



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 15, 2020 – 01:39 pm BST

PDB ID : 2JKV  
Title : Structure of human Phosphogluconate Dehydrogenase in complex with NADPH at 2.53Å  
Authors : Pilka, E.S.; Kavanagh, K.L.; von Delft, F.; Muniz, J.R.C.; Murray, J.; Piccaud, S.; Guo, K.; Edwards, A.; Arrowsmith, C.H.; Weigelt, J.; Bountra, C.; Oppermann, U.  
Deposited on : 2008-09-01  
Resolution : 2.53 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.

---

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 : 2.11  
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) : 2.11

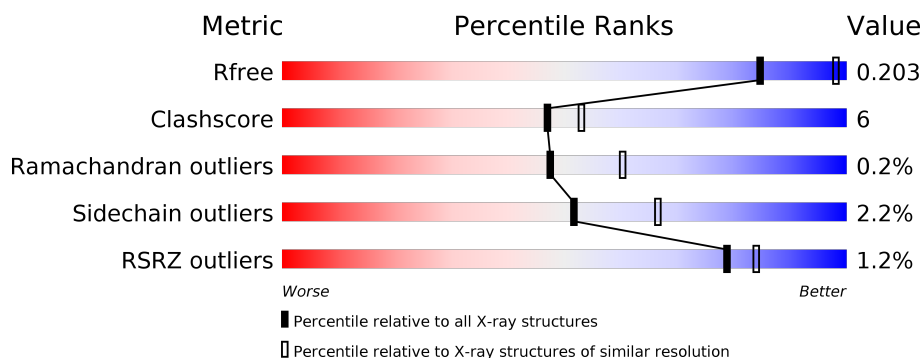
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.53 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	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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	505	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>%</span> <span>81%</span> <span>13%</span> <span>• 5%</span> </div> </div>
1	B	505	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>%</span> <span>83%</span> <span>12%</span> <span>• 5%</span> </div> </div>
1	C	505	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>2%</span> <span>81%</span> <span>14%</span> <span>5%</span> </div> </div>
1	D	505	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>2%</span> <span>80%</span> <span>15%</span> <span>5%</span> </div> </div>
1	E	505	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span></span> <span>82%</span> <span>13%</span> <span>5%</span> </div> </div>
1	F	505	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>%</span> <span>80%</span> <span>13%</span> <span>• 7%</span> </div> </div>

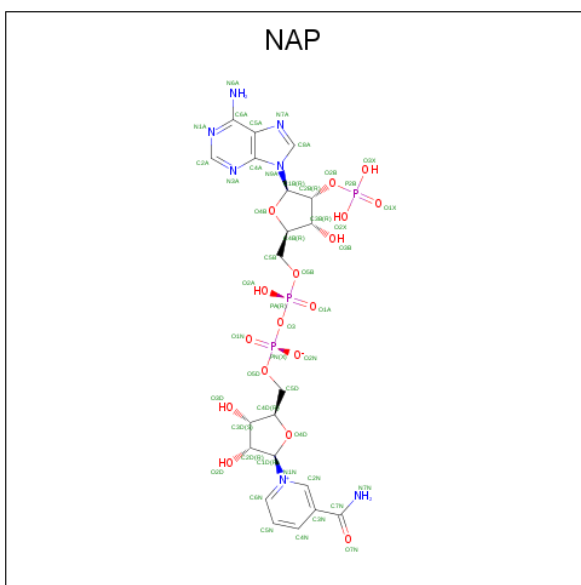


In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 6-PHOSPHOGLUCONATE DEHYDROGENASE, DECARBOXYLATING.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	482	Total 3708	C 2361	N 634	O 691	S 22	0	1	0
1	B	482	Total 3701	C 2358	N 634	O 687	S 22	0	1	0
1	C	482	Total 3689	C 2351	N 629	O 687	S 22	0	0	0
1	D	482	Total 3690	C 2351	N 632	O 685	S 22	0	0	0
1	E	482	Total 3693	C 2354	N 633	O 684	S 22	0	0	0
1	F	471	Total 3640	C 2322	N 626	O 670	S 22	0	0	0

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

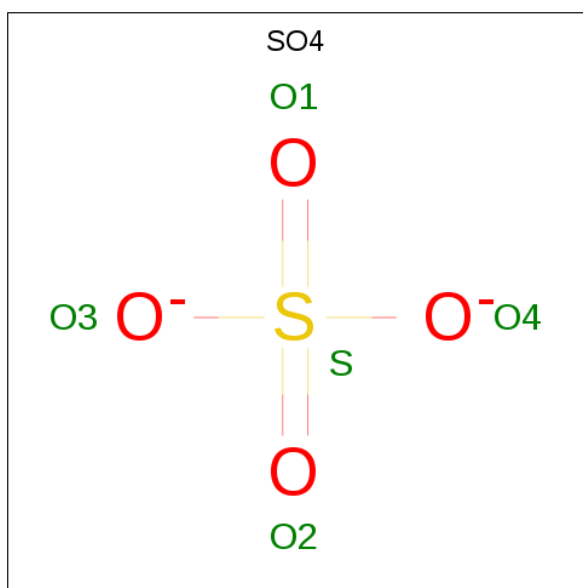


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	E	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	3	Total	Cl	0	0
			3	3		
3	A	3	Total	Cl	0	0
			3	3		
3	D	1	Total	Cl	0	0
			1	1		
3	F	2	Total	Cl	0	0
			2	2		
3	E	2	Total	Cl	0	0
			2	2		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0
4	E	1	Total O S 5 4 1	0	0
4	E	1	Total O S 5 4 1	0	0
4	F	1	Total O S 5 4 1	0	0
4	F	1	Total O S 5 4 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	263	Total O 263 263	0	0
5	B	269	Total O 269 269	0	0
5	C	195	Total O 195 195	0	0
5	D	191	Total O 191 191	0	0
5	E	238	Total O 238 238	0	0
5	F	249	Total O 249 249	0	0

These plots are drawn for all protein, RNA and DNA 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 ( $\text{RSRZ} > 2$ ). 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.

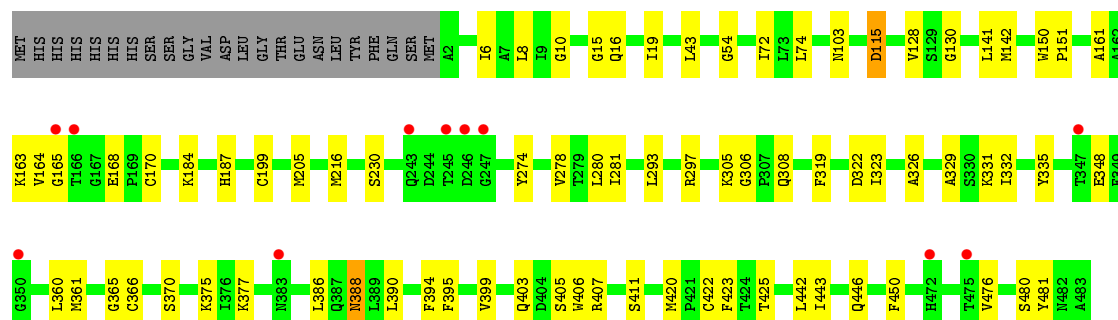
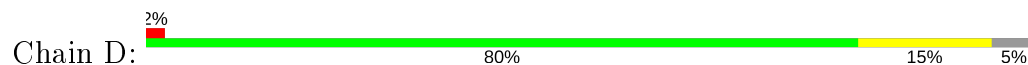
- Chain A:
- 
- 81% 13% 5%
- MET HIS HIS HIS HIS HIS HIS SER SER GLY VAL ASP LEU GLY THR GLU ASN LEU TRP PHE GLN SER MET A2 A7 A8 F27 L43 A44 N45 K48 K51 V52 L53 L65 K66 K67 P68 L74 D82 L88 E105 R111 G131 M142 W150 P151 I156 V164 G165 T166 L167 E168 P169 M185 D194 G199 E200 I235 I239 L251 T267 Y274 G275 V276 P277 V278 I281 G282 G306 K317 D322 Q337 E348 K361 K362 R363 S370 V371 F372 L391 Q403 D404 S405 S406 R407 R408 P421 C422 T425 A426 L427 S428 P439 L442 Q446 Y449 F450 E456 K460 Q463 W469 S479 S480 A483

- Chain B:
- 
- 83% 12% 5%
- MTT HIS HIS HIS HIS HIS HIS SER SER GLY VAL ASP LEU LEU THR GLY GLU ASN LEU LEU TRR PHE GLN MET MET A2 Q3 L8 I9 N23 T50 K51 L73 L74 K119 S129 G130 G131 P139 S140 L141 M142 P143 A161 V164 G165 E168 P169 D172 P104 C199 M205 M216 E227 L228 D229 T245 R255 D256 Y274 V278 T279 L280 I281 Q299 K302 G306 P307 Q308 F319 D322 I323 Y328 E348 M361 K362 R363 R369 S370 V371 F372 K375 N388 I389 L390 L391 F394 Q403 P406 S405 W406 R407 R408 V414 Q415 C422 T425 P439 I443 F450 E456 S479 S480 A483

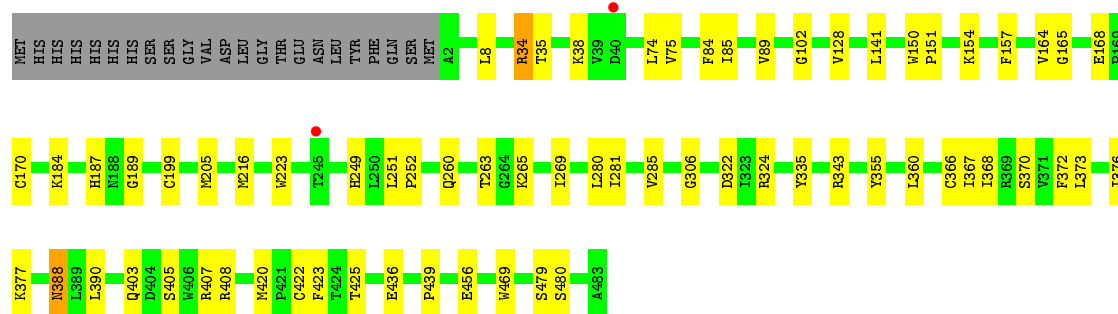
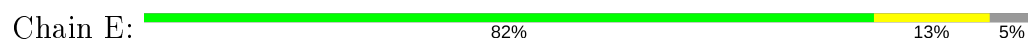
- Chain C:
- 
- | Residue Type | Count |
|--------------|-------|
| MET          | 2     |
| HIS          | 1     |
| HIS          | 1     |
| HIS          | 1     |
| HIS          | 1     |
| HIS          | 1     |
| SER          | 1     |
| SER          | 1     |
| GLY          | 1     |
| VAL          | 1     |
| ASP          | 1     |
| LEU          | 1     |
| GLY          | 1     |
| THR          | 1     |
| GLU          | 1     |
| ASN          | 1     |
| LEU          | 1     |
| TYR          | 1     |
| PHE          | 1     |
| GLN          | 1     |
| SER          | 1     |
| MET          | 1     |
| A2           | 1     |
| I9           | 1     |
| G10          | 1     |
| L11          | 1     |
| G15          | 1     |
| Q16          | 1     |
| N33          | 1     |
| A44          | 1     |
| G49          | 1     |
| L73          | 1     |
| K76          | 1     |
| V89          | 1     |
| N103         | 1     |
| S104         | 1     |
| E105         | 1     |
| L116         | 1     |
| F123         | 1     |
| S129         | 1     |
| G130         | 1     |
| G131         | 1     |
| E132         | 1     |
| E133         | 1     |
| G138         | 1     |
| P139         | 1     |



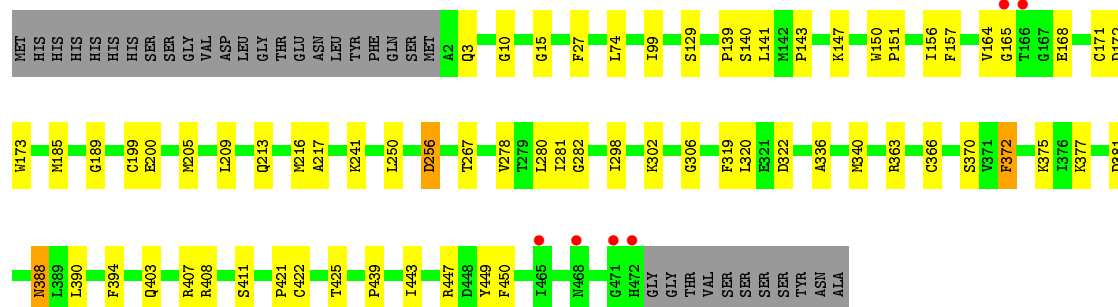
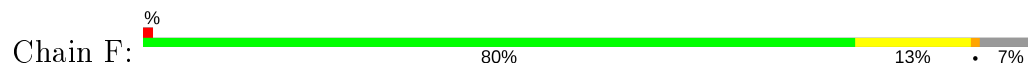
- Molecule 1: 6-PHOSPHOGLUCONATE DEHYDROGENASE, DECARBOXYLATING



- Molecule 1: 6-PHOSPHOGLUCONATE DEHYDROGENASE, DECARBOXYLATING



- Molecule 1: 6-PHOSPHOGLUCONATE DEHYDROGENASE, DECARBOXYLATING



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	56.64Å 204.71Å 170.32Å 90.00° 90.65° 90.00°	Depositor
Resolution (Å)	36.90 – 2.53 36.90 – 2.53	Depositor EDS
% Data completeness (in resolution range)	92.2 (36.90-2.53) 97.8 (36.90-2.53)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.08 (at 2.54Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.156 , 0.207 0.155 , 0.203	Depositor DCC
$R_{free}$ test set	2120 reflections (1.68%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	31.2	Xtriage
Anisotropy	0.515	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 49.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.054 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	23837	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.47% 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: NAP, SO4, CL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.43	0/3784	0.53	0/5105
1	B	0.43	0/3777	0.56	1/5096 (0.0%)
1	C	0.43	0/3765	0.53	0/5083
1	D	0.42	0/3766	0.52	0/5083
1	E	0.43	0/3769	0.57	0/5087
1	F	0.41	0/3715	0.56	1/5010 (0.0%)
All	All	0.42	0/22576	0.55	2/30464 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	256	ASP	N-CA-CB	-7.87	96.44	110.60
1	F	256	ASP	N-CA-CB	-6.79	98.38	110.60

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	3708	0	3652	57	0
1	B	3701	0	3646	47	0
1	C	3689	0	3623	46	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3690	0	3628	55	0
1	E	3693	0	3639	49	0
1	F	3640	0	3614	50	0
2	A	48	0	25	1	0
2	B	48	0	25	0	0
2	C	48	0	25	1	0
2	D	48	0	25	0	0
2	E	48	0	25	0	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
3	D	1	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
4	A	10	0	0	0	0
4	B	10	0	0	0	0
4	C	10	0	0	0	0
4	D	10	0	0	0	0
4	E	10	0	0	1	0
4	F	10	0	0	0	0
5	A	263	0	0	4	0
5	B	269	0	0	3	0
5	C	195	0	0	2	0
5	D	191	0	0	1	0
5	E	238	0	0	1	0
5	F	249	0	0	3	0
All	All	23837	0	21927	275	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 6.

The worst 5 of 275 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:C:388:ASN:HD22	1:C:390:LEU:H	1.10	0.94
1:D:403:GLN:HE21	1:D:407:ARG:HH21	1.12	0.92
1:A:403:GLN:HE21	1:A:407:ARG:HH21	1.13	0.92
1:B:403:GLN:HE21	1:B:407:ARG:HH21	0.98	0.90
1:B:403:GLN:NE2	1:B:407:ARG:HH21	1.69	0.89

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	481/505 (95%)	463 (96%)	17 (4%)	1 (0%)	47	60
1	B	481/505 (95%)	461 (96%)	19 (4%)	1 (0%)	47	60
1	C	480/505 (95%)	466 (97%)	13 (3%)	1 (0%)	47	60
1	D	480/505 (95%)	462 (96%)	16 (3%)	2 (0%)	34	46
1	E	480/505 (95%)	459 (96%)	20 (4%)	1 (0%)	47	60
1	F	469/505 (93%)	453 (97%)	15 (3%)	1 (0%)	47	60
All	All	2871/3030 (95%)	2764 (96%)	100 (4%)	7 (0%)	47	60

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	165	GLY
1	B	165	GLY
1	C	165	GLY
1	D	165	GLY
1	D	386	LEU

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

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	380/410 (93%)	372 (98%)	8 (2%)	53	68
1	B	378/410 (92%)	370 (98%)	8 (2%)	53	68
1	C	376/410 (92%)	366 (97%)	10 (3%)	44	59

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	376/410 (92%)	370 (98%)	6 (2%)	62	77
1	E	377/410 (92%)	369 (98%)	8 (2%)	53	68
1	F	375/410 (92%)	365 (97%)	10 (3%)	44	59
All	All	2262/2460 (92%)	2212 (98%)	50 (2%)	52	66

5 of 50 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	372	PHE
1	D	168	GLU
1	F	370	SER
1	C	388	ASN
1	C	479	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	415	GLN
1	D	308	GLN
1	E	388	ASN
1	C	403	GLN
1	E	403	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 28 ligands modelled in this entry, 11 are monoatomic - leaving 17 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	NAP	C	500	-	45,52,52	1.68	4 (8%)	56,80,80	1.18	4 (7%)
4	SO4	E	1484	-	4,4,4	0.16	0	6,6,6	0.26	0
2	NAP	D	500	-	45,52,52	1.72	4 (8%)	56,80,80	1.16	2 (3%)
2	NAP	E	500	-	45,52,52	1.69	4 (8%)	56,80,80	1.17	2 (3%)
4	SO4	C	1484	-	4,4,4	0.22	0	6,6,6	0.42	0
2	NAP	A	500	-	45,52,52	1.69	3 (6%)	56,80,80	1.13	2 (3%)
2	NAP	B	500	-	45,52,52	1.67	3 (6%)	56,80,80	1.20	3 (5%)
4	SO4	D	1484	-	4,4,4	0.15	0	6,6,6	0.32	0
4	SO4	F	1475	-	4,4,4	0.11	0	6,6,6	0.29	0
4	SO4	A	1485	-	4,4,4	0.12	0	6,6,6	0.41	0
4	SO4	F	1474	-	4,4,4	0.26	0	6,6,6	0.19	0
4	SO4	C	1485	-	4,4,4	0.17	0	6,6,6	0.18	0
4	SO4	E	1485	-	4,4,4	0.18	0	6,6,6	0.60	0
4	SO4	A	1486	-	4,4,4	0.22	0	6,6,6	0.18	0
4	SO4	D	1485	-	4,4,4	0.12	0	6,6,6	0.15	0
4	SO4	B	1486	-	4,4,4	0.20	0	6,6,6	0.61	0
4	SO4	B	1487	-	4,4,4	0.17	0	6,6,6	0.22	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAP	B	500	-	-	6/31/67/67	0/5/5/5
2	NAP	E	500	-	-	6/31/67/67	0/5/5/5
2	NAP	C	500	-	-	6/31/67/67	0/5/5/5
2	NAP	A	500	-	-	6/31/67/67	0/5/5/5
2	NAP	D	500	-	-	6/31/67/67	0/5/5/5

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	500	NAP	O7N-C7N	9.10	1.41	1.24
2	E	500	NAP	O7N-C7N	8.74	1.40	1.24
2	A	500	NAP	O7N-C7N	8.62	1.40	1.24
2	B	500	NAP	O7N-C7N	8.57	1.40	1.24
2	C	500	NAP	O7N-C7N	8.43	1.40	1.24

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	500	NAP	N3A-C2A-N1A	-5.88	119.49	128.68
2	E	500	NAP	N3A-C2A-N1A	-5.85	119.54	128.68
2	C	500	NAP	N3A-C2A-N1A	-5.49	120.10	128.68
2	A	500	NAP	N3A-C2A-N1A	-5.46	120.15	128.68
2	B	500	NAP	N3A-C2A-N1A	-5.37	120.28	128.68

There are no chirality outliers.

5 of 30 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	500	NAP	C2B-O2B-P2B-O1X
2	D	500	NAP	C2B-O2B-P2B-O3X
2	D	500	NAP	O4D-C1D-N1N-C2N
2	D	500	NAP	O4D-C1D-N1N-C6N
2	D	500	NAP	C2D-C1D-N1N-C2N

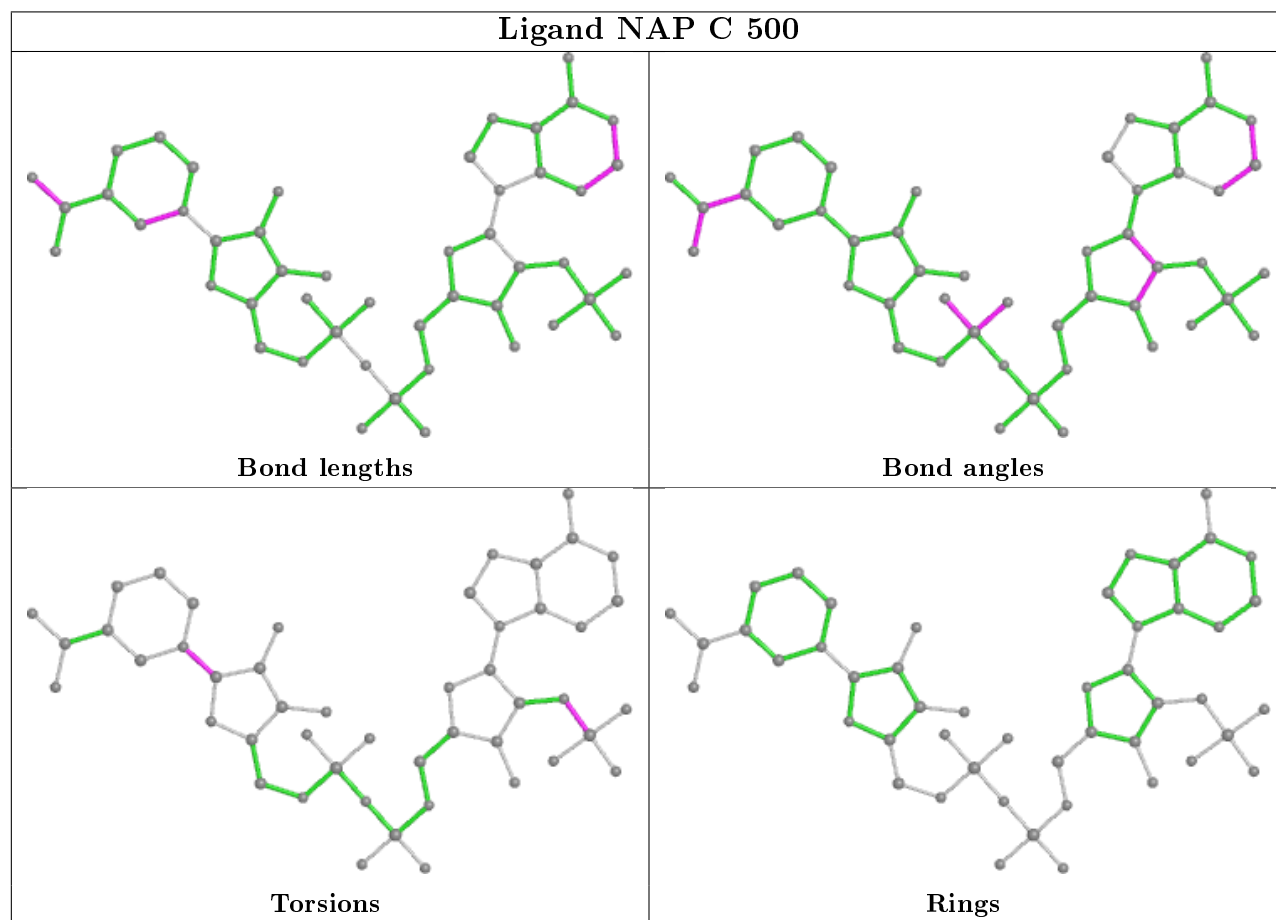
There are no ring outliers.

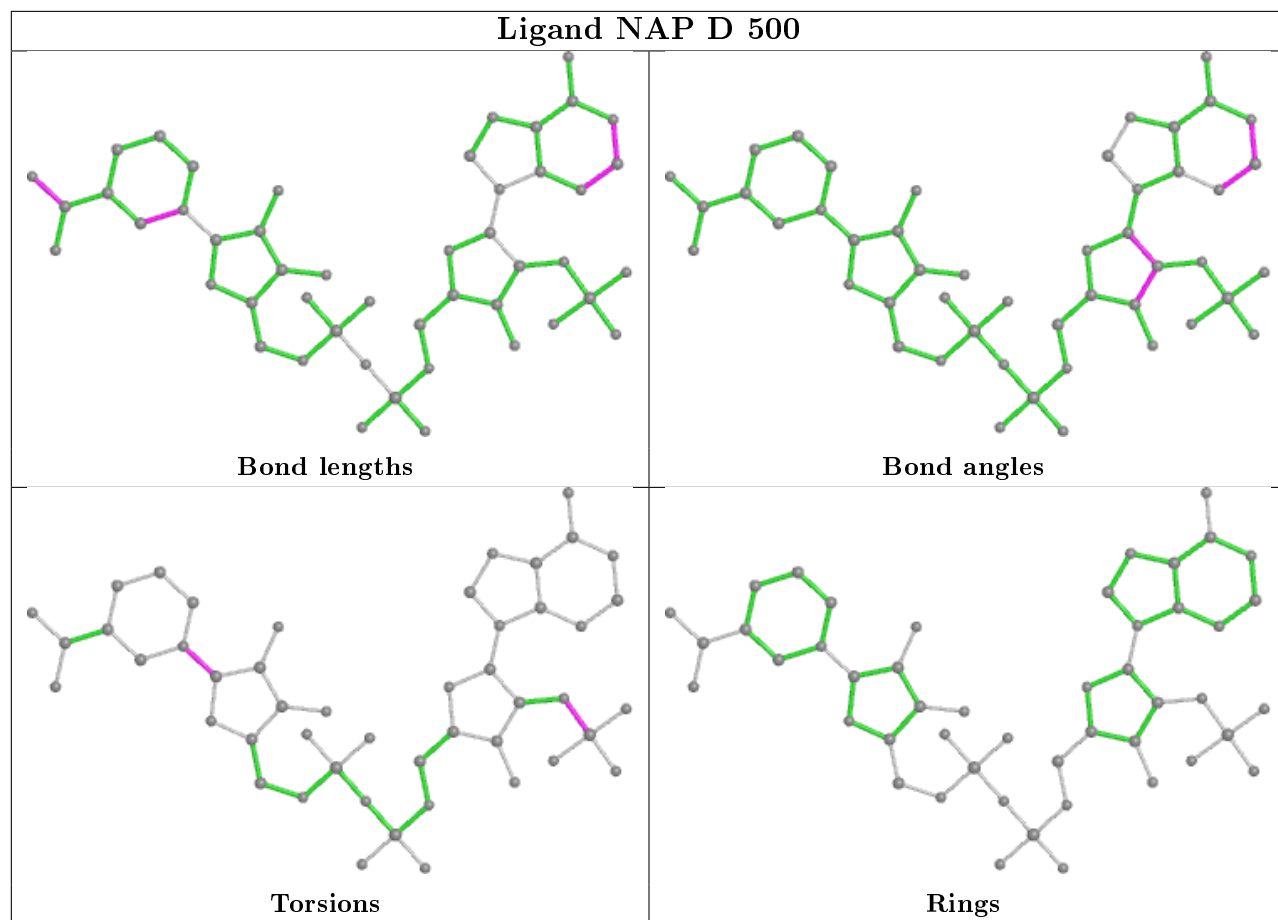
3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	500	NAP	1	0
4	E	1484	SO4	1	0
2	A	500	NAP	1	0

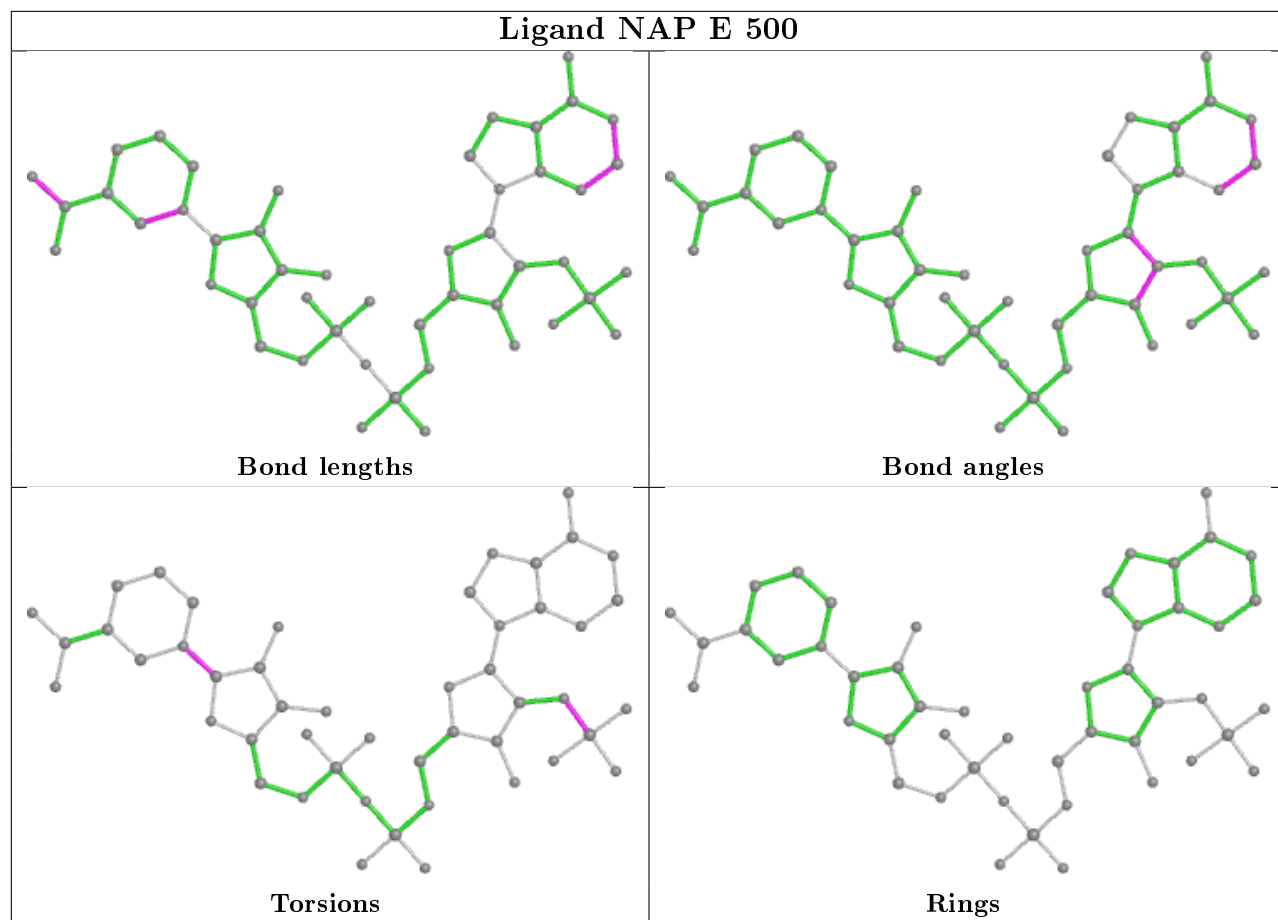
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

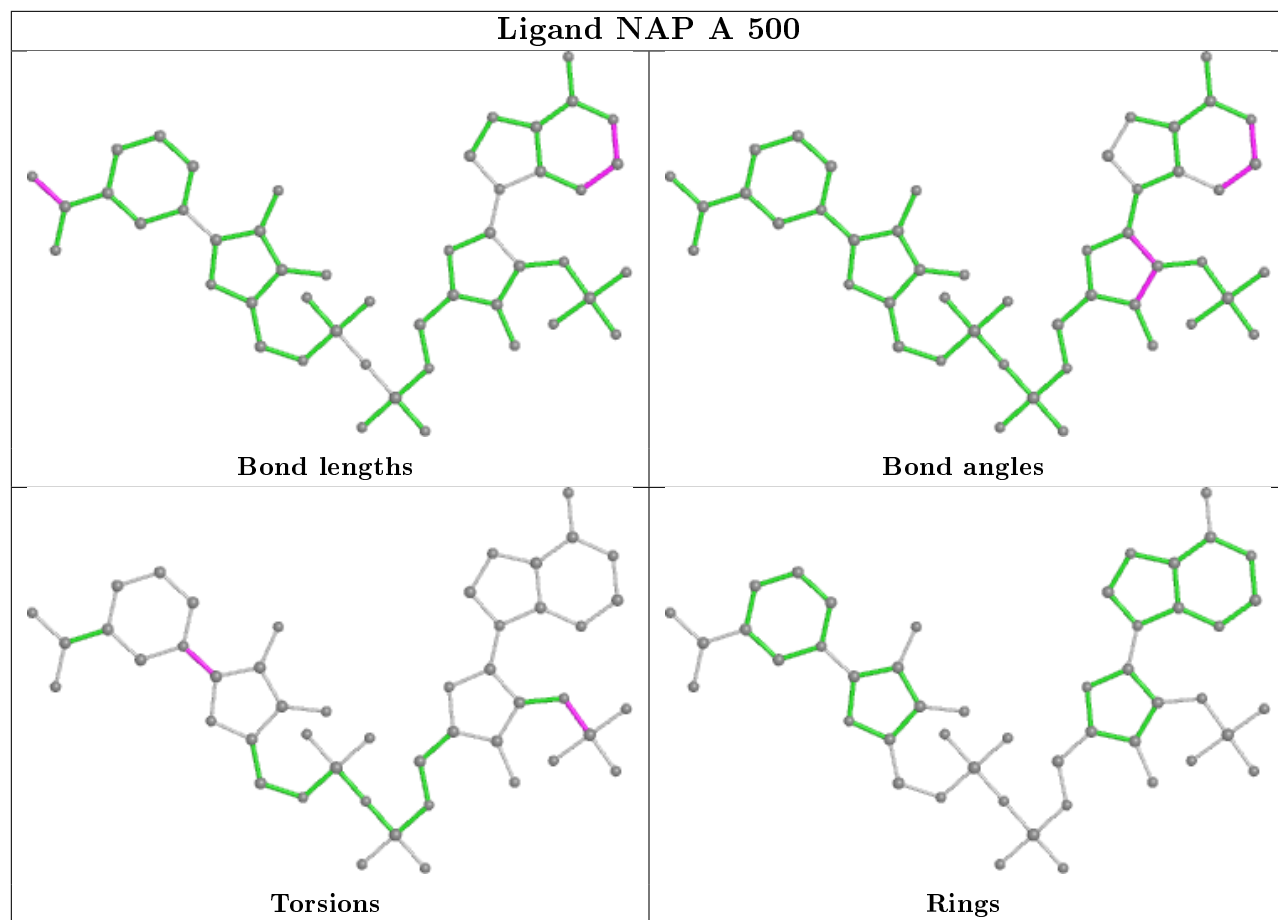
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

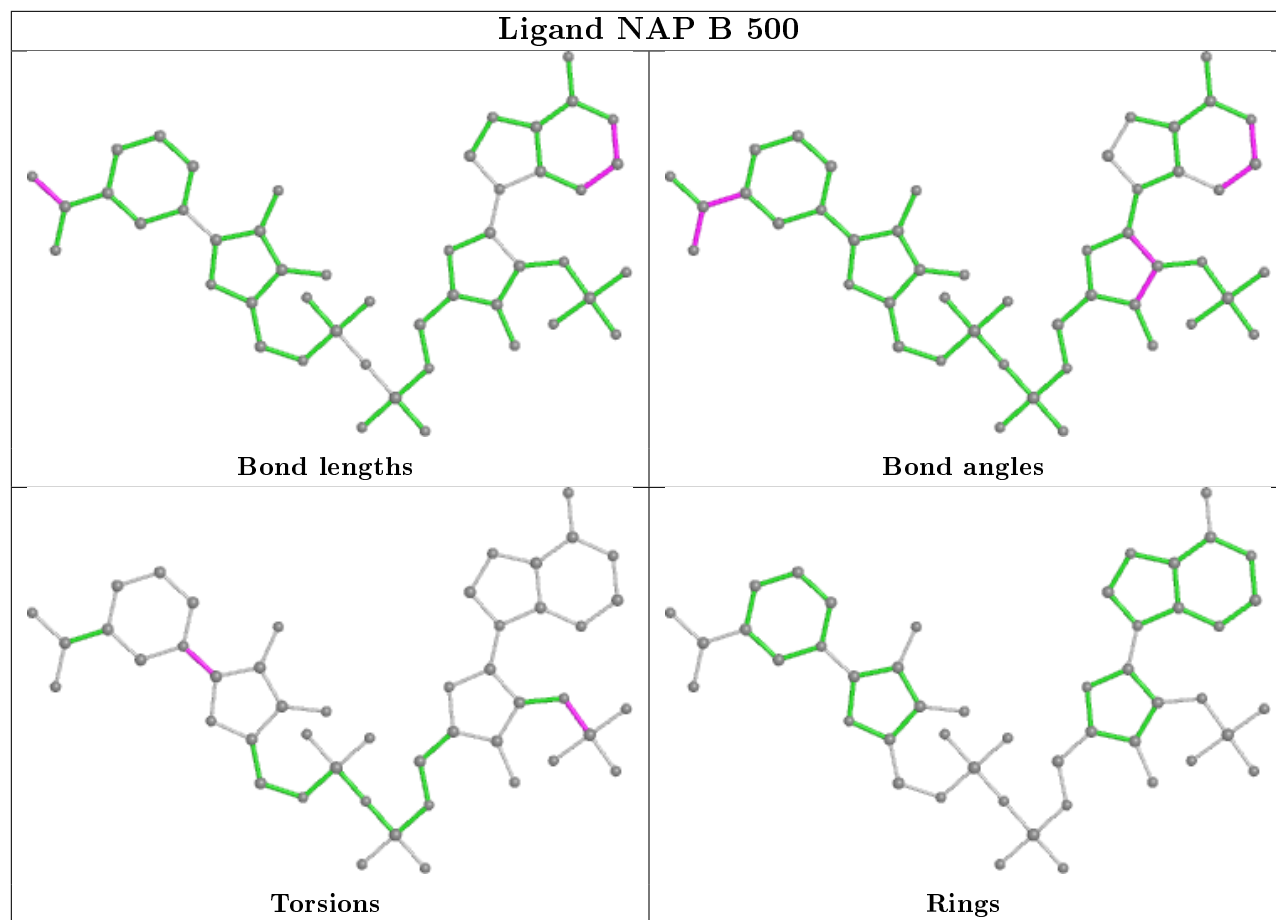












## 5.7 Other polymers [i](#)

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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	482/505 (95%)	-0.46	3 (0%) 89 92	12, 30, 57, 83	0
1	B	482/505 (95%)	-0.35	4 (0%) 86 89	12, 29, 56, 84	0
1	C	482/505 (95%)	-0.24	10 (2%) 63 70	18, 34, 59, 84	0
1	D	482/505 (95%)	-0.21	11 (2%) 60 67	21, 35, 59, 85	0
1	E	482/505 (95%)	-0.44	2 (0%) 92 96	14, 31, 57, 83	0
1	F	471/505 (93%)	-0.42	6 (1%) 77 82	14, 29, 52, 88	0
All	All	2881/3030 (95%)	-0.35	36 (1%) 79 84	12, 31, 58, 88	0

The worst 5 of 36 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	472	HIS	5.3
1	D	472	HIS	4.8
1	F	471	GLY	4.0
1	B	2	ALA	3.8
1	D	245	THR	3.7

### 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 carbohydrates in this entry.

## 6.4 Ligands ⓘ

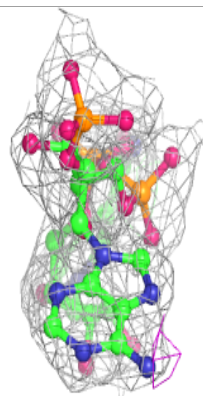
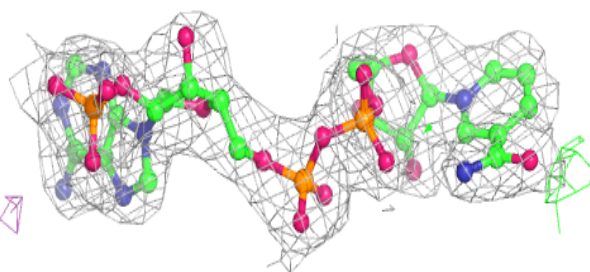
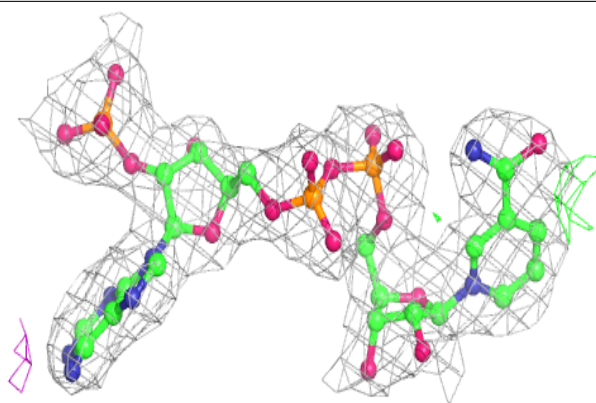
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
3	CL	D	1486	1/1	0.81	0.82	81,81,81,81	0
3	CL	E	1486	1/1	0.88	0.10	67,67,67,67	0
4	SO4	C	1485	5/5	0.90	0.31	75,100,106,115	0
3	CL	A	1487	1/1	0.91	0.09	80,80,80,80	0
3	CL	E	1488	1/1	0.92	0.06	75,75,75,75	0
4	SO4	B	1487	5/5	0.93	0.22	46,67,92,99	0
3	CL	B	1485	1/1	0.94	0.05	56,56,56,56	0
4	SO4	D	1485	5/5	0.94	0.33	91,92,100,116	0
4	SO4	F	1475	5/5	0.95	0.21	69,69,78,85	0
2	NAP	C	500	48/48	0.95	0.13	40,42,44,54	0
4	SO4	A	1486	5/5	0.95	0.17	68,70,83,92	0
3	CL	F	1476	1/1	0.96	0.06	62,62,62,62	0
4	SO4	E	1484	5/5	0.96	0.23	58,97,106,106	0
2	NAP	D	500	48/48	0.96	0.12	28,33,42,46	0
3	CL	A	1488	1/1	0.96	0.07	62,62,62,62	0
2	NAP	A	500	48/48	0.96	0.13	19,29,40,44	0
2	NAP	B	500	48/48	0.97	0.11	23,31,42,50	0
2	NAP	E	500	48/48	0.97	0.12	13,27,36,48	0
3	CL	B	1488	1/1	0.98	0.05	61,61,61,61	0
4	SO4	E	1485	5/5	0.98	0.12	17,25,35,36	0
3	CL	A	1484	1/1	0.98	0.19	37,37,37,37	0
3	CL	B	1484	1/1	0.99	0.22	34,34,34,34	0
4	SO4	C	1484	5/5	0.99	0.15	16,25,42,44	0
3	CL	F	1473	1/1	0.99	0.14	35,35,35,35	0
4	SO4	F	1474	5/5	0.99	0.14	12,15,20,32	0
4	SO4	D	1484	5/5	0.99	0.16	21,27,35,36	0
4	SO4	B	1486	5/5	1.00	0.14	12,19,21,24	0
4	SO4	A	1485	5/5	1.00	0.11	10,18,24,25	0

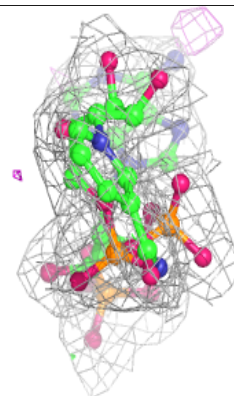
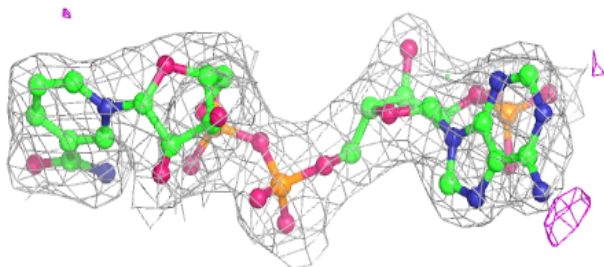
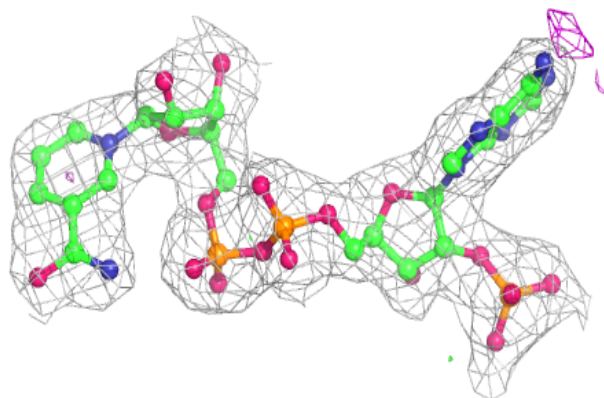
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around NAP 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)

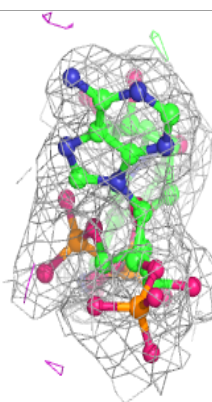
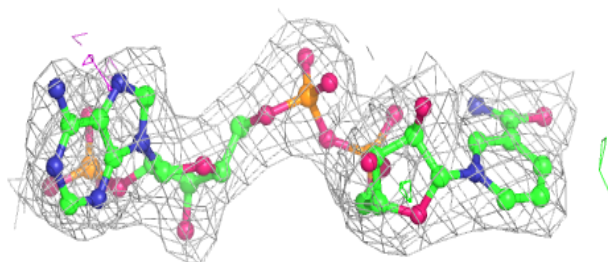
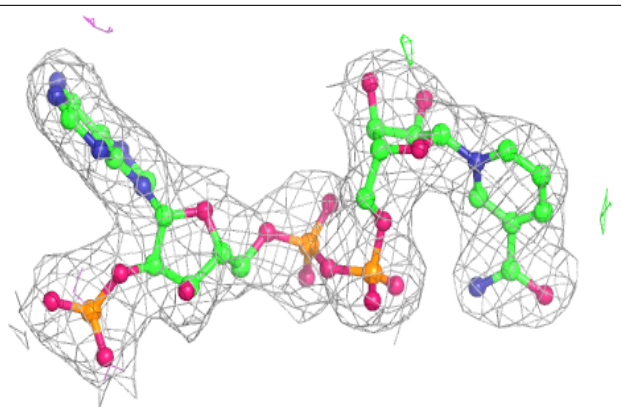
**Electron density around NAP D 500:**

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

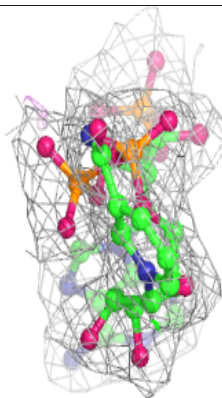
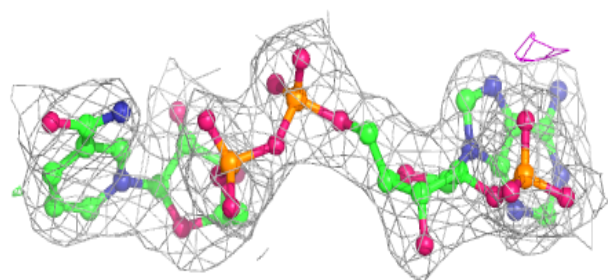
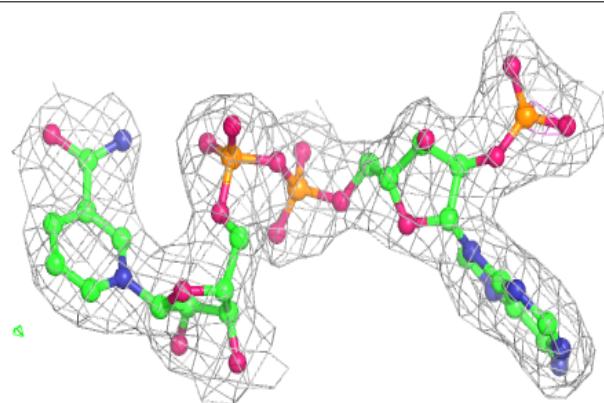


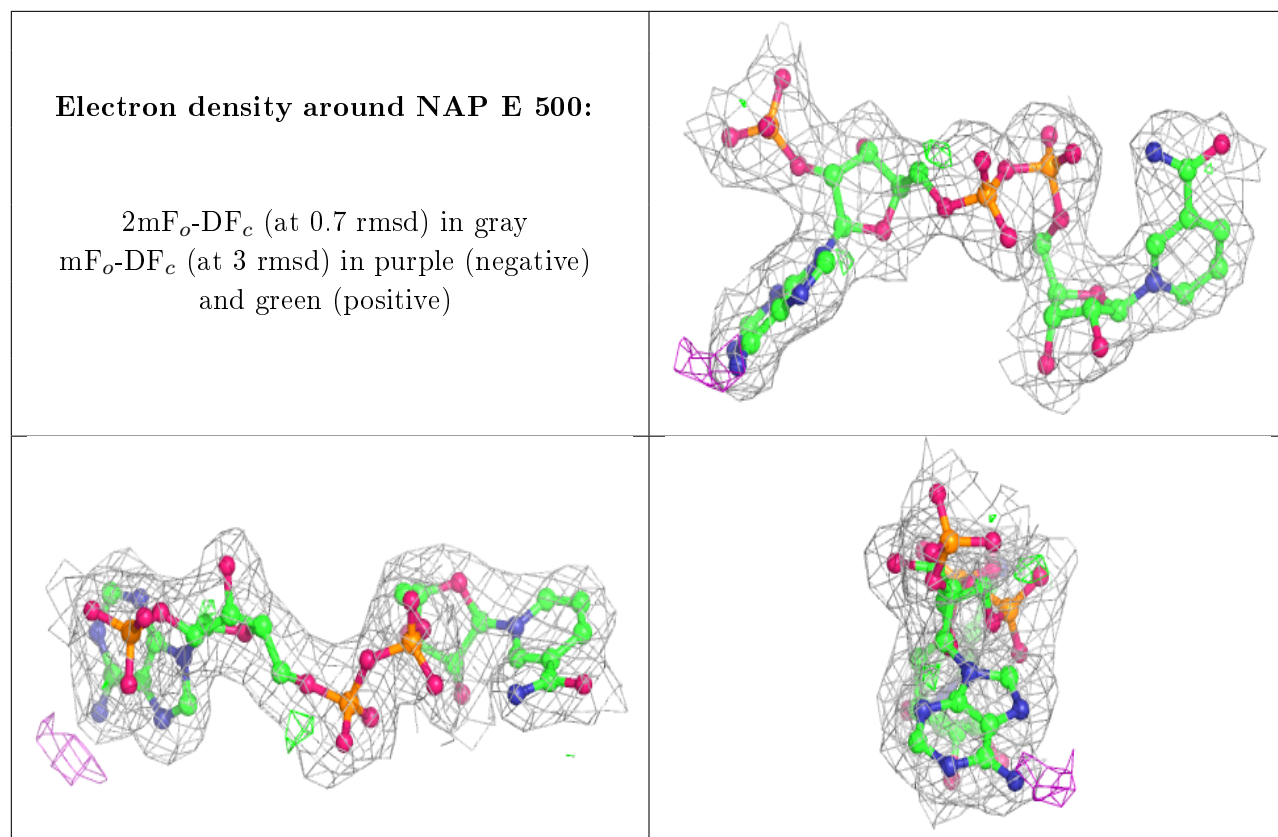
**Electron density around NAP A 500:**

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

**Electron density around NAP 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.