



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 07:06 am GMT

PDB ID : 3NC5  
Title : CYP134A1 structure with an open substrate binding loop  
Authors : Cryle, M.J.; Schlichting, I.  
Deposited on : 2010-06-04  
Resolution : 2.90 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 : 1.7.2 (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

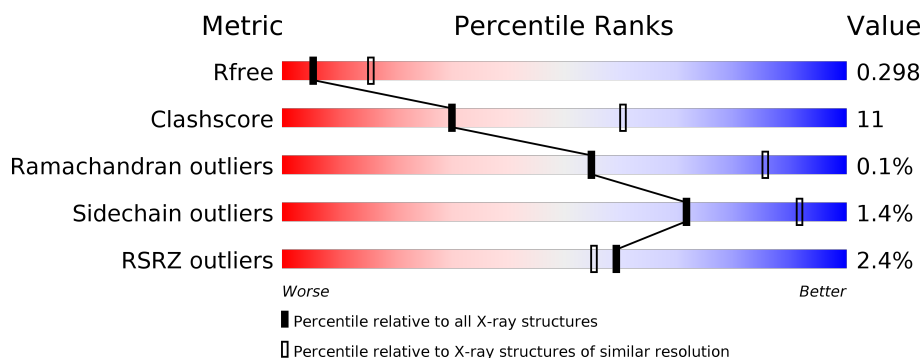
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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	1586 (2.90-2.90)
Clashscore	112137	1807 (2.90-2.90)
Ramachandran outliers	110173	1768 (2.90-2.90)
Sidechain outliers	110143	1770 (2.90-2.90)
RSRZ outliers	101464	1596 (2.90-2.90)

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	441	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%;"></div> <div style="position: absolute; top: 0; left: 0; width: 100%; height: 10px;"> <div style="width: 1%; height: 10px; background-color: red;"></div> <div style="width: 76%, height: 10px; background-color: green;"></div> <div style="width: 10%, height: 10px; background-color: yellow;"></div> <div style="width: 13%, height: 10px; background-color: grey;"></div> </div> </div> </div>
1	B	441	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%;"></div> <div style="position: absolute; top: 0; left: 0; width: 100%; height: 10px;"> <div style="width: 3%, height: 10px; background-color: red;"></div> <div style="width: 69%, height: 10px; background-color: green;"></div> <div style="width: 14%, height: 10px; background-color: yellow;"></div> <div style="width: 15%, height: 10px; background-color: grey;"></div> </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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	MG	A	409	-	-	-	X
4	MG	B	408	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6136 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 Cytochrome P450 cypX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	384	Total	C	N	O	S	0	0	0
			3048	1934	523	575	16			
1	B	373	Total	C	N	O	S	0	0	0
			2955	1876	505	560	14			

There are 74 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-35	MET	-	EXPRESSION TAG	UNP O34926
A	-34	GLY	-	EXPRESSION TAG	UNP O34926
A	-33	SER	-	EXPRESSION TAG	UNP O34926
A	-32	SER	-	EXPRESSION TAG	UNP O34926
A	-31	HIS	-	EXPRESSION TAG	UNP O34926
A	-30	HIS	-	EXPRESSION TAG	UNP O34926
A	-29	HIS	-	EXPRESSION TAG	UNP O34926
A	-28	HIS	-	EXPRESSION TAG	UNP O34926
A	-27	HIS	-	EXPRESSION TAG	UNP O34926
A	-26	HIS	-	EXPRESSION TAG	UNP O34926
A	-25	SER	-	EXPRESSION TAG	UNP O34926
A	-24	SER	-	EXPRESSION TAG	UNP O34926
A	-23	GLY	-	EXPRESSION TAG	UNP O34926
A	-22	LEU	-	EXPRESSION TAG	UNP O34926
A	-21	VAL	-	EXPRESSION TAG	UNP O34926
A	-20	PRO	-	EXPRESSION TAG	UNP O34926
A	-19	ARG	-	EXPRESSION TAG	UNP O34926
A	-18	GLY	-	EXPRESSION TAG	UNP O34926
A	-17	SER	-	EXPRESSION TAG	UNP O34926
A	-16	HIS	-	EXPRESSION TAG	UNP O34926
A	-15	MET	-	EXPRESSION TAG	UNP O34926
A	-14	ALA	-	EXPRESSION TAG	UNP O34926
A	-13	SER	-	EXPRESSION TAG	UNP O34926
A	-12	MET	-	EXPRESSION TAG	UNP O34926
A	-11	THR	-	EXPRESSION TAG	UNP O34926

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	GLY	-	EXPRESSION TAG	UNP O34926
A	-9	GLY	-	EXPRESSION TAG	UNP O34926
A	-8	GLN	-	EXPRESSION TAG	UNP O34926
A	-7	GLN	-	EXPRESSION TAG	UNP O34926
A	-6	MET	-	EXPRESSION TAG	UNP O34926
A	-5	GLY	-	EXPRESSION TAG	UNP O34926
A	-4	ARG	-	EXPRESSION TAG	UNP O34926
A	-3	GLY	-	EXPRESSION TAG	UNP O34926
A	-2	SER	-	EXPRESSION TAG	UNP O34926
A	-1	GLU	-	EXPRESSION TAG	UNP O34926
A	0	PHE	-	EXPRESSION TAG	UNP O34926
A	356	THR	ALA	ENGINEERED MUTATION	UNP O34926
B	-35	MET	-	EXPRESSION TAG	UNP O34926
B	-34	GLY	-	EXPRESSION TAG	UNP O34926
B	-33	SER	-	EXPRESSION TAG	UNP O34926
B	-32	SER	-	EXPRESSION TAG	UNP O34926
B	-31	HIS	-	EXPRESSION TAG	UNP O34926
B	-30	HIS	-	EXPRESSION TAG	UNP O34926
B	-29	HIS	-	EXPRESSION TAG	UNP O34926
B	-28	HIS	-	EXPRESSION TAG	UNP O34926
B	-27	HIS	-	EXPRESSION TAG	UNP O34926
B	-26	HIS	-	EXPRESSION TAG	UNP O34926
B	-25	SER	-	EXPRESSION TAG	UNP O34926
B	-24	SER	-	EXPRESSION TAG	UNP O34926
B	-23	GLY	-	EXPRESSION TAG	UNP O34926
B	-22	LEU	-	EXPRESSION TAG	UNP O34926
B	-21	VAL	-	EXPRESSION TAG	UNP O34926
B	-20	PRO	-	EXPRESSION TAG	UNP O34926
B	-19	ARG	-	EXPRESSION TAG	UNP O34926
B	-18	GLY	-	EXPRESSION TAG	UNP O34926
B	-17	SER	-	EXPRESSION TAG	UNP O34926
B	-16	HIS	-	EXPRESSION TAG	UNP O34926
B	-15	MET	-	EXPRESSION TAG	UNP O34926
B	-14	ALA	-	EXPRESSION TAG	UNP O34926
B	-13	SER	-	EXPRESSION TAG	UNP O34926
B	-12	MET	-	EXPRESSION TAG	UNP O34926
B	-11	THR	-	EXPRESSION TAG	UNP O34926
B	-10	GLY	-	EXPRESSION TAG	UNP O34926
B	-9	GLY	-	EXPRESSION TAG	UNP O34926
B	-8	GLN	-	EXPRESSION TAG	UNP O34926
B	-7	GLN	-	EXPRESSION TAG	UNP O34926
B	-6	MET	-	EXPRESSION TAG	UNP O34926

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-5	GLY	-	EXPRESSION TAG	UNP O34926
B	-4	ARG	-	EXPRESSION TAG	UNP O34926
B	-3	GLY	-	EXPRESSION TAG	UNP O34926
B	-2	SER	-	EXPRESSION TAG	UNP O34926
B	-1	GLU	-	EXPRESSION TAG	UNP O34926
B	0	PHE	-	EXPRESSION TAG	UNP O34926
B	356	THR	ALA	ENGINEERED MUTATION	UNP O34926

- # HEM
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- The diagram illustrates the chemical structure of Hemoglobin (HEM). It features a central iron atom (Fe) coordinated by four nitrogen atoms (N) in a porphyrin-like ring. The ring is substituted with various side chains, including vinyl groups (C8B, C8C), methyl groups (C5, C8), and other functional groups. The structure is labeled with various atoms and bonds, including O1A, O2A, O1D, O2D, C1A, C1B, C1C, C1D, C2A, C2B, C2C, C2D, C3A, C3B, C3C, C3D, C4A, C4B, C4C, C4D, C5A, C5B, C5C, C5D, C6A, C6B, C6C, C6D, C7A, C7B, C7C, C7D, C8A, C8B, C8C, C8D, C9A, C9B, C9C, C9D, C10A, C10B, C10C, C10D, C11A, C11B, C11C, C11D, C12A, C12B, C12C, C12D, C13A, C13B, C13C, C13D, C14A, C14B, C14C, C14D, C15A, C15B, C15C, C15D, C16A, C16B, C16C, C16D, C17A, C17B, C17C, C17D, C18A, C18B, C18C, C18D, C19A, C19B, C19C, C19D, C20A, C20B, C20C, C20D, C21A, C21B, C21C, C21D, C22A, C22B, C22C, C22D, C23A, C23B, C23C, C23D, C24A, C24B, C24C, C24D, C25A, C25B, C25C, C25D, C26A, C26B, C26C, C26D, C27A, C27B, C27C, C27D, C28A, C28B, C28C, C28D, C29A, C29B, C29C, C29D, C30A, C30B, C30C, C30D, C31A, C31B, C31C, C31D, C32A, C32B, C32C, C32D, C33A, C33B, C33C, C33D, C34A, C34B, C34C, C34D, C35A, C35B, C35C, C35D, C36A, C36B, C36C, C36D, C37A, C37B, C37C, C37D, C38A, C38B, C38C, C38D, C39A, C39B, C39C, C39D, C40A, C40B, C40C, C40D, C41A, C41B, C41C, C41D, C42A, C42B, C42C, C42D, C43A, C43B, C43C, C43D, C44A, C44B, C44C, C44D, C45A, C45B, C45C, C45D, C46A, C46B, C46C, C46D, C47A, C47B, C47C, C47D, C48A, C48B, C48C, C48D, C49A, C49B, C49C, C49D, C50A, C50B, C50C, C50D, C51A, C51B, C51C, C51D, C52A, C52B, C52C, C52D, C53A, C53B, C53C, C53D, C54A, C54B, C54C, C54D, C55A, C55B, C55C, C55D, C56A, C56B, C56C, C56D, C57A, C57B, C57C, C57D, C58A, C58B, C58C, C58D, C59A, C59B, C59C, C59D, C60A, C60B, C60C, C60D, C61A, C61B, C61C, C61D, C62A, C62B, C62C, C62D, C63A, C63B, C63C, C63D, C64A, C64B, C64C, C64D, C65A, C65B, C65C, C65D, C66A, C66B, C66C, C66D, C67A, C67B, C67C, C67D, C68A, C68B, C68C, C68D, C69A, C69B, C69C, C69D, C70A, C70B, C70C, C70D, C71A, C71B, C71C, C71D, C72A, C72B, C72C, C72D, C73A, C73B, C73C, C73D, C74A, C74B, C74C, C74D, C75A, C75B, C75C, C75D, C76A, C76B, C76C, C76D, C77A, C77B, C77C, C77D, C78A, C78B, C78C, C78D, C79A, C79B, C79C, C79D, C80A, C80B, C80C, C80D, C81A, C81B, C81C, C81D, C82A, C82B, C82C, C82D, C83A, C83B, C83C, C83D, C84A, C84B, C84C, C84D, C85A, C85B, C85C, C85D, C86A, C86B, C86C, C86D, C87A, C87B, C87C, C87D, C88A, C88B, C88C, C88D, C89A, C89B, C89C, C89D, C90A, C90B, C90C, C90D, C91A, C91B, C91C, C91D, C92A, C92B, C92C, C92D, C93A, C93B, C93C, C93D, C94A, C94B, C94C, C94D, C95A, C95B, C95C, C95D, C96A, C96B, C96C, C96D, C97A, C97B, C97C, C97D, C98A, C98B, C98C, C98D, C99A, C99B, C99C, C99D, C100A, C100B, C100C, C100D.

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

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

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Mg	0	0
			1	1		
4	A	2	Total	Mg	0	0
			2	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	18	Total	O	0	0
			18	18		
5	B	14	Total	O	0	0
			14	14		





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	63.80Å 105.40Å 143.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.62 – 2.90 40.63 – 2.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (40.62-2.90) 98.8 (40.63-2.90)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.51 (at 2.90Å)	Xtriage
Refinement program	REFMAC 5.5.0070	Depositor
R, $R_{free}$	0.231 , 0.306 0.226 , 0.298	Depositor DCC
$R_{free}$ test set	1091 reflections (5.24%)	DCC
Wilson B-factor (Å <sup>2</sup> )	57.4	Xtriage
Anisotropy	0.533	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 45.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	6136	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.74% 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: GOL, MG, HEM

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	0.46	0/3108	0.59	0/4208
1	B	0.42	0/3013	0.60	1/4082 (0.0%)
All	All	0.44	0/6121	0.60	1/8290 (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	B	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	B	65	VAL	N-CA-C	5.96	127.08	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	300	LYS	Peptide

### 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	3048	0	3030	51	0
1	B	2955	0	2932	78	0
2	A	43	0	30	2	0
2	B	43	0	30	1	0
3	A	6	0	8	0	0
3	B	6	0	8	2	0
4	A	2	0	0	0	0
4	B	1	0	0	0	0
5	A	18	0	0	1	0
5	B	14	0	0	1	0
All	All	6136	0	6038	129	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 11.

All (129) 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:211:SER:OG	1:A:212:GLU:HA	1.20	1.25
1:A:211:SER:CB	1:A:212:GLU:HA	1.66	1.22
1:B:62:LYS:HD3	1:B:65:VAL:CG2	1.73	1.18
1:B:63:SER:O	1:B:64:LEU:HD23	1.48	1.12
1:B:65:VAL:HB	1:B:66:GLU:HA	1.10	1.09
1:A:211:SER:OG	1:A:212:GLU:CA	2.02	1.07
1:B:300:LYS:HB3	1:B:301:ASP:HA	1.32	1.07
1:B:62:LYS:CD	1:B:65:VAL:HG21	1.87	1.04
1:B:211:SER:CB	1:B:212:GLU:HA	1.89	1.03
1:B:65:VAL:CB	1:B:66:GLU:HA	1.91	1.00
1:B:62:LYS:HD3	1:B:65:VAL:HG21	1.02	1.00
1:A:135:PHE:CZ	1:A:366:VAL:CG2	2.47	0.97
1:B:65:VAL:HB	1:B:66:GLU:CA	1.96	0.93
1:B:287:LEU:O	1:B:301:ASP:HB2	1.67	0.92
1:B:211:SER:HB2	1:B:212:GLU:HA	1.54	0.90
1:A:211:SER:CB	1:A:212:GLU:CA	2.48	0.89
1:B:300:LYS:CB	1:B:301:ASP:HA	2.03	0.86
1:B:135:PHE:CZ	1:B:366:VAL:HG11	2.12	0.85
1:B:38:ILE:HA	1:B:39:ASP:CB	2.08	0.84
1:A:211:SER:HB2	1:A:212:GLU:HA	1.59	0.84
1:A:38:ILE:HA	1:A:39:ASP:HB2	1.59	0.83
1:B:211:SER:HB2	1:B:212:GLU:CA	2.09	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:ARG:HG2	1:A:333:ILE:HG21	1.61	0.82
1:B:350:ILE:HD13	1:B:350:ILE:H	1.43	0.82
1:B:135:PHE:CZ	1:B:366:VAL:CG1	2.64	0.81
1:A:135:PHE:CZ	1:A:366:VAL:HG21	2.16	0.81
1:A:135:PHE:CE2	1:A:366:VAL:HG21	2.16	0.80
1:B:63:SER:O	1:B:64:LEU:CD2	2.29	0.80
1:A:68:ALA:HB1	1:A:165:ILE:HD11	1.62	0.79
1:B:211:SER:HB3	1:B:212:GLU:HA	1.63	0.79
1:B:38:ILE:HA	1:B:39:ASP:HB2	1.67	0.75
1:A:135:PHE:CZ	1:A:366:VAL:HG22	2.22	0.73
1:B:300:LYS:HB3	1:B:301:ASP:CA	2.17	0.72
1:B:287:LEU:O	1:B:301:ASP:CB	2.38	0.70
1:A:68:ALA:CB	1:A:165:ILE:HD11	2.20	0.70
1:B:268:ARG:HG2	1:B:333:ILE:HD12	1.72	0.70
1:B:135:PHE:CE2	1:B:366:VAL:HG11	2.28	0.69
1:B:283:ILE:HG13	1:B:308:ILE:HD11	1.77	0.66
1:A:242:LEU:HD22	1:A:366:VAL:HG11	1.78	0.65
1:A:67:ARG:HG3	1:A:68:ALA:N	2.11	0.64
1:A:211:SER:HG	1:A:212:GLU:CA	2.07	0.63
1:B:211:SER:HB2	1:B:212:GLU:CB	2.28	0.63
1:A:211:SER:HG	1:A:212:GLU:HA	1.57	0.62
1:B:65:VAL:CB	1:B:66:GLU:CA	2.63	0.61
1:B:63:SER:C	1:B:64:LEU:HD23	2.19	0.60
1:B:350:ILE:HD13	1:B:350:ILE:N	2.16	0.59
1:A:16:GLN:HG3	1:A:390:LEU:HG	1.84	0.58
1:A:68:ALA:HB1	1:A:165:ILE:CD1	2.32	0.57
1:B:350:ILE:CD1	1:B:350:ILE:H	2.14	0.57
1:A:69:GLU:CD	1:A:70:PRO:HD2	2.25	0.57
1:A:268:ARG:HG2	1:A:333:ILE:CG2	2.34	0.57
1:B:256:MET:HA	1:B:256:MET:HE3	1.87	0.56
1:B:328:ARG:HG3	1:B:331:LEU:HB2	1.86	0.56
1:B:49:VAL:HG13	1:B:306:CYS:HB3	1.88	0.55
1:B:354:VAL:O	1:B:354:VAL:HG12	2.05	0.55
1:A:319:GLU:OE1	5:A:420:HOH:O	2.18	0.54
1:A:128:VAL:HG12	1:A:133:LYS:HE2	1.90	0.54
1:A:381:GLU:HA	1:A:381:GLU:OE2	2.06	0.54
1:A:211:SER:OG	1:A:212:GLU:CB	2.56	0.54
1:B:38:ILE:HA	1:B:39:ASP:HB3	1.88	0.54
1:A:38:ILE:CA	1:A:39:ASP:HB2	2.36	0.53
1:B:62:LYS:HB3	1:B:65:VAL:CG2	2.39	0.53
1:B:285:ARG:NH2	2:B:406:HEM:O1A	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:66:GLU:HB2	1:B:229:ASN:OD1	2.10	0.52
1:B:300:LYS:HB3	1:B:302:THR:H	1.75	0.52
1:B:127:LEU:HD11	1:B:374:MET:HE1	1.92	0.52
1:A:67:ARG:CG	1:A:68:ALA:N	2.73	0.52
1:A:211:SER:HB2	1:A:212:GLU:CA	2.29	0.51
1:A:69:GLU:HG3	1:A:70:PRO:HD2	1.93	0.51
1:B:168:ILE:HD11	1:B:390:LEU:HD13	1.92	0.51
1:B:133:LYS:HD2	1:B:239:ASP:OD1	2.09	0.51
1:B:292:VAL:HA	1:B:297:GLU:HA	1.93	0.50
1:B:27:ARG:HH21	1:B:315:PRO:HD3	1.76	0.50
1:B:38:ILE:CA	1:B:39:ASP:CB	2.87	0.50
1:B:135:PHE:CZ	1:B:366:VAL:HG13	2.47	0.49
1:B:50:ARG:O	1:B:54:GLN:CG	2.60	0.49
1:B:36:GLU:O	1:B:37:SER:OG	2.26	0.49
1:B:67:ARG:HD2	1:B:67:ARG:H	1.77	0.49
1:A:69:GLU:CG	1:A:70:PRO:HD2	2.43	0.49
1:A:67:ARG:HG3	1:A:68:ALA:H	1.78	0.49
1:A:9:SER:HB2	1:A:35:GLU:OE1	2.13	0.48
1:B:27:ARG:NH2	1:B:315:PRO:HD3	2.29	0.48
1:B:299:LYS:C	1:B:300:LYS:HG2	2.34	0.48
1:A:317:ALA:O	1:A:342:ARG:NH2	2.44	0.48
1:B:237:PRO:HG3	3:B:407:GOL:O3	2.14	0.47
1:B:242:LEU:HD13	1:B:366:VAL:HG23	1.96	0.47
1:B:268:ARG:CG	1:B:333:ILE:HD12	2.40	0.46
1:B:50:ARG:O	1:B:54:GLN:HG2	2.15	0.46
1:B:62:LYS:HB3	1:B:65:VAL:HG23	1.98	0.46
1:B:244:LEU:HD22	1:B:277:LYS:HB2	1.97	0.46
1:A:242:LEU:CD2	1:A:366:VAL:HG11	2.45	0.46
1:A:67:ARG:CG	1:A:68:ALA:H	2.29	0.46
1:B:67:ARG:NH1	5:B:419:HOH:O	2.47	0.45
1:A:89:ARG:HG2	1:A:216:MET:HG2	1.98	0.45
1:A:283:ILE:HD12	1:A:308:ILE:HD11	1.98	0.45
1:B:366:VAL:HG23	1:B:367:ALA:N	2.32	0.44
1:A:278:PRO:HG3	1:A:308:ILE:HG22	1.99	0.44
1:B:189:LEU:O	1:B:193:ILE:HG12	2.17	0.44
1:B:233:ALA:HA	3:B:407:GOL:H32	1.99	0.44
1:B:354:VAL:CG1	1:B:354:VAL:O	2.65	0.44
1:B:346:PHE:CE2	1:B:356:THR:HG23	2.53	0.44
1:A:263:ARG:NH2	1:A:372:ASP:OD2	2.52	0.43
1:B:98:GLY:O	1:B:101:LEU:HG	2.18	0.43
1:B:211:SER:HB2	1:B:212:GLU:HB2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:275:ARG:O	1:B:312:ASN:HB3	2.18	0.43
1:A:64:LEU:HD12	2:A:406:HEM:O1D	2.19	0.43
1:B:282:LEU:HA	1:B:306:CYS:O	2.19	0.43
1:B:325:ASN:O	1:B:328:ARG:HG2	2.19	0.43
1:B:38:ILE:CA	1:B:39:ASP:HB2	2.44	0.43
1:A:108:ILE:HG12	1:A:108:ILE:H	1.65	0.42
1:A:135:PHE:CE1	1:A:366:VAL:HG22	2.53	0.42
1:B:62:LYS:HD3	1:B:65:VAL:HG22	1.82	0.42
1:B:54:GLN:O	1:B:350:ILE:HD11	2.19	0.42
1:A:18:ASN:OD1	1:A:21:ALA:HB2	2.19	0.42
1:A:234:ALA:HB2	2:A:406:HEM:CAC	2.50	0.42
1:A:211:SER:OG	1:A:212:GLU:HG3	2.20	0.42
1:B:314:ASP:HA	1:B:315:PRO:HD3	1.94	0.41
1:A:253:PRO:O	1:A:256:MET:HB3	2.20	0.41
1:A:328:ARG:HG3	1:A:331:LEU:HB2	2.01	0.41
1:A:374:MET:CE	1:A:377:ILE:HD12	2.50	0.41
1:B:300:LYS:HB3	1:B:302:THR:N	2.34	0.41
1:B:67:ARG:HH22	1:B:228:LEU:HD13	1.86	0.41
1:B:50:ARG:O	1:B:54:GLN:HG3	2.19	0.41
1:B:380:GLU:OE1	1:B:399:LEU:HB3	2.20	0.41
1:A:104:LEU:O	1:A:108:ILE:HG12	2.21	0.40
1:B:38:ILE:HG13	1:B:38:ILE:O	2.21	0.40
1:A:164:PHE:HB2	1:A:178:SER:HB3	2.04	0.40
1:A:133:LYS:HA	1:A:239:ASP:OD2	2.21	0.40
1:B:109:LYS:O	1:B:113:GLU:HG3	2.22	0.40

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	378/441 (86%)	358 (95%)	19 (5%)	1 (0%)	44 77

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	367/441 (83%)	340 (93%)	27 (7%)	0	100	100
All	All	745/882 (84%)	698 (94%)	46 (6%)	1 (0%)	55	85

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	334	LYS

### 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	337/380 (89%)	333 (99%)	4 (1%)	75	93
1	B	327/380 (86%)	322 (98%)	5 (2%)	70	91
All	All	664/760 (87%)	655 (99%)	9 (1%)	71	91

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	SER
1	A	108	ILE
1	A	308	ILE
1	A	381	GLU
1	B	67	ARG
1	B	178	SER
1	B	350	ILE
1	B	377	ILE
1	B	390	LEU

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 ⓘ

Of 7 ligands modelled in this entry, 3 are monoatomic - leaving 4 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	HEM	A	406	1,5	28,50,50	2.18	6 (21%)	17,82,82	1.92	4 (23%)
3	GOL	A	407	-	5,5,5	0.17	0	5,5,5	0.47	0
2	HEM	B	406	1,5	28,50,50	2.13	6 (21%)	17,82,82	2.04	5 (29%)
3	GOL	B	407	-	5,5,5	0.37	0	5,5,5	0.27	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	HEM	A	406	1,5	-	0/6/54/54	0/0/8/8
3	GOL	A	407	-	-	0/4/4/4	0/0/0/0
2	HEM	B	406	1,5	-	0/6/54/54	0/0/8/8
3	GOL	B	407	-	-	0/4/4/4	0/0/0/0

All (12) bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	406	HEM	C3C-C2C	-5.38	1.33	1.40
2	B	406	HEM	C3C-C2C	-5.11	1.33	1.40
2	B	406	HEM	C3B-C2B	-5.01	1.33	1.40
2	A	406	HEM	C3B-C2B	-3.91	1.35	1.40
2	B	406	HEM	C4D-ND	2.15	1.39	1.36
2	A	406	HEM	C3B-CAB	3.11	1.54	1.47
2	B	406	HEM	C3C-CAC	3.25	1.54	1.47
2	B	406	HEM	C3B-CAB	3.49	1.54	1.47
2	A	406	HEM	C4D-ND	3.49	1.40	1.36
2	A	406	HEM	C3C-CAC	3.79	1.55	1.47
2	B	406	HEM	C3D-C2D	4.79	1.51	1.37
2	A	406	HEM	C3D-C2D	5.27	1.53	1.37

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	406	HEM	CBA-CAA-C2A	-4.37	104.13	112.48
2	B	406	HEM	CAD-CBD-CGD	-3.70	106.33	112.66
2	B	406	HEM	CBA-CAA-C2A	-3.44	105.90	112.48
2	B	406	HEM	CAA-CBA-CGA	-3.40	106.85	112.66
2	B	406	HEM	C1D-C2D-C3D	-3.15	104.80	107.00
2	A	406	HEM	C1D-C2D-C3D	-3.02	104.89	107.00
2	A	406	HEM	CMA-C3A-C4A	-2.33	124.89	128.46
2	B	406	HEM	CMC-C2C-C3C	2.06	128.71	124.89
2	A	406	HEM	CMB-C2B-C3B	2.75	129.99	124.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	406	HEM	2	0
2	B	406	HEM	1	0
3	B	407	GOL	2	0

## 5.7 Other polymers [i](#)

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	384/441 (87%)	0.01	6 (1%) 72 70	31, 52, 90, 133	1 (0%)
1	B	373/441 (84%)	0.24	12 (3%) 48 42	33, 57, 96, 115	1 (0%)
All	All	757/882 (85%)	0.12	18 (2%) 59 55	31, 54, 94, 133	2 (0%)

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	218	LEU	3.9
1	A	300	LYS	3.4
1	B	8	PHE	3.4
1	B	28	GLU	3.1
1	B	211	SER	2.9
1	B	7	LEU	2.8
1	B	217	ALA	2.6
1	B	65	VAL	2.6
1	B	212	GLU	2.5
1	B	297	GLU	2.5
1	A	382	ASP	2.4
1	B	303	ILE	2.4
1	B	221	LYS	2.3
1	B	288	SER	2.2
1	A	28	GLU	2.2
1	A	7	LEU	2.0
1	A	296	MET	2.0
1	A	121	GLU	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( $\text{\AA}^2$ )	Q<0.9
4	MG	A	409	1/1	0.91	0.50	13.23	43,43,43,43	0
4	MG	B	408	1/1	0.80	0.29	2.26	41,41,41,41	0
3	GOL	A	407	6/6	0.94	0.19	0.53	33,37,37,39	0
2	HEM	A	406	43/43	0.97	0.18	-0.23	14,18,28,30	0
3	GOL	B	407	6/6	0.92	0.19	-0.48	41,42,43,44	0
2	HEM	B	406	43/43	0.97	0.18	-0.76	14,18,27,30	0
4	MG	A	408	1/1	0.68	0.27	-	54,54,54,54	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.