

# wwPDB X-ray Structure Validation Summary Report (i)

#### Nov 27, 2023 – 06:12 PM JST

PDB ID	:	8JB1
Title	:	Crystal structure of glyceraldehyde-3-phosphate dehydrogenase from
		Corynebacterium glutamicum ATCC13032 in complex with NADP
Authors	:	Son, H.F.; Kim, K.J.
Deposited on	:	2023-05-07
Resolution	:	2.44  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 A user guide is available at https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

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

The following versions of software and data (see references (1)) were used in the production of this report:

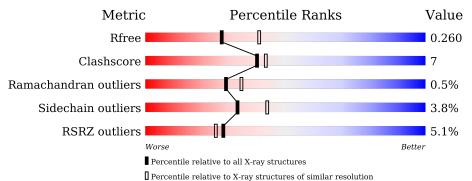
MolProbity Mogul Xtriage (Phenix) EDS	:	4.02b-467 1.8.5 (274361), CSD as541be (2020) 1.13 2.36
buster-report Percentile statistics Refmac	: : :	1.1.7 (2018) 20191225.v01 (using entries in the PDB archive December 25th 2019) 5.8.0158 7.0.044 (Gargrove)
Ideal geometry (DNA, RNA) Validation Pipeline (wwPDB-VP)		Parkinson et al. (1996) 2.36

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $X\text{-}RAY\;DIFFRACTION$ 

The reported resolution of this entry is 2.44 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	$\begin{array}{c} \textbf{Whole archive} \\ (\#\textbf{Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R <sub>free</sub>	130704	$1564 \ (2.46-2.42)$
Clashscore	141614	1631 (2.46-2.42)
Ramachandran outliers	138981	1617 (2.46-2.42)
Sidechain outliers	138945	1617 (2.46-2.42)
RSRZ outliers	127900	1547 (2.46-2.42)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	А	488	6%	19%	·
1	В	488	4%	18%	• •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:



Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	В	502	-	-	Х	-



## 2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 7536 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Δ	468	Total	С	Ν	0	$\mathbf{S}$	0	0	0
	A	408	3651	2288	657	701	5	0	0	0
1	В	468	Total	С	Ν	0	S	0	0	0
	D	400	3641	2282	653	701	5		0	0

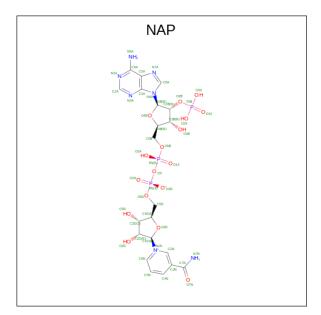
• Molecule 1 is a protein called Glyceraldehyde-3-phosphate dehydrogenase.

Chain	Residue	Modelled	Actual	Comment	Reference
А	481	LEU	-	expression tag	UNP A0A8G0FZM1
А	482	GLU	-	expression tag	UNP A0A8G0FZM1
А	483	HIS	-	expression tag	UNP A0A8G0FZM1
А	484	HIS	-	expression tag	UNP A0A8G0FZM1
А	485	HIS	-	expression tag	UNP A0A8G0FZM1
А	486	HIS	-	expression tag	UNP A0A8G0FZM1
А	487	HIS	-	expression tag	UNP A0A8G0FZM1
А	488	HIS	-	expression tag	UNP A0A8G0FZM1
В	481	LEU	-	expression tag	UNP A0A8G0FZM1
В	482	GLU	-	expression tag	UNP A0A8G0FZM1
В	483	HIS	-	expression tag	UNP A0A8G0FZM1
В	484	HIS	-	expression tag	UNP A0A8G0FZM1
В	485	HIS	-	expression tag	UNP A0A8G0FZM1
В	486	HIS	-	expression tag	UNP A0A8G0FZM1
В	487	HIS	-	expression tag	UNP A0A8G0FZM1
В	488	HIS	-	expression tag	UNP A0A8G0FZM1

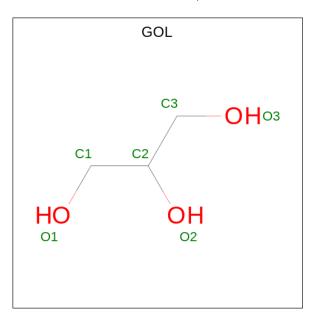
There are 16 discrepancies between the modelled and reference sequences:

• Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (threeletter code: NAP) (formula: C<sub>21</sub>H<sub>28</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	Δ	1	Total	С	Ν	Ο	Р	0	0
	2 A	1	48	21	7	17	3	0	
2	В	1	Total	С	Ν	Ο	Р	0	0
	D		48	21	7	17	3	U	



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
3	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	В	1	Total 6	${ m C} { m 3}$	O 3	0	0

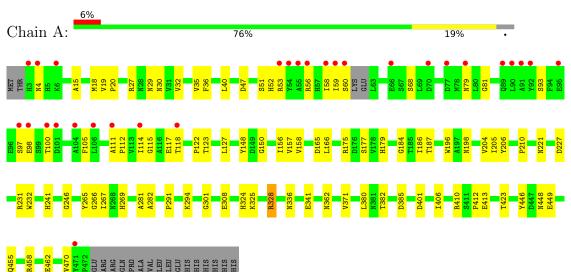
• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	57	$\begin{array}{cc} \text{Total} & \text{O} \\ 57 & 57 \end{array}$	0	0
4	В	73	Total O 73 73	0	0

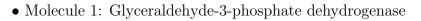


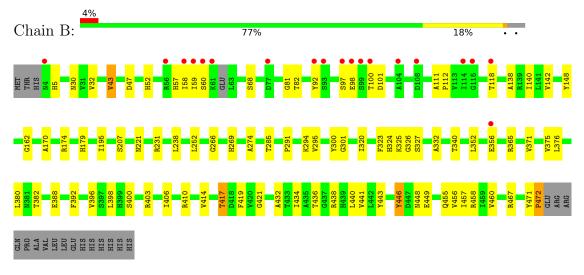
## 3 Residue-property plots (i)

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



• Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase







## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 2 2	Depositor
Cell constants	92.75Å 92.75Å 287.55Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor
Resolution (Å)	31.54 - 2.44	Depositor
Resolution (A)	31.52 - 2.44	EDS
% Data completeness	94.8 (31.54-2.44)	Depositor
(in resolution range)	94.9 (31.52-2.44)	EDS
R <sub>merge</sub>	(Not available)	Depositor
R <sub>sym</sub>	(Not available)	Depositor
$< I/\sigma(I) > 1$	$5.74$ (at $2.45\text{\AA}$ )	Xtriage
Refinement program	REFMAC 5.8.0403	Depositor
D D.	0.192 , $0.262$	Depositor
$R, R_{free}$	0.197 , $0.260$	DCC
$R_{free}$ test set	2189 reflections $(4.85\%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	32.7	Xtriage
Anisotropy	0.362	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.34, 37.0	EDS
L-test for twinning <sup>2</sup>	$ < L >=0.44, < L^2>=0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7536	wwPDB-VP
Average B, all atoms $(Å^2)$	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The analyses of the Patterson function reveals a significant off-origin peak that is 52.23 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.0123e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.

<sup>&</sup>lt;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.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 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, GOL

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	А	0.44	0/3712	0.83	0/5047	
1	В	0.44	0/3701	0.81	0/5032	
All	All	0.44	0/7413	0.82	0/10079	

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	А	0	2
1	В	0	6
All	All	0	8

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	А	336	ASN	Peptide
1	А	410	ARG	Sidechain
1	В	162	GLY	Peptide
1	В	174	ARG	Sidechain
1	В	231	ARG	Sidechain



#### 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	А	3651	0	3642	53	0
1	В	3641	0	3628	59	0
2	А	48	0	25	0	0
2	В	48	0	25	1	0
3	А	6	0	8	1	0
3	В	12	0	16	5	0
4	А	57	0	0	0	0
4	В	73	0	0	1	0
All	All	7536	0	7344	108	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

The worst 5 of 108 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:291:PRO:HB2	1:A:406:ILE:HD11	1.24	1.10
1:B:179:HIS:HD2	3:B:502:GOL:O2	1.49	0.95
1:B:179:HIS:CD2	3:B:502:GOL:O2	2.20	0.95
1:B:30:ASN:HB2	1:B:82:THR:HG22	1.60	0.82
1:A:291:PRO:CB	1:A:406:ILE:HD11	2.11	0.77

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	А	464/488~(95%)	440 (95%)	22~(5%)	2~(0%)	34 4	1	
1	В	464/488~(95%)	428 (92%)	33~(7%)	3 (1%)	25 2	9	
All	All	928/976~(95%)	868 (94%)	55~(6%)	5~(0%)	29 3	4	

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	В	327	SER
1	А	114	ILE
1	В	274	ALA
1	В	371	VAL
1	А	371	VAL

#### 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	А	398/417~(95%)	381 (96%)	17 (4%)	29 38		
1	В	396/417~(95%)	383~(97%)	13 (3%)	38 49		
All	All	794/834~(95%)	764 (96%)	30 (4%)	33 43		

 $5~{\rm of}~30$  residues with a non-rotameric side chain are listed below:

Mol	Chain	Res	Type
1	А	446	TYR
1	В	436	THR
1	В	43	VAL
1	В	472	PRO
1	В	356	GLU

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such side chains are listed below:

Mol	Chain	$\mathbf{Res}$	$\mathbf{Type}$
1	В	297	ASN

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Mol	Chain	Res	Type
1	В	315	ASN
1	А	381	ASN
1	А	324	HIS
1	В	324	HIS

#### 5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

#### 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

#### 5.6 Ligand geometry (i)

5 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	ol Type Chain Res		Res	Link	Bond lengths			Bond angles		
	Mol Type Chain	nes I	LIIIK	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2	
2	NAP	В	501	-	$45,\!52,\!52$	0.71	1 (2%)	$56,\!80,\!80$	1.04	<mark>5 (8%)</mark>
3	GOL	В	502	-	$5,\!5,\!5$	0.28	0	$5,\!5,\!5$	0.64	0
2	NAP	А	501	-	$45,\!52,\!52$	0.75	0	$56,\!80,\!80$	1.11	7 (12%)
3	GOL	В	503	-	$5,\!5,\!5$	0.19	0	$5,\!5,\!5$	0.48	0
3	GOL	А	502	-	$5,\!5,\!5$	0.12	0	$5,\!5,\!5$	0.54	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.



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAP	В	501	-	-	7/31/67/67	0/5/5/5
3	GOL	В	502	-	-	4/4/4/4	-
2	NAP	А	501	-	-	6/31/67/67	0/5/5/5
3	GOL	В	503	-	-	4/4/4/4	-
3	GOL	А	502	-	-	4/4/4/4	-

'-' means no outliers of that kind were identified.

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	В	501	NAP	O4D-C1D	2.04	1.43	1.41

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	А	501	NAP	O2A-PA-O1A	2.88	126.50	112.24
2	В	501	NAP	C5A-C6A-N6A	2.85	124.68	120.35
2	А	501	NAP	C5A-C6A-N6A	2.63	124.34	120.35
2	А	501	NAP	O2B-C2B-C3B	2.53	120.84	111.68
2	В	501	NAP	O3B-C3B-C2B	2.52	118.33	111.17

There are no chirality outliers.

5 of 25 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	А	501	NAP	O4D-C1D-N1N-C2N
2	А	501	NAP	O4D-C1D-N1N-C6N
2	А	501	NAP	C2D-C1D-N1N-C2N
2	А	501	NAP	C2D-C1D-N1N-C6N
2	В	501	NAP	O4D-C1D-N1N-C2N

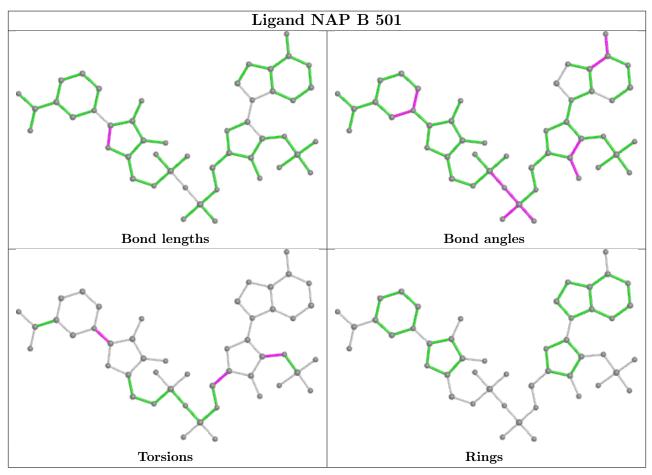
There are no ring outliers.

4 monomers are involved in 7 short contacts:

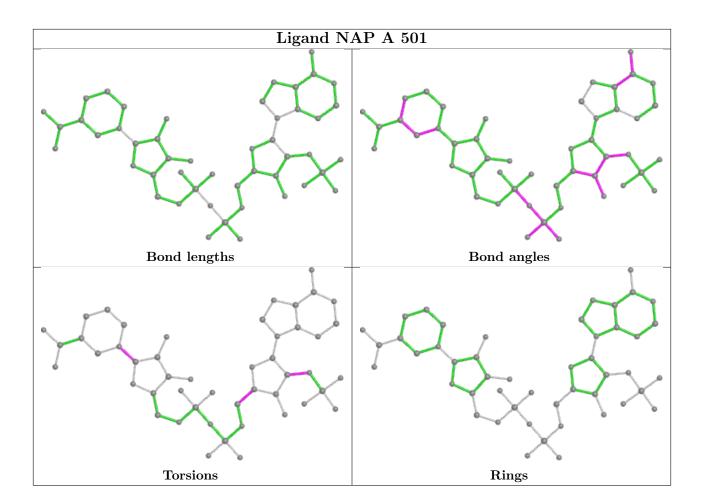
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	В	501	NAP	1	0
3	В	502	GOL	4	0
3	В	503	GOL	1	0
3	А	502	GOL	1	0



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 then 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 sufficient 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,  $95^{th}$  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	$\langle RSRZ \rangle$	#RSRZ>2	$\mathbf{OWAB}(\mathbf{\AA}^2)$	Q < 0.9
1	А	468/488~(95%)	-0.18	29 (6%) 20 17	15, 35, 100, 125	0
1	В	468/488~(95%)	-0.25	19 (4%) 37 34	15, 37, 94, 139	0
All	All	936/976~(95%)	-0.21	48 (5%) 28 25	15, 36, 98, 139	0

The worst 5 of 48 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	60	SER	7.4
1	В	61	LYS	4.7
1	А	471	TYR	4.7
1	А	60	SER	4.4
1	А	100	THR	4.2

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

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

#### 6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

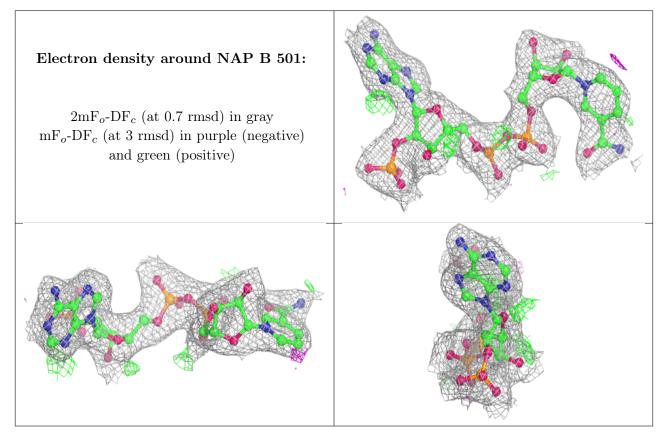
### 6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median,  $95^{th}$  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.

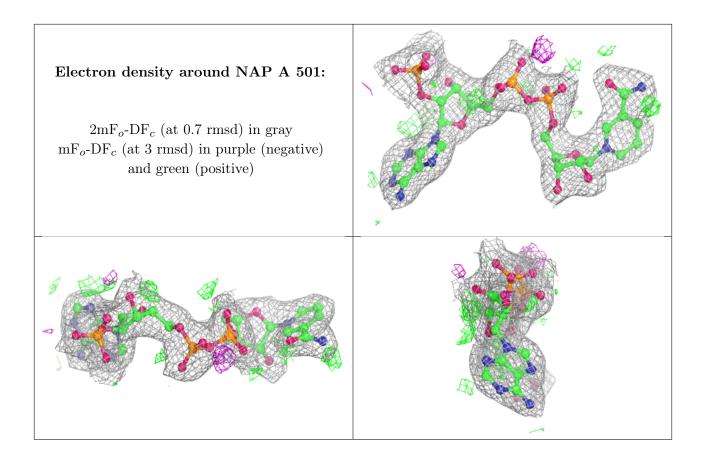


Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q<0.9
3	GOL	В	502	6/6	0.86	0.18	32,41,46,46	0
3	GOL	В	503	6/6	0.92	0.25	52,64,67,69	0
3	GOL	А	502	6/6	0.94	0.13	38,40,43,46	0
2	NAP	В	501	48/48	0.98	0.10	17,26,33,42	0
2	NAP	А	501	48/48	0.98	0.10	14,19,24,27	0

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







## 6.5 Other polymers (i)

There are no such residues in this entry.

