



# wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 17, 2017 – 08:39 PM EDT

PDB ID : 4Z0L  
Title : The murine cyclooxygenase-2 complexed with a nido-dicarbaborate-containing indomethacin derivative  
Authors : Xu, S.; Neumann, W.; Banerjee, S.; Hey-Hawkins, E.; Marnett, L.J.  
Deposited on : unknown  
Resolution : 2.29 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

<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-20029824  
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-20029824



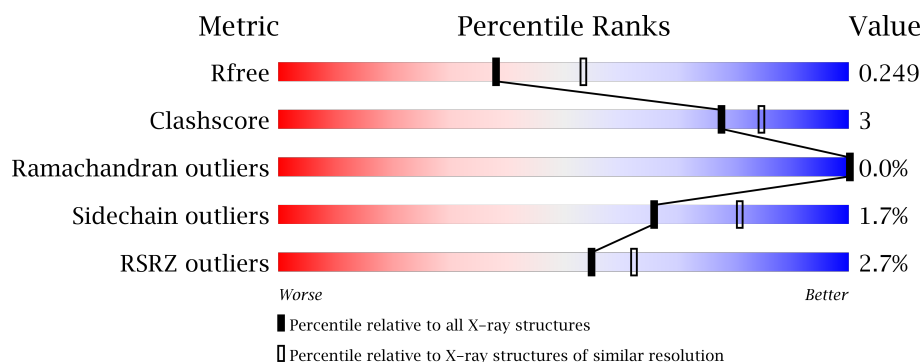
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.29 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	4130 (2.30-2.30)
Clashscore	112137	4751 (2.30-2.30)
Ramachandran outliers	110173	4705 (2.30-2.30)
Sidechain outliers	110143	4704 (2.30-2.30)
RSRZ outliers	101464	4156 (2.30-2.30)

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	587	<div> <div>3%</div> <div> <div></div> <div>87%</div> <div>7%</div> <div>6%</div> </div> </div>
1	B	587	<div> <div>4%</div> <div> <div></div> <div>86%</div> <div>7%</div> <div>6%</div> </div> </div>
1	C	587	<div> <div>2%</div> <div> <div></div> <div>86%</div> <div>7%</div> <div>6%</div> </div> </div>
1	D	587	<div> <div>2%</div> <div> <div></div> <div>87%</div> <div>6%</div> <div>6%</div> </div> </div>

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 crite-



ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	BOG	B	708	-	-	-	X
6	BOG	C	709	-	-	-	X
6	BOG	D	708	-	-	-	X



## 2 Entry composition [i](#)

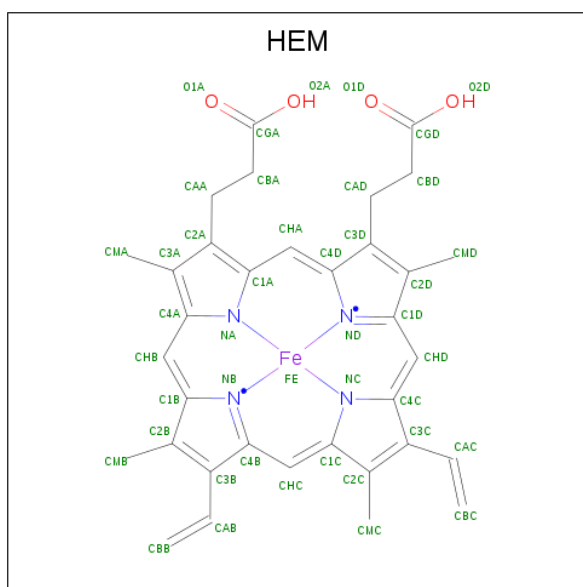
There are 7 unique types of molecules in this entry. The entry contains 19280 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Prostaglandin G/H synthase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	551	Total	C	N	O	S	0	1	0
			4473	2885	751	812	25			
1	B	551	Total	C	N	O	S	0	1	0
			4473	2885	751	812	25			
1	C	551	Total	C	N	O	S	0	1	0
			4473	2885	751	812	25			
1	D	551	Total	C	N	O	S	0	1	0
			4473	2885	751	812	25			

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	Fe	N O	0	0
			43	34	1	4 4		
2	B	1	Total	C	Fe	N O	0	0
			43	34	1	4 4		

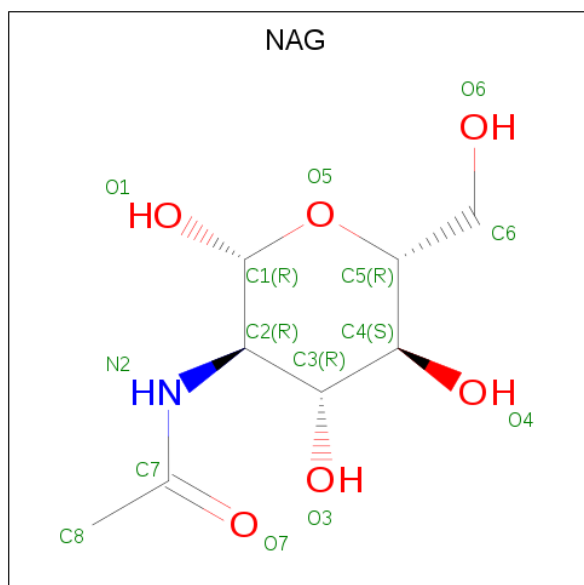
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 3 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		

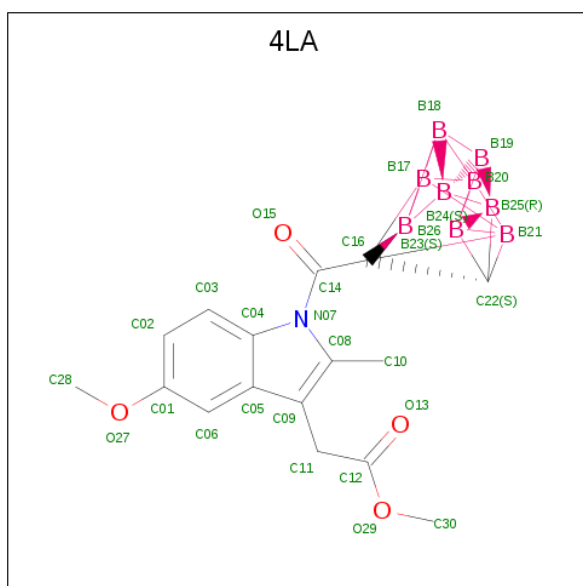
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is (R)-7- {[5-methoxy-2-methyl-3-(methoxycarbonylmethyl)-1H-indolyl]carbonyl}-7,8-dicarba-nido-dodeca-hydrundecaborate (three-letter code: 4LA) (formula: C<sub>16</sub>H<sub>14</sub>B<sub>9</sub>NO<sub>4</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	B	C	N	O	0	1
			30	9	16	1	4		
4	B	1	Total	B	C	N	O	0	1
			30	9	16	1	4		
4	C	1	Total	B	C	N	O	0	1
			30	9	16	1	4		

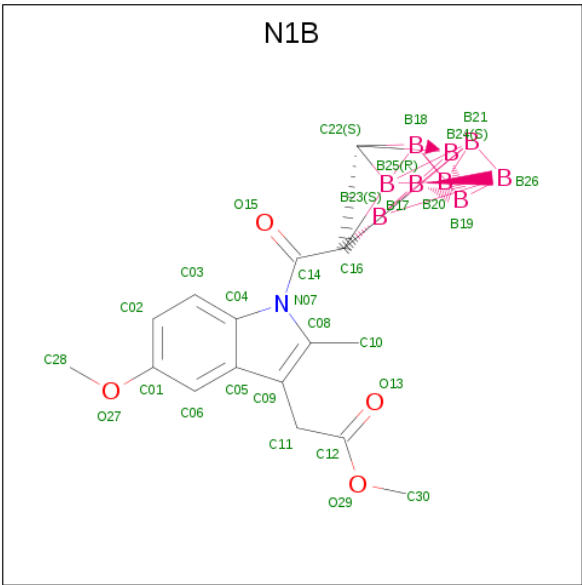
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	D	1	Total	B	C	N	O	0	1
			30	9	16	1	4		

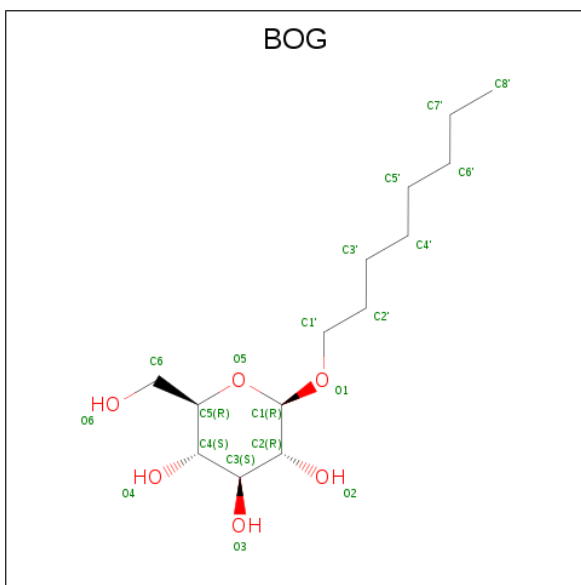
- Molecule 5 is (S)-7-{[5-methoxy-2-methyl-3-(methoxycarbonylmethyl)-1H-indolyl]carbonyl}-7,8-dicarba-nido-dodeca-hydroundecaborate (three-letter code: N1B) (formula: C<sub>16</sub>H<sub>14</sub>B<sub>9</sub>NO<sub>4</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	B	C	N	O	0	1
			30	9	16	1	4		
5	B	1	Total	B	C	N	O	0	1
			30	9	16	1	4		
5	C	1	Total	B	C	N	O	0	1
			30	9	16	1	4		
5	D	1	Total	B	C	N	O	0	1
			30	9	16	1	4		

- Molecule 6 is B-OCTYLGLUCOSIDE (three-letter code: BOG) (formula: C<sub>14</sub>H<sub>28</sub>O<sub>6</sub>).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			20	14	6		
6	B	1	Total	C	O	0	0
			20	14	6		
6	C	1	Total	C	O	0	0
			20	14	6		
6	C	1	Total	C	O	0	0
			20	14	6		
6	D	1	Total	C	O	0	0
			20	14	6		

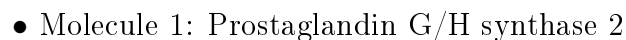
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	162	Total	O	0	0
			162	162		
7	B	153	Total	O	0	0
			153	153		
7	C	162	Total	O	0	0
			162	162		
7	D	175	Total	O	0	0
			175	175		





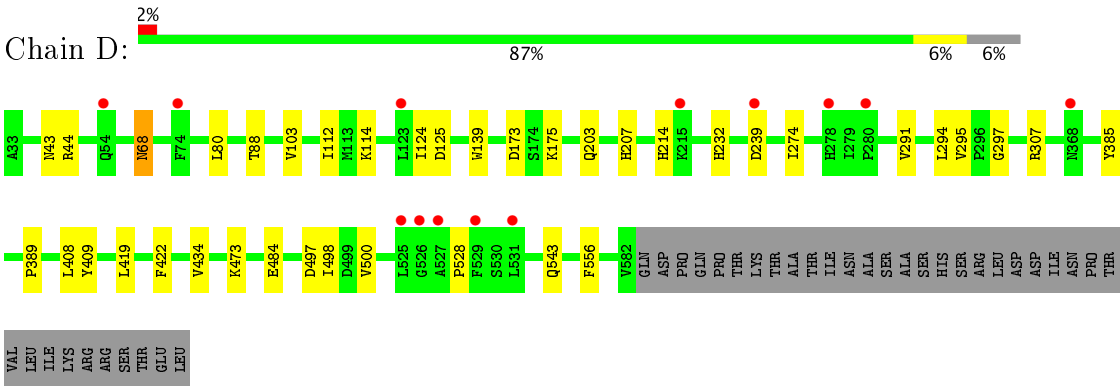
- Molecule 1: Prostaglandin G/H synthase 2





LEU  
ASP  
ASP  
ILE  
ASN  
PRO  
THR  
VAL  
LEU  
ILE  
LYS  
ARG  
ARG  
SER  
THR  
GLU  
LEU

● Molecule 1: Prostaglandin G/H synthase 2





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 <sub>1</sub> 2 <sub>1</sub> 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	180.94Å 135.01Å 124.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.60 – 2.29 49.60 – 2.29	Depositor EDS
% Data completeness (in resolution range)	98.4 (49.60-2.29) 87.2 (49.60-2.29)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.95 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, $R_{free}$	0.210 , 0.250 0.215 , 0.249	Depositor DCC
$R_{free}$ test set	4054 reflections (3.48%)	DCC
Wilson B-factor (Å <sup>2</sup> )	39.0	Xtriage
Anisotropy	0.565	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 31.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	19280	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 48.13 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 8.9865e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: N1B, HEM, 4LA, NAG, BOG

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	0.23	0/4603	0.39	0/6241
1	B	0.23	0/4603	0.39	0/6241
1	C	0.29	0/4603	0.45	4/6241 (0.1%)
1	D	0.23	0/4603	0.39	0/6241
All	All	0.25	0/18412	0.41	4/24964 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	3

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	483	GLY	O-C-N	-11.07	104.98	122.70
1	C	483	GLY	C-N-CA	7.07	139.38	121.70
1	C	483	GLY	CA-C-N	6.75	132.06	117.20
1	C	484	GLU	CA-C-N	-5.28	105.58	117.20

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	483	GLY	Mainchain,Peptide
1	C	484	GLU	Mainchain



## 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	4473	0	4378	21	0
1	B	4473	0	4378	25	0
1	C	4473	0	4377	41	0
1	D	4473	0	4378	23	0
2	A	43	0	30	2	0
2	B	43	0	30	3	0
2	C	43	0	30	0	0
2	D	43	0	30	4	0
3	A	56	0	51	1	0
3	B	56	0	51	0	0
3	C	56	0	51	0	0
3	D	56	0	51	0	0
4	A	30	0	14	2	0
4	B	30	0	14	1	0
4	C	30	0	14	5	0
4	D	30	0	14	1	0
5	A	30	0	14	1	0
5	B	30	0	14	1	0
5	C	30	0	14	3	0
5	D	30	0	14	1	0
6	A	20	0	28	1	0
6	B	20	0	28	0	0
6	C	40	0	56	3	0
6	D	20	0	26	1	0
7	A	162	0	0	2	0
7	B	153	0	0	5	0
7	C	162	0	0	3	0
7	D	175	0	0	4	0
All	All	19280	0	18085	125	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 3.

The worst 5 of 125 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:C:294:LEU:CD2	1:C:295:VAL:HG23	1.74	1.16
1:C:294:LEU:HD23	1:C:295:VAL:CG2	1.89	1.03
1:C:294:LEU:HD23	1:C:295:VAL:HG23	1.02	0.99
1:C:484:GLU:OE2	1:C:487:MET:N	2.07	0.88
1:C:294:LEU:CD2	1:C:295:VAL:CG2	2.48	0.86

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	550/587 (94%)	532 (97%)	18 (3%)	0	100	100
1	B	550/587 (94%)	533 (97%)	17 (3%)	0	100	100
1	C	550/587 (94%)	533 (97%)	16 (3%)	1 (0%)	51	63
1	D	550/587 (94%)	534 (97%)	16 (3%)	0	100	100
All	All	2200/2348 (94%)	2132 (97%)	67 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	484	GLU

### 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	493/525 (94%)	484 (98%)	9 (2%)	64	79
1	B	493/525 (94%)	485 (98%)	8 (2%)	68	82
1	C	493/525 (94%)	485 (98%)	8 (2%)	68	82
1	D	493/525 (94%)	485 (98%)	8 (2%)	68	82
All	All	1972/2100 (94%)	1939 (98%)	33 (2%)	66	81

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

Mol	Chain	Res	Type
1	B	422	PHE
1	C	232	HIS
1	D	422	PHE
1	B	442	ILE
1	B	556	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 ⓘ

33 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	HEM	A	701	1	28,50,50	2.07	9 (32%)	17,82,82	1.32	2 (11%)
3	NAG	A	702	1	14,14,15	0.31	0	15,19,21	0.39	0
3	NAG	A	703	1,3	14,14,15	0.31	0	15,19,21	0.52	0
3	NAG	A	704	3	14,14,15	1.03	0	15,19,21	1.42	3 (20%)
3	NAG	A	705	1	14,14,15	0.19	0	15,19,21	0.45	0
4	4LA	A	706[A]	-	35,46,46	1.45	5 (14%)	83,124,124	1.71	15 (18%)
5	N1B	A	707[B]	-	35,46,46	1.46	5 (14%)	83,124,124	1.74	15 (18%)
6	BOG	A	708	-	20,20,20	1.09	1 (5%)	25,25,25	1.07	2 (8%)
2	HEM	B	701	1,7	28,50,50	1.99	8 (28%)	17,82,82	1.60	2 (11%)
3	NAG	B	702	1	14,14,15	0.30	0	15,19,21	0.38	0
3	NAG	B	703	1,3	14,14,15	0.29	0	15,19,21	0.46	0
3	NAG	B	704	3	14,14,15	0.26	0	15,19,21	0.48	0
3	NAG	B	705	1	14,14,15	0.26	0	15,19,21	0.47	0
4	4LA	B	706[A]	-	35,46,46	1.40	4 (11%)	83,124,124	1.72	14 (16%)
5	N1B	B	707[B]	-	35,46,46	1.40	4 (11%)	83,124,124	1.71	14 (16%)
6	BOG	B	708	-	20,20,20	1.07	1 (5%)	25,25,25	1.15	2 (8%)
2	HEM	C	701	1	28,50,50	1.92	5 (17%)	17,82,82	1.30	2 (11%)
3	NAG	C	702	1	14,14,15	0.31	0	15,19,21	0.39	0
3	NAG	C	703	1,3	14,14,15	0.29	0	15,19,21	0.46	0
3	NAG	C	704	3	14,14,15	0.24	0	15,19,21	0.43	0
3	NAG	C	705	1	14,14,15	0.24	0	15,19,21	0.47	0
4	4LA	C	706[A]	-	35,46,46	1.30	3 (8%)	83,124,124	1.70	14 (16%)
5	N1B	C	707[B]	-	35,46,46	1.35	4 (11%)	83,124,124	1.68	14 (16%)
6	BOG	C	708	-	20,20,20	1.09	1 (5%)	25,25,25	1.04	3 (12%)
6	BOG	C	709	-	20,20,20	1.06	1 (5%)	25,25,25	1.11	2 (8%)
2	HEM	D	701	1	28,50,50	2.02	4 (14%)	17,82,82	1.66	3 (17%)
3	NAG	D	702	1	14,14,15	0.31	0	15,19,21	0.35	0
3	NAG	D	703	1,3	14,14,15	0.32	0	15,19,21	0.47	0
3	NAG	D	704	3	14,14,15	0.23	0	15,19,21	0.47	0
3	NAG	D	705	1	14,14,15	0.19	0	15,19,21	0.45	0
4	4LA	D	706[A]	-	35,46,46	1.35	4 (11%)	83,124,124	1.64	14 (16%)
5	N1B	D	707[B]	-	35,46,46	1.36	3 (8%)	83,124,124	1.64	13 (15%)
6	BOG	D	708	-	20,20,20	1.31	2 (10%)	25,25,25	1.13	2 (8%)

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	HEM	A	701	1	-	0/6/54/54	0/0/8/8
3	NAG	A	702	1	-	0/6/23/26	0/1/1/1
3	NAG	A	703	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	704	3	-	0/6/23/26	0/1/1/1
3	NAG	A	705	1	-	0/6/23/26	0/1/1/1
4	4LA	A	706[A]	-	-	0/8/314/314	0/2/17/17
5	N1B	A	707[B]	-	-	0/8/314/314	0/2/17/17
6	BOG	A	708	-	-	0/11/31/31	0/1/1/1
2	HEM	B	701	1,7	-	0/6/54/54	0/0/8/8
3	NAG	B	702	1	-	0/6/23/26	0/1/1/1
3	NAG	B	703	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	704	3	-	0/6/23/26	0/1/1/1
3	NAG	B	705	1	-	0/6/23/26	0/1/1/1
4	4LA	B	706[A]	-	-	0/8/314/314	0/2/17/17
5	N1B	B	707[B]	-	-	0/8/314/314	0/2/17/17
6	BOG	B	708	-	-	0/11/31/31	0/1/1/1
2	HEM	C	701	1	-	0/6/54/54	0/0/8/8
3	NAG	C	702	1	-	0/6/23/26	0/1/1/1
3	NAG	C	703	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	704	3	-	0/6/23/26	0/1/1/1
3	NAG	C	705	1	-	0/6/23/26	0/1/1/1
4	4LA	C	706[A]	-	-	0/8/314/314	0/2/17/17
5	N1B	C	707[B]	-	-	0/8/314/314	0/2/17/17
6	BOG	C	708	-	-	0/11/31/31	0/1/1/1
6	BOG	C	709	-	-	0/11/31/31	0/1/1/1
2	HEM	D	701	1	-	0/6/54/54	0/0/8/8
3	NAG	D	702	1	-	0/6/23/26	0/1/1/1
3	NAG	D	703	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	704	3	-	0/6/23/26	0/1/1/1
3	NAG	D	705	1	-	0/6/23/26	0/1/1/1
4	4LA	D	706[A]	-	-	0/8/314/314	0/2/17/17
5	N1B	D	707[B]	-	-	0/8/314/314	0/2/17/17
6	BOG	D	708	-	-	0/11/31/31	0/1/1/1

The worst 5 of 64 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	701	HEM	C3B-C2B	-5.95	1.32	1.40
2	A	701	HEM	C3B-C2B	-5.63	1.32	1.40
2	C	701	HEM	C3B-C2B	-5.50	1.33	1.40
2	B	701	HEM	C3B-C2B	-4.53	1.34	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	701	HEM	C1B-NB	-4.22	1.31	1.36

The worst 5 of 136 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	707[B]	N1B	B21-C16-C14	-5.84	109.79	124.46
4	C	706[A]	4LA	B17-C16-C14	-5.66	110.24	124.46
4	A	706[A]	4LA	B17-C16-C14	-5.51	110.61	124.46
5	A	707[B]	N1B	B21-C16-C14	-5.43	110.80	124.46
5	D	707[B]	N1B	B21-C16-C14	-5.33	111.06	124.46

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

16 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	HEM	2	0
3	A	704	NAG	1	0
4	A	706[A]	4LA	2	0
5	A	707[B]	N1B	1	0
6	A	708	BOG	1	0
2	B	701	HEM	3	0
4	B	706[A]	4LA	1	0
5	B	707[B]	N1B	1	0
4	C	706[A]	4LA	5	0
5	C	707[B]	N1B	3	0
6	C	708	BOG	1	0
6	C	709	BOG	2	0
2	D	701	HEM	4	0
4	D	706[A]	4LA	1	0
5	D	707[B]	N1B	1	0
6	D	708	BOG	1	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 [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<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	551/587 (93%)	0.08	16 (2%) 52 59	33, 52, 77, 95	0
1	B	551/587 (93%)	0.12	21 (3%) 41 48	33, 50, 76, 97	0
1	C	551/587 (93%)	0.06	9 (1%) 72 77	32, 49, 73, 99	0
1	D	551/587 (93%)	0.03	13 (2%) 59 66	33, 47, 73, 102	0
All	All	2204/2348 (93%)	0.07	59 (2%) 55 62	32, 50, 75, 102	0

The worst 5 of 59 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	122	TYR	5.4
1	B	96	PHE	4.1
1	B	101	ASN	3.7
1	C	399	ASP	3.6
1	B	278	HIS	3.6

### 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 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(Å <sup>2</sup> )	Q<0.9
6	BOG	B	708	20/20	0.74	0.42	6.18	68,84,104,105	0
6	BOG	D	708	20/20	0.82	0.34	3.99	67,77,82,83	0
6	BOG	C	709	20/20	0.82	0.36	3.42	64,75,79,81	0
3	NAG	C	705	14/15	0.90	0.30	1.56	61,69,76,79	0
6	BOG	C	708	20/20	0.94	0.14	1.42	47,56,58,59	0
3	NAG	A	705	14/15	0.86	0.31	1.22	62,76,80,80	0
5	N1B	B	707[B]	30/30	0.86	0.21	0.53	40,48,56,60	30
4	4LA	B	706[A]	30/30	0.86	0.20	0.43	41,48,56,60	30
3	NAG	B	705	14/15	0.91	0.18	0.24	70,74,78,79	0
3	NAG	D	703	14/15	0.94	0.13	0.15	40,49,54,60	0
3	NAG	D	705	14/15	0.94	0.17	0.07	70,76,78,80	0
3	NAG	A	703	14/15	0.96	0.14	0.03	35,49,54,62	0
4	4LA	C	706[A]	30/30	0.90	0.16	-0.03	40,49,57,61	30
5	N1B	C	707[B]	30/30	0.90	0.16	-0.07	40,49,57,61	30
4	4LA	D	706[A]	30/30	0.94	0.16	-0.21	32,47,58,68	30
5	N1B	D	707[B]	30/30	0.94	0.16	-0.26	32,47,58,68	30
2	HEM	D	701	43/43	0.96	0.13	-0.28	30,41,64,77	0
2	HEM	A	701	43/43	0.95	0.13	-0.33	35,44,64,76	0
2	HEM	B	701	43/43	0.96	0.15	-0.42	35,43,66,75	0
6	BOG	A	708	20/20	0.96	0.11	-0.47	48,52,67,69	0
4	4LA	A	706[A]	30/30	0.94	0.14	-0.54	45,48,54,56	30
5	N1B	A	707[B]	30/30	0.94	0.14	-0.54	44,48,54,56	30
2	HEM	C	701	43/43	0.96	0.12	-0.63	37,41,59,71	0
3	NAG	B	703	14/15	0.93	0.11	-1.06	45,48,56,62	0
3	NAG	C	703	14/15	0.96	0.10	-1.56	37,45,55,62	0
3	NAG	B	702	14/15	0.78	0.24	-	85,92,98,98	0
3	NAG	D	704	14/15	0.92	0.14	-	61,66,72,75	0
3	NAG	A	704	14/15	0.87	0.27	-	67,70,76,76	0
3	NAG	D	702	14/15	0.83	0.21	-	82,86,91,94	0
3	NAG	C	704	14/15	0.93	0.21	-	64,68,72,73	0
3	NAG	B	704	14/15	0.91	0.16	-	62,67,73,75	0
3	NAG	C	702	14/15	0.83	0.26	-	66,76,79,83	0
3	NAG	A	702	14/15	0.81	0.15	-	69,81,84,85	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.