



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 27, 2017 – 12:15 AM EDT

PDB ID : 4WDW  
Title : 17beta-HSD5 in complex with 3,6-dihydropyridin-1(2H)-yl(5-methyl-1H-indol-2-yl)methanone  
Authors : Amano, Y.; Yamaguchi, T.  
Deposited on : unknown  
Resolution : 1.94 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

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030345  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030345

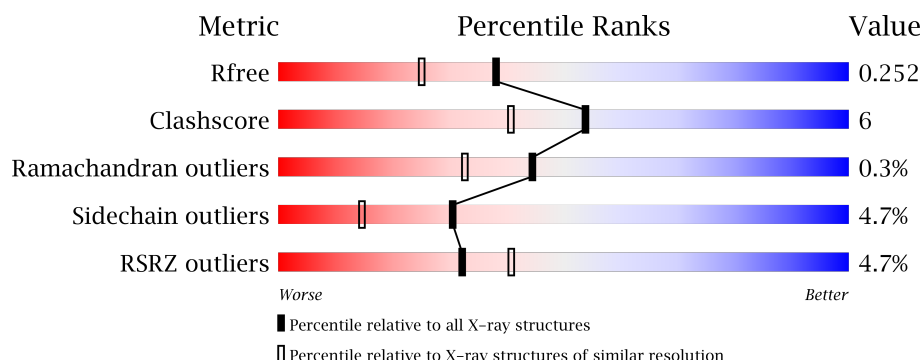
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.94 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))
$R_{free}$	100719	3233 (1.96-1.92)
Clashscore	112137	3430 (1.96-1.92)
Ramachandran outliers	110173	3395 (1.96-1.92)
Sidechain outliers	110143	3395 (1.96-1.92)
RSRZ outliers	101464	3250 (1.96-1.92)

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  $\leq 5\%$ . 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	331	<div> <div>4%</div> <div> <div></div> <div>74%</div> <div>14%</div> <div>••</div> <div>10%</div> </div> </div>
1	B	331	<div> <div>4%</div> <div> <div></div> <div>81%</div> <div>8%</div> <div>•</div> <div>9%</div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5069 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 Aldo-keto reductase family 1 member C3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	298	Total	C	N	O	S	0	0	0
			2380	1518	418	432	12			
1	B	301	Total	C	N	O	S	0	0	0
			2408	1536	423	437	12			

There are 18 discrepancies between the modelled and reference sequences:

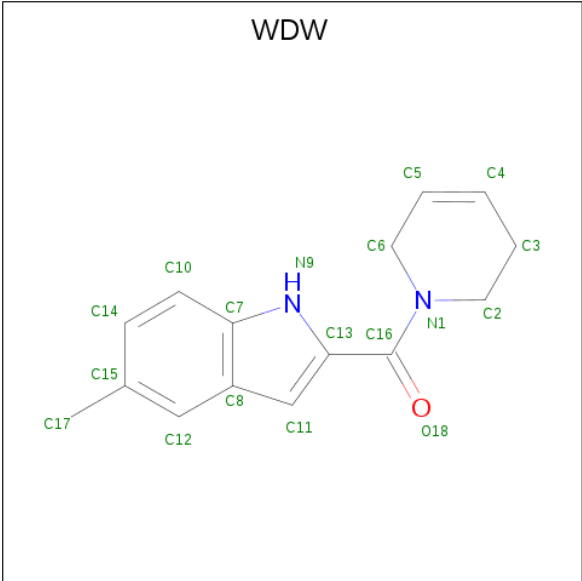
Chain	Residue	Modelled	Actual	Comment	Reference
A	5	GLN	HIS	natural variant	UNP P42330
A	324	LEU	-	expression tag	UNP P42330
A	325	GLU	-	expression tag	UNP P42330
A	326	HIS	-	expression tag	UNP P42330
A	327	HIS	-	expression tag	UNP P42330
A	328	HIS	-	expression tag	UNP P42330
A	329	HIS	-	expression tag	UNP P42330
A	330	HIS	-	expression tag	UNP P42330
A	331	HIS	-	expression tag	UNP P42330
B	5	GLN	HIS	natural variant	UNP P42330
B	324	LEU	-	expression tag	UNP P42330
B	325	GLU	-	expression tag	UNP P42330
B	326	HIS	-	expression tag	UNP P42330
B	327	HIS	-	expression tag	UNP P42330
B	328	HIS	-	expression tag	UNP P42330
B	329	HIS	-	expression tag	UNP P42330
B	330	HIS	-	expression tag	UNP P42330
B	331	HIS	-	expression tag	UNP P42330

- 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	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0
			48	21	7	17	3	
2	B	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 3 is 3,6-dihydropyridin-1(2H)-yl(5-methyl-1H-indol-2-yl)methanone (three-letter code: WDW) (formula: C<sub>15</sub>H<sub>16</sub>N<sub>2</sub>O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			18	15	2	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			18	15	2	1		

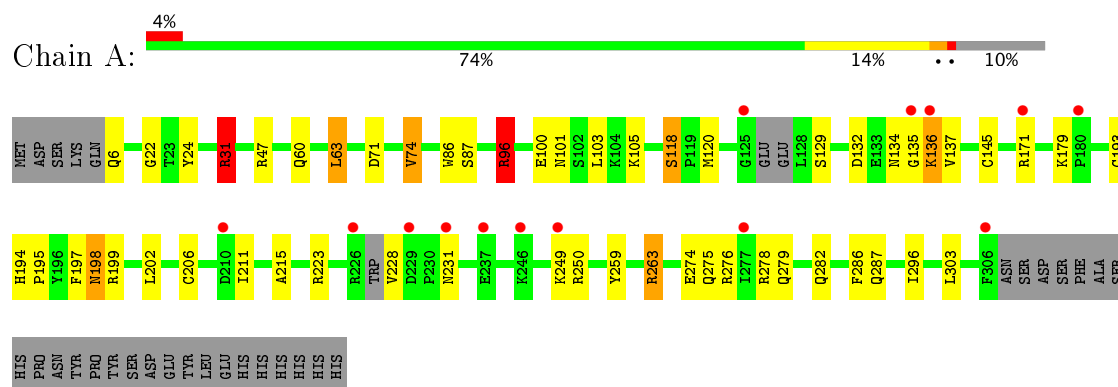
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	74	Total	O	0	0
			74	74		
4	B	75	Total	O	0	0
			75	75		

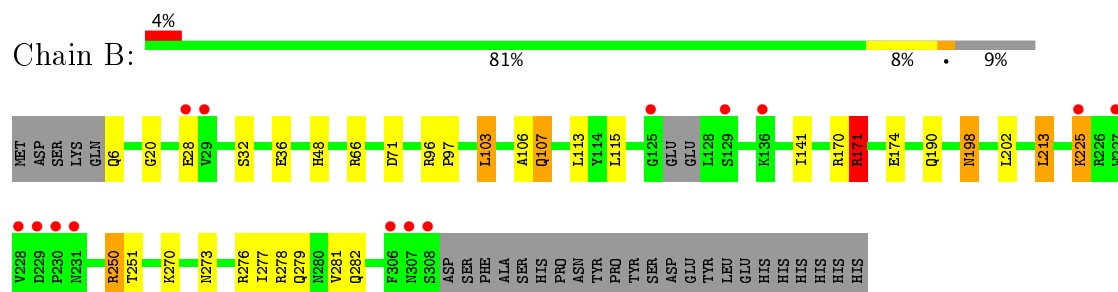
### 3 Residue-property plots [i](#)

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 ( $RSRZ > 2$ ). 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: Aldo-keto reductase family 1 member C3



- Molecule 1: Aldo-keto reductase family 1 member C3



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	55.13Å 57.92Å 60.33Å 81.03° 69.72° 79.11°	Depositor
Resolution (Å)	14.60 – 1.94 14.60 – 1.94	Depositor EDS
% Data completeness (in resolution range)	93.5 (14.60-1.94) 91.4 (14.60-1.94)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.87 (at 1.94Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.199 , 0.253 0.198 , 0.252	Depositor DCC
$R_{free}$ test set	2404 reflections (5.34%)	DCC
Wilson B-factor (Å <sup>2</sup> )	28.3	Xtriage
Anisotropy	0.080	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.49 , 49.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	5069	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.39% 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: NAP, WDW

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	0.94	0/2428	1.08	11/3278 (0.3%)
1	B	0.99	0/2459	1.03	7/3323 (0.2%)
All	All	0.97	0/4887	1.05	18/6601 (0.3%)

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	96	ARG	NE-CZ-NH2	17.00	128.80	120.30
1	A	96	ARG	NE-CZ-NH1	-11.42	114.59	120.30
1	B	250	ARG	NE-CZ-NH2	9.85	125.22	120.30
1	A	199	ARG	NE-CZ-NH2	-7.61	116.50	120.30
1	B	171	ARG	NE-CZ-NH1	-7.44	116.58	120.30
1	B	213	LEU	CA-CB-CG	7.25	131.99	115.30
1	A	31	ARG	NE-CZ-NH1	-7.23	116.69	120.30
1	A	31	ARG	NE-CZ-NH2	6.83	123.72	120.30
1	B	71	ASP	CB-CG-OD1	6.73	124.35	118.30
1	B	103	LEU	CA-CB-CG	6.21	129.59	115.30
1	A	74	VAL	CB-CA-C	-6.20	99.62	111.40
1	A	47	ARG	NE-CZ-NH2	5.89	123.25	120.30
1	A	63	LEU	CB-CG-CD2	-5.66	101.38	111.00
1	B	171	ARG	NE-CZ-NH2	5.56	123.08	120.30
1	A	96	ARG	CD-NE-CZ	5.44	131.22	123.60
1	A	96	ARG	CB-CA-C	5.20	120.80	110.40
1	B	141	ILE	CG1-CB-CG2	-5.17	100.01	111.40
1	A	71	ASP	CB-CG-OD1	5.14	122.93	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	2380	0	2418	29	0
1	B	2408	0	2440	28	0
2	A	48	0	25	3	0
2	B	48	0	25	4	0
3	A	18	0	16	1	0
3	B	18	0	16	3	0
4	A	74	0	0	0	0
4	B	75	0	0	0	0
All	All	5069	0	4940	60	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.

All (60) 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:B:171:ARG:NH1	1:B:174:GLU:HG3	1.90	0.85
1:A:135:GLY:HA3	1:A:136:LYS:HB2	1.60	0.83
3:B:402:WDW:C11	3:B:402:WDW:H12	2.10	0.79
3:B:402:WDW:H4	3:B:402:WDW:H12	1.64	0.78
1:A:279:GLN:NE2	2:A:401:NAP:H62A	1.82	0.77
1:B:198:ASN:C	1:B:198:ASN:HD22	1.90	0.74
1:A:250:ARG:HH11	1:A:282:GLN:HE21	1.35	0.74
1:A:132:ASP:OD1	1:A:136:LYS:HB3	1.88	0.74
1:A:96:ARG:HD2	1:A:100:GLU:OE2	1.88	0.73
1:B:171:ARG:NH1	1:B:174:GLU:OE1	2.22	0.73
1:A:135:GLY:CA	1:A:136:LYS:HB2	2.19	0.71
1:B:171:ARG:HH11	1:B:174:GLU:HG3	1.53	0.70
1:A:259:TYR:O	1:A:263:ARG:HG3	1.93	0.69
1:A:101:ASN:HD21	1:A:105:LYS:HE3	1.60	0.67
1:A:250:ARG:HH11	1:A:282:GLN:NE2	1.95	0.64
1:B:279:GLN:NE2	2:B:401:NAP:H62A	1.95	0.64
1:B:278:ARG:HH21	1:B:278:ARG:HG2	1.62	0.63
1:B:171:ARG:NH1	1:B:174:GLU:CG	2.60	0.61
1:A:198:ASN:HD22	1:A:198:ASN:C	2.07	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:TYR:CD2	3:A:402:WDW:H8	2.39	0.57
1:B:225:LYS:H	1:B:225:LYS:HD2	1.70	0.57
1:B:279:GLN:O	1:B:282:GLN:HB2	2.05	0.56
1:B:270:LYS:HB2	2:B:401:NAP:H52N	1.88	0.56
1:A:101:ASN:ND2	1:A:105:LYS:HE3	2.22	0.54
1:B:66:ARG:CZ	1:B:107:GLN:HG3	2.38	0.54
1:A:274:GLU:O	1:A:278:ARG:HG3	2.09	0.53
1:B:171:ARG:HH11	1:B:174:GLU:CG	2.19	0.53
1:B:32:SER:O	1:B:36:GLU:HG3	2.10	0.52
1:B:278:ARG:O	1:B:281:VAL:HG22	2.11	0.51
1:B:20:GLY:HA2	1:B:48:HIS:HB3	1.93	0.51
1:B:96:ARG:HB3	1:B:97:PRO:HD3	1.92	0.51
1:B:66:ARG:NH1	1:B:107:GLN:HG3	2.27	0.50
1:B:278:ARG:HG2	1:B:278:ARG:NH2	2.25	0.49
1:B:170:ARG:O	1:B:174:GLU:HG2	2.13	0.48
3:B:402:WDW:C2	3:B:402:WDW:C11	2.89	0.47
1:A:259:TYR:HB2	1:A:296:ILE:HD13	1.97	0.47
1:B:28:GLU:H	1:B:28:GLU:CD	2.18	0.45
1:A:145:CYS:HB3	1:A:179:LYS:HD3	1.97	0.45
1:B:276:ARG:HD2	2:B:401:NAP:C5A	2.47	0.45
1:A:22:GLY:HA3	2:A:401:NAP:H4D	1.99	0.45
1:B:106:ALA:C	1:B:107:GLN:HG2	2.34	0.45
1:A:31:ARG:N	1:A:31:ARG:HD2	2.33	0.44
1:A:171:ARG:HD3	1:A:171:ARG:O	2.18	0.43
1:A:194:HIS:HB2	1:A:195:PRO:CD	2.48	0.43
1:A:145:CYS:HB3	1:A:179:LYS:CD	2.48	0.43
1:A:60:GLN:H	1:A:60:GLN:NE2	2.17	0.42
1:A:276:ARG:HD2	2:A:401:NAP:C5A	2.49	0.42
1:B:190:GLN:OE1	2:B:401:NAP:H2N	2.19	0.42
1:B:171:ARG:NH1	1:B:174:GLU:CD	2.72	0.42
1:A:118:SER:OG	1:A:120:MET:HG2	2.19	0.41
1:A:250:ARG:HG3	1:A:286:PHE:CE2	2.55	0.41
1:B:113:LEU:HD21	1:B:115:LEU:HD21	2.02	0.41
1:A:197:PHE:HB2	1:A:303:LEU:O	2.20	0.41
1:A:223:ARG:HA	1:A:228:VAL:HG11	2.01	0.41
1:B:251:THR:OG1	1:B:279:GLN:NE2	2.53	0.41
1:B:198:ASN:C	1:B:198:ASN:ND2	2.67	0.41
1:A:86:TRP:CG	1:A:87:SER:N	2.88	0.41
1:B:273:ASN:O	1:B:277:ILE:HG13	2.20	0.41
1:A:193:CYS:HB3	1:A:215:ALA:CB	2.51	0.41
1:A:206:CYS:HB3	1:A:211:ILE:O	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	292/331 (88%)	281 (96%)	9 (3%)	2 (1%)	25	12
1	B	297/331 (90%)	284 (96%)	13 (4%)	0	100	100
All	All	589/662 (89%)	565 (96%)	22 (4%)	2 (0%)	44	33

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	136	LYS
1	A	137	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	A	263/295 (89%)	247 (94%)	16 (6%)	22	8
1	B	266/295 (90%)	257 (97%)	9 (3%)	42	27
All	All	529/590 (90%)	504 (95%)	25 (5%)	30	15

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	GLN

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Mol	Chain	Res	Type
1	A	31	ARG
1	A	63	LEU
1	A	74	VAL
1	A	96	ARG
1	A	103	LEU
1	A	118	SER
1	A	129	SER
1	A	134	ASN
1	A	198	ASN
1	A	202	LEU
1	A	231	ASN
1	A	249	LYS
1	A	263	ARG
1	A	275	GLN
1	A	287	GLN
1	B	6	GLN
1	B	103	LEU
1	B	107	GLN
1	B	171	ARG
1	B	198	ASN
1	B	202	LEU
1	B	213	LEU
1	B	225	LYS
1	B	250	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	GLN
1	A	101	ASN
1	A	134	ASN
1	A	198	ASN
1	A	279	GLN
1	A	282	GLN
1	B	6	GLN
1	B	56	ASN
1	B	60	GLN
1	B	198	ASN
1	B	279	GLN
1	B	282	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 ⓘ

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
2	NAP	A	401	-	44,52,52	1.19	4 (9%)	51,80,80	1.26	6 (11%)
3	WDW	A	402	-	18,20,20	1.27	1 (5%)	21,28,28	2.10	7 (33%)
2	NAP	B	401	-	44,52,52	1.12	4 (9%)	51,80,80	1.60	7 (13%)
3	WDW	B	402	-	18,20,20	0.92	1 (5%)	21,28,28	2.00	7 (33%)

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	A	401	-	-	0/27/67/67	0/5/5/5
3	WDW	A	402	-	-	0/5/16/16	0/3/3/3
2	NAP	B	401	-	-	0/27/67/67	0/5/5/5
3	WDW	B	402	-	-	0/5/16/16	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	402	WDW	C13-C16	-3.76	1.43	1.50
3	B	402	WDW	C13-C16	-2.59	1.45	1.50
2	A	401	NAP	C3N-C7N	-2.41	1.46	1.50
2	B	401	NAP	O4D-C4D	-2.10	1.40	1.45
2	B	401	NAP	C3N-C7N	-2.09	1.47	1.50
2	A	401	NAP	C7N-N7N	2.16	1.37	1.33
2	A	401	NAP	O4B-C1B	2.18	1.44	1.41
2	B	401	NAP	C7N-N7N	2.25	1.37	1.33
2	B	401	NAP	P2B-O2B	3.47	1.65	1.59
2	A	401	NAP	P2B-O2B	3.79	1.66	1.59

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	NAP	C4B-O4B-C1B	-6.04	103.34	109.77
3	A	402	WDW	C14-C10-C7	-4.82	114.93	120.84
2	B	401	NAP	C3N-C2N-N1N	-4.73	115.67	120.43
3	B	402	WDW	C14-C10-C7	-4.65	115.14	120.84
3	B	402	WDW	C15-C12-C8	-3.26	117.77	121.87
2	A	401	NAP	C4B-O4B-C1B	-3.25	106.31	109.77
3	A	402	WDW	C15-C12-C8	-3.24	117.81	121.87
2	B	401	NAP	O4D-C4D-C3D	-2.85	99.50	105.17
2	B	401	NAP	O2D-C2D-C3D	-2.56	103.61	111.83
2	B	401	NAP	O3B-C3B-C4B	-2.55	103.64	111.09
2	A	401	NAP	O2D-C2D-C3D	-2.42	104.07	111.83
2	B	401	NAP	C6N-C5N-C4N	-2.13	116.23	119.44
3	B	402	WDW	C17-C15-C12	-2.10	116.93	121.75
2	A	401	NAP	O2B-P2B-O1X	-2.00	101.40	109.26
2	A	401	NAP	O3X-P2B-O2X	2.01	115.72	107.61
3	A	402	WDW	C6-N1-C2	2.02	118.95	113.92
3	A	402	WDW	C11-C13-C16	2.03	135.14	128.37
2	A	401	NAP	O5D-C5D-C4D	2.15	116.62	109.00
3	B	402	WDW	O18-C16-C13	2.18	123.40	118.93
2	A	401	NAP	O3X-P2B-O1X	2.36	119.75	110.50
3	B	402	WDW	C14-C15-C12	2.37	121.35	118.47
3	B	402	WDW	C13-C11-C8	2.77	110.01	106.55
3	A	402	WDW	C14-C15-C12	2.94	122.04	118.47
3	A	402	WDW	C3-C2-N1	3.26	116.78	110.58
2	B	401	NAP	C2N-C3N-C4N	3.50	122.25	118.26
3	A	402	WDW	C13-N9-C7	4.08	112.87	104.47
3	B	402	WDW	C13-N9-C7	4.15	113.03	104.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	NAP	3	0
3	A	402	WDW	1	0
2	B	401	NAP	4	0
3	B	402	WDW	3	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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	298/331 (90%)	0.17	14 (4%) 32 41	17, 28, 51, 74	0
1	B	301/331 (90%)	0.11	14 (4%) 32 41	17, 26, 51, 113	0
All	All	599/662 (90%)	0.14	28 (4%) 32 41	17, 27, 51, 113	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	227	TRP	7.9
1	B	307	ASN	6.2
1	A	306	PHE	5.4
1	A	125	GLY	4.6
1	A	231	ASN	4.6
1	B	225	LYS	4.3
1	B	231	ASN	4.0
1	B	308	SER	3.8
1	A	226	ARG	3.7
1	A	229	ASP	3.7
1	A	136	LYS	3.4
1	B	228	VAL	2.8
1	B	230	PRO	2.7
1	A	249	LYS	2.6
1	B	129	SER	2.5
1	B	28	GLU	2.5
1	A	180	PRO	2.4
1	B	125	GLY	2.4
1	B	229	ASP	2.3
1	A	246	LYS	2.2
1	A	237	GLU	2.2
1	B	136	LYS	2.2
1	A	277	ILE	2.2
1	A	210	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	29	VAL	2.1
1	B	306	PHE	2.1
1	A	171	ARG	2.0
1	A	135	GLY	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	WDW	A	402	18/18	0.81	0.18	0.79	38,60,65,66	0
2	NAP	A	401	48/48	0.95	0.10	0.08	23,28,33,37	0
3	WDW	B	402	18/18	0.89	0.16	0.06	30,46,65,68	0
2	NAP	B	401	48/48	0.96	0.08	-0.55	18,24,31,40	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.