



# wwPDB X-ray Structure Validation Summary Report

Feb 14, 2017 – 06:37 pm GMT

PDB ID : 1PGF  
Title : PROSTAGLANDIN H2 SYNTHASE-1 COMPLEXED WITH 1-(4-IODOBE NZOYL)-5-METHOXY-2-METHYLINDOLE-3-ACETIC ACID (IODOIN- DOMETHACIN), CIS MODEL  
Authors : Loll, P.J.; Picot, D.; Garavito, R.M.  
Deposited on : 1995-12-02  
Resolution : 4.50 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 : trunk28620  
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) : recalc28949

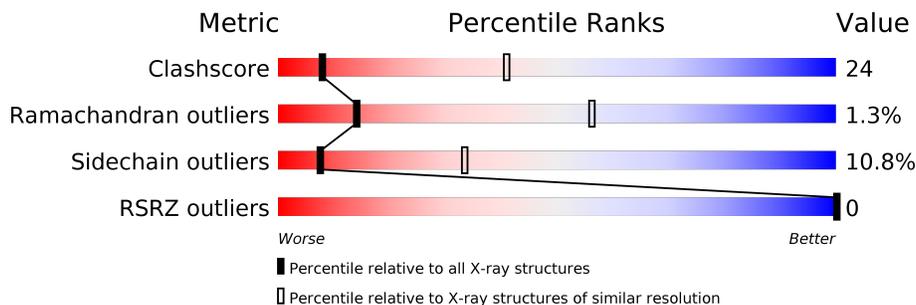
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.50 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	112137	1029 (5.30-3.70)
Ramachandran outliers	110173	1025 (5.30-3.66)
Sidechain outliers	110143	1006 (5.30-3.66)
RSRZ outliers	101464	1015 (5.30-3.64)

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	576	 55% 34% 6% . .
1	B	576	 54% 35% 6% . .

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	B	681	-	-	-	X
5	IMM	A	800	-	-	X	X

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<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Chirality</b>	<b>Geometry</b>	<b>Clashes</b>	<b>Electron density</b>
5	IMM	B	800	-	-	X	X

## 2 Entry composition [i](#)

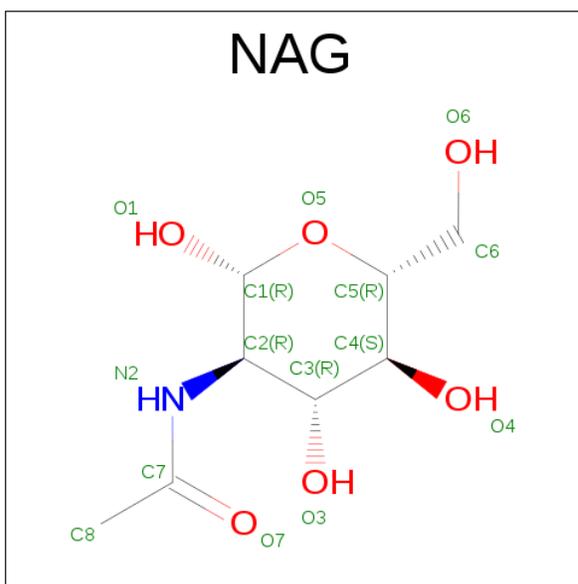
There are 5 unique types of molecules in this entry. The entry contains 9202 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 H2 SYNTHASE-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	551	Total 4477	C 2903	N 758	O 788	S 28	0	0	0
1	B	551	Total 4477	C 2903	N 758	O 788	S 28	0	0	0

- Molecule 2 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).

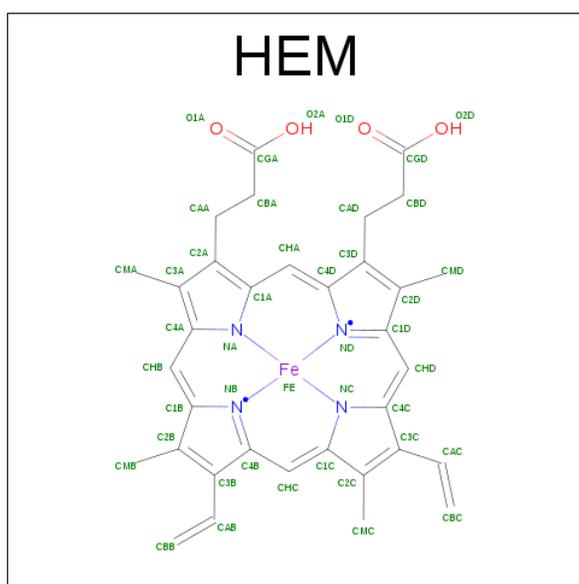


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	Total 14	C 8	N 1	O 5	0	0
2	A	1	Total 14	C 8	N 1	O 5	0	0
2	B	1	Total 14	C 8	N 1	O 5	0	0
2	B	1	Total 14	C 8	N 1	O 5	0	0

- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

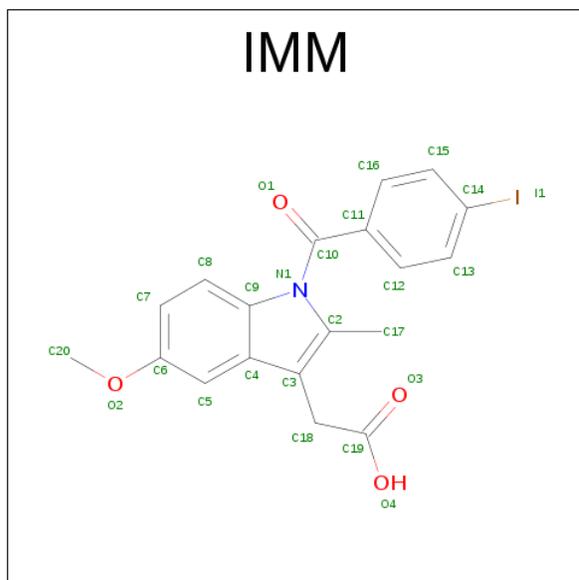
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	2	Total	C	N	O	0	0
			28	16	2	10		
3	B	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 4 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



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

- Molecule 5 is 1-(4-iodobenzoyle)-5-methoxy-2-methyl indole-3-acetic acid (three-letter code: IMM) (formula:  $C_{19}H_{16}INO_4$ ).

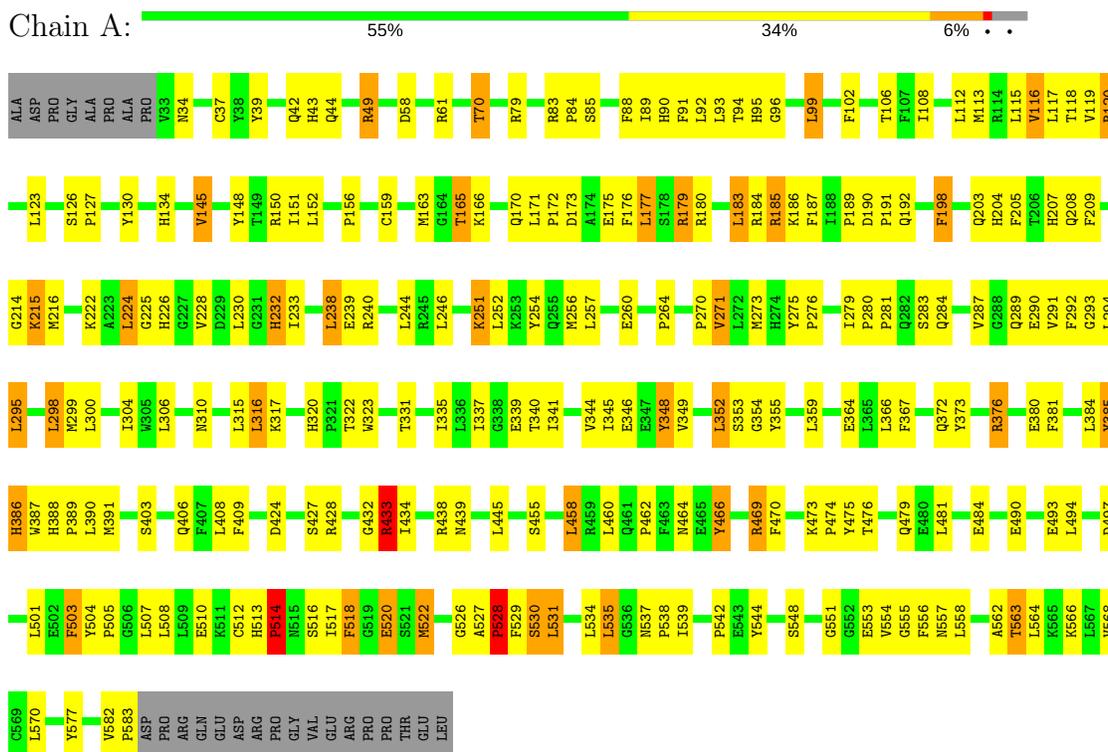


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	I	N			O
5	A	1	Total	19	1	1	4	0	0
5	B	1	Total	19	1	1	4	0	0

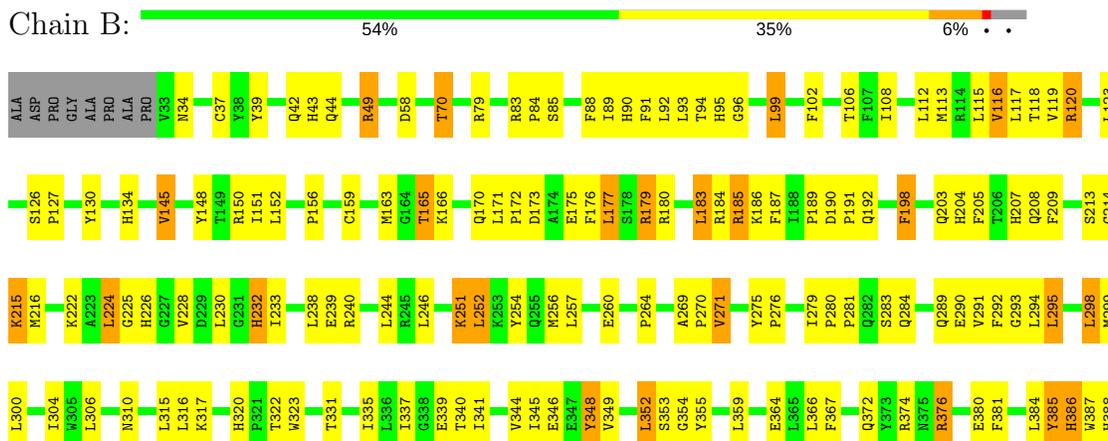
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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 H2 SYNTHASE-1



- Molecule 1: PROSTAGLANDIN H2 SYNTHASE-1



P389	F608	C575
L390	Y504	P576
M391	P505	Y577
P392	G506	Y582
S403	L507	P583
L508	L508	ASP
S406	L509	PRO
F407	E510	ARG
L408	K511	GLN
F409	C512	GLU
D424	H513	ASP
S427	P514	ARG
R428	M516	PRO
G432	S516	GLY
R433	I517	VAL
I434	F518	GLU
R438	G519	ARG
N439	E520	PRO
L445	S521	PRO
S455	M522	THR
L458	G526	LEU
R459	A527	
L460	P528	
R461	F529	
P462	S530	
F463	S531	
N464	L534	
E465	L535	
Y466	R536	
R469	M537	
F470	P538	
K473	I539	
P474	P542	
Y475	F543	
T476	Y544	
Q479	S548	
E480	G551	
L481	G552	
E484	E553	
E490	V554	
L494	G555	
D497	F556	
L501	N557	
E502	L558	
	A562	
	T563	
	L564	
	K565	
	K566	
	I567	
	V568	
	C569	
	L570	

## 4 Data and refinement statistics i

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	99.22Å 208.99Å 232.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 4.50 15.11 – 4.50	Depositor EDS
% Data completeness (in resolution range)	79.2 (8.00-4.50) 78.2 (15.11-4.50)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.54 (at 4.46Å)	Xtrriage
Refinement program	X-PLOR 3.1	Depositor
R, $R_{free}$	0.254 , 0.267 0.247 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	80.6	Xtrriage
Anisotropy	0.740	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.23 , 52.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	9202	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.16% 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: HEM, IMM, NAG

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	0.69	0/4615	0.87	9/6264 (0.1%)
1	B	0.70	0/4615	0.87	9/6264 (0.1%)
All	All	0.69	0/9230	0.87	18/12528 (0.1%)

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	A	0	2
1	B	0	2
All	All	0	4

There are no bond length outliers.

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	93	LEU	CA-CB-CG	-7.17	98.80	115.30
1	A	93	LEU	CA-CB-CG	-7.16	98.84	115.30
1	A	433	ARG	NE-CZ-NH1	6.40	123.50	120.30
1	B	433	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	B	408	LEU	N-CA-C	6.30	128.01	111.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	39	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	A	466	TYR	Sidechain
1	B	39	TYR	Sidechain
1	B	466	TYR	Sidechain

## 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	4477	0	4383	220	0
1	B	4477	0	4383	220	0
2	A	28	0	26	0	0
2	B	28	0	26	0	0
3	A	28	0	25	1	0
3	B	28	0	25	1	0
4	A	43	0	30	6	0
4	B	43	0	30	6	0
5	A	25	0	15	16	0
5	B	25	0	15	18	0
All	All	9202	0	8958	434	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 24.

The worst 5 of 434 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:391:MET:HG3	4:A:601:HEM:HAB	1.41	1.00
1:B:391:MET:HG3	4:B:601:HEM:HAB	1.41	0.99
1:A:384:LEU:HD21	1:A:526:GLY:HA2	1.46	0.97
1:B:91:PHE:HD1	1:B:92:LEU:HD12	1.34	0.93
1:A:152:LEU:HD21	1:A:469:ARG:HG2	1.49	0.92

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	549/576 (95%)	490 (89%)	52 (10%)	7 (1%)	14	56
1	B	549/576 (95%)	490 (89%)	52 (10%)	7 (1%)	14	56
All	All	1098/1152 (95%)	980 (89%)	104 (10%)	14 (1%)	14	56

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	386	HIS
1	A	514	PRO
1	A	520	GLU
1	B	386	HIS
1	B	514	PRO

### 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	486/506 (96%)	434 (89%)	52 (11%)	8	33
1	B	486/506 (96%)	433 (89%)	53 (11%)	7	33
All	All	972/1012 (96%)	867 (89%)	105 (11%)	7	33

5 of 105 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	531	LEU

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Mol	Chain	Res	Type
1	B	165	THR
1	B	522	MET
1	A	535	LEU
1	B	70	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	513	HIS
1	B	170	GLN
1	B	513	HIS
1	A	557	ASN
1	B	134	HIS

### 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](#)

4 carbohydrates 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	$\# Z  > 2$
3	NAG	A	671	1,3	14,14,15	0.54	0	15,19,21	1.13	1 (6%)
3	NAG	A	672	3	14,14,15	1.12	1 (7%)	15,19,21	1.34	2 (13%)
3	NAG	B	671	1,3	14,14,15	0.54	0	15,19,21	1.13	1 (6%)
3	NAG	B	672	3	14,14,15	1.11	1 (7%)	15,19,21	1.35	2 (13%)

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	NAG	A	671	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	672	3	-	0/6/23/26	0/1/1/1
3	NAG	B	671	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	672	3	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	672	NAG	C4-C5	2.33	1.58	1.53
3	A	672	NAG	C4-C5	2.34	1.58	1.53

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	672	NAG	C4-C3-C2	-3.14	106.41	111.02
3	A	672	NAG	C4-C3-C2	-3.14	106.41	111.02
3	A	672	NAG	O5-C1-C2	-2.64	107.80	111.47
3	B	672	NAG	O5-C1-C2	-2.64	107.80	111.47
3	B	671	NAG	C6-C5-C4	-2.44	107.29	113.00

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	672	NAG	1	0
3	B	672	NAG	1	0

## 5.6 Ligand geometry

8 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
4	HEM	A	601	1	28,50,50	2.80	9 (32%)	17,82,82	2.38	4 (23%)
2	NAG	A	661	1	14,14,15	0.76	0	15,19,21	1.29	1 (6%)
2	NAG	A	681	1	14,14,15	0.76	0	15,19,21	0.88	0
5	IMM	A	800	-	21,27,27	1.89	5 (23%)	26,39,39	1.13	3 (11%)
4	HEM	B	601	1	28,50,50	2.80	10 (35%)	17,82,82	2.38	4 (23%)
2	NAG	B	661	1	14,14,15	0.76	0	15,19,21	1.28	1 (6%)
2	NAG	B	681	1	14,14,15	0.76	0	15,19,21	0.88	0
5	IMM	B	800	-	21,27,27	1.89	5 (23%)	26,39,39	1.14	3 (11%)

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
4	HEM	A	601	1	-	0/6/54/54	0/0/8/8
2	NAG	A	661	1	-	0/6/23/26	0/1/1/1
2	NAG	A	681	1	-	0/6/23/26	0/1/1/1
5	IMM	A	800	-	-	0/8/14/14	0/3/3/3
4	HEM	B	601	1	-	0/6/54/54	0/0/8/8
2	NAG	B	661	1	-	0/6/23/26	0/1/1/1
2	NAG	B	681	1	-	0/6/23/26	0/1/1/1
5	IMM	B	800	-	-	0/8/14/14	0/3/3/3

The worst 5 of 29 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	601	HEM	C3B-C2B	-7.65	1.30	1.40
4	A	601	HEM	C3B-C2B	-7.60	1.30	1.40
4	A	601	HEM	C3C-CAC	-7.02	1.33	1.47
4	B	601	HEM	C3C-CAC	-7.01	1.33	1.47
4	B	601	HEM	C3C-C2C	-5.91	1.32	1.40

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	661	NAG	C2-N2-C7	-4.17	116.86	122.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	661	NAG	C2-N2-C7	-4.15	116.89	122.94
5	A	800	IMM	C19-C18-C3	-2.54	111.19	116.14
5	B	800	IMM	C19-C18-C3	-2.54	111.21	116.14
5	A	800	IMM	O2-C6-C5	-2.37	118.27	124.49

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 46 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	601	HEM	6	0
5	A	800	IMM	16	0
4	B	601	HEM	6	0
5	B	800	IMM	18	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 [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	551/576 (95%)	-0.69	0 100 100	4, 18, 53, 91	0
1	B	551/576 (95%)	-0.71	0 100 100	4, 18, 53, 91	0
All	All	1102/1152 (95%)	-0.70	0 100 100	4, 18, 53, 91	0

There are no RSRZ outliers to report.

### 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](#)

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
3	NAG	B	672	14/15	0.86	0.34	1.00	19,37,47,59	0
3	NAG	A	672	14/15	0.91	0.25	-0.07	19,37,47,59	0
3	NAG	B	671	14/15	0.92	0.20	-0.29	4,22,31,34	0
3	NAG	A	671	14/15	0.93	0.20	-0.35	4,22,31,34	0

### 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	681	14/15	0.85	0.32	4.81	15,22,38,44	0
5	IMM	B	800	25/25	0.86	0.31	3.78	15,15,15,15	0
5	IMM	A	800	25/25	0.90	0.29	2.96	15,15,15,15	0
4	HEM	B	601	43/43	0.93	0.25	1.70	7,17,43,67	0
2	NAG	A	681	14/15	0.82	0.32	1.19	15,22,38,44	0
4	HEM	A	601	43/43	0.93	0.23	0.68	7,17,43,67	0
2	NAG	A	661	14/15	0.86	0.23	0.42	33,43,61,66	0
2	NAG	B	661	14/15	0.91	0.19	-0.51	33,43,61,66	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.