



wwPDB X-ray Structure Validation Summary Report i

Feb 26, 2014 – 09:26 PM GMT

PDB ID : 1PGF
Title : PROSTAGLANDIN H2 SYNTHASE-1 COMPLEXED WITH 1-(4-IODOBENZYL)-5-METHOXY-2-METHYLINDOLE-3-ACETICACID (IODOMETHACIN), 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 validation summary report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

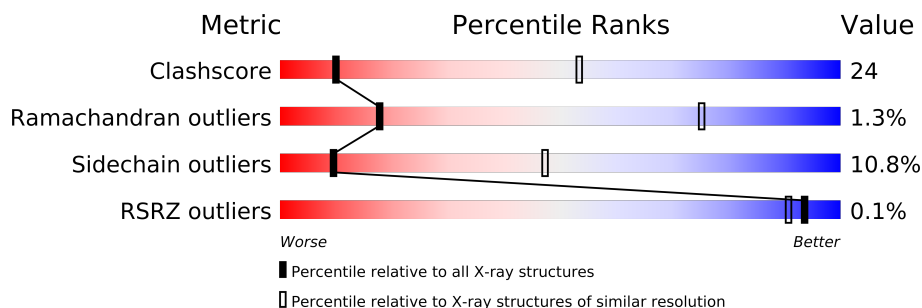
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

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	79885	1300 (5.50-3.50)
Ramachandran outliers	78287	1222 (5.50-3.50)
Sidechain outliers	78261	1203 (5.50-3.50)
RSRZ outliers	66119	1028 (5.50-3.50)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	576	
1	B	576	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	NAG	A	661	-	X
2	NAG	B	681	-	X
5	IMM	A	800	-	X
5	IMM	B	800	-	X

2 Entry composition i

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

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
1	A	551	Total	C	N	O	S	0	0	0
			4477	2903	758	788	28			
1	B	551	Total	C	N	O	S	0	0	0
			4477	2903	758	788	28			

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

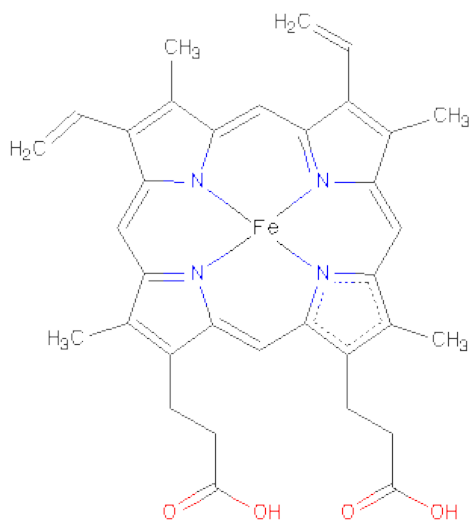


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		

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

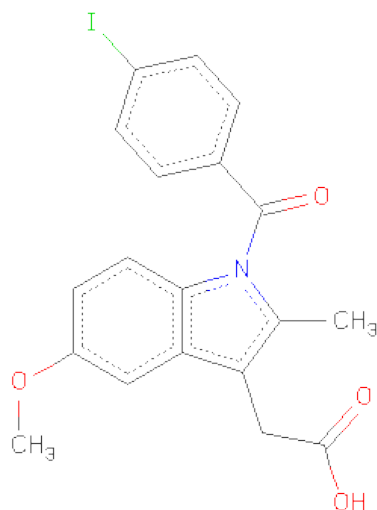
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	2	Total	C	N	O	0	0
			28	16	2	10		
3	B	2	Total	C	N	O	0	0
			28	16	2	10		

- 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
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-IODOBENZOYL)-5-METHOXY-2-METHYLINDOLE-3-ACETIC ACID (three-letter code: IMM) (formula: $C_{19}H_{16}INO_4$).



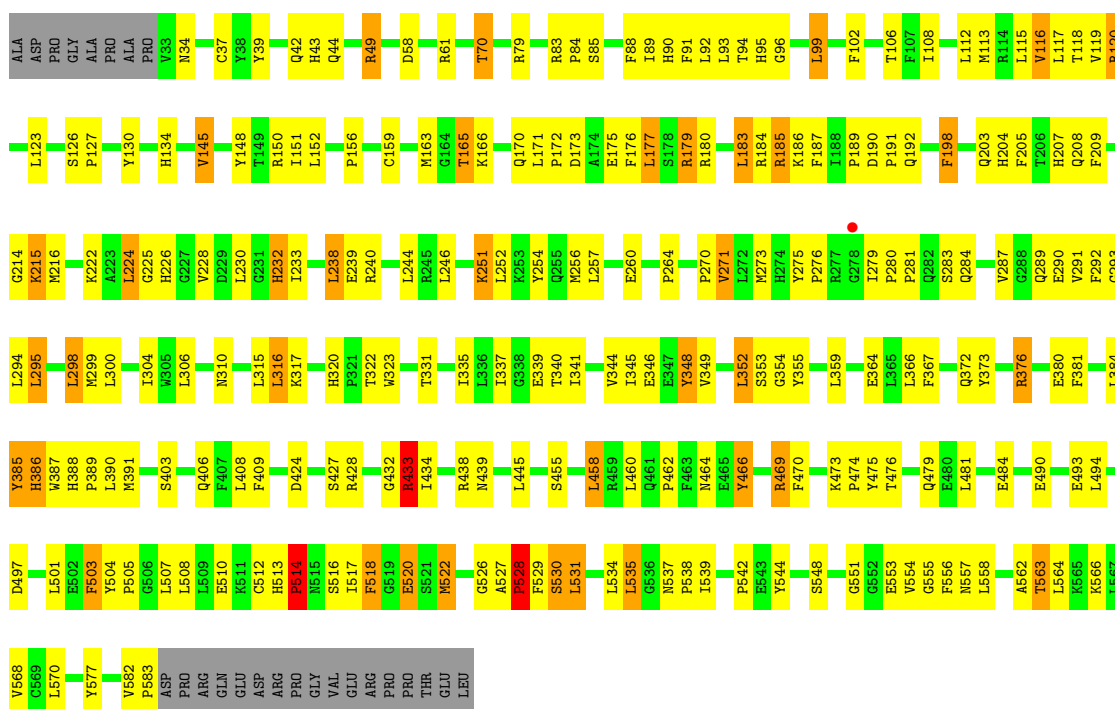
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	I	N	O	0	0
			25	19	1	1	4		
5	B	1	Total	C	I	N	O	0	0
			25	19	1	1	4		

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.

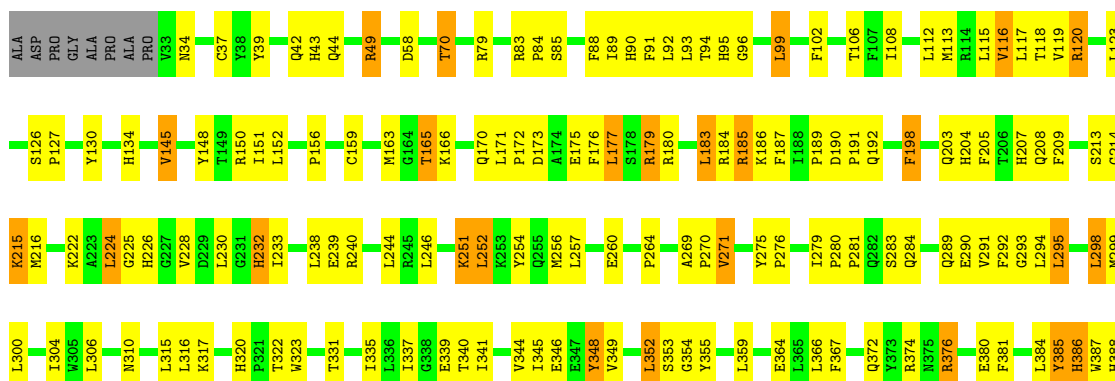
• Molecule 1: PROSTAGLANDIN H2 SYNTHASE-1

Chain A:



• Molecule 1: PROSTAGLANDIN H2 SYNTHASE-1

Chain B:



C575	F503	P389
P576	Y504	L390
Y577	P505	N391
	G506	P392
V582	L507	
P583	L508	S403
ASP	L509	
PRO	E510	Q406
ARG	K511	F407
GLN	C512	L408
GLU	H513	F409
ASP	P514	
ARG	N515	D424
PRO	S516	
GLY	I517	S427
VAL	G518	R428
GLU	G519	
ARG	E520	G432
PRO	S521	R433
PRO	M522	I434
THR		
GLU	G526	R438
LEU	A527	N439
	P528	
	F529	L445
	S530	
	L531	S455
	L534	L458
	L535	R459
	G536	L460
	N537	Q461
	P538	P462
	I539	F463
		N464
	P542	E465
	E543	Y466
	Y544	
	S548	R469
		F470
	G551	K473
	G552	P474
	E553	Y475
	V554	T476
	G555	
	F556	Q479
	N557	E480
	L558	L481
	A562	E484
	T563	
	L564	E490
	K565	
	K566	L494
	L567	
	V568	D497
	G569	
	L570	L501
		E502

4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	5.54 (at 4.46Å)	Xtriage
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 ²)	80.6	Xtriage
Anisotropy	0.740	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 6.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 11169 reflections (0.009%)	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	9202	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage'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.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 24.

The worst 5 of 434 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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

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	549/576 (95%)	490 (89%)	52 (10%)	7 (1%)	18	75
1	B	549/576 (95%)	490 (89%)	52 (10%)	7 (1%)	18	75
All	All	1098/1152 (95%)	980 (89%)	104 (10%)	14 (1%)	18	75

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 ⓘ

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%)	10	48
1	B	486/506 (96%)	433 (89%)	53 (11%)	9	46
All	All	972/1012 (96%)	867 (89%)	105 (11%)	9	47

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

Mol	Chain	Res	Type
1	A	531	LEU
1	B	165	THR
1	B	522	MET
1	A	535	LEU

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Mol	Chain	Res	Type
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 ⓘ

There are no RNA chains 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 ⓘ

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	12,14,15	0.62	0	15,19,21	1.15	2 (13%)
3	NAG	A	672	3	12,14,15	1.07	1 (8%)	15,19,21	1.19	3 (20%)
3	NAG	B	671	1,3	12,14,15	0.62	0	15,19,21	1.15	2 (13%)
3	NAG	B	672	3	12,14,15	1.07	1 (8%)	15,19,21	1.19	3 (20%)

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	A	672	NAG	C4-C5	2.27	1.58	1.53
3	B	672	NAG	C4-C5	2.26	1.58	1.53

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	671	NAG	C6-C5-C4	-2.36	107.29	113.00
3	A	671	NAG	C6-C5-C4	-2.36	107.29	113.00
3	A	672	NAG	C3-C2-N2	2.29	115.25	111.76
3	B	672	NAG	C3-C2-N2	2.28	115.24	111.76
3	B	672	NAG	O5-C5-C6	-2.18	104.69	106.98

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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	49,50,50	5.35	19 (38%)	46,82,82	2.60	14 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	A	661	1	12,14,15	0.77	0	15,19,21	1.21	2 (13%)
2	NAG	A	681	1	12,14,15	0.78	0	15,19,21	0.84	0
5	IMM	A	800	-	27,27,27	1.71	6 (22%)	38,39,39	1.30	5 (13%)
4	HEM	B	601	1	49,50,50	5.37	19 (38%)	46,82,82	2.60	14 (30%)
2	NAG	B	661	1	12,14,15	0.79	0	15,19,21	1.20	2 (13%)
2	NAG	B	681	1	12,14,15	0.79	0	15,19,21	0.84	0
5	IMM	B	800	-	27,27,27	1.72	6 (22%)	38,39,39	1.30	5 (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
4	HEM	A	601	1	-	0/14/114/114	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	-	-	0/10/14/14	0/1/3/3
4	HEM	B	601	1	-	0/14/114/114	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	-	-	0/10/14/14	0/1/3/3

The worst 5 of 50 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	601	HEM	C2B-C1B	28.17	1.51	1.44
4	A	601	HEM	C2B-C1B	27.93	1.51	1.44
4	B	601	HEM	C2D-C1D	14.94	1.48	1.44
4	A	601	HEM	C2D-C1D	14.93	1.48	1.44
4	A	601	HEM	C3B-C4B	8.81	1.54	1.44

The worst 5 of 42 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	601	HEM	CHC-C4B-NB	-8.02	117.92	124.58
4	A	601	HEM	CHC-C4B-NB	-8.02	117.92	124.58
4	A	601	HEM	C1A-C2A-C3A	-6.47	100.22	106.92
4	B	601	HEM	C1A-C2A-C3A	-6.47	100.22	106.92
4	A	601	HEM	CBA-CAA-C2A	6.12	123.48	112.69

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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

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, 95th 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 ²)	Q<0.9
1	A	551/576 (95%)	-0.14	1 (0%) 93 89	4, 18, 53, 91	0
1	B	551/576 (95%)	-0.14	0 100 100	4, 18, 53, 91	0
All	All	1102/1152 (95%)	-0.14	1 (0%) 93 91	4, 18, 53, 91	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	278	GLY	2.2

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

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, 95th 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	NAG	A	672	14/15	0.30	1.60	19,37,47,59	0
3	NAG	B	672	14/15	0.36	0.88	19,37,47,59	0
3	NAG	A	671	14/15	0.21	-0.00	4,22,31,34	0
3	NAG	B	671	14/15	0.19	-0.45	4,22,31,34	0

6.4 Ligands ⓘ

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, 95th 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	NAG	B	681	14/15	0.32	3.46	15,22,38,44	0
5	IMM	B	800	25/25	0.31	3.00	15,15,15,15	0
5	IMM	A	800	25/25	0.29	2.21	15,15,15,15	0
2	NAG	A	661	14/15	0.32	2.10	33,43,61,66	0
4	HEM	B	601	43/43	0.24	1.06	7,17,43,67	0
4	HEM	A	601	43/43	0.24	0.79	7,17,43,67	0
2	NAG	A	681	14/15	0.32	0.69	15,22,38,44	0
2	NAG	B	661	14/15	0.24	-0.02	33,43,61,66	0

6.5 Other polymers ⓘ

There are no such residues in this entry.