

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

#### Aug 22, 2023 – 09:41 PM EDT

PDB ID	:	3BUR
Title	:	Crystal structure of Delta(4)-3-ketosteroid 5-beta-reductase in complex with
		NADP and TESTOSTERONE. RESOLUTION: 1.62 A.
Authors	:	Di Costanzo, L.; Christianson, D.W.
Deposited on	:	2008-01-03
Resolution	:	1.62  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:

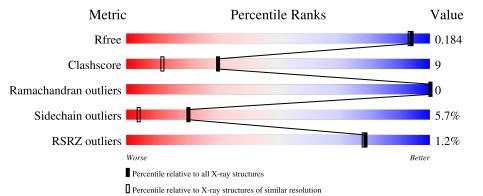
MolProbity	:	4.02b-467
	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)		
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

# 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 1.62 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	$\begin{array}{c} \textbf{Whole archive} \\ (\#\textbf{Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
$R_{free}$	130704	4693 (1.64-1.60)
Clashscore	141614	5002 (1.64-1.60)
Ramachandran outliers	138981	4888 (1.64-1.60)
Sidechain outliers	138945	4887 (1.64-1.60)
RSRZ outliers	127900	4609 (1.64-1.60)

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	326	<sup>2%</sup> 74%	20%	6%
1	В	326	85%		13% •

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
4	GOL	А	338	-	-	-	Х



# 2 Entry composition (i)

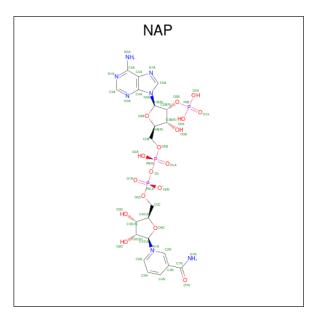
There are 5 unique types of molecules in this entry. The entry contains 5950 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 3-oxo-5-beta-steroid 4-dehydrogenase.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace	
1	А	325	Total	С	N	0	S	0	0	0	
			2627	1680	455	481	11				
1	В	395	325 Total C N O S		$\mathbf{S}$	0	0	0			
	D	525	2627	1680	455	481	11	0	0	U	

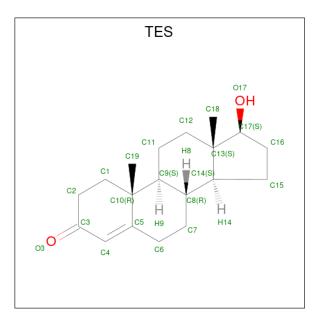
• Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: C<sub>21</sub>H<sub>28</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>).



Mol	Chain	Residues		Ate	oms			ZeroOcc	AltConf
0	٨	1	Total	С	Ν	Ο	Р	0	0
	A	1	48	21	7	17	3	0	0
0	р	1	Total	С	Ν	Ο	Р	0	0
	D	1	48	21	7	17	3	0	0

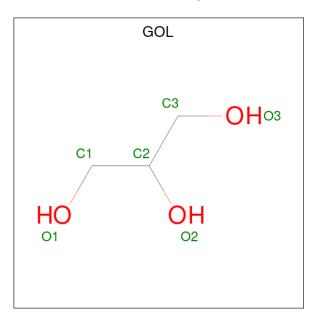
• Molecule 3 is TESTOSTERONE (three-letter code: TES) (formula:  $C_{19}H_{28}O_2$ ).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	Total         C         O           21         19         2	0	0
3	В	1	Total         C         O           21         19         2	0	0

• Molecule 4 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

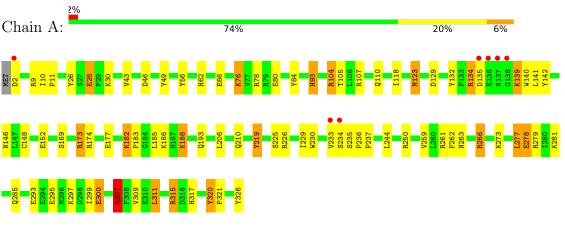
• Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	242	Total         O           242         242	0	0
5	В	256	Total         O           256         256	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: 3-oxo-5-beta-steroid 4-dehydrogenase

• Molecule 1: 3-oxo-5-beta-steroid 4-dehydrogenase

Chair	ain B: 85%															139	%	•														
MET D2 R9		D14	Y26	52/ E28	P29 #20	S31	K34		T39	V43	Y49	R50	K71	E74	G75	N/O	Y84	N89	R99	P100	1118	1131	R134	D135 F136	1 7	2013	S169	R173	K182	<mark>զ193</mark>	P198	F208
H212 1216	Y219	N227	P228	K253		ACZ A	R266	K273	1.277	E278	K281	F289		V309 E310	L311 1040	L312 M313	W314 P315	CT CH	1320													



# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	49.82Å 109.98Å 128.91Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor
Resolution (Å)	50.00 - 1.62	Depositor
Resolution (A)	46.47 - 1.62	EDS
% Data completeness	(Not available) $(50.00-1.62)$	Depositor
(in resolution range)	95.0(46.47 - 1.62)	EDS
R <sub>merge</sub>	0.10	Depositor
R <sub>sym</sub>	(Not available)	Depositor
$< I/\sigma(I) > 1$	2.78 (at $1.63$ Å)	Xtriage
Refinement program	SHELXL-97	Depositor
B B.	0.228 , $0.248$	Depositor
$R, R_{free}$	0.182 , $0.184$	DCC
$R_{free}$ test set	4317 reflections $(5.03%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	15.1	Xtriage
Anisotropy	0.169	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.36 , $65.9$	EDS
L-test for twinning <sup>2</sup>	$ \langle L  \rangle = 0.49, \langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	5950	wwPDB-VP
Average B, all atoms $(Å^2)$	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.44% of the height of the origin peak. No significant pseudotranslation is detected.

<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: GOL, TES, 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	Bo	nd lengths	Bo	ond angles
	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	А	0.44	1/2692~(0.0%)	1.20	17/3649~(0.5%)
1	В	0.39	0/2692	1.07	12/3649~(0.3%)
All	All	0.42	1/5384~(0.0%)	1.14	29/7298~(0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	А	326	TYR	C-OXT	9.95	1.42	1.23

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	104	ARG	CD-NE-CZ	23.65	156.71	123.60
1	А	266	ARG	NE-CZ-NH1	12.71	126.65	120.30
1	А	104	ARG	NE-CZ-NH1	11.11	125.86	120.30
1	А	266	ARG	CD-NE-CZ	10.79	138.71	123.60
1	А	104	ARG	NE-CZ-NH2	-10.77	114.92	120.30

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	А	2627	0	2622	67	0
1	В	2627	0	2622	25	0
2	А	48	0	25	4	0
2	В	48	0	25	5	0
3	А	21	0	28	3	0
3	В	21	0	28	4	0
4	А	36	0	48	11	0
4	В	24	0	32	3	0
5	А	242	0	0	9	0
5	В	256	0	0	2	0
All	All	5950	0	5430	101	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 9.

The worst 5 of 101 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)
2:B:327:NAP:H5N	3:B:340:TES:H62	1.54	0.87
1:A:152:GLU:OE1	1:A:182:LYS:HE3	1.84	0.77
1:A:229:ILE:HG21	4:A:331:GOL:H32	1.66	0.77
1:A:188:LYS:HG3	5:A:1226:HOH:O	1.84	0.77
1:A:206:LEU:O	1:A:210:GLN:HG3	1.83	0.76

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	Perce	entiles
1	А	323/326~(99%)	311 (96%)	12~(4%)	0	100	100
1	В	323/326~(99%)	315~(98%)	8 (2%)	0	100	100
All	All	646/652~(99%)	626 (97%)	20 (3%)	0	100	100



There are no Ramachandran outliers to report.

#### 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	289/290~(100%)	267~(92%)	22 (8%)	13 2
1	В	289/290~(100%)	278~(96%)	11 (4%)	33 9
All	All	578/580~(100%)	545~(94%)	33 (6%)	20 4

5 of 33 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	В	216	ILE
1	В	219	TYR
1	В	315	ARG
1	А	182	LYS
1	А	173	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	92	ASN
1	А	93	HIS
1	А	110	GLN
1	А	146	ASN
1	В	212	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)

#### 14 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	B	ond leng	gths	B	ond ang	gles
	туре	Unam	nes	LIIIK	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	GOL	А	331	-	$5,\!5,\!5$	0.53	0	$5,\!5,\!5$	0.78	0
4	GOL	А	334	-	$5,\!5,\!5$	0.62	0	$5,\!5,\!5$	0.76	0
4	GOL	В	336	-	$5,\!5,\!5$	0.59	0	$5,\!5,\!5$	0.75	0
4	GOL	А	332	-	$5,\!5,\!5$	0.56	0	$5,\!5,\!5$	0.48	0
4	GOL	В	330	-	$5,\!5,\!5$	0.45	0	$5,\!5,\!5$	1.10	0
2	NAP	В	327	-	45,52,52	2.27	17 (37%)	56,80,80	2.14	17 (30%)
4	GOL	А	338	-	$5,\!5,\!5$	0.68	0	$5,\!5,\!5$	0.82	0
4	GOL	В	329	-	$5,\!5,\!5$	0.51	0	$5,\!5,\!5$	0.71	0
4	GOL	В	337	-	$5,\!5,\!5$	0.50	0	$5,\!5,\!5$	0.61	0
3	TES	А	339	-	24,24,24	0.74	0	39,39,39	0.90	0
2	NAP	А	328	-	45,52,52	2.14	13 (28%)	56,80,80	1.94	12 (21%)
4	GOL	А	335	-	$5,\!5,\!5$	0.43	0	$5,\!5,\!5$	0.67	0
4	GOL	А	333	-	$5,\!5,\!5$	0.60	0	$5,\!5,\!5$	0.88	0
3	TES	В	340	-	24,24,24	0.79	0	39,39,39	1.44	5 (12%)

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
4	GOL	А	331	-	-	2/4/4/4	-
4	GOL	А	334	-	-	2/4/4/4	-
4	GOL	В	336	-	-	2/4/4/4	-
4	GOL	А	332	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	В	330	-	-	4/4/4/4	-
2	NAP	В	327	-	-	6/31/67/67	0/5/5/5
4	GOL	А	338	-	-	4/4/4/4	-
4	GOL	В	329	-	-	1/4/4/4	-
4	GOL	В	337	-	-	3/4/4/4	-
3	TES	А	339	-	-	-	0/4/4/4
2	NAP	А	328	-	-	7/31/67/67	0/5/5/5
4	GOL	А	335	-	-	2/4/4/4	-
4	GOL	А	333	-	-	1/4/4/4	-
3	TES	В	340	-	-	-	0/4/4/4

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The worst 5 of 30 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	Observed(A)	Ideal(Å)
2	В	327	NAP	C4A-N3A	6.42	1.44	1.35
2	А	328	NAP	C4A-N3A	5.72	1.43	1.35
2	В	327	NAP	C6N-N1N	5.32	1.48	1.35
2	А	328	NAP	C6N-N1N	5.08	1.47	1.35
2	В	327	NAP	C2N-N1N	4.67	1.40	1.35

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
2	А	328	NAP	C5A-C6A-N6A	6.83	130.73	120.35
2	В	327	NAP	PN-O3-PA	6.45	154.97	132.83
2	А	328	NAP	PN-O3-PA	6.45	154.94	132.83
3	В	340	TES	C16-C17-C13	-5.59	100.09	104.53
2	В	327	NAP	C5A-C6A-N6A	5.30	128.41	120.35

There are no chirality outliers.

5 of 36 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	А	328	NAP	C5D-O5D-PN-O2N
2	А	328	NAP	O4D-C1D-N1N-C6N
2	В	327	NAP	C5D-O5D-PN-O2N
2	В	327	NAP	O4D-C1D-N1N-C6N
4	А	331	GOL	O1-C1-C2-O2

There are no ring outliers.

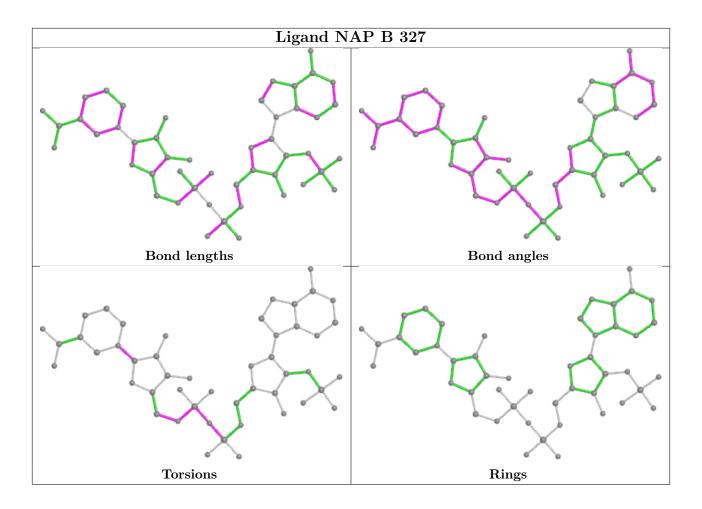


Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	А	331	GOL	2	0
4	А	334	GOL	2	0
4	В	336	GOL	1	0
4	А	332	GOL	3	0
4	В	330	GOL	1	0
2	В	327	NAP	5	0
4	А	338	GOL	2	0
4	В	329	GOL	1	0
4	В	337	GOL	1	0
3	А	339	TES	3	0
2	А	328	NAP	4	0
4	А	335	GOL	3	0
4	А	333	GOL	1	0
3	В	340	TES	4	0

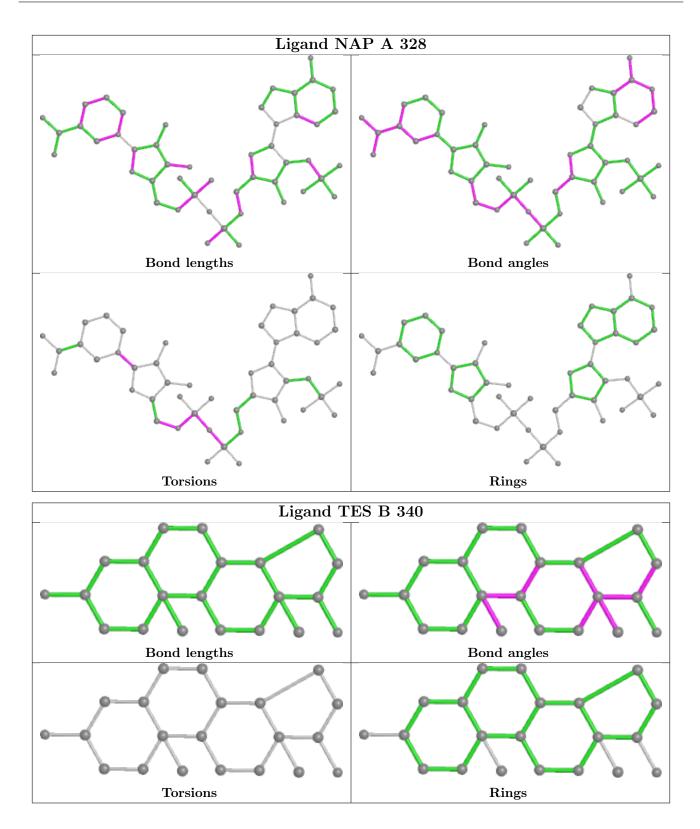
14 monomers are involved in 26 short contacts:

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	$OWAB(A^2)$	Q<0.9
1	А	325/326~(99%)	-0.09	7 (2%) 62 60	9, 18, 45, 87	0
1	В	325/326~(99%)	-0.38	1 (0%) 94 93	10, 16, 33, 71	0
All	All	650/652~(99%)	-0.24	8 (1%) 79 78	9, 17, 39, 87	0

The worst 5 of 8 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	234	SER	4.3
1	В	2	ASP	3.2
1	А	137	ASN	3.1
1	А	135	ASP	2.6
1	А	2	ASP	2.6

#### 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.

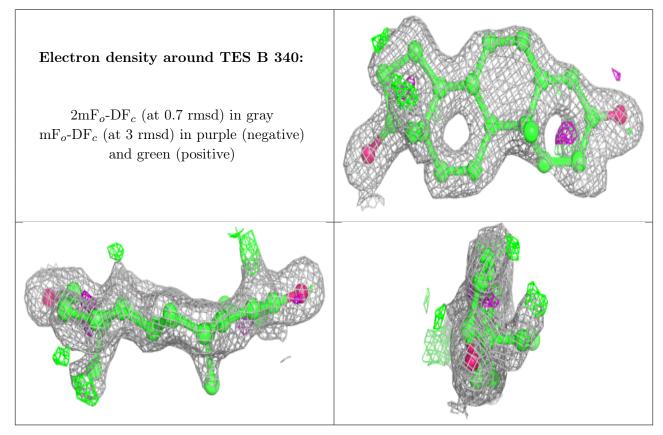
### 6.4 Ligands (i)

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.

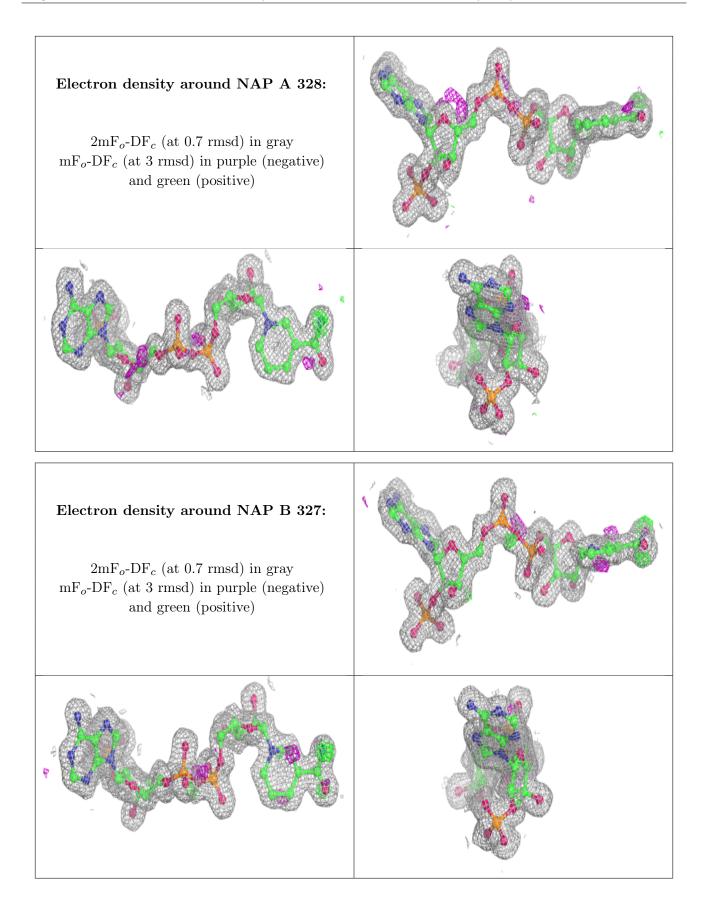


Mol	Type	Chain	Res	Atoms	RSCC	RSR	$B-factors(A^2)$	Q<0.9
4	GOL	А	334	6/6	0.38	0.33	35,39,44,46	6
4	GOL	А	331	6/6	0.65	0.34	21,26,32,38	6
4	GOL	А	338	6/6	0.67	0.42	19,24,26,28	6
4	GOL	А	332	6/6	0.76	0.26	39,54,62,76	0
4	GOL	В	336	6/6	0.76	0.21	30,40,51,60	6
3	TES	В	340	21/21	0.80	0.20	$27,\!35,\!49,\!51$	0
4	GOL	А	335	6/6	0.80	0.31	34,38,39,50	0
4	GOL	В	329	6/6	0.81	0.16	26, 36, 41, 57	0
4	GOL	В	330	6/6	0.84	0.15	20,38,47,62	0
3	TES	А	339	21/21	0.88	0.13	21,29,34,40	0
4	GOL	А	333	6/6	0.88	0.18	37,51,53,53	0
4	GOL	В	337	6/6	0.90	0.13	27,44,48,50	0
2	NAP	А	328	48/48	0.97	0.08	9,14,18,22	0
2	NAP	В	327	48/48	0.97	0.08	9,12,16,19	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.

