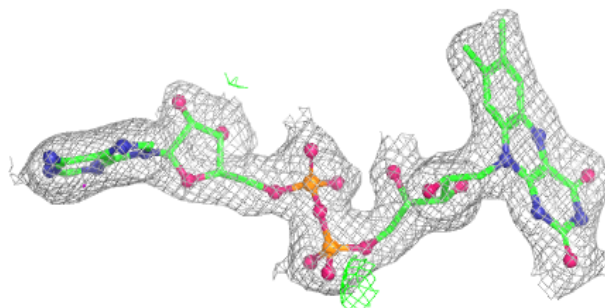


Electron density around NAP A 502:

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

**Electron density around FDA A 501:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.