



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 6, 2025 – 04:13 PM EDT

PDB ID : 9YIT / pdb\_00009yit  
Title : Crystal structure of glutamate dehydrogenase from Babesia microti in complex with NADP  
Authors : Seattle Structural Genomics Center for Infectious Disease (SSGCID)  
Deposited on : 2025-10-02  
Resolution : 2.28 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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 : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
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) : 2.46

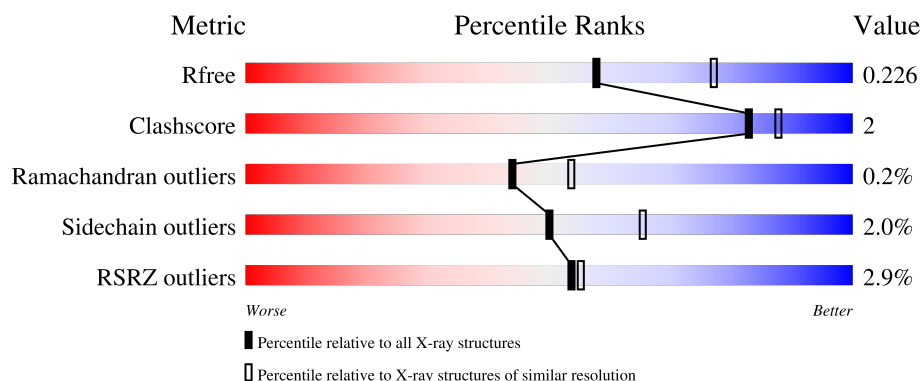
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.28 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))
$R_{free}$	164625	8487 (2.30-2.26)
Clashscore	180529	9437 (2.30-2.26)
Ramachandran outliers	177936	9341 (2.30-2.26)
Sidechain outliers	177891	9342 (2.30-2.26)
RSRZ outliers	164620	8487 (2.30-2.26)

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  $\geq 3$ , 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	487	<div> <div></div> <div>90% 5% .</div> </div>
1	B	487	<div> <div></div> <div>90% 5% . .</div> </div>
1	C	487	<div> <div></div> <div>90% 6% .</div> </div>
1	D	487	<div> <div>13%</div> <div>87% 7% . 6%</div> </div>
1	E	487	<div> <div></div> <div>90% 6% . .</div> </div>

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	487	<div><div><div>%</div><div><div></div></div><div>89%</div><div><div>6%</div><div>• •</div></div></div></div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 21896 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 Glutamate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	467	Total	C	N	O	S	0	0	0
			3575	2267	606	683	19			
1	B	466	Total	C	N	O	S	0	0	0
			3579	2272	607	681	19			
1	C	467	Total	C	N	O	S	0	0	0
			3581	2272	607	683	19			
1	D	460	Total	C	N	O	S	0	0	0
			3392	2152	579	645	16			
1	E	466	Total	C	N	O	S	0	0	0
			3575	2269	606	681	19			
1	F	466	Total	C	N	O	S	0	0	0
			3575	2269	606	681	19			

There are 126 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP A0A0K3AUK4
A	-18	ALA	-	expression tag	UNP A0A0K3AUK4
A	-17	HIS	-	expression tag	UNP A0A0K3AUK4
A	-16	HIS	-	expression tag	UNP A0A0K3AUK4
A	-15	HIS	-	expression tag	UNP A0A0K3AUK4
A	-14	HIS	-	expression tag	UNP A0A0K3AUK4
A	-13	HIS	-	expression tag	UNP A0A0K3AUK4
A	-12	HIS	-	expression tag	UNP A0A0K3AUK4
A	-11	MET	-	expression tag	UNP A0A0K3AUK4
A	-10	GLY	-	expression tag	UNP A0A0K3AUK4
A	-9	THR	-	expression tag	UNP A0A0K3AUK4
A	-8	LEU	-	expression tag	UNP A0A0K3AUK4
A	-7	GLU	-	expression tag	UNP A0A0K3AUK4
A	-6	ALA	-	expression tag	UNP A0A0K3AUK4
A	-5	GLN	-	expression tag	UNP A0A0K3AUK4
A	-4	THR	-	expression tag	UNP A0A0K3AUK4
A	-3	GLN	-	expression tag	UNP A0A0K3AUK4

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP A0A0K3AUK4
A	-1	PRO	-	expression tag	UNP A0A0K3AUK4
A	0	GLY	-	expression tag	UNP A0A0K3AUK4
A	1	SER	-	expression tag	UNP A0A0K3AUK4
B	-19	MET	-	initiating methionine	UNP A0A0K3AUK4
B	-18	ALA	-	expression tag	UNP A0A0K3AUK4
B	-17	HIS	-	expression tag	UNP A0A0K3AUK4
B	-16	HIS	-	expression tag	UNP A0A0K3AUK4
B	-15	HIS	-	expression tag	UNP A0A0K3AUK4
B	-14	HIS	-	expression tag	UNP A0A0K3AUK4
B	-13	HIS	-	expression tag	UNP A0A0K3AUK4
B	-12	HIS	-	expression tag	UNP A0A0K3AUK4
B	-11	MET	-	expression tag	UNP A0A0K3AUK4
B	-10	GLY	-	expression tag	UNP A0A0K3AUK4
B	-9	THR	-	expression tag	UNP A0A0K3AUK4
B	-8	LEU	-	expression tag	UNP A0A0K3AUK4
B	-7	GLU	-	expression tag	UNP A0A0K3AUK4
B	-6	ALA	-	expression tag	UNP A0A0K3AUK4
B	-5	GLN	-	expression tag	UNP A0A0K3AUK4
B	-4	THR	-	expression tag	UNP A0A0K3AUK4
B	-3	GLN	-	expression tag	UNP A0A0K3AUK4
B	-2	GLY	-	expression tag	UNP A0A0K3AUK4
B	-1	PRO	-	expression tag	UNP A0A0K3AUK4
B	0	GLY	-	expression tag	UNP A0A0K3AUK4
B	1	SER	-	expression tag	UNP A0A0K3AUK4
C	-19	MET	-	initiating methionine	UNP A0A0K3AUK4
C	-18	ALA	-	expression tag	UNP A0A0K3AUK4
C	-17	HIS	-	expression tag	UNP A0A0K3AUK4
C	-16	HIS	-	expression tag	UNP A0A0K3AUK4
C	-15	HIS	-	expression tag	UNP A0A0K3AUK4
C	-14	HIS	-	expression tag	UNP A0A0K3AUK4
C	-13	HIS	-	expression tag	UNP A0A0K3AUK4
C	-12	HIS	-	expression tag	UNP A0A0K3AUK4
C	-11	MET	-	expression tag	UNP A0A0K3AUK4
C	-10	GLY	-	expression tag	UNP A0A0K3AUK4
C	-9	THR	-	expression tag	UNP A0A0K3AUK4
C	-8	LEU	-	expression tag	UNP A0A0K3AUK4
C	-7	GLU	-	expression tag	UNP A0A0K3AUK4
C	-6	ALA	-	expression tag	UNP A0A0K3AUK4
C	-5	GLN	-	expression tag	UNP A0A0K3AUK4
C	-4	THR	-	expression tag	UNP A0A0K3AUK4
C	-3	GLN	-	expression tag	UNP A0A0K3AUK4

*Continued on next page...*

*Continued from previous page...*

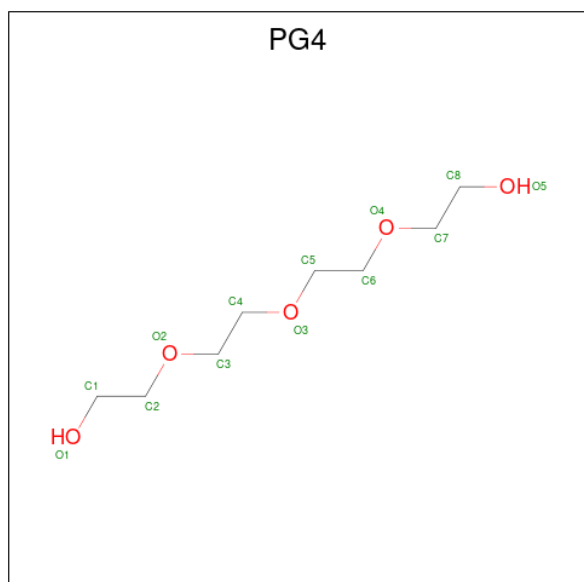
Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	GLY	-	expression tag	UNP A0A0K3AUK4
C	-1	PRO	-	expression tag	UNP A0A0K3AUK4
C	0	GLY	-	expression tag	UNP A0A0K3AUK4
C	1	SER	-	expression tag	UNP A0A0K3AUK4
D	-19	MET	-	initiating methionine	UNP A0A0K3AUK4
D	-18	ALA	-	expression tag	UNP A0A0K3AUK4
D	-17	HIS	-	expression tag	UNP A0A0K3AUK4
D	-16	HIS	-	expression tag	UNP A0A0K3AUK4
D	-15	HIS	-	expression tag	UNP A0A0K3AUK4
D	-14	HIS	-	expression tag	UNP A0A0K3AUK4
D	-13	HIS	-	expression tag	UNP A0A0K3AUK4
D	-12	HIS	-	expression tag	UNP A0A0K3AUK4
D	-11	MET	-	expression tag	UNP A0A0K3AUK4
D	-10	GLY	-	expression tag	UNP A0A0K3AUK4
D	-9	THR	-	expression tag	UNP A0A0K3AUK4
D	-8	LEU	-	expression tag	UNP A0A0K3AUK4
D	-7	GLU	-	expression tag	UNP A0A0K3AUK4
D	-6	ALA	-	expression tag	UNP A0A0K3AUK4
D	-5	GLN	-	expression tag	UNP A0A0K3AUK4
D	-4	THR	-	expression tag	UNP A0A0K3AUK4
D	-3	GLN	-	expression tag	UNP A0A0K3AUK4
D	-2	GLY	-	expression tag	UNP A0A0K3AUK4
D	-1	PRO	-	expression tag	UNP A0A0K3AUK4
D	0	GLY	-	expression tag	UNP A0A0K3AUK4
D	1	SER	-	expression tag	UNP A0A0K3AUK4
E	-19	MET	-	initiating methionine	UNP A0A0K3AUK4
E	-18	ALA	-	expression tag	UNP A0A0K3AUK4
E	-17	HIS	-	expression tag	UNP A0A0K3AUK4
E	-16	HIS	-	expression tag	UNP A0A0K3AUK4
E	-15	HIS	-	expression tag	UNP A0A0K3AUK4
E	-14	HIS	-	expression tag	UNP A0A0K3AUK4
E	-13	HIS	-	expression tag	UNP A0A0K3AUK4
E	-12	HIS	-	expression tag	UNP A0A0K3AUK4
E	-11	MET	-	expression tag	UNP A0A0K3AUK4
E	-10	GLY	-	expression tag	UNP A0A0K3AUK4
E	-9	THR	-	expression tag	UNP A0A0K3AUK4
E	-8	LEU	-	expression tag	UNP A0A0K3AUK4
E	-7	GLU	-	expression tag	UNP A0A0K3AUK4
E	-6	ALA	-	expression tag	UNP A0A0K3AUK4
E	-5	GLN	-	expression tag	UNP A0A0K3AUK4
E	-4	THR	-	expression tag	UNP A0A0K3AUK4
E	-3	GLN	-	expression tag	UNP A0A0K3AUK4

*Continued on next page...*

Continued from previous page...

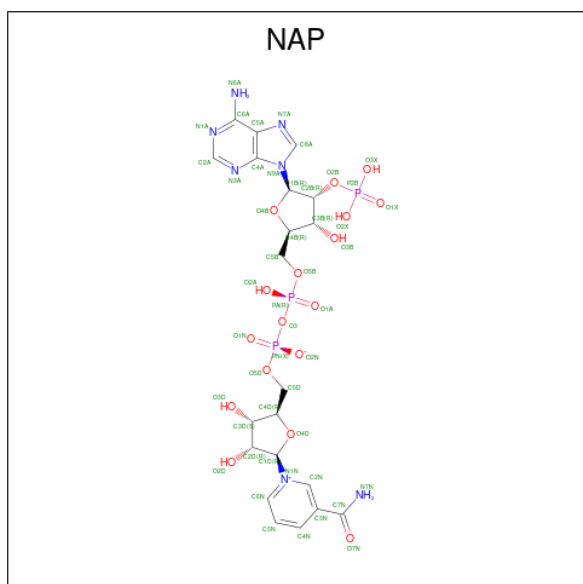
Chain	Residue	Modelled	Actual	Comment	Reference
E	-2	GLY	-	expression tag	UNP A0A0K3AUK4
E	-1	PRO	-	expression tag	UNP A0A0K3AUK4
E	0	GLY	-	expression tag	UNP A0A0K3AUK4
E	1	SER	-	expression tag	UNP A0A0K3AUK4
F	-19	MET	-	initiating methionine	UNP A0A0K3AUK4
F	-18	ALA	-	expression tag	UNP A0A0K3AUK4
F	-17	HIS	-	expression tag	UNP A0A0K3AUK4
F	-16	HIS	-	expression tag	UNP A0A0K3AUK4
F	-15	HIS	-	expression tag	UNP A0A0K3AUK4
F	-14	HIS	-	expression tag	UNP A0A0K3AUK4
F	-13	HIS	-	expression tag	UNP A0A0K3AUK4
F	-12	HIS	-	expression tag	UNP A0A0K3AUK4
F	-11	MET	-	expression tag	UNP A0A0K3AUK4
F	-10	GLY	-	expression tag	UNP A0A0K3AUK4
F	-9	THR	-	expression tag	UNP A0A0K3AUK4
F	-8	LEU	-	expression tag	UNP A0A0K3AUK4
F	-7	GLU	-	expression tag	UNP A0A0K3AUK4
F	-6	ALA	-	expression tag	UNP A0A0K3AUK4
F	-5	GLN	-	expression tag	UNP A0A0K3AUK4
F	-4	THR	-	expression tag	UNP A0A0K3AUK4
F	-3	GLN	-	expression tag	UNP A0A0K3AUK4
F	-2	GLY	-	expression tag	UNP A0A0K3AUK4
F	-1	PRO	-	expression tag	UNP A0A0K3AUK4
F	0	GLY	-	expression tag	UNP A0A0K3AUK4
F	1	SER	-	expression tag	UNP A0A0K3AUK4

- Molecule 2 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: C<sub>8</sub>H<sub>18</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 13	C 8	O 5	0	0
2	B	1	Total 13	C 8	O 5	0	0
2	C	1	Total 13	C 8	O 5	0	0
2	D	1	Total 13	C 8	O 5	0	0
2	E	1	Total 13	C 8	O 5	0	0
2	F	1	Total 13	C 8	O 5	0	0

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula:  $C_{21}H_{28}N_7O_{17}P_3$ ) (labeled as "Ligand of Interest" by depositor).



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

*Continued on next page...*



*Continued from previous page...*

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

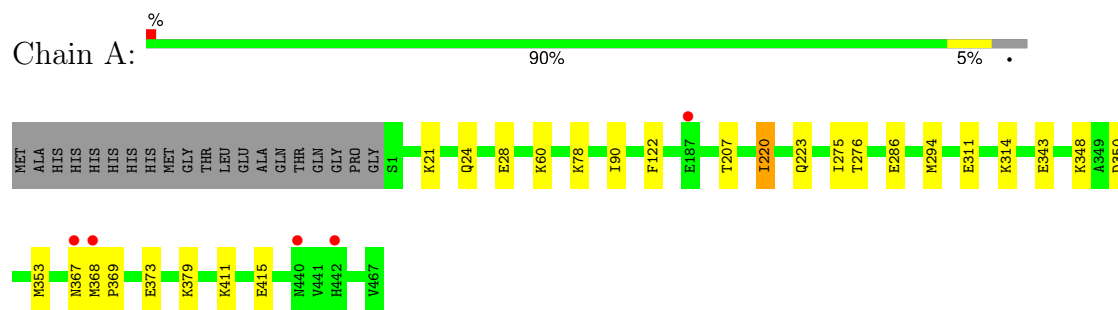
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	48	Total	O	0	0
			48	48		
4	B	59	Total	O	0	0
			59	59		
4	C	40	Total	O	0	0
			40	40		
4	D	25	Total	O	0	0
			25	25		
4	E	38	Total	O	0	0
			38	38		
4	F	43	Total	O	0	0
			43	43		

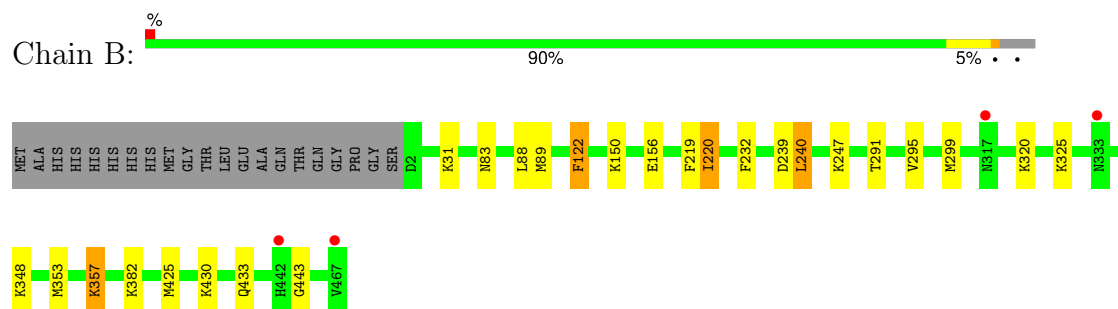
### 3 Residue-property plots [i](#)

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.

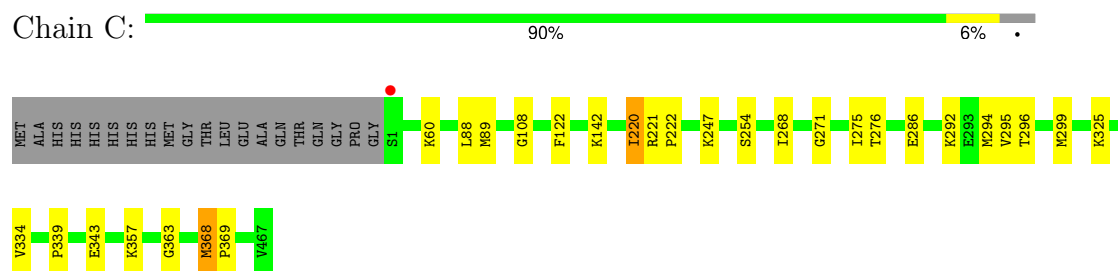
- Molecule 1: Glutamate dehydrogenase



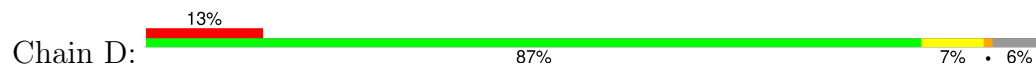
- Molecule 1: Glutamate dehydrogenase

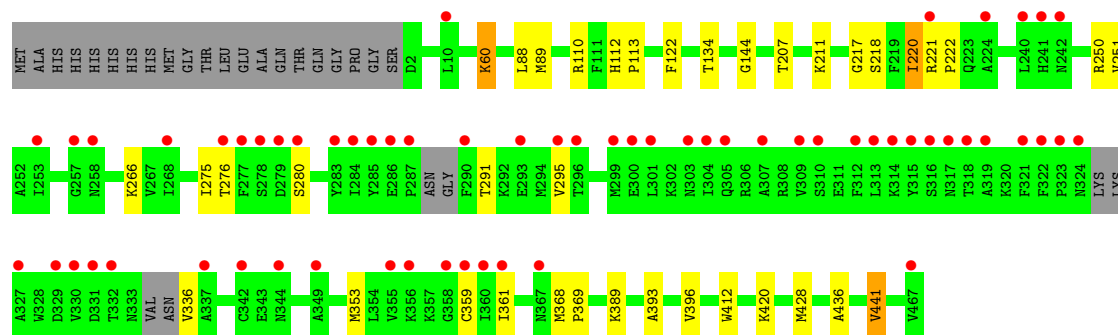


- Molecule 1: Glutamate dehydrogenase

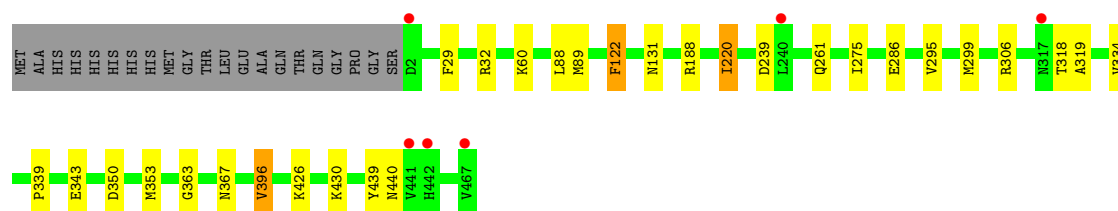
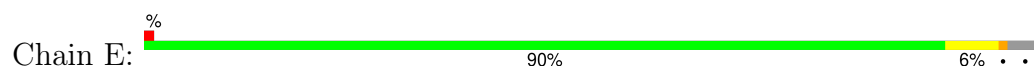


- Molecule 1: Glutamate dehydrogenase

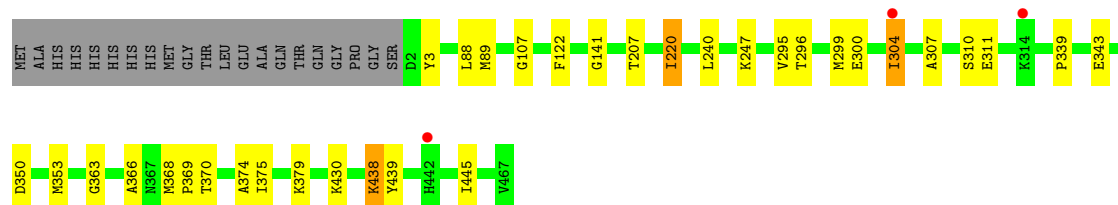
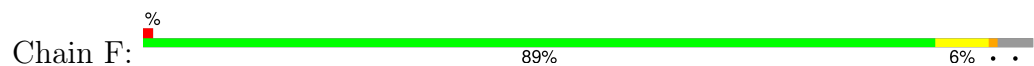




● Molecule 1: Glutamate dehydrogenase



● Molecule 1: Glutamate dehydrogenase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	105.67Å 125.31Å 123.71Å 90.00° 100.29° 90.00°	Depositor
Resolution (Å)	48.02 – 2.28 48.02 – 2.28	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.02-2.28) 99.9 (48.02-2.28)	Depositor EDS
$R_{merge}$	0.18	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.82 (at 2.29Å)	Xtriage
Refinement program	PHENIX (dev_5438: ???)	Depositor
R, $R_{free}$	0.190 , 0.224 0.196 , 0.226	Depositor DCC
$R_{free}$ test set	7172 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	36.2	Xtriage
Anisotropy	0.193	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 34.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	21896	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.84% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: PG4, 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	0.20	0/3649	0.41	0/4926
1	B	0.21	0/3653	0.41	0/4929
1	C	0.20	0/3655	0.39	0/4933
1	D	0.18	0/3459	0.38	0/4684
1	E	0.20	0/3649	0.39	0/4925
1	F	0.20	0/3649	0.40	0/4925
All	All	0.20	0/21714	0.40	0/29322

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	3575	0	3519	17	0
1	B	3579	0	3540	11	0
1	C	3581	0	3537	15	0
1	D	3392	0	3218	21	0
1	E	3575	0	3529	20	0
1	F	3575	0	3529	17	0
2	A	13	0	18	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	13	0	18	0	0
2	C	13	0	18	0	0
2	D	13	0	18	0	0
2	E	13	0	18	0	0
2	F	13	0	18	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
3	E	48	0	25	1	0
3	F	48	0	25	0	0
4	A	48	0	0	0	0
4	B	59	0	0	0	0
4	C	40	0	0	0	0
4	D	25	0	0	0	0
4	E	38	0	0	0	0
4	F	43	0	0	0	0
All	All	21896	0	21130	100	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 (100) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:307:ALA:HB1	1:F:311:GLU:HG3	1.71	0.73
1:B:240:LEU:HD11	1:B:443:GLY:HA2	1.73	0.71
1:E:286:GLU:OE2	1:E:319:ALA:HB2	1.92	0.70
1:E:426:LYS:O	1:E:430:LYS:HG2	1.94	0.67
1:D:275:ILE:HG13	1:D:276:THR:HG23	1.76	0.67
1:F:295:VAL:HG12	1:F:299:MET:HE2	1.77	0.66
1:D:218:SER:H	1:D:221:ARG:NH2	1.95	0.65
1:D:250:ARG:HB3	1:D:275:ILE:HD13	1.79	0.65
1:C:286:GLU:HG2	1:C:294:MET:HE1	1.79	0.64
1:D:412:TRP:CZ3	1:D:420:LYS:HD2	2.33	0.62
1:E:261:GLN:HB3	1:E:299:MET:HE2	1.80	0.62
1:E:275:ILE:HD11	1:E:334:VAL:HG12	1.80	0.62
1:A:78:LYS:HD2	1:A:90:ILE:HD12	1.81	0.61
1:D:291:THR:O	1:D:295:VAL:HG23	2.02	0.60
1:A:286:GLU:CD	1:A:294:MET:HE1	2.28	0.59
1:F:300:GLU:HG2	1:F:304:ILE:HD12	1.84	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:348:LYS:HB2	1:A:373:GLU:HG3	1.85	0.58
1:A:78:LYS:HG3	1:A:90:ILE:HG23	1.86	0.57
1:C:334:VAL:HG22	1:C:357:LYS:HB3	1.86	0.56
1:D:251:VAL:HG13	1:D:336:VAL:HG12	1.87	0.56
1:E:239:ASP:CG	1:E:430:LYS:HZ3	2.13	0.56
1:E:239:ASP:OD2	1:E:430:LYS:NZ	2.33	0.56
1:E:88:LEU:O	1:E:89:MET:HE2	2.07	0.55
1:F:220:ILE:HG22	1:F:220:ILE:O	2.07	0.54
1:B:232:PHE:HB2	1:B:425:MET:HE2	1.89	0.54
1:A:275:ILE:HG13	1:A:276:THR:HG23	1.90	0.54
1:A:220:ILE:HG22	1:A:220:ILE:O	2.08	0.53
1:C:295:VAL:HG12	1:C:299:MET:HE2	1.89	0.53
1:F:366:ALA:HB3	1:F:369:PRO:HG3	1.91	0.53
1:D:88:LEU:O	1:D:89:MET:HE2	2.09	0.53
1:D:221:ARG:HB3	1:D:222:PRO:HD3	1.91	0.52
1:C:339:PRO:HD2	1:C:363:GLY:O	2.11	0.51
1:A:348:LYS:HB2	1:A:373:GLU:CG	2.42	0.50
1:C:220:ILE:O	1:C:220:ILE:HG22	2.12	0.49
1:E:239:ASP:CG	1:E:430:LYS:NZ	2.70	0.49
1:E:350:ASP:HA	1:E:353:MET:HE3	1.94	0.49
1:F:296:THR:HA	1:F:299:MET:HE3	1.94	0.49
1:F:350:ASP:HA	1:F:353:MET:HE3	1.94	0.49
1:C:296:THR:HA	1:C:299:MET:HE3	1.95	0.49
1:C:368:MET:N	1:C:369:PRO:HD3	2.27	0.49
1:B:220:ILE:HG22	1:B:220:ILE:O	2.12	0.49
1:D:220:ILE:O	1:D:220:ILE:HG22	2.13	0.48
1:E:295:VAL:HG12	1:E:299:MET:HE3	1.95	0.48
1:B:88:LEU:O	1:B:89:MET:HE2	2.13	0.48
1:E:220:ILE:HG22	1:E:220:ILE:O	2.12	0.48
1:C:88:LEU:O	1:C:89:MET:HE2	2.13	0.48
1:B:239:ASP:HB3	1:B:433:GLN:OE1	2.14	0.48
1:C:268:ILE:HG21	1:C:292:LYS:HG2	1.97	0.47
1:C:254:SER:OG	1:C:339:PRO:HA	2.13	0.47
1:A:78:LYS:HG3	1:A:90:ILE:CG2	2.44	0.47
1:A:368:MET:N	1:A:369:PRO:HD3	2.30	0.47
1:D:211:LYS:O	1:D:217:GLY:HA3	2.15	0.47
1:B:295:VAL:HG12	1:B:299:MET:HE2	1.96	0.46
1:C:108:GLY:O	1:C:142:LYS:HD3	2.16	0.46
1:E:286:GLU:OE2	1:E:319:ALA:CB	2.61	0.46
1:F:368:MET:N	1:F:369:PRO:HD3	2.31	0.46
1:B:219:PHE:O	1:B:220:ILE:HB	2.16	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:131:ASN:OD1	1:E:396:VAL:HG11	2.16	0.45
1:F:240:LEU:HD11	1:F:445:ILE:HD11	1.98	0.45
1:C:221:ARG:HB3	1:C:222:PRO:HD3	1.99	0.45
1:F:88:LEU:O	1:F:89:MET:HE2	2.17	0.45
1:D:60:LYS:HB3	1:D:60:LYS:HE2	1.43	0.45
1:E:29:PHE:HD1	1:E:32:ARG:NH2	2.15	0.45
1:A:311:GLU:OE2	1:A:314:LYS:HD2	2.16	0.45
1:D:393:ALA:O	1:D:396:VAL:HG22	2.16	0.45
1:A:415:GLU:CD	1:A:415:GLU:H	2.26	0.44
1:C:275:ILE:HD11	1:C:334:VAL:HG12	2.00	0.44
1:D:368:MET:N	1:D:369:PRO:HD3	2.32	0.44
1:C:247:LYS:HD2	1:C:271:GLY:HA3	2.00	0.44
1:D:436:ALA:HB1	1:D:441:VAL:O	2.18	0.44
1:B:353:MET:O	1:B:357:LYS:HD3	2.18	0.44
1:E:188:ARG:HD3	1:F:3:TYR:CD1	2.53	0.44
1:A:207:THR:HG22	1:A:207:THR:O	2.18	0.43
1:D:412:TRP:CH2	1:D:420:LYS:HE3	2.54	0.43
1:E:367:ASN:OD1	3:E:502:NAP:H6N	2.18	0.43
1:B:122:PHE:CD1	1:B:122:PHE:C	2.96	0.43
1:E:439:TYR:O	1:E:440:ASN:HB2	2.18	0.43
1:D:218:SER:H	1:D:221:ARG:HH22	1.65	0.43
1:D:110:ARG:O	1:D:144:GLY:HA3	2.19	0.43
1:B:83:ASN:HB2	1:B:156:GLU:OE2	2.19	0.42
1:F:339:PRO:HD2	1:F:363:GLY:O	2.19	0.42
1:A:24:GLN:O	1:A:28:GLU:HG2	2.20	0.42
1:A:350:ASP:HA	1:A:353:MET:HE3	2.00	0.42
1:A:220:ILE:HA	1:A:223:GLN:OE1	2.19	0.42
1:A:311:GLU:CD	1:A:314:LYS:HD2	2.44	0.42
1:E:339:PRO:HD2	1:E:363:GLY:O	2.20	0.42
1:A:78:LYS:CG	1:A:90:ILE:HG23	2.47	0.42
1:C:275:ILE:HG13	1:C:276:THR:HG23	2.02	0.41
1:E:122:PHE:CD1	1:E:122:PHE:C	2.98	0.41
1:F:370:THR:HG22	1:F:374:ALA:HB3	2.01	0.41
1:F:207:THR:O	1:F:207:THR:HG22	2.20	0.41
1:F:438:LYS:HD3	1:F:439:TYR:CE2	2.56	0.41
1:B:291:THR:O	1:B:295:VAL:HG23	2.21	0.41
1:F:375:ILE:CG2	1:F:379:LYS:HE2	2.51	0.41
1:D:207:THR:O	1:D:207:THR:HG22	2.21	0.41
1:D:134:THR:HA	1:D:428:MET:HE2	2.02	0.41
1:D:112:HIS:CG	1:D:113:PRO:HD2	2.56	0.41
1:E:239:ASP:OD1	1:E:430:LYS:NZ	2.54	0.40

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:217:GLY:CA	1:D:221:ARG:HH22	2.34	0.40
1:F:107:GLY:HA3	1:F:141:GLY:O	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	465/487 (96%)	457 (98%)	7 (2%)	1 (0%)	44	53
1	B	464/487 (95%)	455 (98%)	8 (2%)	1 (0%)	44	53
1	C	465/487 (96%)	457 (98%)	7 (2%)	1 (0%)	44	53
1	D	452/487 (93%)	446 (99%)	5 (1%)	1 (0%)	44	53
1	E	464/487 (95%)	456 (98%)	7 (2%)	1 (0%)	44	53
1	F	464/487 (95%)	454 (98%)	9 (2%)	1 (0%)	44	53
All	All	2774/2922 (95%)	2725 (98%)	43 (2%)	6 (0%)	44	53

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	220	ILE
1	B	220	ILE
1	C	220	ILE
1	E	220	ILE
1	D	220	ILE
1	F	220	ILE

### 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	382/401 (95%)	375 (98%)	7 (2%)	54	68
1	B	384/401 (96%)	373 (97%)	11 (3%)	37	51
1	C	384/401 (96%)	379 (99%)	5 (1%)	65	77
1	D	338/401 (84%)	329 (97%)	9 (3%)	40	54
1	E	383/401 (96%)	377 (98%)	6 (2%)	58	72
1	F	383/401 (96%)	376 (98%)	7 (2%)	54	68
All	All	2254/2406 (94%)	2209 (98%)	45 (2%)	50	65

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	LYS
1	A	60	LYS
1	A	122	PHE
1	A	343	GLU
1	A	367	ASN
1	A	379	LYS
1	A	411	LYS
1	B	31	LYS
1	B	122	PHE
1	B	150	LYS
1	B	240	LEU
1	B	247	LYS
1	B	320	LYS
1	B	325	LYS
1	B	348	LYS
1	B	357	LYS
1	B	382	LYS
1	B	430	LYS
1	C	60	LYS
1	C	122	PHE
1	C	325	LYS
1	C	343	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	368	MET
1	D	60	LYS
1	D	122	PHE
1	D	266	LYS
1	D	280	SER
1	D	353	MET
1	D	359	CYS
1	D	361	ILE
1	D	389	LYS
1	D	441	VAL
1	E	60	LYS
1	E	122	PHE
1	E	306	ARG
1	E	318	THR
1	E	343	GLU
1	E	396	VAL
1	F	122	PHE
1	F	247	LYS
1	F	304	ILE
1	F	310	SER
1	F	343	GLU
1	F	430	LYS
1	F	438	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	127	GLN
1	A	155	ASN
1	A	317	ASN
1	B	155	ASN
1	C	155	ASN
1	D	22	HIS
1	D	24	GLN
1	D	42	GLN
1	D	234	GLN
1	D	464	GLN
1	E	155	ASN
1	E	238	ASN
1	E	464	GLN
1	F	155	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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

12 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	NAP	A	502	-	46,52,52	1.95	4 (8%)	61,80,80	1.21	3 (4%)
3	NAP	E	502	-	46,52,52	1.84	4 (8%)	61,80,80	1.17	6 (9%)
2	PG4	D	501	-	12,12,12	0.32	0	11,11,11	0.26	0
2	PG4	A	501	-	12,12,12	0.30	0	11,11,11	0.28	0
3	NAP	D	502	-	46,52,52	1.85	5 (10%)	61,80,80	1.19	6 (9%)
2	PG4	C	501	-	12,12,12	0.31	0	11,11,11	0.32	0
3	NAP	C	502	-	46,52,52	1.90	5 (10%)	61,80,80	1.18	6 (9%)
2	PG4	E	501	-	12,12,12	0.31	0	11,11,11	0.27	0
2	PG4	B	501	-	12,12,12	0.31	0	11,11,11	0.26	0
3	NAP	B	502	-	46,52,52	1.97	4 (8%)	61,80,80	1.21	4 (6%)
2	PG4	F	501	-	12,12,12	0.29	0	11,11,11	0.30	0
3	NAP	F	502	-	46,52,52	1.91	5 (10%)	61,80,80	1.16	6 (9%)

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	NAP	A	502	-	-	5/31/67/67	0/5/5/5
3	NAP	E	502	-	-	7/31/67/67	0/5/5/5
2	PG4	D	501	-	-	1/10/10/10	-
2	PG4	A	501	-	-	3/10/10/10	-
3	NAP	D	502	-	-	5/31/67/67	0/5/5/5
2	PG4	C	501	-	-	3/10/10/10	-
3	NAP	C	502	-	-	9/31/67/67	0/5/5/5
2	PG4	E	501	-	-	2/10/10/10	-
2	PG4	B	501	-	-	2/10/10/10	-
3	NAP	B	502	-	-	9/31/67/67	0/5/5/5
2	PG4	F	501	-	-	2/10/10/10	-
3	NAP	F	502	-	-	9/31/67/67	0/5/5/5

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	502	NAP	P2B-O2B	8.91	1.75	1.59
3	F	502	NAP	P2B-O2B	8.70	1.74	1.59
3	C	502	NAP	P2B-O2B	8.70	1.74	1.59
3	D	502	NAP	P2B-O2B	8.35	1.74	1.59
3	A	502	NAP	P2B-O2B	8.20	1.73	1.59
3	E	502	NAP	P2B-O2B	8.16	1.73	1.59
3	A	502	NAP	PA-O3	6.14	1.66	1.59
3	A	502	NAP	PN-O3	5.87	1.65	1.59
3	B	502	NAP	PA-O3	5.44	1.65	1.59
3	B	502	NAP	PN-O3	5.37	1.65	1.59
3	C	502	NAP	PN-O3	5.36	1.65	1.59
3	F	502	NAP	PN-O3	5.32	1.65	1.59
3	D	502	NAP	PA-O3	5.30	1.65	1.59
3	D	502	NAP	PN-O3	5.24	1.65	1.59
3	E	502	NAP	PA-O3	5.22	1.65	1.59
3	F	502	NAP	PA-O3	5.16	1.65	1.59
3	C	502	NAP	PA-O3	5.12	1.65	1.59
3	E	502	NAP	PN-O3	5.01	1.64	1.59
3	C	502	NAP	C8A-N7A	-2.47	1.30	1.34
3	B	502	NAP	C8A-N7A	-2.27	1.30	1.34
3	A	502	NAP	C8A-N7A	-2.26	1.30	1.34
3	E	502	NAP	C8A-N7A	-2.26	1.30	1.34
3	F	502	NAP	O4D-C1D	-2.25	1.37	1.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	502	NAP	C8A-N7A	-2.18	1.30	1.34
3	D	502	NAP	C8A-N7A	-2.06	1.30	1.34
3	C	502	NAP	C1B-N9A	-2.04	1.44	1.49
3	D	502	NAP	O4D-C1D	-2.04	1.38	1.40

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	NAP	O4B-C1B-N9A	4.48	114.69	108.75
3	E	502	NAP	O4B-C1B-N9A	3.63	113.56	108.75
3	A	502	NAP	P2B-O2B-C2B	-3.61	113.78	123.43
3	D	502	NAP	O4B-C1B-N9A	3.61	113.53	108.75
3	B	502	NAP	O4B-C1B-N9A	3.57	113.48	108.75
3	E	502	NAP	P2B-O2B-C2B	-3.48	114.13	123.43
3	F	502	NAP	P2B-O2B-C2B	-3.24	114.77	123.43
3	F	502	NAP	O4B-C1B-N9A	3.24	113.04	108.75
3	B	502	NAP	P2B-O2B-C2B	-3.23	114.81	123.43
3	C	502	NAP	P2B-O2B-C2B	-3.20	114.89	123.43
3	D	502	NAP	C1B-N9A-C4A	-3.04	121.30	126.64
3	D	502	NAP	P2B-O2B-C2B	-2.74	116.10	123.43
3	C	502	NAP	C1B-N9A-C4A	-2.69	121.92	126.64
3	F	502	NAP	C1B-N9A-C4A	-2.54	122.19	126.64
3	B	502	NAP	C1B-N9A-C4A	-2.52	122.21	126.64
3	E	502	NAP	O3X-P2B-O2X	2.41	116.86	107.80
3	A	502	NAP	O3X-P2B-O2X	2.37	116.70	107.80
3	B	502	NAP	O2A-PA-O1A	2.33	123.28	112.44
3	E	502	NAP	C1B-N9A-C4A	-2.31	122.59	126.64
3	E	502	NAP	O2A-PA-O1A	2.17	122.54	112.44
3	C	502	NAP	O2A-PA-O1A	2.15	122.46	112.44
3	D	502	NAP	O3X-P2B-O2X	2.14	115.83	107.80
3	C	502	NAP	O7N-C7N-N7N	2.11	125.67	122.62
3	C	502	NAP	O3X-P2B-O2X	2.10	115.67	107.80
3	F	502	NAP	O7N-C7N-N7N	2.08	125.63	122.62
3	C	502	NAP	O2N-PN-O1N	2.07	122.06	112.44
3	D	502	NAP	O2A-PA-O1A	2.04	121.95	112.44
3	E	502	NAP	O2N-PN-O1N	2.04	121.92	112.44
3	D	502	NAP	O2N-PN-O1N	2.03	121.87	112.44
3	F	502	NAP	O2N-PN-O1N	2.00	121.77	112.44
3	F	502	NAP	O2A-PA-O1A	2.00	121.76	112.44

There are no chirality outliers.

All (57) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502	NAP	O4D-C1D-N1N-C2N
3	B	502	NAP	O4D-C4D-C5D-O5D
3	C	502	NAP	C5D-O5D-PN-O1N
3	C	502	NAP	C5D-O5D-PN-O2N
3	C	502	NAP	O4D-C1D-N1N-C2N
3	D	502	NAP	O4D-C1D-N1N-C2N
3	E	502	NAP	O4D-C1D-N1N-C2N
3	F	502	NAP	O4D-C4D-C5D-O5D
3	B	502	NAP	C3D-C4D-C5D-O5D
3	C	502	NAP	O4D-C4D-C5D-O5D
3	C	502	NAP	C3D-C4D-C5D-O5D
3	D	502	NAP	O4D-C4D-C5D-O5D
3	E	502	NAP	O4D-C4D-C5D-O5D
2	A	501	PG4	O1-C1-C2-O2
2	C	501	PG4	O1-C1-C2-O2
3	F	502	NAP	C3D-C4D-C5D-O5D
2	B	501	PG4	O1-C1-C2-O2
3	D	502	NAP	C3D-C4D-C5D-O5D
3	E	502	NAP	C3D-C4D-C5D-O5D
3	A	502	NAP	O4D-C4D-C5D-O5D
2	E	501	PG4	O1-C1-C2-O2
2	E	501	PG4	C3-C4-O3-C5
2	C	501	PG4	C3-C4-O3-C5
2	D	501	PG4	C3-C4-O3-C5
2	F	501	PG4	O1-C1-C2-O2
2	A	501	PG4	C4-C3-O2-C2
2	F	501	PG4	C3-C4-O3-C5
3	B	502	NAP	C5D-O5D-PN-O3
3	B	502	NAP	C5D-O5D-PN-O1N
3	B	502	NAP	C5D-O5D-PN-O2N
3	C	502	NAP	C5D-O5D-PN-O3
3	E	502	NAP	C5D-O5D-PN-O1N
3	F	502	NAP	C5D-O5D-PN-O1N
2	A	501	PG4	C3-C4-O3-C5
3	F	502	NAP	C4N-C3N-C7N-O7N
3	F	502	NAP	C4N-C3N-C7N-N7N
2	C	501	PG4	C4-C3-O2-C2
3	B	502	NAP	C4N-C3N-C7N-N7N
2	B	501	PG4	C3-C4-O3-C5
3	A	502	NAP	C3D-C4D-C5D-O5D
3	A	502	NAP	O4D-C1D-N1N-C6N
3	B	502	NAP	O4D-C1D-N1N-C6N
3	C	502	NAP	O4D-C1D-N1N-C6N

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
3	D	502	NAP	O4D-C1D-N1N-C6N
3	E	502	NAP	O4D-C1D-N1N-C6N
3	F	502	NAP	C2B-O2B-P2B-O1X
3	F	502	NAP	C2N-C3N-C7N-O7N
3	F	502	NAP	C2N-C3N-C7N-N7N
3	B	502	NAP	C4N-C3N-C7N-O7N
3	A	502	NAP	C2B-O2B-P2B-O3X
3	E	502	NAP	C2B-O2B-P2B-O3X
3	B	502	NAP	C2N-C3N-C7N-N7N
3	C	502	NAP	PA-O3-PN-O2N
3	C	502	NAP	O4B-C4B-C5B-O5B
3	D	502	NAP	O4B-C4B-C5B-O5B
3	E	502	NAP	O4B-C4B-C5B-O5B
3	F	502	NAP	O4B-C4B-C5B-O5B

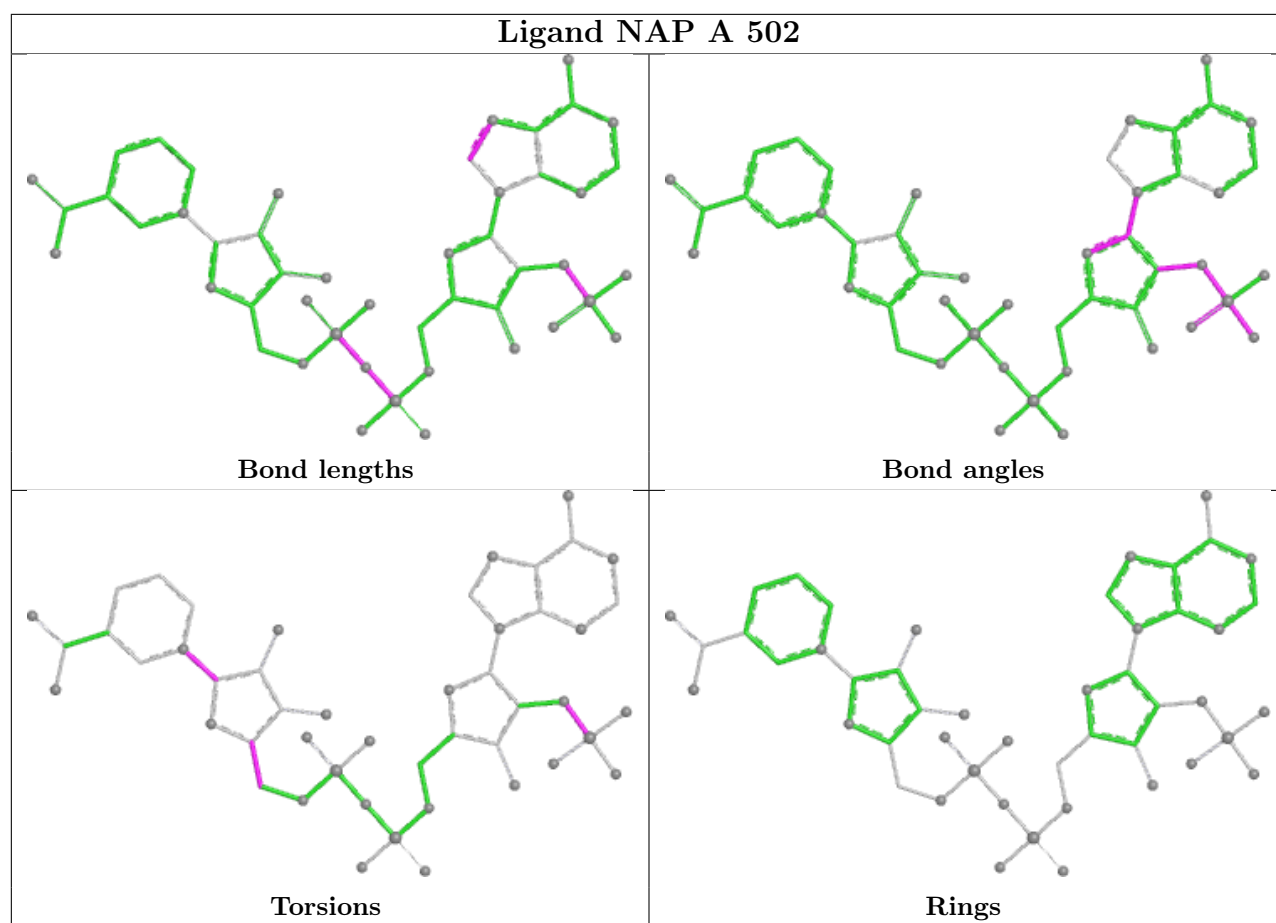
There are no ring outliers.

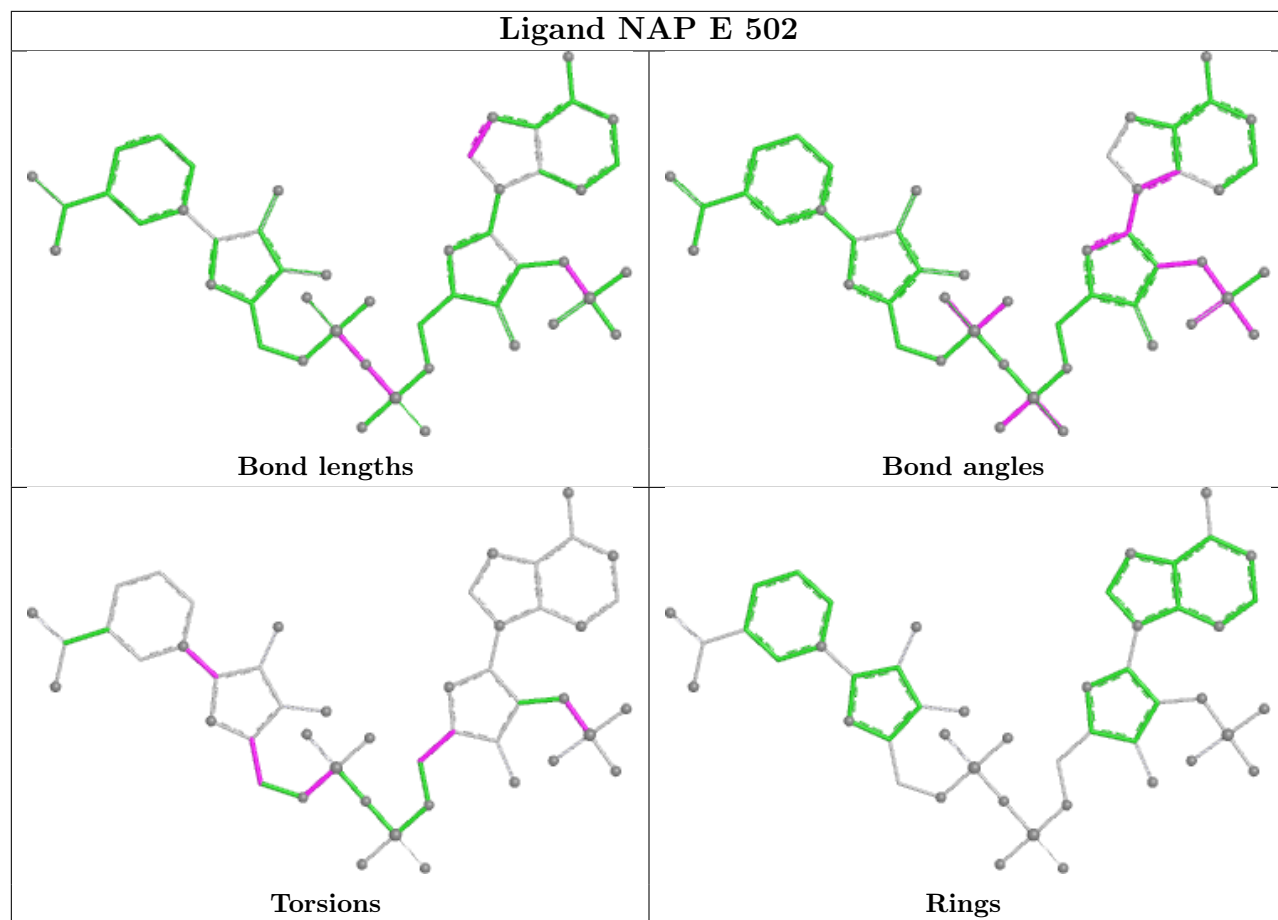
1 monomer is involved in 1 short contact:

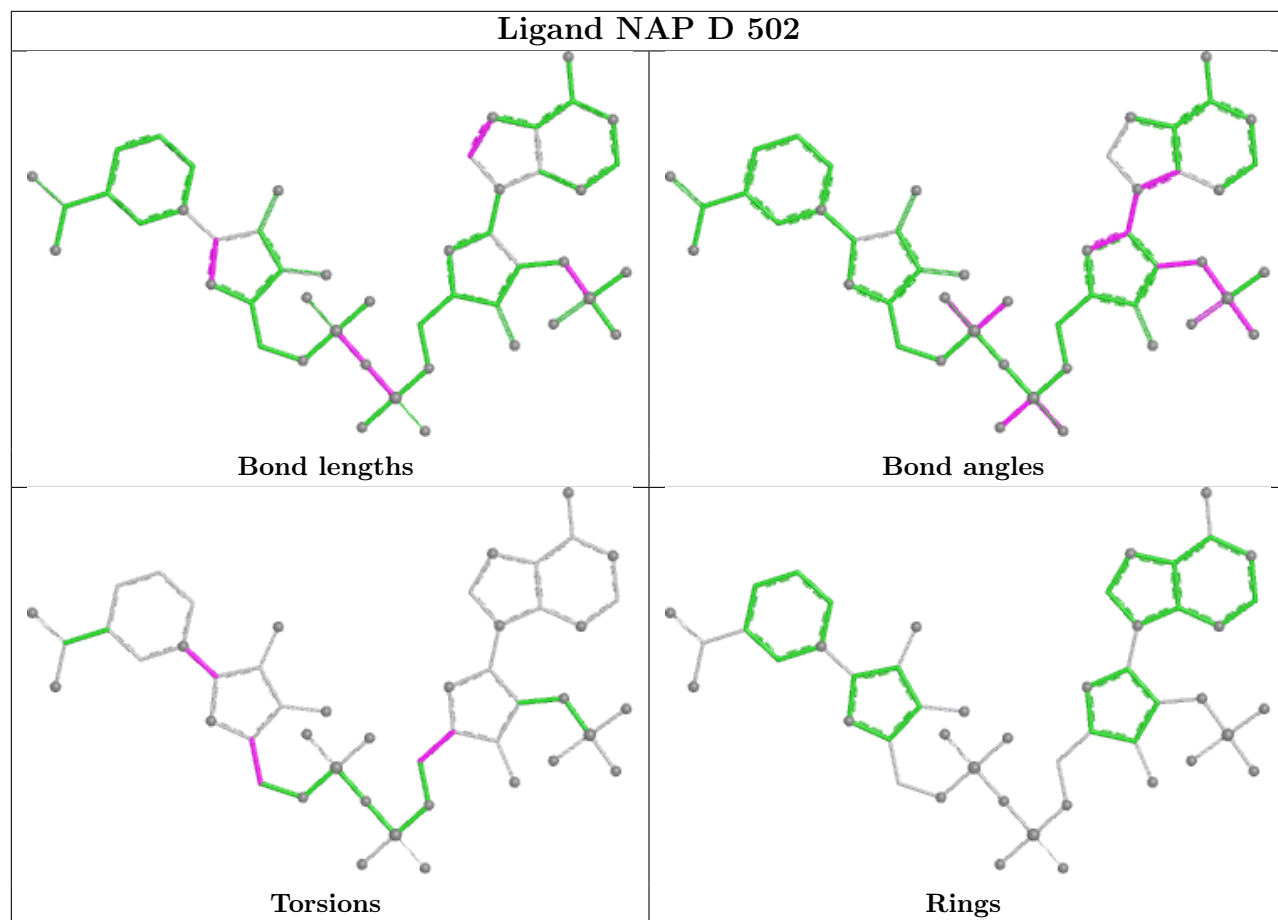
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	502	NAP	1	0

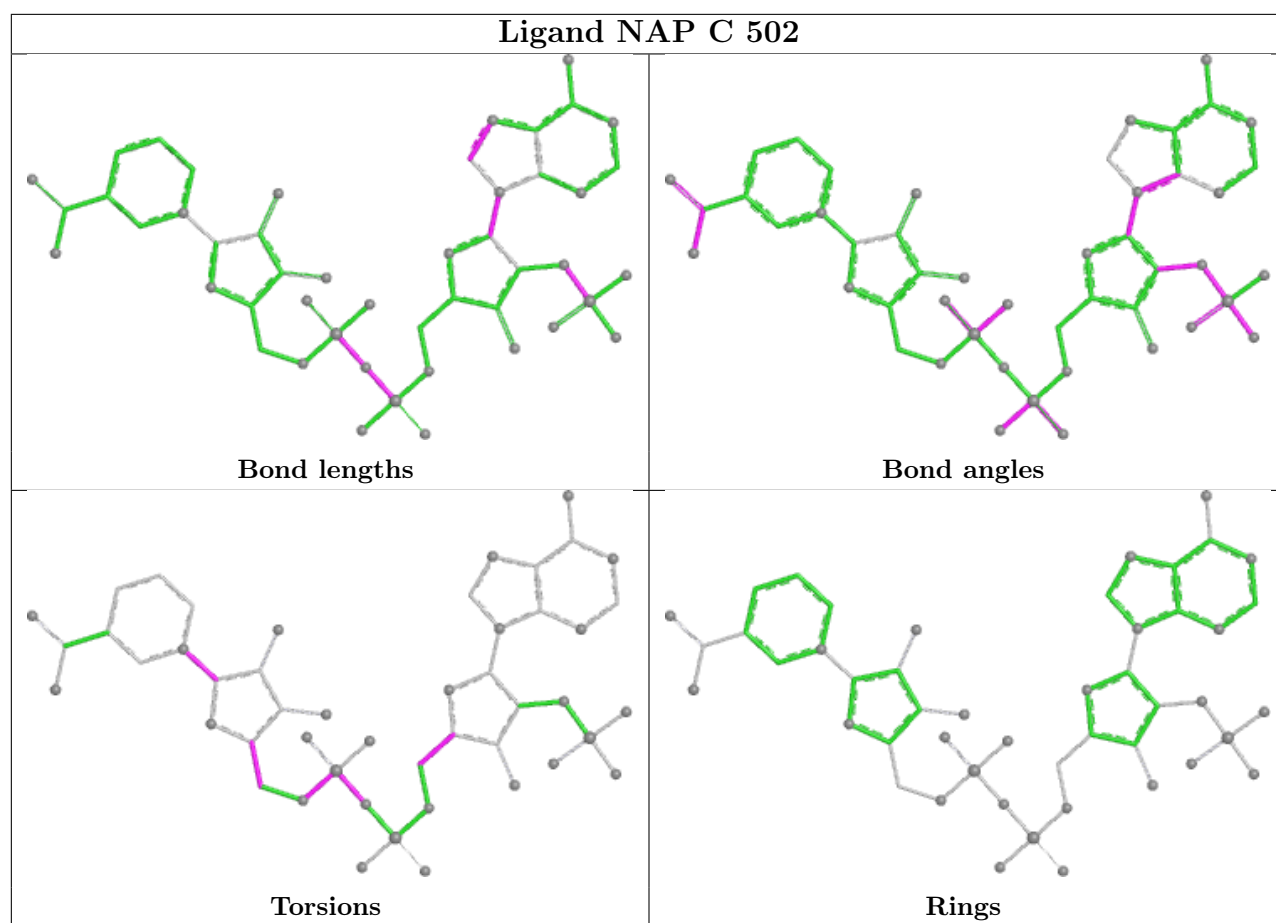
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

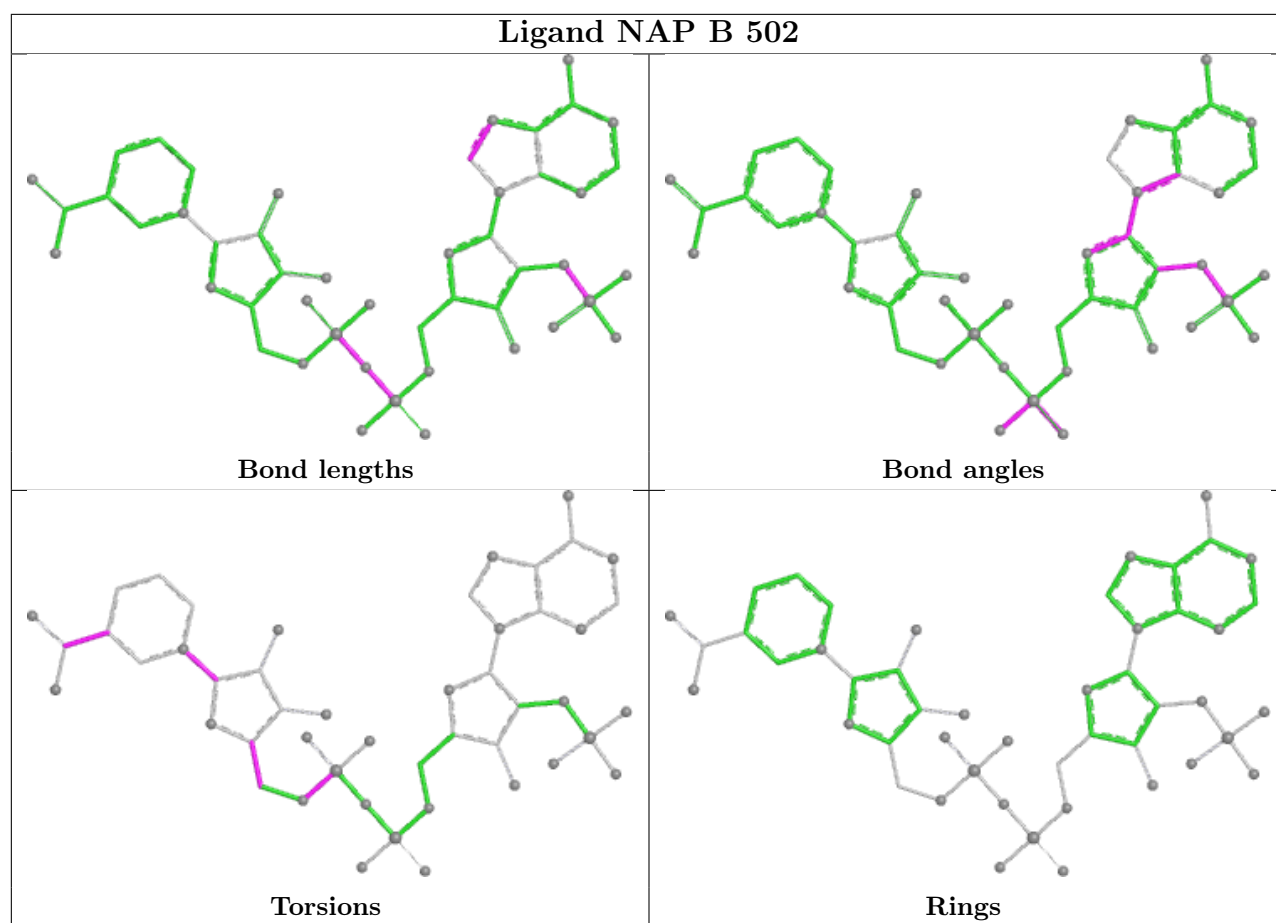


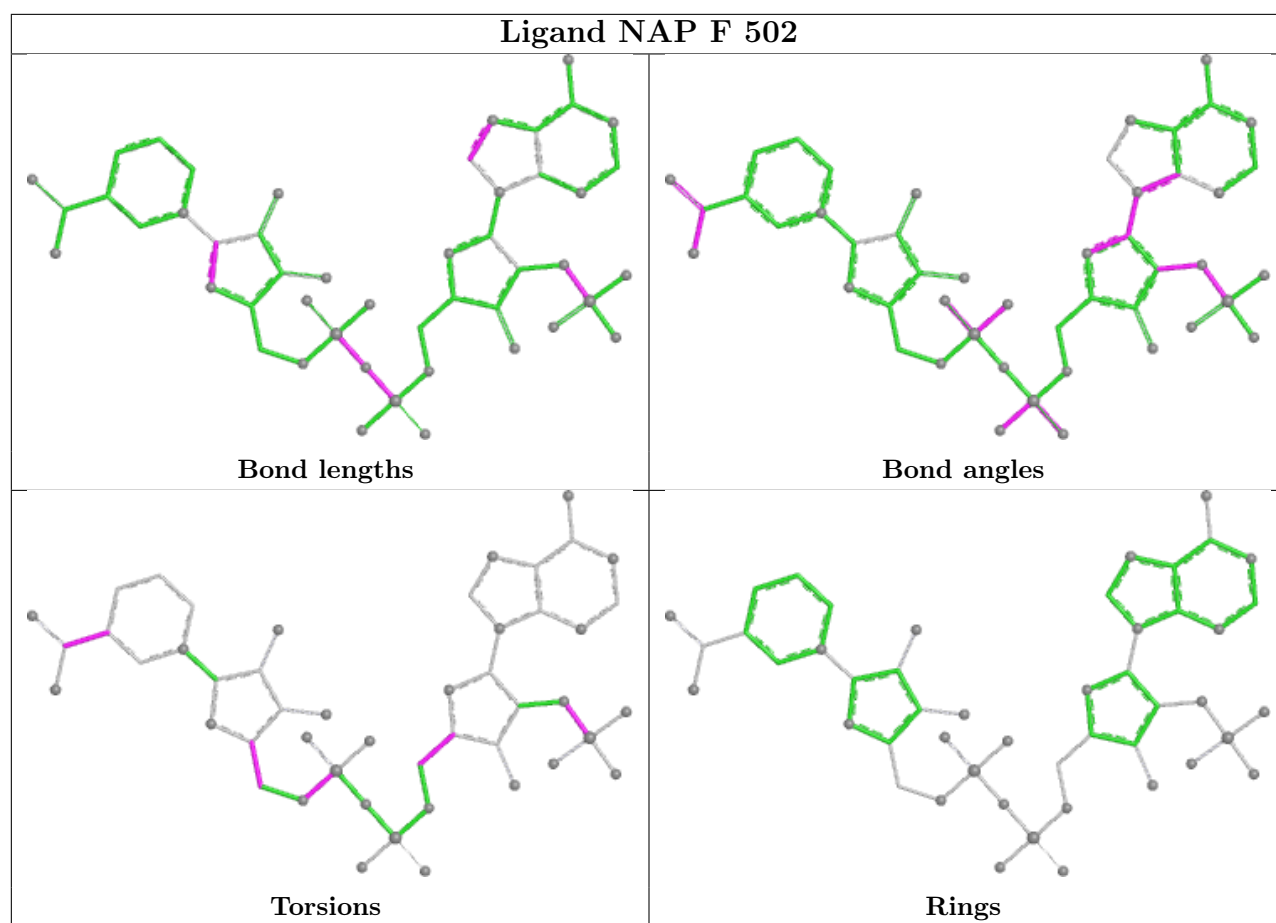












## 5.7 Other polymers [i](#)

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	467/487 (95%)	-0.06	5 (1%) 77 78	28, 40, 67, 80	0
1	B	466/487 (95%)	-0.29	4 (0%) 81 82	24, 34, 51, 79	0
1	C	467/487 (95%)	-0.11	1 (0%) 92 92	28, 40, 62, 81	0
1	D	460/487 (94%)	0.59	62 (13%) 8 9	30, 51, 127, 161	0
1	E	466/487 (95%)	0.09	6 (1%) 74 75	28, 46, 73, 90	0
1	F	466/487 (95%)	-0.13	3 (0%) 85 86	27, 39, 59, 77	0
All	All	2792/2922 (95%)	0.01	81 (2%) 54 55	24, 40, 79, 161	0

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	310	SER	4.9
1	D	283	TYR	3.7
1	D	277	PHE	3.7
1	D	287	PRO	3.6
1	D	349	ALA	3.6
1	D	284	ILE	3.5
1	D	290	PHE	3.5
1	D	312	PHE	3.5
1	D	330	VAL	3.5
1	D	279	ASP	3.4
1	D	321	PHE	3.3
1	D	358	GLY	3.3
1	D	329	ASP	3.2
1	F	304	ILE	3.2
1	D	316	SER	3.1
1	D	317	ASN	3.1
1	D	342	CYS	3.1
1	D	360	ILE	3.1
1	A	367	ASN	3.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	D	309	VAL	3.1
1	D	315	TYR	3.1
1	D	221	ARG	3.0
1	D	327	ALA	3.0
1	D	304	ILE	2.9
1	D	318	THR	2.9
1	D	280	SER	2.9
1	D	467	VAL	2.9
1	D	359	CYS	2.8
1	B	467	VAL	2.8
1	D	331	ASP	2.8
1	D	324	ASN	2.8
1	D	303	ASN	2.7
1	D	356	LYS	2.7
1	D	322	PHE	2.7
1	D	295	VAL	2.7
1	D	323	PRO	2.6
1	B	317	ASN	2.6
1	D	10	LEU	2.5
1	E	442	HIS	2.5
1	D	240	LEU	2.5
1	D	301	LEU	2.5
1	B	442	HIS	2.5
1	D	258	ASN	2.5
1	D	314	LYS	2.4
1	D	307	ALA	2.4
1	A	187	GLU	2.4
1	C	1	SER	2.4
1	D	361	ILE	2.4
1	B	333	ASN	2.4
1	D	278	SER	2.4
1	D	355	VAL	2.4
1	A	368	MET	2.4
1	D	299	MET	2.3
1	D	296	THR	2.3
1	D	257	GLY	2.3
1	D	300	GLU	2.3
1	D	319	ALA	2.3
1	E	441	VAL	2.2
1	D	305	GLN	2.2
1	D	286	GLU	2.2
1	E	317	ASN	2.2

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	F	442	HIS	2.2
1	D	253	ILE	2.2
1	D	268	ILE	2.2
1	E	467	VAL	2.2
1	D	313	LEU	2.2
1	D	367	ASN	2.2
1	D	224	ALA	2.2
1	D	276	THR	2.2
1	F	314	LYS	2.1
1	E	2	ASP	2.1
1	D	293	GLU	2.1
1	D	241	HIS	2.1
1	E	240	LEU	2.1
1	D	285	TYR	2.0
1	A	442	HIS	2.0
1	A	440	ASN	2.0
1	D	332	THR	2.0
1	D	337	ALA	2.0
1	D	242	ASN	2.0
1	D	344	ASN	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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

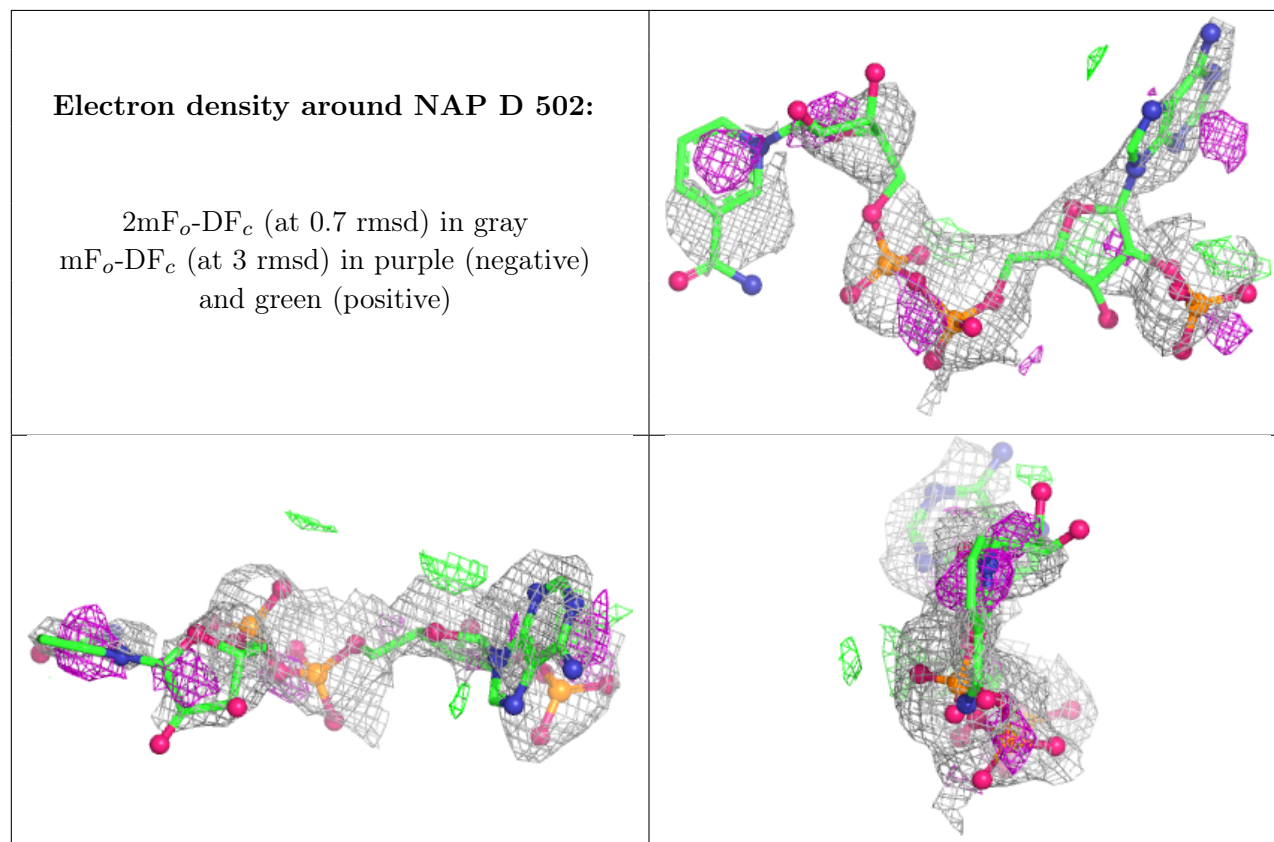
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	NAP	D	502	48/48	0.50	0.17	80,107,116,119	0
2	PG4	A	501	13/13	0.84	0.14	35,44,51,53	0
2	PG4	E	501	13/13	0.87	0.11	35,45,51,52	0

*Continued on next page...*

*Continued from previous page...*

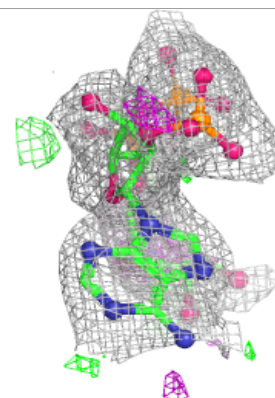
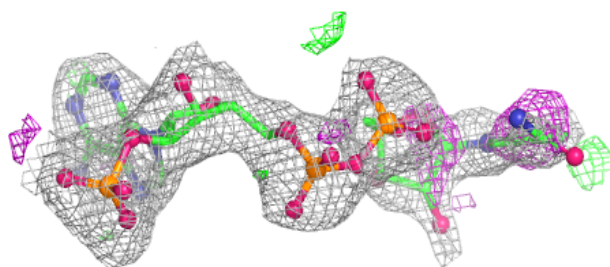
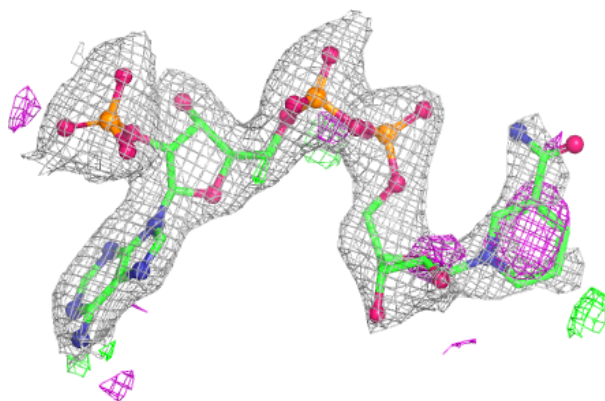
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NAP	A	502	48/48	0.88	0.11	46,58,67,71	0
3	NAP	C	502	48/48	0.89	0.11	36,47,60,66	0
2	PG4	C	501	13/13	0.89	0.10	35,42,46,53	0
2	PG4	F	501	13/13	0.90	0.12	41,44,53,54	0
2	PG4	B	501	13/13	0.91	0.10	34,39,53,53	0
3	NAP	E	502	48/48	0.91	0.11	38,50,61,66	0
2	PG4	D	501	13/13	0.92	0.11	41,46,51,52	0
3	NAP	F	502	48/48	0.93	0.10	34,46,62,68	0
3	NAP	B	502	48/48	0.95	0.09	31,39,56,60	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.

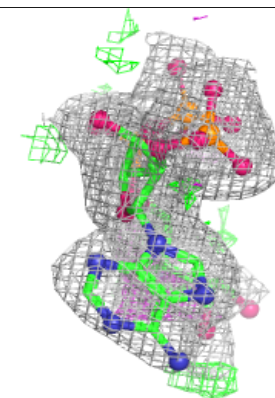
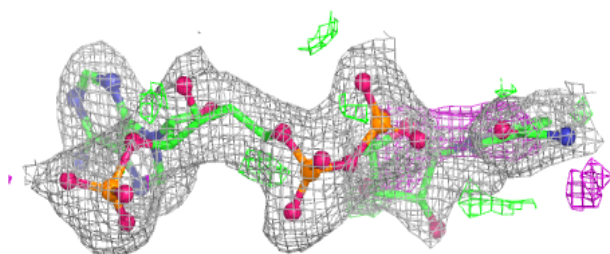
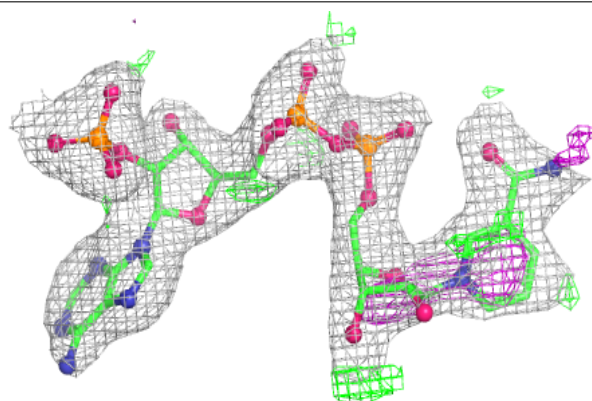


**Electron density around NAP A 502:**

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

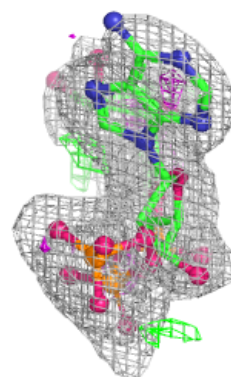
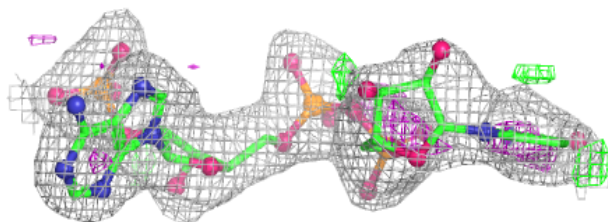
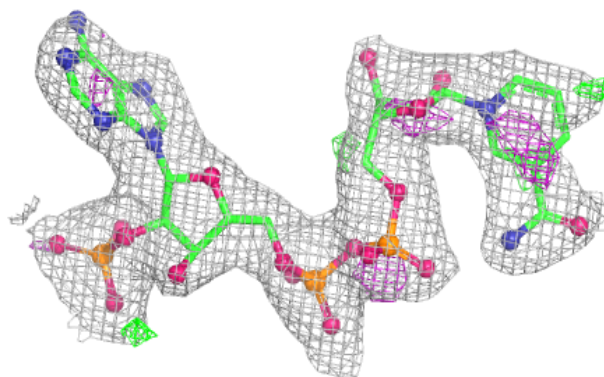
**Electron density around NAP C 502:**

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

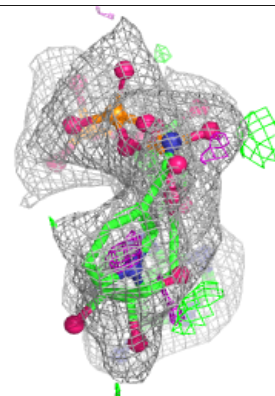
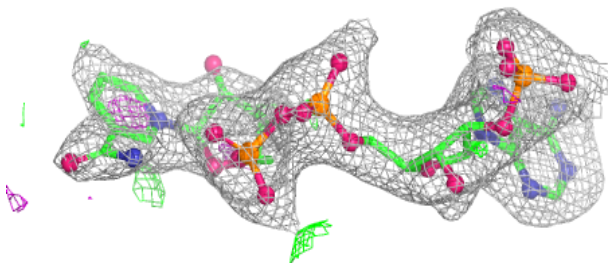
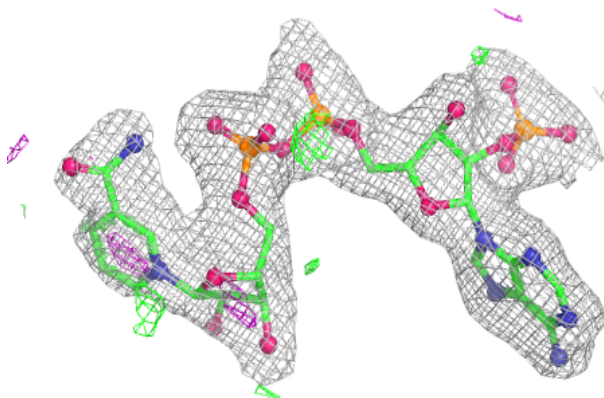


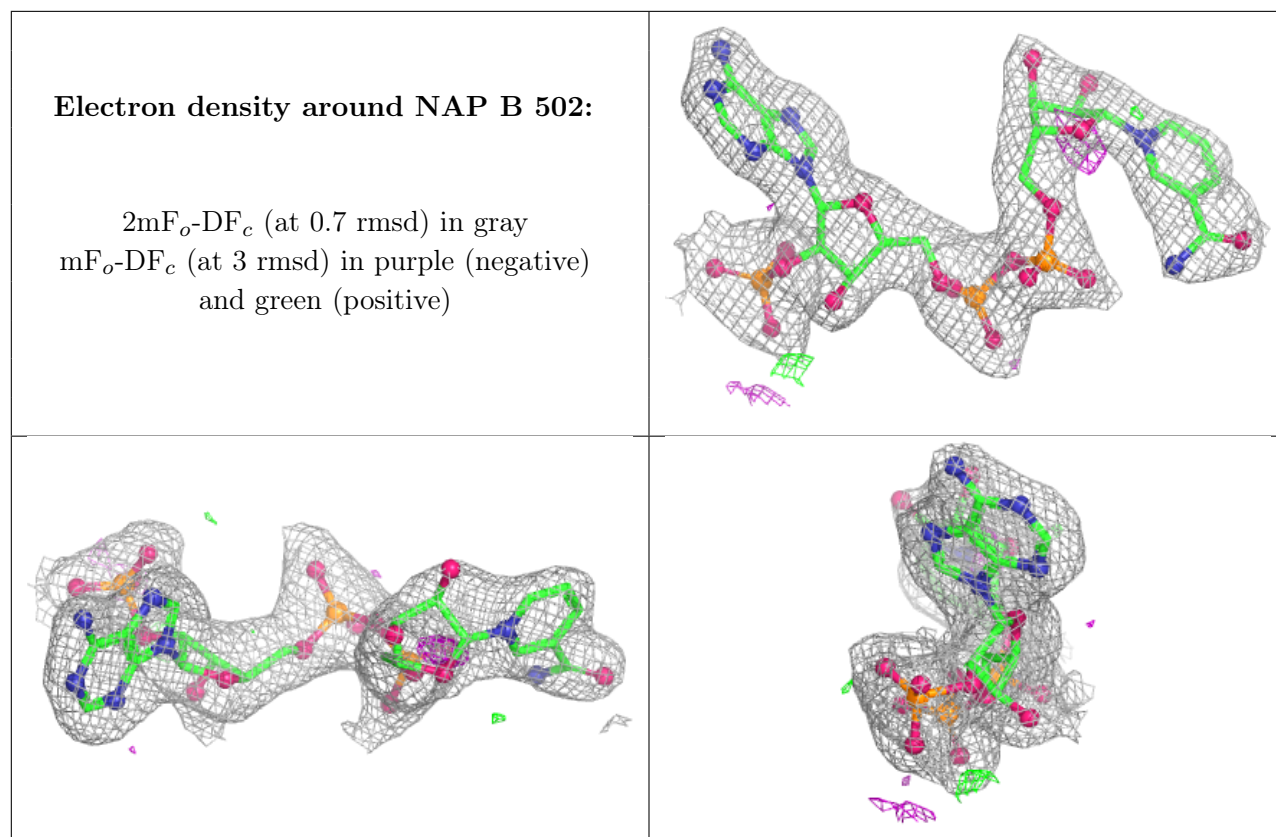
**Electron density around NAP E 502:**

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

**Electron density around NAP F 502:**

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





## 6.5 Other polymers [i](#)

There are no such residues in this entry.