



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:05 PM GMT

PDB ID : 1S2A  
Title : Crystal structures of prostaglandin D2 11-ketoreductase in complex with the non-steroidal anti-inflammatory drugs flufenamic acid and indomethacin  
Authors : Lovering, A.L.; Ride, J.P.; Bunce, C.M.; Desmond, J.C.; Cummings, S.M.; White, S.A.  
Deposited on : 2004-01-08  
Resolution : 1.70 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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

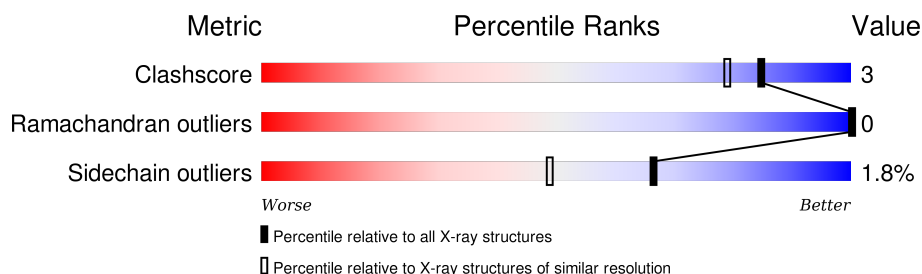
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.70 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	102246	3585 (1.70-1.70)
Ramachandran outliers	100387	3527 (1.70-1.70)
Sidechain outliers	100360	3527 (1.70-1.70)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	331	 88% 7% 5%

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 2963 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
			Total	C	N	O	S			
1	A	315	2524	1609	440	463	12	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

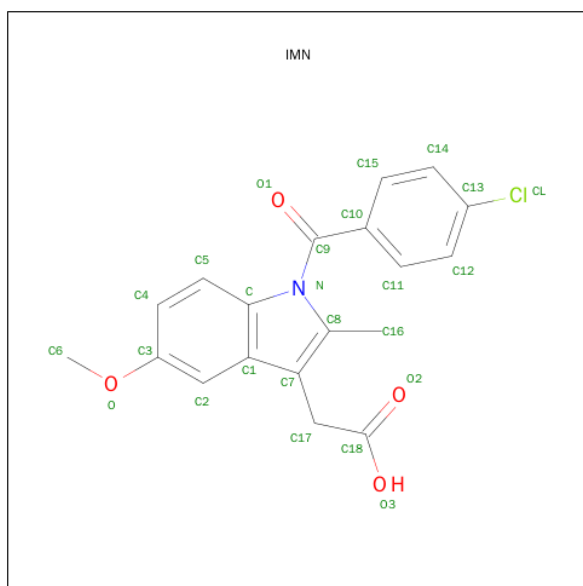
Chain	Residue	Modelled	Actual	Comment	Reference
A	324	LEU	-	EXPRESSION TAG	UNP P42330
A	325	GLU	-	EXPRESSION TAG	UNP P42330
A	326	HIS	-	EXPRESSION TAG	UNP P42330
A	327	HIS	-	EXPRESSION TAG	UNP P42330
A	328	HIS	-	EXPRESSION TAG	UNP P42330
A	329	HIS	-	EXPRESSION TAG	UNP P42330
A	330	HIS	-	EXPRESSION TAG	UNP P42330
A	331	HIS	-	EXPRESSION TAG	UNP P42330

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula:  $C_{21}H_{28}N_7O_{17}P_3$ ).



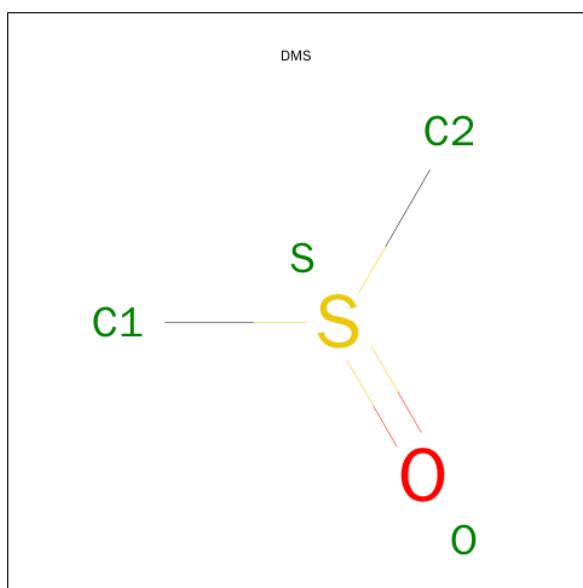
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is INDOMETHACIN (three-letter code: IMN) (formula:  $C_{19}H_{16}ClNO_4$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	0	0
			25	19	1	1	4		

- Molecule 4 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula:  $C_2H_6OS$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 5 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	X	0	0
			1	1		

- Molecule 6 is water.


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	361	Total	O	0	0
			361	361		

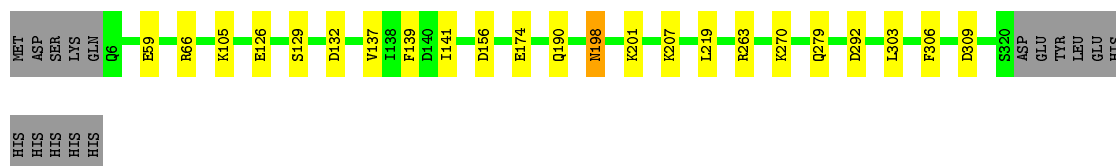
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

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

Chain A: 



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	55.81Å 63.07Å 96.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.70	Depositor
% Data completeness (in resolution range)	97.8 (20.00-1.70)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.05	Depositor
Refinement program	REFMAC 5.1.19	Depositor
R, $R_{free}$	0.172 , 0.198	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2963	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

## 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: UNX, NAP, DMS, IMN

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	0.42	0/2582	0.71	6/3494 (0.2%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	132	ASP	CB-CG-OD2	6.32	123.99	118.30
1	A	309	ASP	CB-CG-OD2	6.05	123.74	118.30
1	A	156	ASP	CB-CG-OD2	5.94	123.64	118.30
1	A	263	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	A	292	ASP	CB-CG-OD2	5.43	123.19	118.30
1	A	263	ARG	NE-CZ-NH2	-5.11	117.75	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	2524	0	2530	13	2
2	A	48	0	25	6	0
3	A	25	0	15	3	0
4	A	4	0	6	0	0
5	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	361	0	0	5	3
All	All	2963	0	2576	15	3

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 3.

All (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:219:LEU:HB2	2:A:1001:NAP:H51A	1.81	0.63
1:A:207:LYS:NZ	6:A:2353:HOH:O	2.19	0.63
1:A:198:ASN:HD22	1:A:198:ASN:C	2.04	0.61
1:A:270:LYS:O	2:A:1001:NAP:H8A	2.05	0.55
1:A:279:GLN:NE2	2:A:1001:NAP:H62A	2.06	0.53
2:A:1001:NAP:H4N	3:A:2001:IMN:C5	2.40	0.52
1:A:59:GLU:HG3	1:A:105:LYS:HG3	1.93	0.49
1:A:174:GLU:CD	6:A:2359:HOH:O	2.54	0.45
1:A:139:PHE:HB3	6:A:2250:HOH:O	2.16	0.44
1:A:141:ILE:CD1	6:A:2239:HOH:O	2.66	0.43
1:A:137:VAL:HB	6:A:2335:HOH:O	2.19	0.42
1:A:219:LEU:HB2	2:A:1001:NAP:C5B	2.47	0.42
3:A:2001:IMN:O1	3:A:2001:IMN:H161	2.20	0.41
1:A:190:GLN:OE1	2:A:1001:NAP:H2N	2.20	0.41
1:A:306:PHE:HB2	3:A:2001:IMN:O	2.21	0.41

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:2139:HOH:O	6:A:2242:HOH:O[4_446]	1.93	0.27
1:A:126:GLU:OE1	6:A:2358:HOH:O[3_646]	2.13	0.07
1:A:59:GLU:OE1	6:A:2239:HOH:O[3_646]	2.13	0.07

## 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	313/331 (95%)	309 (99%)	4 (1%)	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	279/295 (95%)	274 (98%)	5 (2%)	66	49

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	ARG
1	A	129	SER
1	A	198	ASN
1	A	201	LYS
1	A	303	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	ASN
1	A	101	ASN
1	A	107	GLN
1	A	198	ASN
1	A	279	GLN
1	A	287	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 ⓘ

Of 4 ligands modelled in this entry, 1 is unknown - leaving 3 for Mogul analysis.

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	1001	-	42,52,52	1.43	5 (11%)	54,80,80	2.29	8 (14%)
3	IMN	A	2001	-	21,27,27	2.61	5 (23%)	26,39,39	2.45	4 (15%)
4	DMS	A	2002	-	3,3,3	0.71	0	3,3,3	0.60	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	1001	-	-	0/27/67/67	0/5/5/5
3	IMN	A	2001	-	-	0/8/14/14	0/3/3/3
4	DMS	A	2002	-	-	0/0/0/0	0/0/0/0

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2001	IMN	C-N	-4.43	1.33	1.39
2	A	1001	NAP	O5B-C5B	-2.89	1.33	1.44
2	A	1001	NAP	O4B-C4B	-2.54	1.39	1.45
3	A	2001	IMN	C13-CL	2.34	1.79	1.74
2	A	1001	NAP	C2A-N1A	2.52	1.38	1.33
3	A	2001	IMN	C17-C7	3.60	1.57	1.52
2	A	1001	NAP	C2A-N3A	3.62	1.38	1.32
3	A	2001	IMN	C7-C1	5.12	1.50	1.41
2	A	1001	NAP	O7N-C7N	6.09	1.37	1.24
3	A	2001	IMN	C8-C7	8.09	1.54	1.39

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1001	NAP	N3A-C2A-N1A	-11.09	120.41	128.89
3	A	2001	IMN	C18-C17-C7	-9.05	99.01	116.31
2	A	1001	NAP	O3-PA-O5B	-6.81	84.86	102.94
2	A	1001	NAP	O4B-C4B-C5B	-5.85	88.41	109.32
3	A	2001	IMN	O1-C9-C10	-3.22	114.06	120.17
3	A	2001	IMN	C5-C-C1	-2.50	117.49	120.93
2	A	1001	NAP	O7N-C7N-C3N	-2.28	117.10	119.59
2	A	1001	NAP	O5B-C5B-C4B	2.02	116.57	109.12
2	A	1001	NAP	O4D-C1D-N1N	2.37	110.74	108.13
2	A	1001	NAP	O5B-PA-O1A	2.70	120.10	109.62
2	A	1001	NAP	C3N-C7N-N7N	3.39	121.53	117.82
3	A	2001	IMN	C10-C9-N	6.08	125.84	118.02

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	NAP	6	0
3	A	2001	IMN	3	0

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.