



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2018 – 09:30 am GMT

PDB ID : 1A80  
Title : Native 2,5-DIKETO-D-GLUCONIC acid reductase a from CORYNBACTERIUM SP. complexed with nadph  
Authors : Khurana, S.; Powers, D.B.; Anderson, S.; Blaber, M.  
Deposited on : 1998-03-31  
Resolution : 2.10 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.

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

MolProbity : 4.02b-467  
Mogul : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : trunk30967  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30967

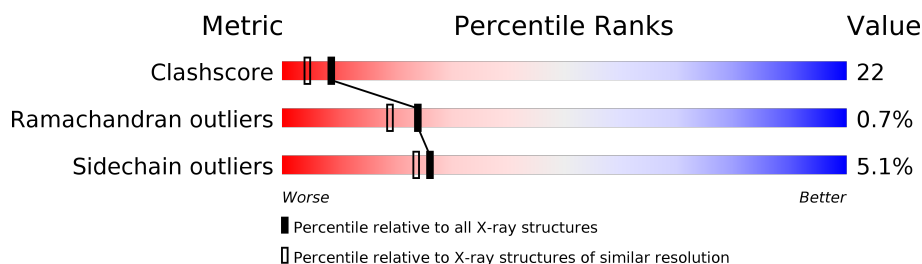
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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))
Clashscore	122126	5109 (2.10-2.10)
Ramachandran outliers	120053	5059 (2.10-2.10)
Sidechain outliers	120020	5060 (2.10-2.10)

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. 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	277	

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 2275 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 2,5-DIKETO-D-GLUCONIC ACID REDUCTASE A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	277	Total	C	N	O	S	0	0	0
			2122	1341	370	409	2			

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula:  $C_{21}H_{30}N_7O_{17}P_3$ ).



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

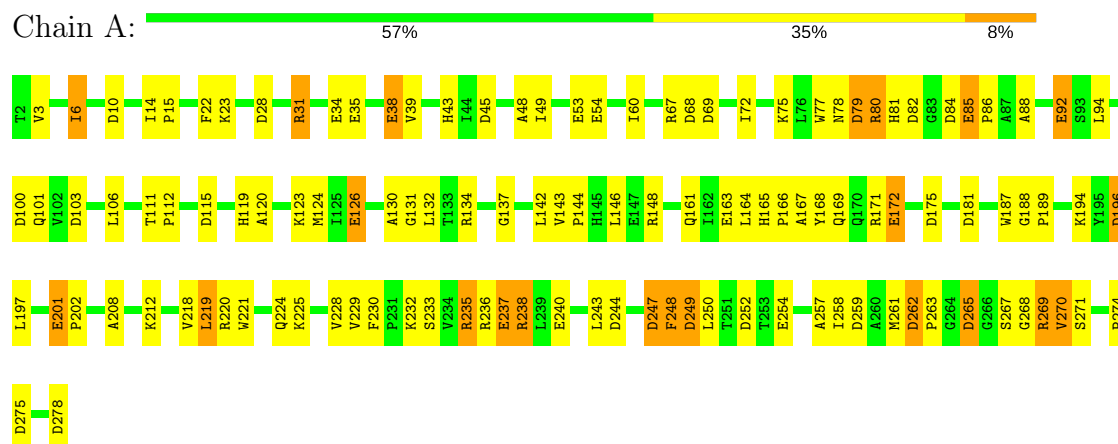
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	105	Total	O	0	0
			105	105		

### 3 Residue-property plots

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. 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. 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: 2,5-DIKETO-D-GLUCONIC ACID REDUCTASE A



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	35.70Å 55.80Å 74.70Å 90.00° 92.20° 90.00°	Depositor
Resolution (Å)	60.00 – 2.10 35.67 – 2.09	Depositor EDS
% Data completeness (in resolution range)	85.0 (60.00-2.10) 79.0 (35.67-2.09)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.12	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.60 (at 2.08Å)	Xtriage
Refinement program	TNT 5E	Depositor
R, $R_{free}$	(Not available) , (Not available) 0.180 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	16.3	Xtriage
Anisotropy	0.823	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 87.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.039 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	2275	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.02% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

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

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	0.88	13/2174 (0.6%)	1.26	44/2971 (1.5%)

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	254	GLU	CD-OE2	6.11	1.32	1.25
1	A	237	GLU	CD-OE2	5.87	1.32	1.25
1	A	126	GLU	CD-OE2	5.66	1.31	1.25
1	A	38	GLU	CD-OE2	5.63	1.31	1.25
1	A	85	GLU	CD-OE2	5.46	1.31	1.25
1	A	172	GLU	CD-OE2	5.45	1.31	1.25
1	A	201	GLU	CD-OE2	5.43	1.31	1.25
1	A	34	GLU	CD-OE2	5.38	1.31	1.25
1	A	240	GLU	CD-OE2	5.34	1.31	1.25
1	A	92	GLU	CD-OE2	5.33	1.31	1.25
1	A	54	GLU	CD-OE2	5.23	1.31	1.25
1	A	163	GLU	CD-OE2	5.20	1.31	1.25
1	A	35	GLU	CD-OE2	5.01	1.31	1.25

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	84	ASP	CB-CG-OD2	-7.64	111.42	118.30
1	A	79	ASP	CB-CG-OD2	-7.10	111.91	118.30
1	A	275	ASP	CB-CG-OD1	7.08	124.67	118.30
1	A	259	ASP	CB-CG-OD2	-7.02	111.98	118.30
1	A	69	ASP	CB-CG-OD2	-6.97	112.03	118.30
1	A	275	ASP	CB-CG-OD2	-6.90	112.09	118.30
1	A	196	ASP	CB-CG-OD2	-6.89	112.10	118.30
1	A	249	ASP	CB-CG-OD2	-6.82	112.17	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	244	ASP	CB-CG-OD2	-6.77	112.21	118.30
1	A	28	ASP	CB-CG-OD2	-6.54	112.41	118.30
1	A	79	ASP	CB-CG-OD1	6.48	124.13	118.30
1	A	100	ASP	CB-CG-OD2	-6.34	112.59	118.30
1	A	181	ASP	CB-CG-OD1	6.33	124.00	118.30
1	A	259	ASP	CB-CG-OD1	6.22	123.90	118.30
1	A	262	ASP	CB-CG-OD2	-6.18	112.73	118.30
1	A	68	ASP	CB-CG-OD2	-6.17	112.75	118.30
1	A	69	ASP	CB-CG-OD1	6.13	123.82	118.30
1	A	84	ASP	CB-CG-OD1	5.96	123.67	118.30
1	A	181	ASP	CB-CG-OD2	-5.96	112.93	118.30
1	A	196	ASP	CB-CG-OD1	5.87	123.58	118.30
1	A	82	ASP	CB-CG-OD2	-5.81	113.07	118.30
1	A	244	ASP	CB-CG-OD1	5.79	123.51	118.30
1	A	235	ARG	NE-CZ-NH1	5.79	123.19	120.30
1	A	45	ASP	CB-CG-OD2	-5.76	113.12	118.30
1	A	175	ASP	CB-CG-OD2	-5.73	113.14	118.30
1	A	252	ASP	CB-CG-OD2	-5.68	113.19	118.30
1	A	265	ASP	CB-CG-OD2	-5.63	113.24	118.30
1	A	80	ARG	NE-CZ-NH1	5.61	123.10	120.30
1	A	249	ASP	CB-CG-OD1	5.53	123.28	118.30
1	A	45	ASP	CB-CG-OD1	5.50	123.25	118.30
1	A	100	ASP	CB-CG-OD1	5.45	123.21	118.30
1	A	269	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	A	148	ARG	NE-CZ-NH1	5.43	123.01	120.30
1	A	262	ASP	CB-CG-OD1	5.42	123.17	118.30
1	A	247	ASP	CB-CG-OD2	-5.37	113.47	118.30
1	A	115	ASP	CB-CG-OD2	-5.35	113.49	118.30
1	A	115	ASP	CB-CG-OD1	5.32	123.09	118.30
1	A	175	ASP	CB-CG-OD1	5.21	122.99	118.30
1	A	28	ASP	CB-CG-OD1	5.19	122.97	118.30
1	A	278	ASP	CB-CG-OD2	-5.18	113.64	118.30
1	A	238	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	A	10	ASP	CB-CG-OD2	-5.16	113.66	118.30
1	A	278	ASP	CB-CG-OD1	5.14	122.92	118.30
1	A	10	ASP	CB-CG-OD1	5.08	122.87	118.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2122	0	2051	91	0
2	A	48	0	26	8	0
3	A	105	0	0	9	0
All	All	2275	0	2077	93	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 22.

All (93) 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:224:GLN:HE22	1:A:250:LEU:H	1.08	1.02
1:A:220:ARG:HG3	1:A:224:GLN:HE21	1.29	0.98
1:A:6:ILE:HD11	1:A:228:VAL:HG22	1.56	0.88
1:A:212:LYS:HE3	1:A:248:PHE:CD1	2.10	0.85
1:A:221:TRP:CZ2	1:A:225:LYS:HE2	2.14	0.82
1:A:161:GLN:OE1	2:A:300:NDP:H2N	1.87	0.75
1:A:15:PRO:HG2	1:A:43:HIS:HB2	1.70	0.71
1:A:164:LEU:HD23	1:A:165:HIS:N	2.06	0.70
1:A:224:GLN:HE22	1:A:250:LEU:N	1.87	0.69
1:A:248:PHE:H	1:A:248:PHE:HD1	1.38	0.69
1:A:232:LYS:O	2:A:300:NDP:H8A	1.92	0.69
1:A:233:SER:HA	2:A:300:NDP:O3X	1.93	0.69
1:A:212:LYS:HZ1	1:A:247:ASP:HB2	1.59	0.68
1:A:142:LEU:HD21	1:A:274:PRO:HG2	1.74	0.67
2:A:300:NDP:H42N	3:A:332:HOH:O	1.95	0.66
1:A:165:HIS:HB2	1:A:166:PRO:HD2	1.78	0.66
1:A:130:ALA:HB3	1:A:132:LEU:HD23	1.78	0.65
1:A:212:LYS:NZ	1:A:247:ASP:HB2	2.12	0.64
1:A:38:GLU:OE1	1:A:236:ARG:NH2	2.31	0.63
1:A:31:ARG:HG2	3:A:329:HOH:O	1.97	0.63
1:A:224:GLN:NE2	1:A:250:LEU:H	1.89	0.63
1:A:134:ARG:HD2	3:A:319:HOH:O	1.99	0.62
1:A:6:ILE:CD1	1:A:228:VAL:HG22	2.29	0.61
1:A:166:PRO:HG2	1:A:197:LEU:HD11	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:LYS:HD3	3:A:368:HOH:O	2.00	0.60
2:A:300:NDP:H6N	2:A:300:NDP:H3D	1.84	0.59
1:A:220:ARG:HG3	1:A:224:GLN:NE2	2.11	0.59
1:A:79:ASP:OD1	1:A:80:ARG:HG2	2.06	0.55
1:A:221:TRP:NE1	1:A:225:LYS:HD2	2.22	0.55
1:A:88:ALA:O	1:A:92:GLU:HG2	2.07	0.54
1:A:49:ILE:HG13	1:A:49:ILE:O	2.08	0.54
1:A:221:TRP:CE2	1:A:225:LYS:HE2	2.42	0.54
1:A:235:ARG:NH1	1:A:238:ARG:NH1	2.56	0.53
1:A:187:TRP:HH2	1:A:271:SER:HB3	1.74	0.53
1:A:188:GLY:N	1:A:189:PRO:HD3	2.23	0.52
1:A:81:HIS:O	1:A:119:HIS:HD2	1.92	0.52
1:A:14:ILE:HD11	1:A:43:HIS:CE1	2.44	0.52
1:A:130:ALA:CB	1:A:132:LEU:HD23	2.40	0.52
1:A:111:THR:N	1:A:112:PRO:HD3	2.23	0.52
1:A:194:LYS:HB2	1:A:270:VAL:CG2	2.39	0.52
1:A:208:ALA:HB2	3:A:388:HOH:O	2.10	0.51
1:A:250:LEU:N	1:A:250:LEU:HD12	2.25	0.51
1:A:60:ILE:HD11	1:A:72:ILE:CD1	2.41	0.51
1:A:235:ARG:HH11	1:A:238:ARG:CZ	2.23	0.51
1:A:168:TYR:CE2	1:A:269:ARG:HG3	2.45	0.51
1:A:67:ARG:NH2	1:A:103:ASP:OD2	2.42	0.50
1:A:218:VAL:O	1:A:221:TRP:HB3	2.12	0.50
1:A:169:GLN:NE2	1:A:262:ASP:HB2	2.27	0.49
1:A:123:LYS:HE2	1:A:126:GLU:OE1	2.12	0.49
1:A:67:ARG:HH22	1:A:103:ASP:CG	2.15	0.49
1:A:123:LYS:HE2	1:A:123:LYS:HA	1.95	0.48
1:A:232:LYS:C	1:A:232:LYS:HD3	2.34	0.48
1:A:258:ILE:O	1:A:261:MET:HG3	2.14	0.48
1:A:194:LYS:HD2	1:A:270:VAL:HG13	1.96	0.47
1:A:85:GLU:N	1:A:86:PRO:HD2	2.29	0.47
1:A:106:LEU:HA	1:A:137:GLY:O	2.14	0.47
1:A:167:ALA:O	1:A:268:GLY:HA3	2.16	0.46
1:A:187:TRP:CH2	1:A:271:SER:HB3	2.50	0.46
1:A:171:ARG:HH21	1:A:262:ASP:HB3	1.78	0.46
1:A:202:PRO:HB3	1:A:257:ALA:HB1	1.97	0.46
1:A:219:LEU:HA	1:A:219:LEU:HD12	1.65	0.46
1:A:85:GLU:N	1:A:86:PRO:CD	2.79	0.45
1:A:77:TRP:CG	1:A:78:ASN:N	2.84	0.45
1:A:79:ASP:O	1:A:80:ARG:HD2	2.17	0.45
1:A:48:ALA:HA	1:A:53:GLU:OE1	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:ARG:NH1	3:A:361:HOH:O	2.49	0.45
1:A:92:GLU:HG3	3:A:311:HOH:O	2.16	0.45
1:A:188:GLY:N	1:A:189:PRO:CD	2.79	0.45
1:A:67:ARG:CZ	1:A:134:ARG:NH2	2.80	0.44
1:A:60:ILE:HD11	1:A:72:ILE:HD12	1.99	0.44
1:A:126:GLU:HB2	3:A:402:HOH:O	2.18	0.44
1:A:194:LYS:HB2	1:A:270:VAL:HG21	1.98	0.44
1:A:250:LEU:CD1	1:A:250:LEU:N	2.80	0.44
1:A:143:VAL:N	1:A:144:PRO:CD	2.80	0.44
1:A:75:LYS:HE2	2:A:300:NDP:N7N	2.33	0.44
1:A:221:TRP:CD1	1:A:225:LYS:HD2	2.53	0.43
1:A:265:ASP:OD1	1:A:267:SER:OG	2.30	0.43
1:A:261:MET:O	1:A:263:PRO:HD3	2.18	0.42
1:A:22:PHE:O	1:A:23:LYS:HB2	2.19	0.42
1:A:233:SER:HB2	2:A:300:NDP:C8A	2.50	0.42
1:A:39:VAL:HG12	1:A:243:LEU:CD2	2.50	0.42
1:A:171:ARG:NH2	3:A:338:HOH:O	2.53	0.42
1:A:120:ALA:O	1:A:124:MET:HG2	2.20	0.41
1:A:194:LYS:HB2	1:A:270:VAL:HG22	2.02	0.41
1:A:101:GLN:NE2	1:A:131:GLY:O	2.53	0.41
1:A:39:VAL:HG12	1:A:243:LEU:HD23	2.02	0.41
1:A:143:VAL:HA	1:A:146:LEU:HD12	2.03	0.41
1:A:123:LYS:O	1:A:126:GLU:HB2	2.20	0.41
1:A:60:ILE:HD11	1:A:72:ILE:HD11	2.03	0.41
1:A:94:LEU:HD23	1:A:94:LEU:HA	1.81	0.41
1:A:75:LYS:HE2	2:A:300:NDP:H71N	1.85	0.40
1:A:123:LYS:CE	1:A:123:LYS:HA	2.52	0.40
1:A:165:HIS:HB2	1:A:166:PRO:CD	2.49	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	275/277 (99%)	260 (94%)	13 (5%)	2 (1%)	24 19

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	VAL
1	A	196	ASP

### 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	216/216 (100%)	205 (95%)	11 (5%)	26 24

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ILE
1	A	31	ARG
1	A	172	GLU
1	A	201	GLU
1	A	219	LEU
1	A	229	VAL
1	A	230	PHE
1	A	237	GLU
1	A	248	PHE
1	A	249	ASP
1	A	270	VAL

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

Mol	Chain	Res	Type
1	A	30	GLN
1	A	101	GLN
1	A	224	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 ⓘ

1 ligand is 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$
2	NDP	A	300	1	45,52,52	1.46	5 (11%)	54,80,80	1.59	3 (5%)

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	NDP	A	300	1	-	0/30/77/77	0/5/5/5

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	300	NDP	P2B-O2B	-5.75	1.48	1.59
2	A	300	NDP	C4N-C5N	-3.33	1.41	1.49
2	A	300	NDP	PN-O5D	-2.14	1.50	1.59
2	A	300	NDP	PA-O5B	-2.05	1.51	1.59

*Continued on next page...*

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	300	NDP	C6N-C5N	4.19	1.40	1.33

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	300	NDP	C1B-N9A-C4A	-9.24	110.67	126.64
2	A	300	NDP	C1D-N1N-C2N	-3.82	114.65	121.10
2	A	300	NDP	C1D-N1N-C6N	2.26	125.72	120.80

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	300	NDP	8	0

## 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](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.3 Carbohydrates [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.4 Ligands [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.5 Other polymers [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.