



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 7, 2018 – 03:54 am GMT

PDB ID : 4Z3K  
Title : Human sepiapterin reductase in complex with the cofactor NADP<sup>+</sup> and the tryptophan metabolite xanthurenic acid  
Authors : Johnsson, K.  
Deposited on : 2015-03-31  
Resolution : 2.35 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 : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : trunk30967  
Percentile statistics : (not set)  
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

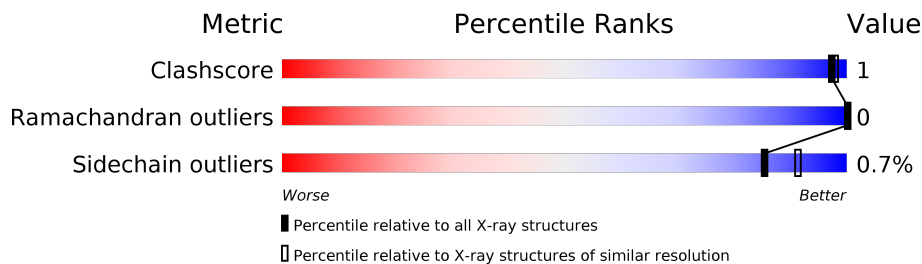
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.35 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	1081 (2.36-2.36)
Ramachandran outliers	120053	1066 (2.36-2.36)
Sidechain outliers	120020	1067 (2.36-2.36)

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	275	91% 7%
1	B	275	92% 7%
1	C	275	91% 7%
1	D	275	90% 7%

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8214 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 Sepiapterin reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	257	Total	C	N	O	S	0	1	0
			1942	1223	344	365	10			
1	B	257	Total	C	N	O	S	0	1	0
			1942	1223	344	365	10			
1	C	257	Total	C	N	O	S	0	1	0
			1942	1223	344	365	10			
1	D	257	Total	C	N	O	S	0	1	0
			1942	1223	344	365	10			

There are 56 discrepancies between the modelled and reference sequences:

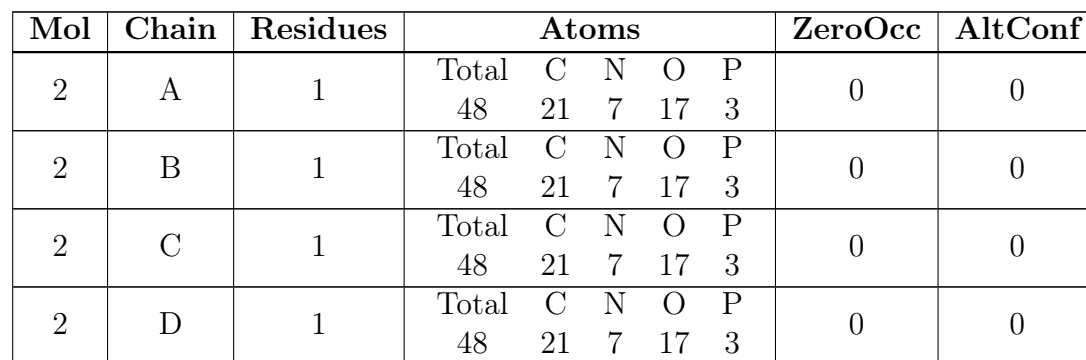
Chain	Residue	Modelled	Actual	Comment	Reference
A	-16	MET	-	initiating methionine	UNP P35270
A	-15	HIS	-	expression tag	UNP P35270
A	-14	HIS	-	expression tag	UNP P35270
A	-13	HIS	-	expression tag	UNP P35270
A	-12	HIS	-	expression tag	UNP P35270
A	-11	HIS	-	expression tag	UNP P35270
A	-10	HIS	-	expression tag	UNP P35270
A	-9	GLU	-	expression tag	UNP P35270
A	-8	ASN	-	expression tag	UNP P35270
A	-7	LEU	-	expression tag	UNP P35270
A	-6	TYR	-	expression tag	UNP P35270
A	-5	PHE	-	expression tag	UNP P35270
A	-4	GLN	-	expression tag	UNP P35270
A	-3	GLY	-	expression tag	UNP P35270
B	-16	MET	-	initiating methionine	UNP P35270
B	-15	HIS	-	expression tag	UNP P35270
B	-14	HIS	-	expression tag	UNP P35270
B	-13	HIS	-	expression tag	UNP P35270
B	-12	HIS	-	expression tag	UNP P35270
B	-11	HIS	-	expression tag	UNP P35270
B	-10	HIS	-	expression tag	UNP P35270

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
B	-9	GLU	-	expression tag	UNP P35270
B	-8	ASN	-	expression tag	UNP P35270
B	-7	LEU	-	expression tag	UNP P35270
B	-6	TYR	-	expression tag	UNP P35270
B	-5	PHE	-	expression tag	UNP P35270
B	-4	GLN	-	expression tag	UNP P35270
B	-3	GLY	-	expression tag	UNP P35270
C	-16	MET	-	initiating methionine	UNP P35270
C	-15	HIS	-	expression tag	UNP P35270
C	-14	HIS	-	expression tag	UNP P35270
C	-13	HIS	-	expression tag	UNP P35270
C	-12	HIS	-	expression tag	UNP P35270
C	-11	HIS	-	expression tag	UNP P35270
C	-10	HIS	-	expression tag	UNP P35270
C	-9	GLU	-	expression tag	UNP P35270
C	-8	ASN	-	expression tag	UNP P35270
C	-7	LEU	-	expression tag	UNP P35270
C	-6	TYR	-	expression tag	UNP P35270
C	-5	PHE	-	expression tag	UNP P35270
C	-4	GLN	-	expression tag	UNP P35270
C	-3	GLY	-	expression tag	UNP P35270
D	-16	MET	-	initiating methionine	UNP P35270
D	-15	HIS	-	expression tag	UNP P35270
D	-14	HIS	-	expression tag	UNP P35270
D	-13	HIS	-	expression tag	UNP P35270
D	-12	HIS	-	expression tag	UNP P35270
D	-11	HIS	-	expression tag	UNP P35270
D	-10	HIS	-	expression tag	UNP P35270
D	-9	GLU	-	expression tag	UNP P35270
D	-8	ASN	-	expression tag	UNP P35270
D	-7	LEU	-	expression tag	UNP P35270
D	-6	TYR	-	expression tag	UNP P35270
D	-5	PHE	-	expression tag	UNP P35270
D	-4	GLN	-	expression tag	UNP P35270
D	-3	GLY	-	expression tag	UNP P35270

- 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>).



- 4KL
- 
- The chemical structure of 4KL (4-ketolactone) is shown. It consists of a central pyridine ring. The nitrogen atom at the top of the ring is labeled 'NAG' in green. The ring is substituted with several groups: a hydroxyl group ('OH' in red) at the top-left position, labeled 'OAK' in green; a carboxylate group ('OH' in red, 'O' in red, 'OAO' in green) at the top-right position, labeled 'OAN' in green; a hydroxyl group ('OH' in red) at the bottom position, labeled 'OAL' in green; and a carboxylate group ('OH' in red, 'O' in red, 'OAO' in green) at the bottom-right position, labeled 'OAM' in green. The pyridine ring is fused to a benzene ring on the left. The benzene ring has three substituents: 'CAB' in green at the top-left, 'CAF' in green at the bottom-left, and 'CAI' in green at the bottom-right. The pyridine ring has two additional substituents: 'CAD' in green at the top-right and 'CAE' in green at the bottom-left. The overall structure is a complex polycyclic molecule with multiple functional groups.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			15	10	1	4		
3	B	1	Total	C	N	O	0	0
			15	10	1	4		
3	C	1	Total	C	N	O	0	0
			15	10	1	4		
3	D	1	Total	C	N	O	0	0
			15	10	1	4		

- 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	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			4	2	2		


- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	46	Total	O	0	0
			46	46		
6	B	29	Total	O	0	0
			29	29		
6	C	37	Total	O	0	0
			37	37		
6	D	48	Total	O	0	0
			48	48		

### 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. 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.

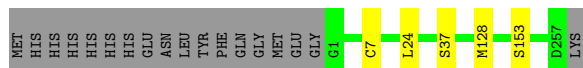
- Molecule 1: Sepiapterin reductase

Chain A:  91% 7%



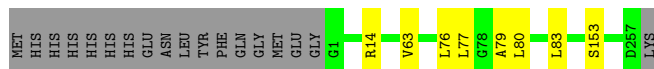
- Molecule 1: Sepiapterin reductase

Chain B:  92% 7%




- Molecule 1: Sepiapterin reductase

Chain C:  91% 7%



- Molecule 1: Sepiapterin reductase

Chain D:  90% 7%





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	143.96Å 143.96Å 180.74Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	124.68 – 2.35 47.12 – 1.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (124.68-2.35) 99.5 (47.12-1.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	-0.13 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.8.0107	Depositor
R, $R_{free}$	0.181 , 0.214 0.203 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	23.8	Xtriage
Anisotropy	0.085	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 34.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.044 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	8214	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.07% 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: 4KL, EDO, NAP, SO4

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	0.98	0/1969	0.70	0/2664
1	B	0.89	1/1969 (0.1%)	0.63	0/2664
1	C	1.07	0/1969	0.73	1/2664 (0.0%)
1	D	0.97	0/1969	0.69	0/2664
All	All	0.98	1/7876 (0.0%)	0.69	1/10656 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	37	SER	CB-OG	5.38	1.49	1.42

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	14	ARG	NE-CZ-NH1	6.47	123.53	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	A	1942	0	2007	2	0
1	B	1942	0	2007	2	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1942	0	2007	6	0
1	D	1942	0	2007	5	0
2	A	48	0	25	0	0
2	B	48	0	25	1	0
2	C	48	0	25	1	0
2	D	48	0	25	1	0
3	A	15	0	6	0	0
3	B	15	0	6	0	0
3	C	15	0	5	0	0
3	D	15	0	5	0	0
4	A	5	0	0	0	0
4	B	10	0	0	0	0
4	C	10	0	0	0	0
4	D	5	0	0	0	0
5	B	4	0	6	0	0
6	A	46	0	0	0	0
6	B	29	0	0	0	0
6	C	37	0	0	0	0
6	D	48	0	0	0	0
All	All	8214	0	8156	15	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 1.

The worst 5 of 15 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:7[B]:CYS:SG	1:A:24:LEU:HD21	2.33	0.68
1:C:79:ALA:O	1:C:83:LEU:HD12	1.94	0.66
1:C:80:LEU:HA	1:C:83:LEU:CD1	2.25	0.65
1:A:2:LEU:O	1:A:91:ARG:HD2	1.99	0.63
1:B:7[B]:CYS:SG	1:B:24:LEU:HD21	2.39	0.62

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	256/275 (93%)	251 (98%)	5 (2%)	0	100	100
1	B	256/275 (93%)	252 (98%)	4 (2%)	0	100	100
1	C	256/275 (93%)	252 (98%)	4 (2%)	0	100	100
1	D	256/275 (93%)	253 (99%)	3 (1%)	0	100	100
All	All	1024/1100 (93%)	1008 (98%)	16 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	210/225 (93%)	207 (99%)	3 (1%)	69	80
1	B	210/225 (93%)	209 (100%)	1 (0%)	90	94
1	C	210/225 (93%)	210 (100%)	0	100	100
1	D	210/225 (93%)	208 (99%)	2 (1%)	78	86
All	All	840/900 (93%)	834 (99%)	6 (1%)	85	91

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	142	SER
1	D	220	GLN
1	B	128	MET

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	137	LYS
1	D	142	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	220	GLN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

15 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	801	-	44,52,52	1.16	3 (6%)	53,80,80	1.63	5 (9%)
3	4KL	A	802	-	13,16,16	1.18	1 (7%)	17,23,23	1.48	2 (11%)
4	SO4	A	803	-	4,4,4	0.50	0	6,6,6	0.23	0
2	NAP	B	301	-	44,52,52	1.12	4 (9%)	53,80,80	1.47	4 (7%)
3	4KL	B	302	-	13,16,16	1.11	0	17,23,23	1.38	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	SO4	B	303	-	4,4,4	0.52	0	6,6,6	0.46	0
4	SO4	B	304	-	4,4,4	0.54	0	6,6,6	0.38	0
5	EDO	B	305	-	3,3,3	0.61	0	2,2,2	0.27	0
2	NAP	C	301	-	44,52,52	1.00	3 (6%)	53,80,80	1.53	5 (9%)
3	4KL	C	302	-	13,16,16	1.50	2 (15%)	17,23,23	1.36	2 (11%)
4	SO4	C	303	-	4,4,4	0.58	0	6,6,6	0.18	0
4	SO4	C	304	-	4,4,4	0.33	0	6,6,6	0.36	0
2	NAP	D	301	-	44,52,52	1.37	4 (9%)	53,80,80	1.58	5 (9%)
3	4KL	D	302	-	13,16,16	1.45	0	17,23,23	1.63	2 (11%)
4	SO4	D	303	-	4,4,4	0.45	0	6,6,6	0.34	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	A	801	-	-	0/27/67/67	0/5/5/5
3	4KL	A	802	-	-	0/0/4/4	0/2/2/2
4	SO4	A	803	-	-	0/0/0/0	0/0/0/0
2	NAP	B	301	-	-	0/27/67/67	0/5/5/5
3	4KL	B	302	-	-	0/0/4/4	0/2/2/2
4	SO4	B	303	-	-	0/0/0/0	0/0/0/0
4	SO4	B	304	-	-	0/0/0/0	0/0/0/0
5	EDO	B	305	-	-	0/1/1/1	0/0/0/0
2	NAP	C	301	-	-	0/27/67/67	0/5/5/5
3	4KL	C	302	-	-	0/0/4/4	0/2/2/2
4	SO4	C	303	-	-	0/0/0/0	0/0/0/0
4	SO4	C	304	-	-	0/0/0/0	0/0/0/0
2	NAP	D	301	-	-	0/27/67/67	0/5/5/5
3	4KL	D	302	-	-	0/0/4/4	0/2/2/2
4	SO4	D	303	-	-	0/0/0/0	0/0/0/0

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	NAP	C3B-C2B	-2.39	1.47	1.53
2	D	301	NAP	P2B-O3X	-2.27	1.45	1.54
2	C	301	NAP	O7N-C7N	-2.11	1.19	1.24
2	B	301	NAP	O4B-C4B	-2.09	1.40	1.45
2	A	801	NAP	C2A-N1A	2.02	1.37	1.33

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	NAP	N3A-C2A-N1A	-8.77	121.36	128.86
2	B	301	NAP	N3A-C2A-N1A	-7.57	122.38	128.86
2	D	301	NAP	N3A-C2A-N1A	-7.23	122.67	128.86
2	C	301	NAP	N3A-C2A-N1A	-6.93	122.93	128.86
2	C	301	NAP	O7N-C7N-C3N	-3.43	115.33	119.62

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	301	NAP	1	0
2	C	301	NAP	1	0
2	D	301	NAP	1	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 ⓘ

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

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

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

### 6.3 Carbohydrates ⓘ

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

### 6.4 Ligands ⓘ

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

### 6.5 Other polymers ⓘ

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