



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 20, 2020 – 09:27 PM BST

PDB ID : 4AUB  
Title : the complex Structure of the bacterial aldo-keto reductase AKR14A1 with NADP and citrate  
Authors : Zhu, X.; Ellis, E.M.; Lapthorn, A.  
Deposited on : 2012-05-16  
Resolution : 2.05 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

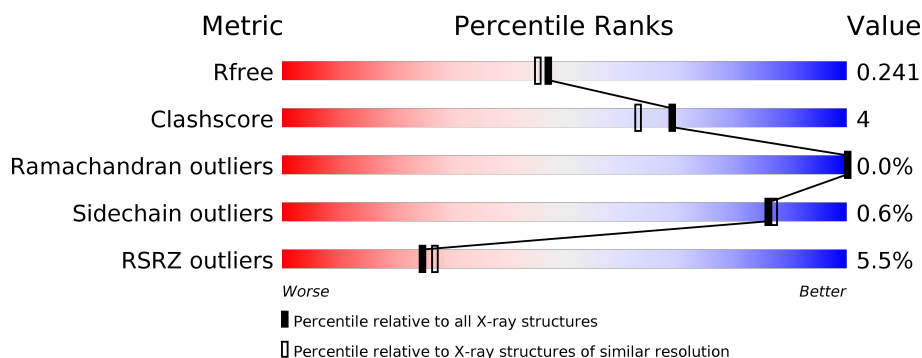
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.05 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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

Mol	Chain	Length	Quality of chain
1	A	366	<div> <div>2%</div> <div>78% 7% 15%</div> </div>
1	B	366	<div> <div>9%</div> <div>82% 9% 8%</div> </div>
1	C	366	<div> <div>7%</div> <div>83% 7% 10%</div> </div>
1	D	366	<div> <div></div> <div>81% • 16%</div> </div>
1	E	366	<div> <div>8%</div> <div>75% 5% • 19%</div> </div>
1	F	366	<div> <div>%</div> <div>75% 5% • 19%</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	366	<div><div>5%</div><div><div></div><div>84%</div><div>7% • 8%</div></div></div>
1	H	366	<div><div>5%</div><div><div></div><div>77%</div><div>• 19%</div></div></div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 21483 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 AKR14A1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	312	Total	C	N	O	S	0	2	0
			2472	1561	436	465	10			
1	B	335	Total	C	N	O	S	0	1	0
			2655	1673	470	500	12			
1	C	330	Total	C	N	O	S	0	1	0
			2608	1646	457	493	12			
1	D	308	Total	C	N	O	S	0	0	0
			2430	1535	427	458	10			
1	E	297	Total	C	N	O	S	0	0	0
			2345	1484	411	440	10			
1	F	298	Total	C	N	O	S	0	0	0
			2359	1493	416	440	10			
1	G	335	Total	C	N	O	S	0	3	0
			2665	1681	471	501	12			
1	H	297	Total	C	N	O	S	0	0	0
			2348	1485	411	442	10			

There are 160 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP Q46851
A	-18	GLY	-	expression tag	UNP Q46851
A	-17	SER	-	expression tag	UNP Q46851
A	-16	SER	-	expression tag	UNP Q46851
A	-15	HIS	-	expression tag	UNP Q46851
A	-14	HIS	-	expression tag	UNP Q46851
A	-13	HIS	-	expression tag	UNP Q46851
A	-12	HIS	-	expression tag	UNP Q46851
A	-11	HIS	-	expression tag	UNP Q46851
A	-10	HIS	-	expression tag	UNP Q46851
A	-9	SER	-	expression tag	UNP Q46851
A	-8	SER	-	expression tag	UNP Q46851
A	-7	GLY	-	expression tag	UNP Q46851

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	LEU	-	expression tag	UNP Q46851
A	-5	VAL	-	expression tag	UNP Q46851
A	-4	PRO	-	expression tag	UNP Q46851
A	-3	ARG	-	expression tag	UNP Q46851
A	-2	GLY	-	expression tag	UNP Q46851
A	-1	SER	-	expression tag	UNP Q46851
A	0	HIS	-	expression tag	UNP Q46851
B	-19	MET	-	expression tag	UNP Q46851
B	-18	GLY	-	expression tag	UNP Q46851
B	-17	SER	-	expression tag	UNP Q46851
B	-16	SER	-	expression tag	UNP Q46851
B	-15	HIS	-	expression tag	UNP Q46851
B	-14	HIS	-	expression tag	UNP Q46851
B	-13	HIS	-	expression tag	UNP Q46851
B	-12	HIS	-	expression tag	UNP Q46851
B	-11	HIS	-	expression tag	UNP Q46851
B	-10	HIS	-	expression tag	UNP Q46851
B	-9	SER	-	expression tag	UNP Q46851
B	-8	SER	-	expression tag	UNP Q46851
B	-7	GLY	-	expression tag	UNP Q46851
B	-6	LEU	-	expression tag	UNP Q46851
B	-5	VAL	-	expression tag	UNP Q46851
B	-4	PRO	-	expression tag	UNP Q46851
B	-3	ARG	-	expression tag	UNP Q46851
B	-2	GLY	-	expression tag	UNP Q46851
B	-1	SER	-	expression tag	UNP Q46851
B	0	HIS	-	expression tag	UNP Q46851
C	-19	MET	-	expression tag	UNP Q46851
C	-18	GLY	-	expression tag	UNP Q46851
C	-17	SER	-	expression tag	UNP Q46851
C	-16	SER	-	expression tag	UNP Q46851
C	-15	HIS	-	expression tag	UNP Q46851
C	-14	HIS	-	expression tag	UNP Q46851
C	-13	HIS	-	expression tag	UNP Q46851
C	-12	HIS	-	expression tag	UNP Q46851
C	-11	HIS	-	expression tag	UNP Q46851
C	-10	HIS	-	expression tag	UNP Q46851
C	-9	SER	-	expression tag	UNP Q46851
C	-8	SER	-	expression tag	UNP Q46851
C	-7	GLY	-	expression tag	UNP Q46851
C	-6	LEU	-	expression tag	UNP Q46851
C	-5	VAL	-	expression tag	UNP Q46851

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	PRO	-	expression tag	UNP Q46851
C	-3	ARG	-	expression tag	UNP Q46851
C	-2	GLY	-	expression tag	UNP Q46851
C	-1	SER	-	expression tag	UNP Q46851
C	0	HIS	-	expression tag	UNP Q46851
D	-19	MET	-	expression tag	UNP Q46851
D	-18	GLY	-	expression tag	UNP Q46851
D	-17	SER	-	expression tag	UNP Q46851
D	-16	SER	-	expression tag	UNP Q46851
D	-15	HIS	-	expression tag	UNP Q46851
D	-14	HIS	-	expression tag	UNP Q46851
D	-13	HIS	-	expression tag	UNP Q46851
D	-12	HIS	-	expression tag	UNP Q46851
D	-11	HIS	-	expression tag	UNP Q46851
D	-10	HIS	-	expression tag	UNP Q46851
D	-9	SER	-	expression tag	UNP Q46851
D	-8	SER	-	expression tag	UNP Q46851
D	-7	GLY	-	expression tag	UNP Q46851
D	-6	LEU	-	expression tag	UNP Q46851
D	-5	VAL	-	expression tag	UNP Q46851
D	-4	PRO	-	expression tag	UNP Q46851
D	-3	ARG	-	expression tag	UNP Q46851
D	-2	GLY	-	expression tag	UNP Q46851
D	-1	SER	-	expression tag	UNP Q46851
D	0	HIS	-	expression tag	UNP Q46851
E	-19	MET	-	expression tag	UNP Q46851
E	-18	GLY	-	expression tag	UNP Q46851
E	-17	SER	-	expression tag	UNP Q46851
E	-16	SER	-	expression tag	UNP Q46851
E	-15	HIS	-	expression tag	UNP Q46851
E	-14	HIS	-	expression tag	UNP Q46851
E	-13	HIS	-	expression tag	UNP Q46851
E	-12	HIS	-	expression tag	UNP Q46851
E	-11	HIS	-	expression tag	UNP Q46851
E	-10	HIS	-	expression tag	UNP Q46851
E	-9	SER	-	expression tag	UNP Q46851
E	-8	SER	-	expression tag	UNP Q46851
E	-7	GLY	-	expression tag	UNP Q46851
E	-6	LEU	-	expression tag	UNP Q46851
E	-5	VAL	-	expression tag	UNP Q46851
E	-4	PRO	-	expression tag	UNP Q46851
E	-3	ARG	-	expression tag	UNP Q46851

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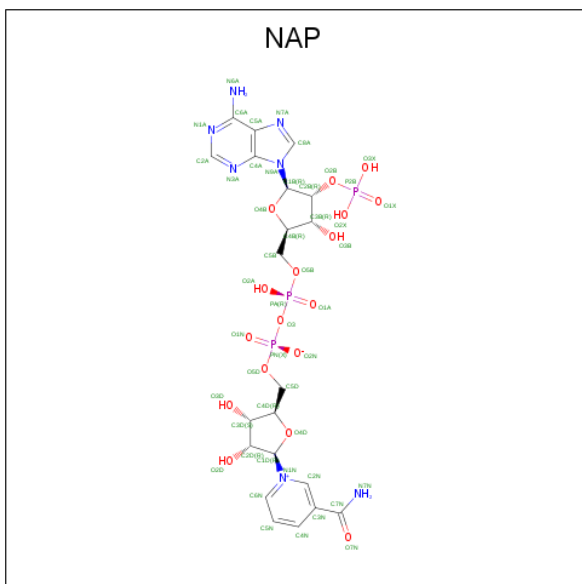
Chain	Residue	Modelled	Actual	Comment	Reference
E	-2	GLY	-	expression tag	UNP Q46851
E	-1	SER	-	expression tag	UNP Q46851
E	0	HIS	-	expression tag	UNP Q46851
F	-19	MET	-	expression tag	UNP Q46851
F	-18	GLY	-	expression tag	UNP Q46851
F	-17	SER	-	expression tag	UNP Q46851
F	-16	SER	-	expression tag	UNP Q46851
F	-15	HIS	-	expression tag	UNP Q46851
F	-14	HIS	-	expression tag	UNP Q46851
F	-13	HIS	-	expression tag	UNP Q46851
F	-12	HIS	-	expression tag	UNP Q46851
F	-11	HIS	-	expression tag	UNP Q46851
F	-10	HIS	-	expression tag	UNP Q46851
F	-9	SER	-	expression tag	UNP Q46851
F	-8	SER	-	expression tag	UNP Q46851
F	-7	GLY	-	expression tag	UNP Q46851
F	-6	LEU	-	expression tag	UNP Q46851
F	-5	VAL	-	expression tag	UNP Q46851
F	-4	PRO	-	expression tag	UNP Q46851
F	-3	ARG	-	expression tag	UNP Q46851
F	-2	GLY	-	expression tag	UNP Q46851
F	-1	SER	-	expression tag	UNP Q46851
F	0	HIS	-	expression tag	UNP Q46851
G	-19	MET	-	expression tag	UNP Q46851
G	-18	GLY	-	expression tag	UNP Q46851
G	-17	SER	-	expression tag	UNP Q46851
G	-16	SER	-	expression tag	UNP Q46851
G	-15	HIS	-	expression tag	UNP Q46851
G	-14	HIS	-	expression tag	UNP Q46851
G	-13	HIS	-	expression tag	UNP Q46851
G	-12	HIS	-	expression tag	UNP Q46851
G	-11	HIS	-	expression tag	UNP Q46851
G	-10	HIS	-	expression tag	UNP Q46851
G	-9	SER	-	expression tag	UNP Q46851
G	-8	SER	-	expression tag	UNP Q46851
G	-7	GLY	-	expression tag	UNP Q46851
G	-6	LEU	-	expression tag	UNP Q46851
G	-5	VAL	-	expression tag	UNP Q46851
G	-4	PRO	-	expression tag	UNP Q46851
G	-3	ARG	-	expression tag	UNP Q46851
G	-2	GLY	-	expression tag	UNP Q46851
G	-1	SER	-	expression tag	UNP Q46851

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Chain	Residue	Modelled	Actual	Comment	Reference
G	0	HIS	-	expression tag	UNP Q46851
H	-19	MET	-	expression tag	UNP Q46851
H	-18	GLY	-	expression tag	UNP Q46851
H	-17	SER	-	expression tag	UNP Q46851
H	-16	SER	-	expression tag	UNP Q46851
H	-15	HIS	-	expression tag	UNP Q46851
H	-14	HIS	-	expression tag	UNP Q46851
H	-13	HIS	-	expression tag	UNP Q46851
H	-12	HIS	-	expression tag	UNP Q46851
H	-11	HIS	-	expression tag	UNP Q46851
H	-10	HIS	-	expression tag	UNP Q46851
H	-9	SER	-	expression tag	UNP Q46851
H	-8	SER	-	expression tag	UNP Q46851
H	-7	GLY	-	expression tag	UNP Q46851
H	-6	LEU	-	expression tag	UNP Q46851
H	-5	VAL	-	expression tag	UNP Q46851
H	-4	PRO	-	expression tag	UNP Q46851
H	-3	ARG	-	expression tag	UNP Q46851
H	-2	GLY	-	expression tag	UNP Q46851
H	-1	SER	-	expression tag	UNP Q46851
H	0	HIS	-	expression tag	UNP Q46851

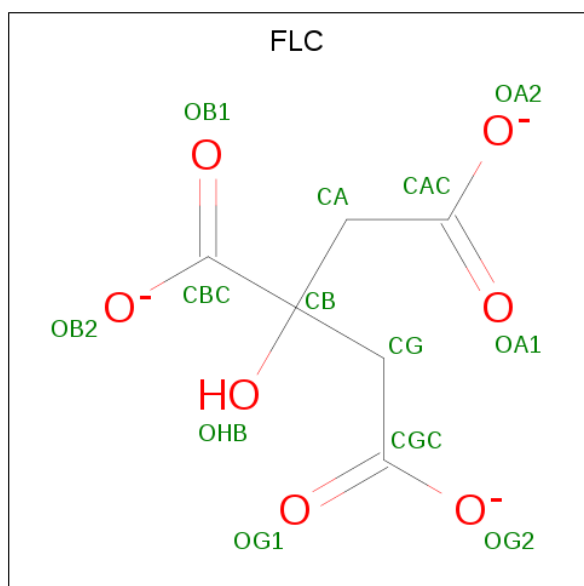
- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula:  $C_{21}H_{28}N_7O_{17}P_3$ ).





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

- Molecule 3 is CITRATE ANION (three-letter code: FLC) (formula:  $C_6H_5O_7$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			13	6	7		
3	B	1	Total	C	O	0	0
			13	6	7		
3	C	1	Total	C	O	0	0
			13	6	7		
3	D	1	Total	C	O	0	0
			13	6	7		
3	E	1	Total	C	O	0	0
			13	6	7		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	F	1	Total	C	O	0	0
			13	6	7		
3	G	1	Total	C	O	0	0
			13	6	7		
3	H	1	Total	C	O	0	0
			13	6	7		

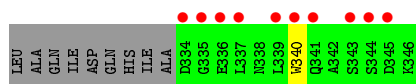
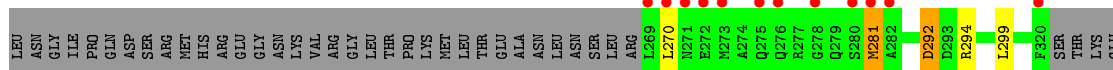
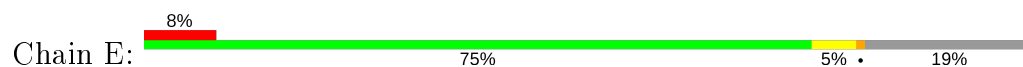
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	181	Total	O	0	0
			181	181		
4	B	155	Total	O	0	0
			155	155		
4	C	142	Total	O	0	0
			142	142		
4	D	161	Total	O	0	0
			161	161		
4	E	121	Total	O	0	0
			121	121		
4	F	156	Total	O	0	0
			156	156		
4	G	132	Total	O	0	0
			132	132		
4	H	113	Total	O	0	0
			113	113		

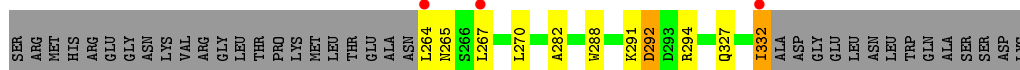
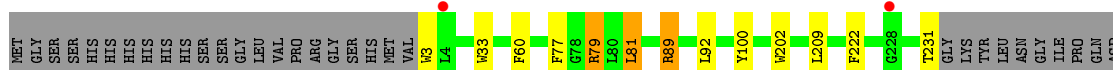
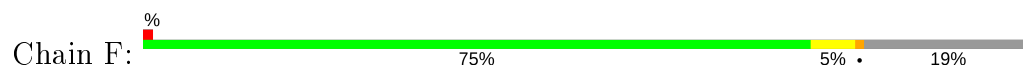




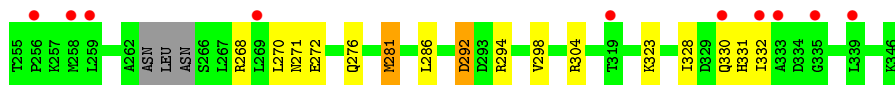
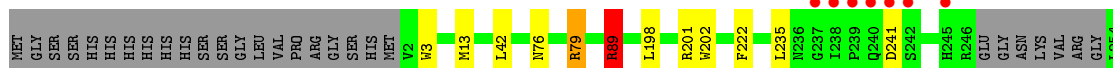
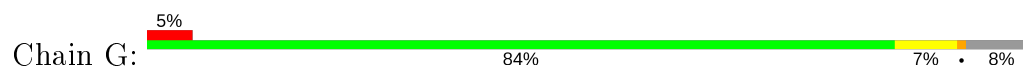
• Molecule 1: ALDO-KETO REDUCTASE AKR14A1



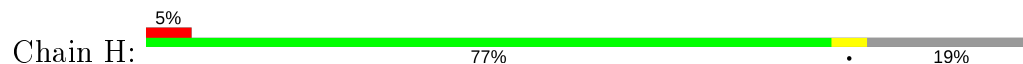
• Molecule 1: ALDO-KETO REDUCTASE AKR14A1



• Molecule 1: ALDO-KETO REDUCTASE AKR14A1



• Molecule 1: ALDO-KETO REDUCTASE AKR14A1



I340
Q341
A342
S343
S344
I345
I346

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	91.81Å 191.09Å 97.30Å 90.00° 105.97° 90.00°	Depositor
Resolution (Å)	95.35 – 2.05 48.87 – 2.05	Depositor EDS
% Data completeness (in resolution range)	92.2 (95.35-2.05) 92.2 (48.87-2.05)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.34 (at 2.05Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.202 , 0.238 0.203 , 0.241	Depositor DCC
$R_{free}$ test set	9319 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.0	Xtriage
Anisotropy	0.080	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 45.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	21483	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.57% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

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

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	0.97	2/2528 (0.1%)	0.88	2/3421 (0.1%)
1	B	0.93	5/2716 (0.2%)	0.84	2/3672 (0.1%)
1	C	0.94	2/2664 (0.1%)	0.85	2/3601 (0.1%)
1	D	1.01	1/2480 (0.0%)	0.90	4/3358 (0.1%)
1	E	0.87	2/2395 (0.1%)	0.86	3/3239 (0.1%)
1	F	0.92	4/2409 (0.2%)	0.87	3/3261 (0.1%)
1	G	0.93	2/2733 (0.1%)	0.92	7/3694 (0.2%)
1	H	0.89	4/2398 (0.2%)	0.85	3/3243 (0.1%)
All	All	0.93	22/20323 (0.1%)	0.87	26/27489 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
1	C	0	2
1	D	0	1
1	E	0	1
1	F	0	1
1	G	0	1
All	All	0	9

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	202	TRP	CD2-CE2	8.72	1.51	1.41
1	B	202	TRP	CD2-CE2	6.96	1.49	1.41
1	H	3	TRP	CD2-CE2	6.76	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	202	TRP	CD2-CE2	6.49	1.49	1.41
1	B	33	TRP	CD2-CE2	6.39	1.49	1.41

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	292	ASP	CB-CG-OD1	9.55	126.90	118.30
1	B	292	ASP	CB-CG-OD1	8.81	126.23	118.30
1	E	292	ASP	CB-CG-OD1	8.73	126.16	118.30
1	G	79	ARG	NE-CZ-NH1	8.16	124.38	120.30
1	E	89	ARG	CG-CD-NE	7.62	127.80	111.80

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	89	ARG	Sidechain
1	B	136	TYR	Peptide
1	B	89	ARG	Sidechain
1	C	136	TYR	Peptide
1	C	89	ARG	Sidechain

## 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	2472	0	2446	24	0
1	B	2655	0	2617	28	0
1	C	2608	0	2577	21	0
1	D	2430	0	2396	7	0
1	E	2345	0	2305	19	0
1	F	2359	0	2332	17	0
1	G	2665	0	2634	31	0
1	H	2348	0	2307	7	0
2	A	48	0	25	6	0
2	B	48	0	25	1	0
2	C	48	0	25	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	48	0	25	2	0
2	F	48	0	25	2	0
2	G	48	0	25	1	0
2	H	48	0	25	1	0
3	A	13	0	5	0	0
3	B	13	0	5	0	0
3	C	13	0	5	0	0
3	D	13	0	5	0	0
3	E	13	0	5	1	0
3	F	13	0	5	3	0
3	G	13	0	5	1	0
3	H	13	0	5	1	0
4	A	181	0	0	3	0
4	B	155	0	0	2	0
4	C	142	0	0	3	0
4	D	161	0	0	2	0
4	E	121	0	0	0	0
4	F	156	0	0	1	0
4	G	132	0	0	1	0
4	H	113	0	0	0	0
All	All	21483	0	19829	147	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 4.

The worst 5 of 147 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:B:180:GLU:HG2	4:B:2124:HOH:O	1.59	1.02
1:B:328:ILE:HG23	1:B:332:ILE:HD12	1.40	1.02
1:D:142:GLU:HB3	4:D:2095:HOH:O	1.63	0.97
1:A:79:ARG:NH1	1:G:79:ARG:CZ	2.27	0.97
1:F:292:ASP:HB3	1:F:294:ARG:HG2	1.50	0.93

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	310/366 (85%)	300 (97%)	10 (3%)	0	100	100
1	B	332/366 (91%)	322 (97%)	10 (3%)	0	100	100
1	C	325/366 (89%)	314 (97%)	11 (3%)	0	100	100
1	D	304/366 (83%)	297 (98%)	7 (2%)	0	100	100
1	E	291/366 (80%)	282 (97%)	9 (3%)	0	100	100
1	F	294/366 (80%)	287 (98%)	7 (2%)	0	100	100
1	G	332/366 (91%)	322 (97%)	10 (3%)	0	100	100
1	H	291/366 (80%)	283 (97%)	7 (2%)	1 (0%)	41	31
All	All	2479/2928 (85%)	2407 (97%)	71 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	194	PRO

### 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	262/307 (85%)	260 (99%)	2 (1%)	81	82
1	B	282/307 (92%)	280 (99%)	2 (1%)	84	84
1	C	278/307 (91%)	278 (100%)	0	100	100
1	D	257/307 (84%)	256 (100%)	1 (0%)	91	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	247/307 (80%)	246 (100%)	1 (0%)	91	91
1	F	250/307 (81%)	247 (99%)	3 (1%)	71	70
1	G	284/307 (92%)	281 (99%)	3 (1%)	73	73
1	H	248/307 (81%)	247 (100%)	1 (0%)	91	91
All	All	2108/2456 (86%)	2095 (99%)	13 (1%)	86	87

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	281	MET
1	F	81	LEU
1	G	268	ARG
1	D	89	ARG
1	G	89	ARG

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

Mol	Chain	Res	Type
1	B	240	GLN
1	B	245	HIS
1	B	263	ASN

### 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	FLC	G	501	-	3,12,12	1.06	0	3,17,17	1.17	0
3	FLC	B	501	-	3,12,12	1.23	0	3,17,17	1.76	1 (33%)
3	FLC	A	501	-	3,12,12	1.62	1 (33%)	3,17,17	2.25	2 (66%)
3	FLC	D	501	-	3,12,12	1.36	1 (33%)	3,17,17	0.85	0
3	FLC	C	501	-	3,12,12	1.31	0	3,17,17	1.02	0
2	NAP	G	500	-	45,52,52	1.20	4 (8%)	56,80,80	1.48	8 (14%)
3	FLC	H	501	-	3,12,12	0.56	0	3,17,17	1.16	0
2	NAP	F	500	-	45,52,52	1.28	7 (15%)	56,80,80	1.36	8 (14%)
2	NAP	C	500	-	45,52,52	1.20	5 (11%)	56,80,80	1.47	12 (21%)
2	NAP	E	500	-	45,52,52	0.97	4 (8%)	56,80,80	1.47	11 (19%)
2	NAP	B	500	-	45,52,52	1.32	8 (17%)	56,80,80	1.49	8 (14%)
2	NAP	A	500	-	45,52,52	1.23	7 (15%)	56,80,80	1.47	10 (17%)
2	NAP	H	500	-	45,52,52	1.10	4 (8%)	56,80,80	1.40	6 (10%)
3	FLC	F	501	-	3,12,12	1.53	0	3,17,17	3.91	2 (66%)
3	FLC	E	501	-	3,12,12	1.81	2 (66%)	3,17,17	2.58	1 (33%)

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	FLC	G	501	-	-	0/6/16/16	-
3	FLC	B	501	-	-	0/6/16/16	-
3	FLC	A	501	-	-	0/6/16/16	-
3	FLC	D	501	-	-	2/6/16/16	-
3	FLC	C	501	-	-	2/6/16/16	-
2	NAP	G	500	-	-	2/31/67/67	0/5/5/5
3	FLC	H	501	-	-	2/6/16/16	-
2	NAP	F	500	-	-	3/31/67/67	0/5/5/5
2	NAP	C	500	-	-	2/31/67/67	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAP	E	500	-	-	5/31/67/67	0/5/5/5
2	NAP	B	500	-	-	3/31/67/67	0/5/5/5
2	NAP	A	500	-	-	5/31/67/67	0/5/5/5
2	NAP	H	500	-	-	3/31/67/67	0/5/5/5
3	FLC	F	501	-	-	2/6/16/16	-
3	FLC	E	501	-	-	0/6/16/16	-

The worst 5 of 43 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	500	NAP	O4D-C1D	3.75	1.46	1.41
2	G	500	NAP	O4D-C1D	3.52	1.46	1.41
2	B	500	NAP	C5A-C4A	3.16	1.49	1.40
2	B	500	NAP	O4B-C1B	3.01	1.45	1.41
2	G	500	NAP	C2A-N3A	2.93	1.36	1.32

The worst 5 of 69 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	501	FLC	CB-CA-CAC	-5.80	105.70	114.98
2	G	500	NAP	C3N-C7N-N7N	4.72	123.41	117.75
2	H	500	NAP	N3A-C2A-N1A	-4.58	121.52	128.68
2	E	500	NAP	N3A-C2A-N1A	-4.38	121.83	128.68
2	B	500	NAP	C3N-C7N-N7N	4.29	122.90	117.75

There are no chirality outliers.

5 of 31 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	501	FLC	CAC-CA-CB-CBC
2	C	500	NAP	PN-O3-PA-O5B
3	D	501	FLC	OHB-CB-CG-CGC
2	F	500	NAP	PN-O3-PA-O1A
2	B	500	NAP	PN-O3-PA-O1A

There are no ring outliers.

11 monomers are involved in 23 short contacts:

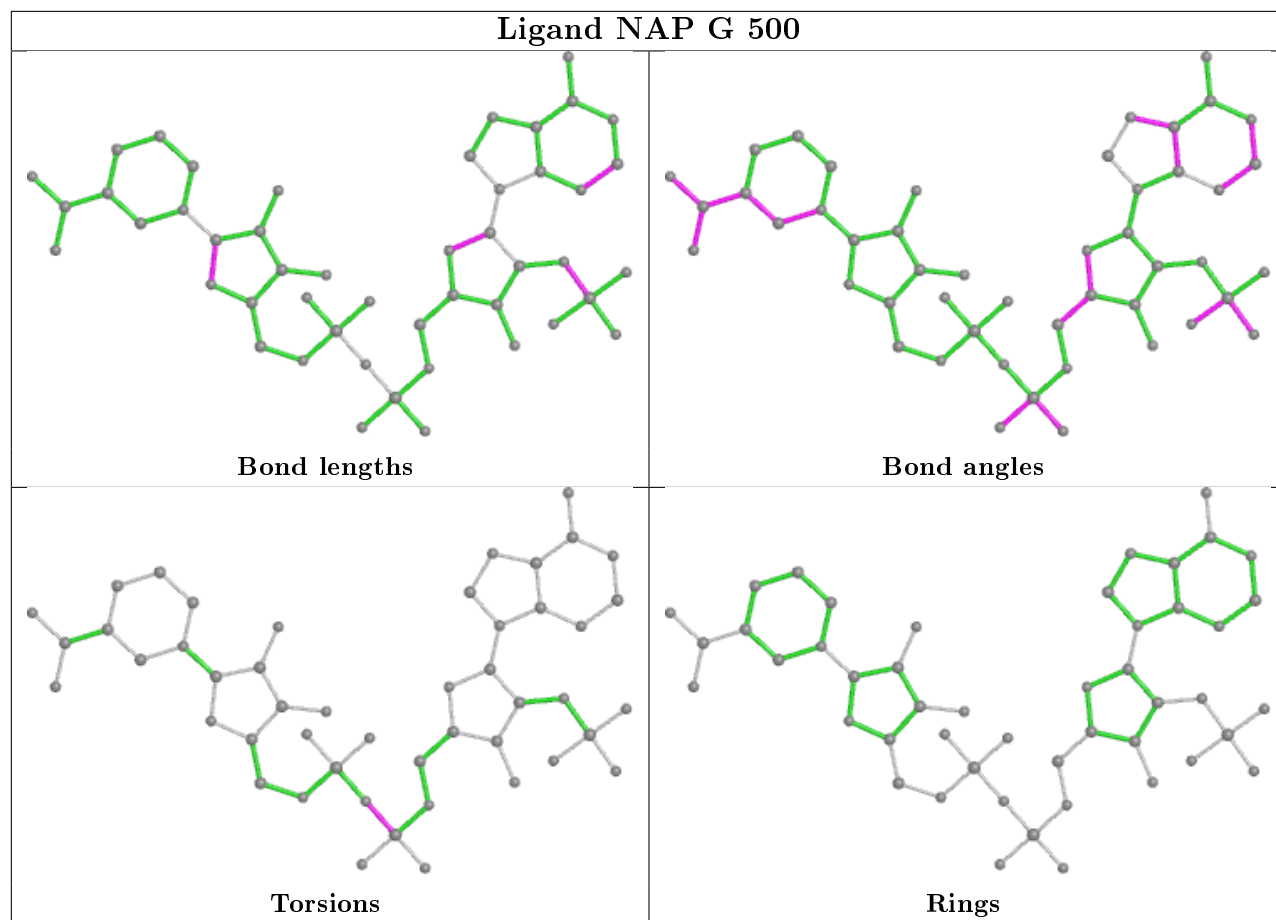
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	501	FLC	1	0

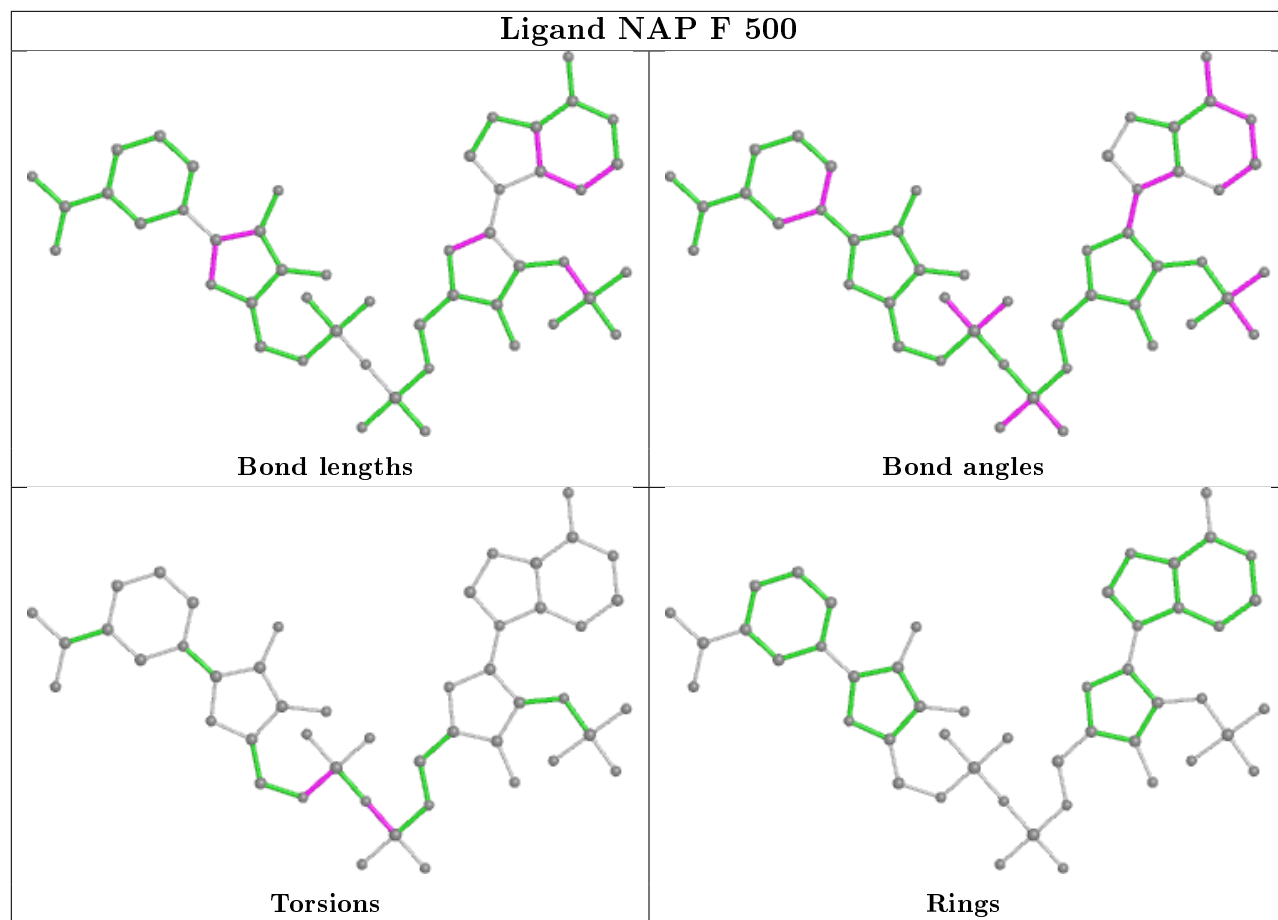
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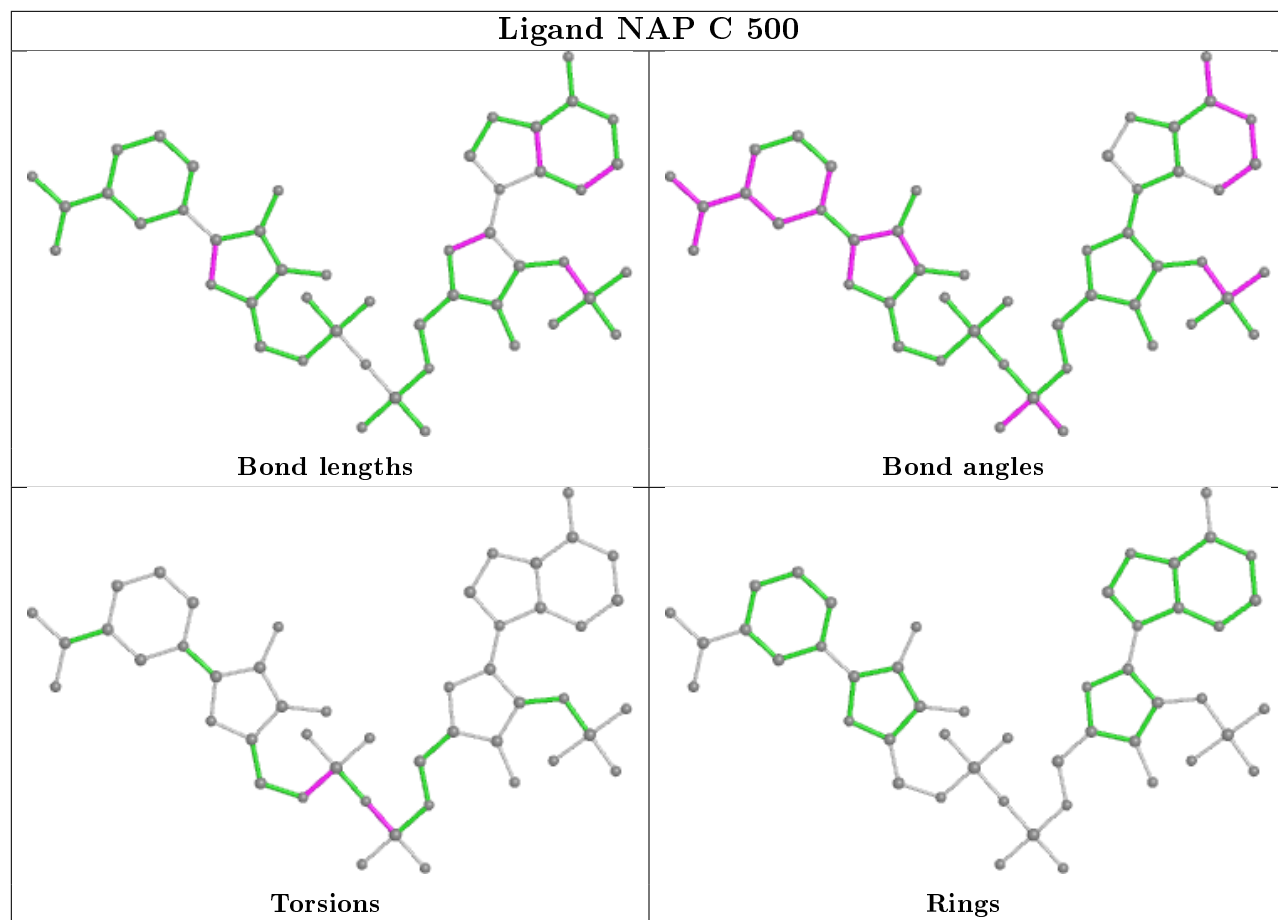
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	500	NAP	1	0
3	H	501	FLC	1	0
2	F	500	NAP	2	0
2	C	500	NAP	5	0
2	E	500	NAP	2	0
2	B	500	NAP	1	0
2	A	500	NAP	6	0
2	H	500	NAP	1	0
3	F	501	FLC	3	0
3	E	501	FLC	1	0

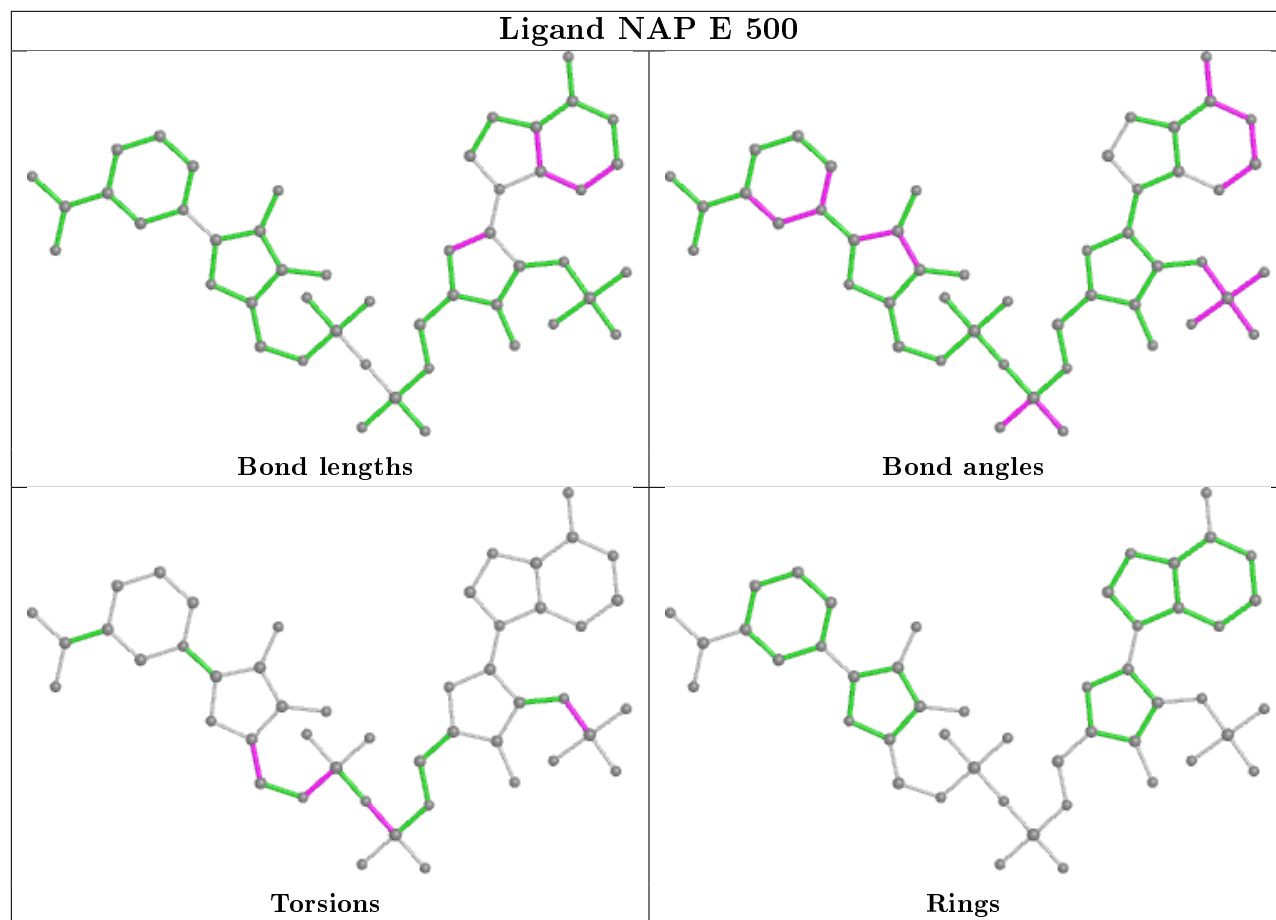
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

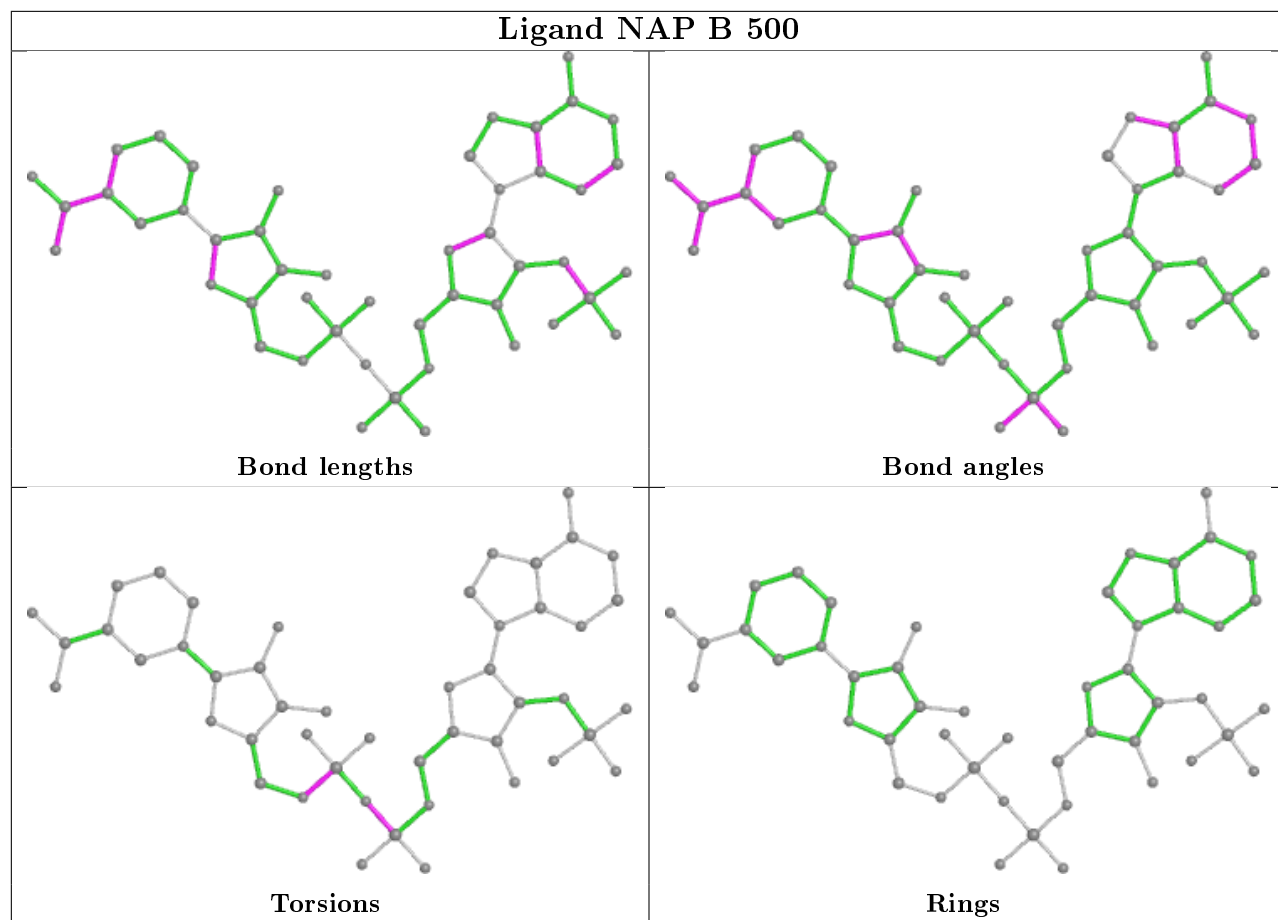


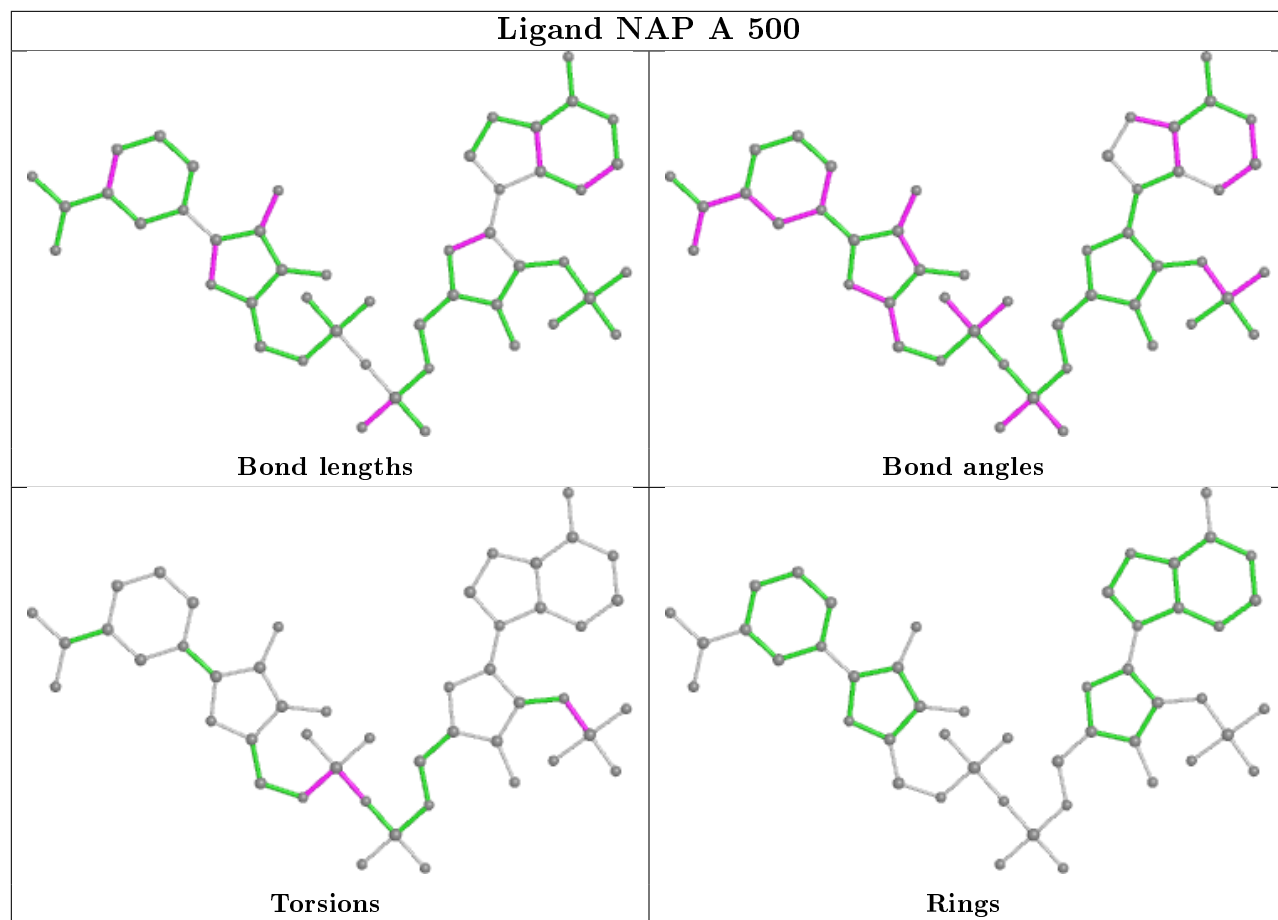


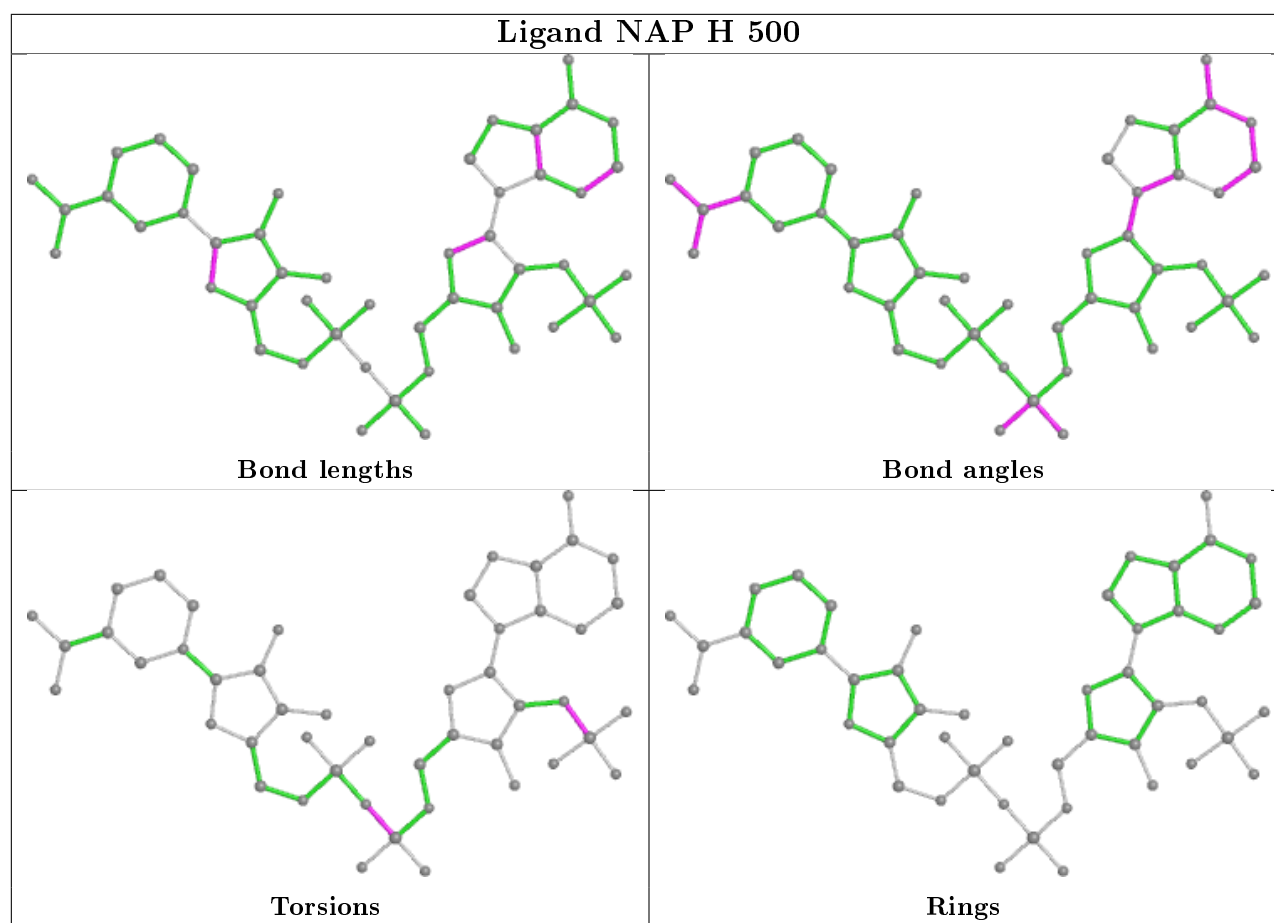












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	312/366 (85%)	0.08	9 (2%) 51 56	12, 21, 47, 77	1 (0%)
1	B	335/366 (91%)	0.33	33 (9%) 7 8	14, 26, 73, 97	1 (0%)
1	C	330/366 (90%)	0.30	26 (7%) 12 13	13, 24, 67, 98	1 (0%)
1	D	308/366 (84%)	-0.14	1 (0%) 94 94	12, 20, 41, 55	1 (0%)
1	E	297/366 (81%)	0.43	28 (9%) 8 9	16, 28, 65, 81	0
1	F	298/366 (81%)	-0.05	5 (1%) 70 73	13, 22, 48, 78	1 (0%)
1	G	335/366 (91%)	0.18	17 (5%) 28 30	14, 24, 59, 84	0
1	H	297/366 (81%)	0.29	20 (6%) 17 19	15, 26, 59, 79	2 (0%)
All	All	2512/2928 (85%)	0.18	139 (5%) 25 27	12, 24, 59, 98	7 (0%)

The worst 5 of 139 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	228	GLY	7.5
1	C	237	GLY	7.4
1	C	262	ALA	6.9
1	B	263	ASN	6.6
1	C	260	THR	6.6

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

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

### 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 6.4 Ligands

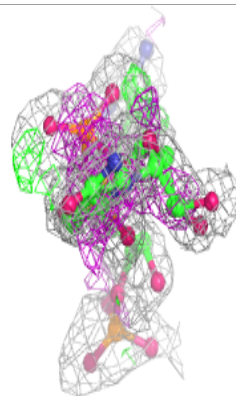
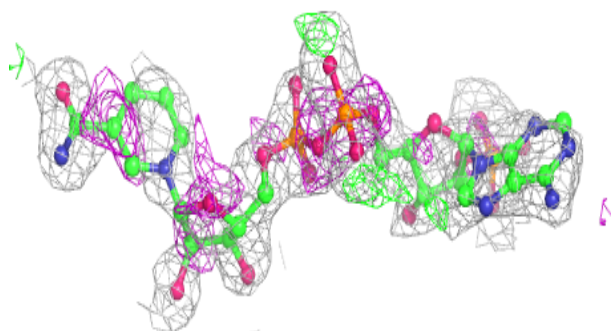
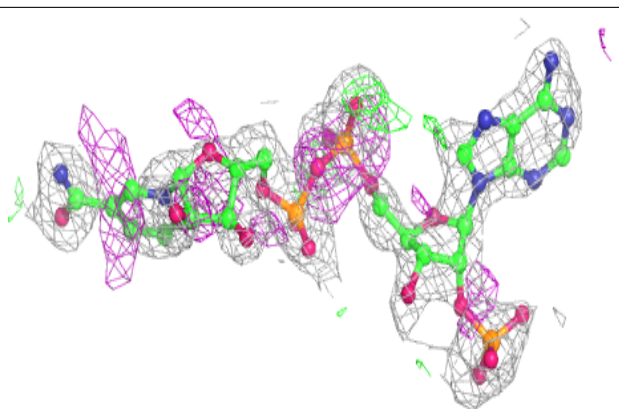
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	NAP	A	500	48/48	0.73	0.38	28,55,79,82	0
3	FLC	D	501	13/13	0.79	0.22	42,51,56,59	0
3	FLC	A	501	13/13	0.82	0.37	46,57,63,65	0
2	NAP	F	500	48/48	0.86	0.22	22,43,56,60	0
3	FLC	F	501	13/13	0.86	0.19	32,43,49,50	0
3	FLC	B	501	13/13	0.89	0.19	34,37,45,51	0
3	FLC	C	501	13/13	0.89	0.19	33,42,48,58	0
3	FLC	H	501	13/13	0.89	0.19	38,46,49,49	0
2	NAP	H	500	48/48	0.90	0.20	33,44,50,52	0
2	NAP	C	500	48/48	0.91	0.17	19,40,51,53	0
3	FLC	G	501	13/13	0.91	0.18	34,39,46,51	0
3	FLC	E	501	13/13	0.91	0.22	38,42,48,50	0
2	NAP	E	500	48/48	0.92	0.21	28,43,50,57	0
2	NAP	B	500	48/48	0.92	0.21	27,43,58,61	0
2	NAP	G	500	48/48	0.96	0.14	21,30,37,40	0

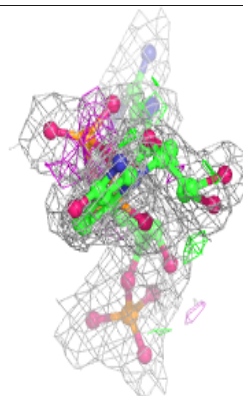
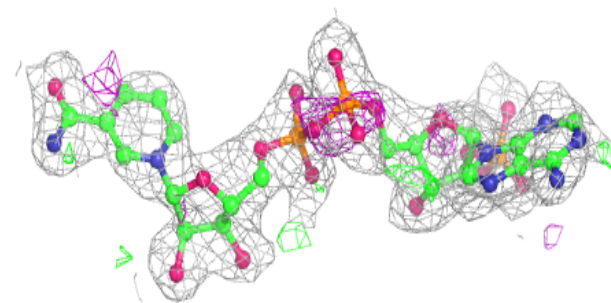
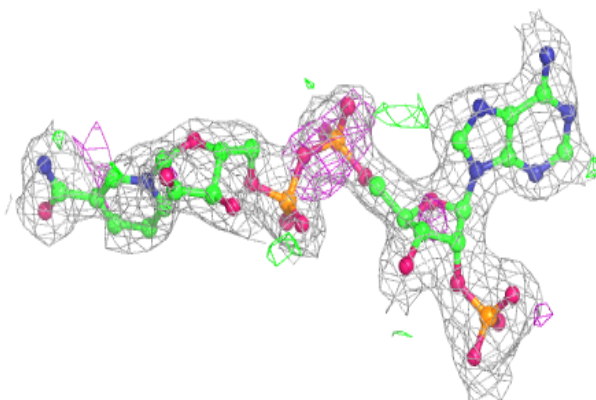
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around NAP A 500:**

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

**Electron density around NAP F 500:**

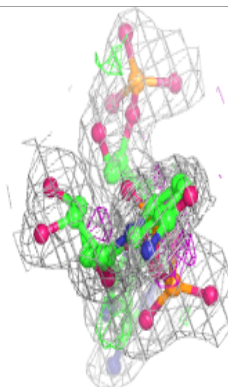
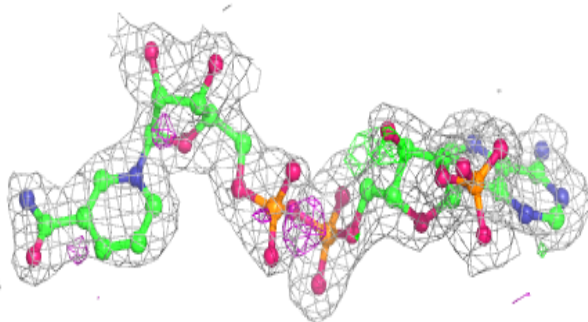
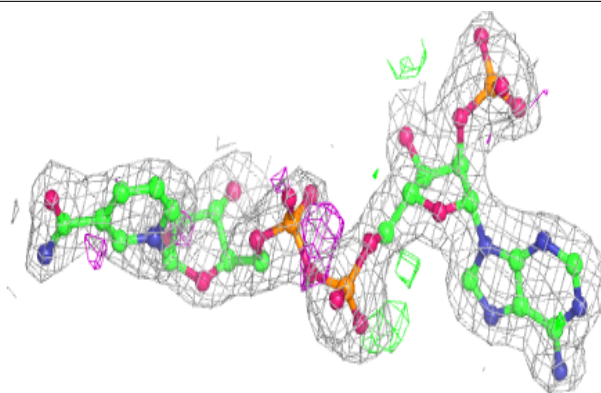
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



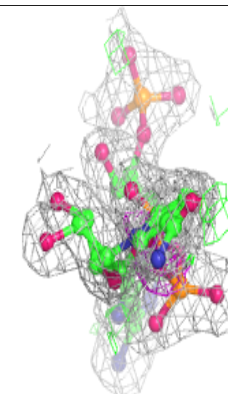
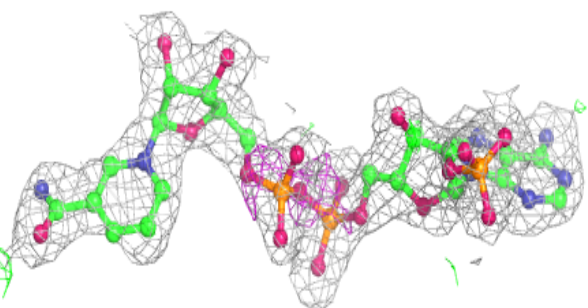
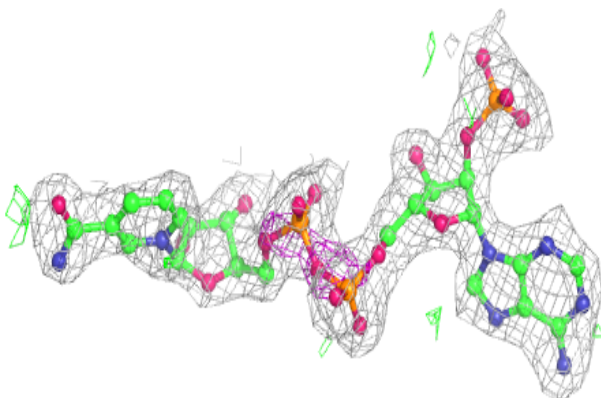


**Electron density around NAP H 500:**

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

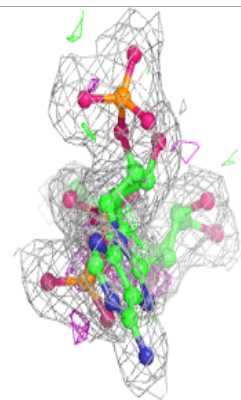
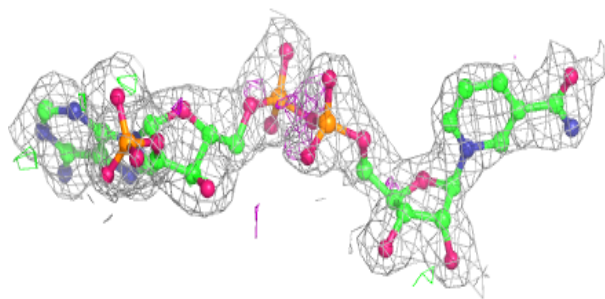
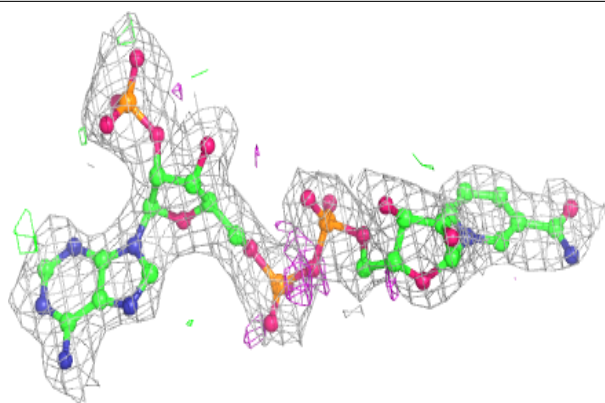
**Electron density around NAP C 500:**

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

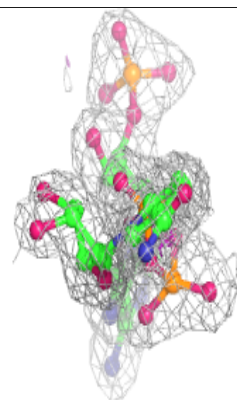
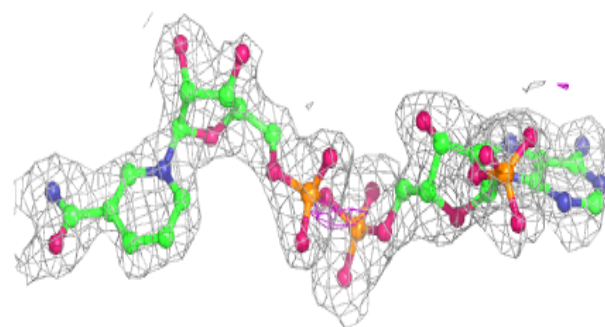
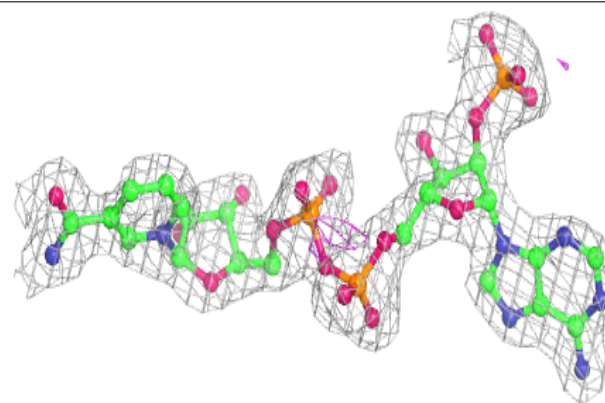


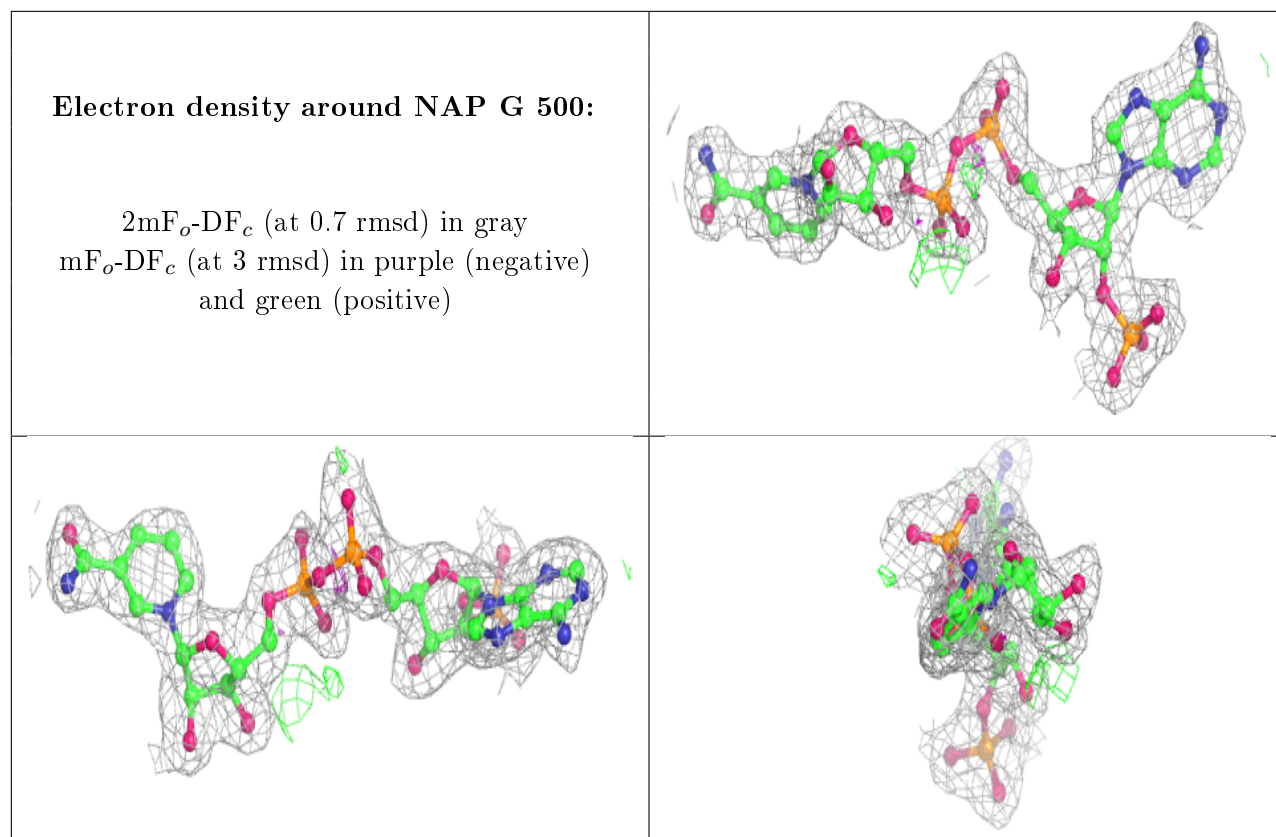
**Electron density around NAP E 500:**

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

**Electron density around NAP B 500:**

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





## 6.5 Other polymers [i](#)

There are no such residues in this entry.