



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 31, 2017 – 09:28 AM EDT

PDB ID : 3NT1  
Title : High resolution structure of naproxen:COX-2 complex.  
Authors : Duggan, K.C.; Musee, J.; Walters, M.J.; Harp, J.M.; Kiefer, J.R.; Oates, J.A.;  
Marnett, L.J.  
Deposited on : unknown  
Resolution : 1.73 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.

---

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

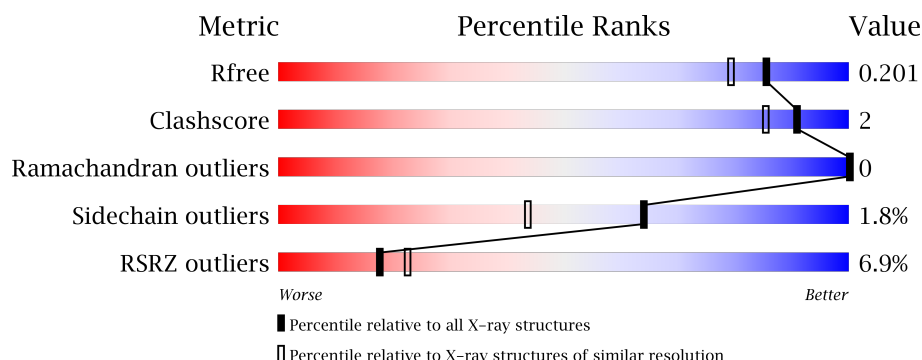
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.73 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	2694 (1.76-1.72)
Clashscore	112137	2854 (1.76-1.72)
Ramachandran outliers	110173	2824 (1.76-1.72)
Sidechain outliers	110143	2824 (1.76-1.72)
RSRZ outliers	101464	2705 (1.76-1.72)

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>6%</div> <div>89%</div> <div>6%</div> </div>
1	B	587	<div> <div>7%</div> <div>88%</div> <div>5%</div> <div>6%</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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	A	661	X	-	-	-
2	NAG	B	9	-	-	-	X
3	BOG	A	620	-	-	-	X

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 10338 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-endoperoxide synthase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	552	Total	C	N	O	S	0	3	0
			4499	2899	756	819	25			
1	B	552	Total	C	N	O	S	0	0	0
			4474	2885	750	814	25			

- Molecule 2 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



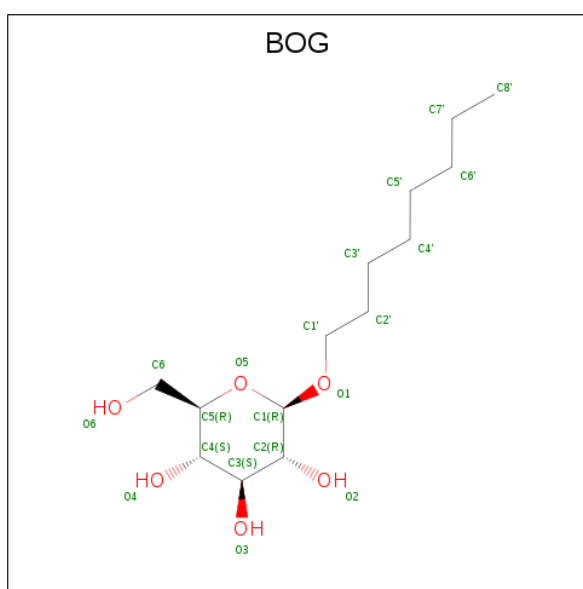
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		

*Continued on next page...*

*Continued from previous page...*

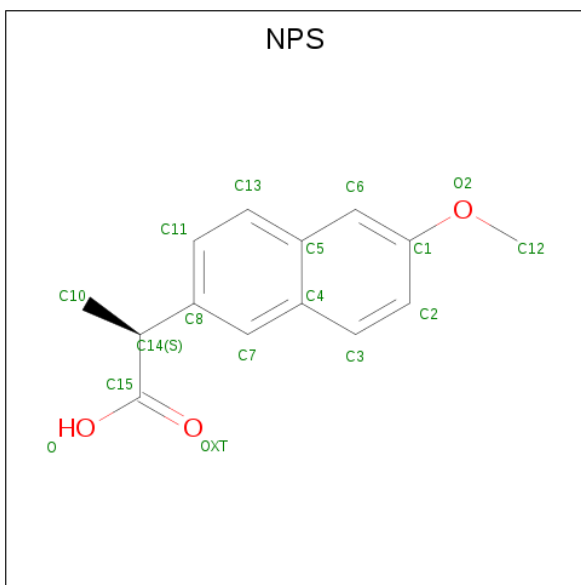
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is B-OCTYLGLUCOSIDE (three-letter code: BOG) (formula:  $C_{14}H_{28}O_6$ ).



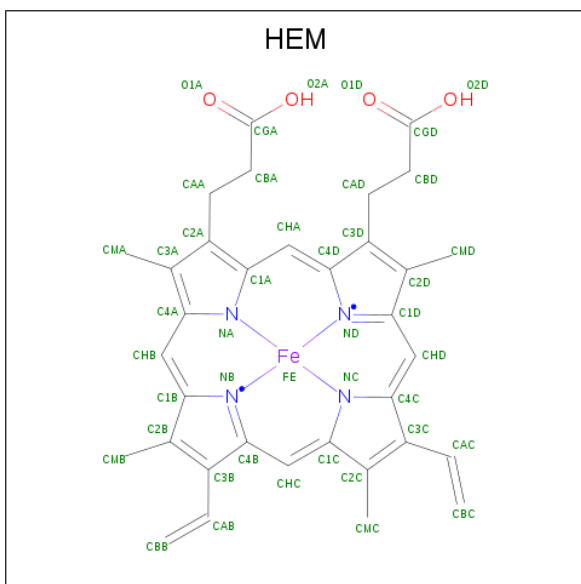
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			20	14	6		
3	A	1	Total	C	O	0	0
			20	14	6		
3	A	1	Total	C	O	0	0
			20	14	6		
3	B	1	Total	C	O	0	0
			20	14	6		

- Molecule 4 is (2S)-2-(6-methoxynaphthalen-2-yl)propanoic acid (three-letter code: NPS) (formula:  $C_{14}H_{14}O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			17	14	3		
4	B	1	Total	C	O	0	0
			17	14	3		

- Molecule 5 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



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

*Continued on next page...*

*Continued from previous page...*

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

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Cl		
			1	1	0	0
6	A	1	Total	Cl		
			1	1	0	0

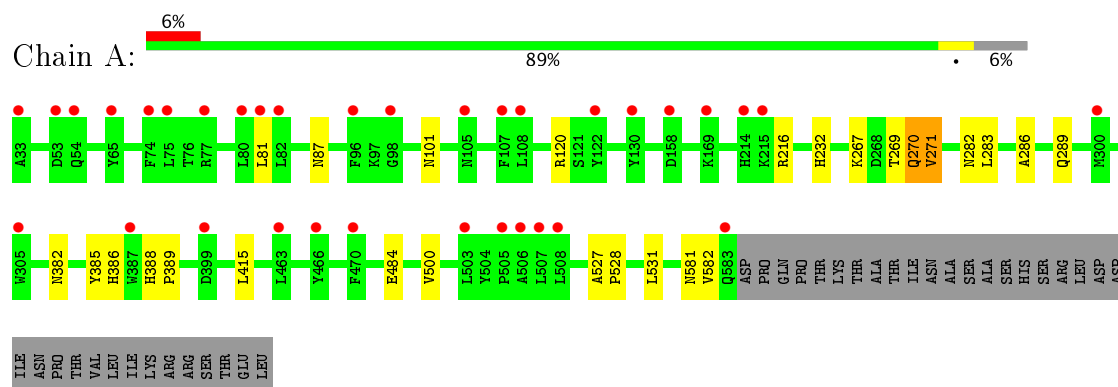
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	527	Total	O		
			527	527	0	0
7	B	524	Total	O		
			524	524	0	0

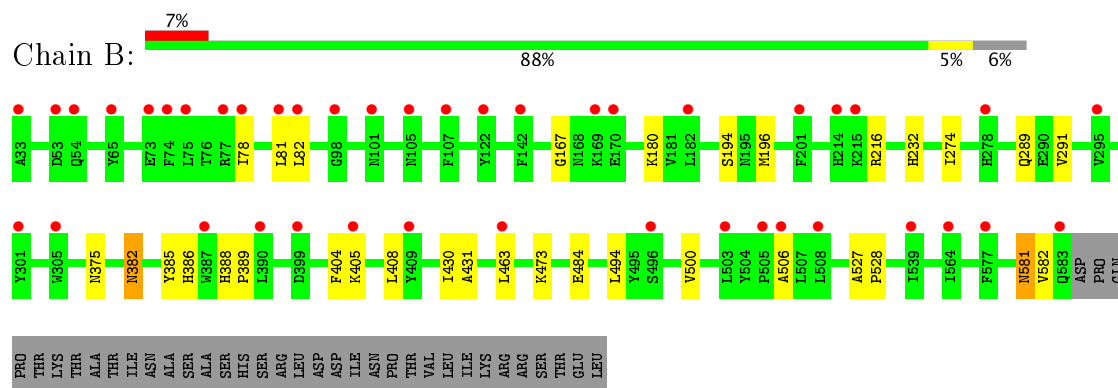
### 3 Residue-property plots [i](#)

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: Prostaglandin-endoperoxide synthase 2



- Molecule 1: Prostaglandin-endoperoxide synthase 2





## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	122.30 Å   133.23 Å   181.27 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	30.00 – 1.73 28.51 – 1.73	Depositor EDS
% Data completeness (in resolution range)	98.2 (30.00-1.73) 98.2 (28.51-1.73)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.48 (at 1.73 Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.167   ,   0.186 0.183   ,   0.201	Depositor DCC
$R_{free}$ test set	7592 reflections (5.31%)	DCC
Wilson B-factor (Å <sup>2</sup> )	22.8	Xtriage
Anisotropy	0.091	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 42.9	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	0.96	EDS
Total number of atoms	10338	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.32% 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: HEM, BOG, NAG, NPS, CL

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	0.34	0/4629	0.51	0/6276
1	B	0.34	0/4601	0.52	0/6239
All	All	0.34	0/9230	0.51	0/12515

There are no bond length outliers.

There are no bond angle outliers.

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	4499	0	4396	17	0
1	B	4474	0	4373	18	0
2	A	56	0	51	1	0
2	B	56	0	51	1	0
3	A	60	0	84	3	0
3	B	20	0	28	0	0
4	A	17	0	13	0	0
4	B	17	0	13	0	0
5	A	43	0	30	1	0
5	B	43	0	30	1	0
6	A	1	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	1	0	0	0	0
7	A	527	0	0	0	0
7	B	524	0	0	1	0
All	All	10338	0	9069	36	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 2.

All (36) 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:283:LEU:HD21	1:A:415:LEU:HD12	1.48	0.95
1:A:87:ASN:HD22	3:A:620:BOG:H62	1.37	0.89
1:A:581[B]:ASN:HD22	1:A:582:VAL:N	1.88	0.72
1:A:283:LEU:CD2	1:A:415:LEU:HD12	2.21	0.69
1:B:382:ASN:HD21	5:B:619:HEM:HAD2	1.57	0.68
1:A:271:VAL:HG22	1:A:286:ALA:HB1	1.78	0.65
1:B:81:LEU:HD22	1:B:82:LEU:HD12	1.78	0.65
1:A:271:VAL:CG2	1:A:286:ALA:HB1	2.32	0.59
1:B:375:ASN:ND2	7:B:832:HOH:O	2.21	0.58
1:A:87:ASN:HD22	3:A:620:BOG:C6	2.12	0.58
1:B:274:ILE:HD12	1:B:291:VAL:HG12	1.88	0.55
1:B:581:ASN:HD22	1:B:582:VAL:N	2.07	0.52
1:A:120:ARG:HG3	1:A:531:LEU:HD12	1.91	0.52
1:A:500:VAL:HG12	1:A:500:VAL:O	2.09	0.51
1:B:196:MET:CE	1:B:431:ALA:HB2	2.41	0.51
1:B:382:ASN:O	1:B:386:HIS:HD2	1.94	0.51
1:A:87:ASN:ND2	3:A:620:BOG:H62	2.16	0.50
1:A:270:GLN:HE21	1:A:270:GLN:N	2.09	0.50
1:B:180:LYS:HD2	1:B:494:LEU:HD11	1.94	0.49
1:B:167:GLY:HA3	1:B:500:VAL:HG21	1.96	0.47
1:B:527:ALA:HB3	1:B:528:PRO:HD3	1.96	0.47
1:A:500:VAL:CG1	1:A:500:VAL:O	2.63	0.47
1:B:194:SER:O	1:B:430:ILE:HD12	2.15	0.47
1:A:527:ALA:HB3	1:A:528:PRO:HD3	1.97	0.46
1:A:216:ARG:NH1	2:A:672:NAG:O7	2.49	0.46
1:A:382:ASN:O	1:A:386:HIS:HD2	1.99	0.45
1:A:269:THR:HB	1:A:271:VAL:HG13	1.99	0.45
1:A:388:HIS:N	1:A:389:PRO:CD	2.81	0.43
1:B:78:ILE:O	1:B:82:LEU:HD13	2.19	0.42
1:B:404:PHE:O	1:B:408:LEU:HD13	2.20	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:388:HIS:N	1:B:389:PRO:CD	2.83	0.41
1:B:463:LEU:HD22	1:B:506:ALA:CB	2.50	0.41
1:B:382:ASN:HD22	1:B:382:ASN:C	2.24	0.41
1:B:167:GLY:CA	1:B:500:VAL:HG21	2.51	0.41
1:B:216:ARG:NH1	2:B:671:NAG:O4	2.54	0.41
5:A:619:HEM:HBB2	5:A:619:HEM:HHC	2.04	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	553/587 (94%)	542 (98%)	11 (2%)	0	100	100
1	B	550/587 (94%)	539 (98%)	11 (2%)	0	100	100
All	All	1103/1174 (94%)	1081 (98%)	22 (2%)	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	A	496/525 (94%)	486 (98%)	10 (2%)	60	37
1	B	493/525 (94%)	485 (98%)	8 (2%)	68	49

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	989/1050 (94%)	971 (98%)	18 (2%)	64	44

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	81	LEU
1	A	101	ASN
1	A	232	HIS
1	A	267	LYS
1	A	270	GLN
1	A	271	VAL
1	A	282	ASN
1	A	289	GLN
1	A	385	TYR
1	A	484	GLU
1	B	232	HIS
1	B	289	GLN
1	B	382	ASN
1	B	385	TYR
1	B	405	LYS
1	B	473	LYS
1	B	484	GLU
1	B	581	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	ASN
1	A	270	GLN
1	A	282	ASN
1	A	369	GLN
1	A	421	GLN
1	B	101	ASN
1	B	369	GLN
1	B	382	ASN
1	B	386	HIS
1	B	388	HIS
1	B	581	ASN

### 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 18 ligands modelled in this entry, 2 are monoatomic - leaving 16 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$
3	BOG	A	3	-	20,20,20	0.61	0	25,25,25	0.89	1 (4%)
4	NPS	A	5	-	15,18,18	1.06	0	21,25,25	0.83	1 (4%)
3	BOG	A	6	-	20,20,20	0.71	1 (5%)	25,25,25	0.83	1 (4%)
5	HEM	A	619	1,7	28,50,50	2.25	7 (25%)	17,82,82	1.46	2 (11%)
3	BOG	A	620	-	20,20,20	0.80	1 (5%)	25,25,25	1.58	3 (12%)
2	NAG	A	661	1	14,14,15	0.75	0	15,19,21	0.99	1 (6%)
2	NAG	A	671	1,2	14,14,15	0.54	0	15,19,21	0.99	1 (6%)
2	NAG	A	672	2	14,14,15	0.49	0	15,19,21	0.93	1 (6%)
2	NAG	A	681	1	14,14,15	0.47	0	15,19,21	0.96	1 (6%)
3	BOG	B	3	-	20,20,20	0.75	1 (5%)	25,25,25	0.85	2 (8%)
4	NPS	B	4	-	15,18,18	1.06	0	21,25,25	0.84	1 (4%)
5	HEM	B	619	1,7	28,50,50	2.22	6 (21%)	17,82,82	1.51	2 (11%)
2	NAG	B	671	1,2	14,14,15	0.56	0	15,19,21	0.91	1 (6%)
2	NAG	B	672	2	14,14,15	0.49	0	15,19,21	1.36	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAG	B	681	1	14,14,15	0.52	0	15,19,21	0.69	0
2	NAG	B	9	1	14,14,15	0.55	0	15,19,21	0.81	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
3	BOG	A	3	-	-	0/11/31/31	0/1/1/1
4	NPS	A	5	-	-	0/6/10/10	0/2/2/2
3	BOG	A	6	-	-	0/11/31/31	0/1/1/1
5	HEM	A	619	1,7	-	0/6/54/54	0/0/8/8
3	BOG	A	620	-	-	0/11/31/31	0/1/1/1
2	NAG	A	661	1	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	A	671	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	672	2	-	0/6/23/26	0/1/1/1
2	NAG	A	681	1	-	0/6/23/26	0/1/1/1
3	BOG	B	3	-	-	0/11/31/31	0/1/1/1
4	NPS	B	4	-	-	0/6/10/10	0/2/2/2
5	HEM	B	619	1,7	-	0/6/54/54	0/0/8/8
2	NAG	B	671	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	672	2	-	0/6/23/26	0/1/1/1
2	NAG	B	681	1	-	0/6/23/26	0/1/1/1
2	NAG	B	9	1	-	0/6/23/26	0/1/1/1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	619	HEM	C3B-C2B	-5.32	1.33	1.40
5	B	619	HEM	C3B-C2B	-4.88	1.33	1.40
5	A	619	HEM	C3C-C2C	-4.76	1.34	1.40
5	B	619	HEM	C3C-C2C	-4.72	1.34	1.40
3	B	3	BOG	O1-C1	2.06	1.43	1.40
5	A	619	HEM	C1C-NC	2.08	1.39	1.36
5	B	619	HEM	C4D-ND	2.10	1.39	1.36
3	A	6	BOG	O1-C1	2.12	1.43	1.40
5	A	619	HEM	C4D-ND	2.35	1.39	1.36
3	A	620	BOG	O1-C1	2.83	1.45	1.40
5	A	619	HEM	C3B-CAB	3.29	1.54	1.47
5	B	619	HEM	C3B-CAB	3.43	1.54	1.47
5	A	619	HEM	C3C-CAC	3.70	1.55	1.47

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	619	HEM	C3C-CAC	3.74	1.55	1.47
5	B	619	HEM	C3D-C2D	5.17	1.53	1.37
5	A	619	HEM	C3D-C2D	5.21	1.53	1.37

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	620	BOG	O5-C1-O1	-4.17	100.12	110.02
5	B	619	HEM	CBD-CAD-C3D	-3.33	106.11	112.47
5	A	619	HEM	CBD-CAD-C3D	-3.02	106.71	112.47
3	A	3	BOG	C1'-O1-C1	-3.00	108.71	113.87
5	A	619	HEM	C1D-C2D-C3D	-2.85	105.02	107.00
2	B	672	NAG	O5-C1-C2	-2.44	108.08	111.47
4	B	4	NPS	C15-C14-C8	-2.43	107.37	112.12
5	B	619	HEM	C1D-C2D-C3D	-2.39	105.33	107.00
2	A	661	NAG	O5-C1-C2	-2.29	108.29	111.47
4	A	5	NPS	C15-C14-C8	-2.13	107.95	112.12
3	B	3	BOG	O1-C1-C2	-2.03	104.92	108.23
3	A	6	BOG	O5-C5-C4	2.09	113.51	109.66
2	B	672	NAG	C8-C7-N2	2.10	119.89	116.11
2	B	671	NAG	C1-O5-C5	2.19	115.19	112.17
3	B	3	BOG	O5-C5-C4	2.28	113.86	109.66
2	A	672	NAG	C4-C3-C2	2.28	114.36	111.02
2	A	681	NAG	C1-O5-C5	2.54	115.66	112.17
2	A	671	NAG	C1-O5-C5	2.68	115.86	112.17
3	A	620	BOG	O5-C5-C4	2.89	114.98	109.66
2	B	672	NAG	C2-N2-C7	3.02	127.34	122.94
3	A	620	BOG	O1-C1-C2	4.57	115.68	108.23

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	661	NAG	C1

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	619	HEM	1	0
3	A	620	BOG	3	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	672	NAG	1	0
5	B	619	HEM	1	0
2	B	671	NAG	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 ⓘ

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	552/587 (94%)	0.27	34 (6%)	21 27	16, 25, 40, 50	0
1	B	552/587 (94%)	0.28	42 (7%)	15 19	16, 25, 41, 55	0
All	All	1104/1174 (94%)	0.28	76 (6%)	18 23	16, 25, 40, 55	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	74	PHE	6.8
1	A	81	LEU	6.6
1	B	81	LEU	5.3
1	A	75	LEU	4.9
1	A	583	GLN	4.7
1	B	583	GLN	4.5
1	B	75	LEU	4.4
1	A	74	PHE	4.3
1	B	33	ALA	4.0
1	A	169	LYS	4.0
1	B	77	ARG	3.9
1	A	80	LEU	3.8
1	B	169	LYS	3.6
1	B	577	PHE	3.5
1	B	82	LEU	3.4
1	B	122	TYR	3.4
1	A	506	ALA	3.3
1	A	503	LEU	3.3
1	A	77	ARG	3.3
1	A	107	PHE	3.2
1	B	503	LEU	3.2
1	A	33	ALA	3.0
1	A	507	LEU	3.0
1	B	409	TYR	3.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	82	LEU	2.9
1	B	215	LYS	2.8
1	A	122	TYR	2.8
1	B	107	PHE	2.8
1	A	463	LEU	2.7
1	B	78	ILE	2.6
1	B	405	LYS	2.6
1	B	65	TYR	2.6
1	A	305	TRP	2.6
1	A	65	TYR	2.6
1	B	98	GLY	2.6
1	A	215	LYS	2.6
1	A	53	ASP	2.5
1	A	96	PHE	2.5
1	A	505	PRO	2.5
1	B	101	ASN	2.5
1	A	470	PHE	2.5
1	B	170	GLU	2.5
1	A	399	ASP	2.5
1	A	98	GLY	2.5
1	B	564	ILE	2.5
1	B	399	ASP	2.5
1	A	158	ASP	2.5
1	B	305	TRP	2.5
1	A	54	GLN	2.4
1	B	182	LEU	2.4
1	B	463	LEU	2.4
1	A	466	TYR	2.4
1	B	73	GLU	2.4
1	B	508	LEU	2.3
1	A	387	TRP	2.3
1	B	387	TRP	2.3
1	B	505	PRO	2.3
1	B	390	LEU	2.2
1	A	130	TYR	2.2
1	B	496	SER	2.2
1	A	108	LEU	2.2
1	B	539	ILE	2.2
1	B	53	ASP	2.2
1	A	214	HIS	2.2
1	A	300	MET	2.1
1	B	295	VAL	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	105	ASN	2.1
1	B	214	HIS	2.1
1	B	201	PHE	2.1
1	B	54	GLN	2.1
1	B	506	ALA	2.1
1	A	508	LEU	2.1
1	B	142	PHE	2.0
1	B	278	HIS	2.0
1	B	301	TYR	2.0
1	A	105	ASN	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(Å <sup>2</sup> )	Q<0.9
2	NAG	B	9	14/15	0.82	0.29	4.22	37,42,45,45	0
3	BOG	A	620	20/20	0.65	0.25	2.95	54,58,59,59	0
3	BOG	B	3	20/20	0.84	0.14	1.88	43,45,50,50	0
2	NAG	A	681	14/15	0.85	0.20	1.26	32,35,38,38	0
3	BOG	A	6	20/20	0.84	0.13	1.12	41,42,46,46	0
4	NPS	A	5	17/17	0.96	0.13	1.11	20,21,23,24	0
2	NAG	B	681	14/15	0.89	0.23	1.00	33,36,38,39	0
2	NAG	A	671	14/15	0.91	0.10	0.54	22,27,29,31	0
3	BOG	A	3	20/20	0.92	0.11	0.47	30,33,43,43	0
5	HEM	A	619	43/43	0.93	0.11	0.21	26,28,38,41	0
5	HEM	B	619	43/43	0.94	0.11	-0.01	26,28,37,42	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	NPS	B	4	17/17	0.97	0.10	-0.13	20,21,24,25	0
2	NAG	B	671	14/15	0.95	0.08	-0.19	22,26,28,33	0
6	CL	A	1	1/1	0.99	0.04	-2.67	25,25,25,25	0
6	CL	B	1	1/1	0.99	0.03	-3.60	26,26,26,26	0
2	NAG	B	672	14/15	0.75	0.27	-	38,42,44,45	0
2	NAG	A	661	14/15	0.70	0.30	-	38,44,46,47	0
2	NAG	A	672	14/15	0.83	0.22	-	35,38,40,40	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.