



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:50 AM GMT

PDB ID : 3NC3  
Title : CYP134A1 structure with a closed substrate binding loop  
Authors : Cryle, M.J.; Schlichting, I.  
Deposited on : 2010-06-04  
Resolution : 2.66 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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

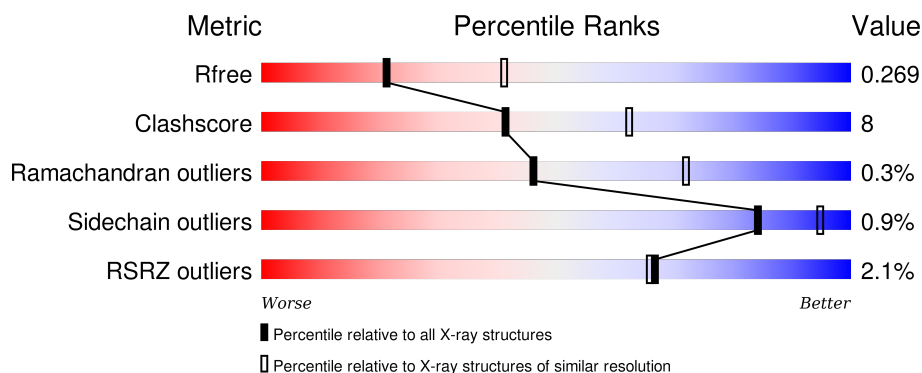
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.66 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))
$R_{free}$	91344	3152 (2.70-2.62)
Clashscore	102246	3524 (2.70-2.62)
Ramachandran outliers	100387	3469 (2.70-2.62)
Sidechain outliers	100360	3469 (2.70-2.62)
RSRZ outliers	91569	3161 (2.70-2.62)

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>3%</div> <div>72%</div> <div>15%</div> <div>14%</div> </div>
1	B	441	<div> <div>%</div> <div>70%</div> <div>17%</div> <div>13%</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
3	GOL	B	407	-	-	-	X
4	MG	A	408	-	-	-	X
4	MG	A	410	-	-	-	X

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 6209 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	380	Total	C	N	O	S	0	2	0
			3018	1914	522	567	15			
1	B	385	Total	C	N	O	S	0	1	0
			3041	1929	523	574	15			

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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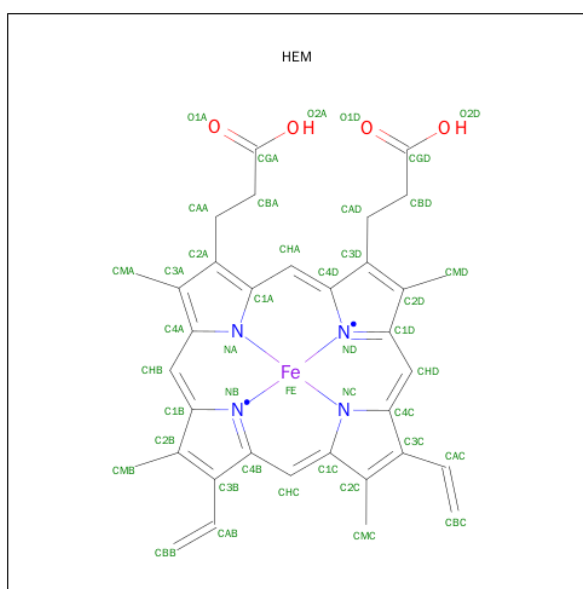
Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	GLY	-	EXPRESSION TAG	UNP O34926
A	-9	GLY	-	EXPRESSION TAG	UNP O34926
A	-8	GLN	-	EXPRESSION TAG	UNP O34926
A	-7	GLN	-	EXPRESSION TAG	UNP O34926
A	-6	MET	-	EXPRESSION TAG	UNP O34926
A	-5	GLY	-	EXPRESSION TAG	UNP O34926
A	-4	ARG	-	EXPRESSION TAG	UNP 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

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



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

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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	2	Total	Mg	0	0
			2	2		
4	A	4	Total	Mg	0	0
			4	4		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	22	Total	O	0	0
			22	22		
5	B	24	Total	O	0	0
			24	24		

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 ( $\text{RSRZ} > 2$ ). 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.

Chain A:

72% 15% 14%

1 MET GLY SER HIS HIS HIS HIS HIS HIS HIS SER SER GLY VAL PRO ARG GLY SER HIS MET ALA SER MET THR GLY GLN MET GLY ARG GLY SER PHE MET SER GLN SER I5 F8 N18 P19 Y20 A21 S24 F28 I38 D39 S40 R50 Q54

V65 E66 V71 M72 R73 GLY PRO VAL LEU ALA GLN MET HIS GLY LYS GLU SER HIS A87 K88 R89 R90 I91 V92 F96 D102 K109 T291 V292 E113 D126 N129 D130 K133 H158 T166 M190 P191 K194 L204 I205 S206 L208 C209 T210 S211

TTR GLU MET A217 L218 S219 D220 L227 L231 E236 P237 A238 D239 R263 R268 K277 P278 L283 P284 R285 Q289 D290 T291 V292 V293 G294 K300 L308 P315 E316 A317 F318 R328 L331 G332 I333 R342 R351 R352 A359 I369

D372 K373 M374 G389 L390 Y391 T392 R393 D403 GLY ALA

Chain B:

Amino Acid	Frequency (%)
MET	70%
GLY	70%
SER	70%
HIS	70%
HIS	70%
HIS	70%
HIS	70%
HIS	70%
SER	70%
GLY	70%
LEU	70%
VAL	70%
PRO	17%
ARG	17%
GLY	17%
SER	17%
HIS	17%
HIS	17%
MET	17%
ALA	17%
SER	17%
MET	17%
THR	17%
GLY	17%
GLY	17%
GLN	17%
GLN	17%
MET	17%
GLY	17%
GLY	17%
SER	17%
GLU	17%
PHE	17%
MET	17%
SER	17%
GLN	17%
SER	17%
ILE	13%
P19	13%
P20	13%
R27	13%
V32	13%
I38	13%
D39	13%
I43	13%
L64	13%
A68	13%
E69	13%
P70	13%
V74	13%



## 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)	47.74 – 2.66 47.74 – 2.66	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.74-2.66) 92.9 (47.74-2.66)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.43 (at 2.65Å)	Xtriage
Refinement program	REFMAC 5.5.0070	Depositor
R, $R_{free}$	0.219 , 0.273 0.213 , 0.269	Depositor DCC
$R_{free}$ test set	1064 reflections (4.18%)	DCC
Wilson B-factor (Å <sup>2</sup> )	52.6	Xtriage
Anisotropy	0.178	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 47.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 26503 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6209	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 20.61 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 8.3773e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.49	0/3083	0.62	0/4176
1	B	0.51	0/3105	0.65	0/4207
All	All	0.50	0/6188	0.63	0/8383

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	3018	0	2997	46	0
1	B	3041	0	3010	57	0
2	A	43	0	30	1	0
2	B	43	0	30	1	0
3	A	6	0	8	0	0
3	B	6	0	8	2	0
4	A	4	0	0	0	0
4	B	2	0	0	0	0
5	A	22	0	0	0	0
5	B	24	0	0	1	0
All	All	6209	0	6083	104	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 8.

All (104) 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:B:268:ARG:HG2	1:B:333:ILE:CD1	1.81	1.10
1:B:38:ILE:HG22	1:B:39:ASP:H	1.10	1.08
1:B:268:ARG:HG2	1:B:333:ILE:HD12	1.29	1.07
1:A:38:ILE:HG22	1:A:39:ASP:N	1.71	1.06
1:B:68:ALA:HB2	1:B:165:ILE:HD11	1.40	1.03
1:A:89[B]:ARG:HB3	1:A:89[B]:ARG:NH1	1.73	1.01
1:B:38:ILE:HG22	1:B:39:ASP:N	1.75	0.96
1:A:38:ILE:CG2	1:A:39:ASP:H	1.80	0.95
1:B:38:ILE:CG2	1:B:39:ASP:H	1.79	0.94
1:A:38:ILE:HG22	1:A:39:ASP:H	1.23	0.93
1:B:96:PHE:CD1	1:B:207:ILE:HD12	2.06	0.91
1:A:38:ILE:CG2	1:A:39:ASP:N	2.38	0.87
1:B:96:PHE:HD1	1:B:207:ILE:HD12	1.47	0.80
1:A:89[B]:ARG:HB3	1:A:89[B]:ARG:HH11	1.46	0.78
1:B:68:ALA:HB2	1:B:165:ILE:CD1	2.16	0.74
1:A:205:ILE:HG23	1:A:227:ILE:HD11	1.71	0.72
1:B:268:ARG:HG2	1:B:333:ILE:HD13	1.73	0.71
1:A:50:ARG:O	1:A:54:GLN:HG2	1.90	0.70
1:A:89[B]:ARG:HB3	1:A:89[B]:ARG:CZ	2.22	0.69
1:A:72:MET:HE1	1:A:391:TYR:HB2	1.75	0.67
1:B:362:GLU:O	1:B:366:VAL:HG23	1.93	0.67
1:B:249:LEU:O	1:B:256:MET:HB2	1.97	0.65
1:A:317:ALA:O	1:A:342:ARG:NH2	2.31	0.63
1:B:43:ILE:HD12	1:B:304:VAL:HB	1.81	0.63
1:B:268:ARG:CG	1:B:333:ILE:CD1	2.70	0.61
1:B:109:LYS:HG3	1:B:369:ILE:HD11	1.83	0.61
1:B:20:TYR:CZ	1:B:277:LYS:HD3	2.36	0.60
1:A:278:PRO:HG3	1:A:308:ILE:HG22	1.84	0.59
1:A:328:ARG:HG3	1:A:331:LEU:HB2	1.84	0.58
1:B:64:LEU:HD11	3:B:407:GOL:H2	1.85	0.58
1:B:228:LEU:O	1:B:232:LEU:HD23	2.05	0.57
1:A:89[B]:ARG:HH11	1:A:89[B]:ARG:CB	2.16	0.57
1:A:268:ARG:HA	1:A:333:ILE:HD13	1.87	0.57
1:B:278:PRO:HG3	1:B:308:ILE:HG22	1.87	0.57
1:A:268:ARG:NH2	1:A:328:ARG:O	2.38	0.56
1:A:18:ASN:ND2	1:A:21:ALA:HB2	2.21	0.56
1:A:72:MET:CE	1:A:391:TYR:HB2	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:269:ALA:HA	1:B:326:ILE:HG22	1.90	0.54
1:B:190:MET:HB3	1:B:191:PRO:HD3	1.90	0.54
1:B:284:PRO:HB3	1:B:305:PHE:CE1	2.44	0.53
1:B:73:ARG:HH11	1:B:75:PRO:HG2	1.73	0.53
1:B:328:ARG:HG3	1:B:331:LEU:HB2	1.92	0.52
1:B:68:ALA:CB	1:B:165:ILE:HD11	2.26	0.52
1:B:89:ARG:O	1:B:92:VAL:HG22	2.10	0.52
1:B:152:GLU:O	1:B:156:GLU:HG3	2.10	0.52
1:B:201:GLY:H	1:B:206:SER:CB	2.23	0.52
1:B:263:ARG:NH2	1:B:372:ASP:OD2	2.43	0.51
1:B:244:LEU:HG	1:B:395:PRO:HD3	1.92	0.51
1:B:256:MET:CE	1:B:260:LEU:HG	2.41	0.51
1:B:135:PHE:CZ	1:B:366:VAL:HG22	2.46	0.51
1:A:263:ARG:NH2	1:A:372:ASP:OD2	2.44	0.50
1:B:91:ILE:O	1:B:91:ILE:CG2	2.60	0.50
1:B:256:MET:HE2	1:B:260:LEU:HG	1.93	0.50
1:B:219:SER:O	1:B:223:ILE:HG13	2.12	0.49
2:B:406:HEM:HBC2	2:B:406:HEM:CMC	2.42	0.49
1:A:89[A]:ARG:HD3	1:A:218:LEU:HD21	1.94	0.49
1:A:109:LYS:HG3	1:A:369:ILE:HD11	1.95	0.48
1:A:91:ILE:HD12	1:A:91:ILE:H	1.78	0.48
1:B:109:LYS:NZ	1:B:109:LYS:HB2	2.29	0.48
1:A:38:ILE:HG21	1:A:40:SER:OG	2.13	0.48
1:A:204:LEU:HA	1:A:207:ILE:HD12	1.95	0.48
1:B:359:ALA:O	1:B:363:ILE:HD12	2.14	0.47
1:B:38:ILE:CG2	1:B:39:ASP:N	2.45	0.47
1:A:38:ILE:HD11	1:A:72:MET:O	2.13	0.47
1:B:99:ASP:O	1:B:103:HIS:ND1	2.32	0.47
1:A:166:THR:HG23	1:A:391:TYR:HB3	1.97	0.47
1:B:101:LEU:HD13	1:B:358:PHE:HA	1.97	0.47
1:A:236:GLU:HB2	1:A:237:PRO:HD3	1.97	0.46
1:A:113:GLU:HG2	1:A:373:LYS:NZ	2.30	0.46
1:B:91:ILE:HG22	1:B:91:ILE:O	2.16	0.46
1:A:359:ALA:HB1	2:A:406:HEM:HAB	1.98	0.46
1:A:289:GLN:HA	1:A:300:LYS:HG2	1.96	0.45
1:B:90:ARG:CZ	1:B:354:VAL:HG12	2.46	0.45
1:A:38:ILE:CD1	1:A:72:MET:O	2.64	0.45
1:A:194:LYS:HE2	1:A:220:ASP:CG	2.37	0.45
1:A:71:VAL:HG21	1:A:391:TYR:CD1	2.52	0.44
1:A:38:ILE:CG2	1:A:40:SER:OG	2.66	0.44
1:B:163:ASP:O	1:B:167:SER:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:64:LEU:HD21	3:B:407:GOL:H32	1.99	0.44
1:A:374:MET:HE2	1:A:374:MET:HB3	1.89	0.43
1:B:196:ARG:HD3	1:B:206:SER:OG	2.18	0.43
1:A:283:ILE:HD12	1:A:308:ILE:HD11	2.01	0.43
1:B:19:PRO:HD2	1:B:393:ARG:NH2	2.34	0.43
1:A:389:GLY:O	1:A:393:ARG:NH1	2.52	0.43
1:A:129:ASN:OD1	1:A:133:LYS:NZ	2.52	0.42
1:A:158:HIS:HB2	1:A:231:LEU:HD21	2.02	0.42
1:B:71:VAL:O	1:B:71:VAL:HG13	2.19	0.42
1:A:20:TYR:CZ	1:A:277:LYS:HD3	2.54	0.42
1:B:27:ARG:NH1	1:B:310:ALA:O	2.54	0.41
1:B:160:GLY:HA3	1:B:181:CYS:SG	2.60	0.41
1:B:205:ILE:HG23	1:B:227:ILE:HD11	2.03	0.41
1:B:269:ALA:HA	1:B:326:ILE:CG2	2.50	0.41
1:B:32:VAL:HG21	1:B:293:VAL:O	2.21	0.41
1:B:278:PRO:HA	1:B:279:PRO:HD3	1.97	0.41
1:A:209:CYS:O	1:A:210:THR:HG23	2.20	0.41
1:B:284:PRO:O	1:B:285:ARG:HD3	2.21	0.41
1:A:285:ARG:HD3	1:A:285:ARG:HA	1.80	0.41
1:A:190:MET:N	1:A:191:PRO:CD	2.84	0.41
1:B:333:ILE:C	1:B:335:SER:H	2.24	0.41
1:A:315:PRO:HA	1:A:318:PHE:O	2.21	0.40
1:A:126:ASP:O	1:A:130:ASP:HB2	2.21	0.40
1:B:100:ALA:O	1:B:103:HIS:N	2.53	0.40
1:B:403:ASP:HB2	5:B:426:HOH:O	2.20	0.40
1:A:290:ASP:OD1	1:A:300:LYS:HG3	2.21	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	376/441 (85%)	351 (93%)	25 (7%)	0	100	100
1	B	380/441 (86%)	359 (94%)	19 (5%)	2 (0%)	34	59
All	All	756/882 (86%)	710 (94%)	44 (6%)	2 (0%)	46	72

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	101	LEU
1	B	294	GLY

### 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	332/380 (87%)	327 (98%)	5 (2%)	72	90
1	B	334/380 (88%)	333 (100%)	1 (0%)	94	99
All	All	666/760 (88%)	660 (99%)	6 (1%)	84	95

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	SER
1	A	102	ASP
1	A	239	ASP
1	A	351	HIS
1	A	352	ASN
1	B	296	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	286	GLN
1	A	352	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 10 ligands modelled in this entry, 6 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	30,50,50	2.00	6 (20%)	24,82,82	2.54	9 (37%)
3	GOL	A	407	-	5,5,5	0.35	0	5,5,5	0.53	0
2	HEM	B	406	1,5	30,50,50	2.03	8 (26%)	24,82,82	2.54	11 (45%)
3	GOL	B	407	-	5,5,5	0.35	0	5,5,5	0.32	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	-	0/10/54/54	0/0/8/8
3	GOL	A	407	-	-	0/4/4/4	0/0/0/0
2	HEM	B	406	1,5	-	0/10/54/54	0/0/8/8
3	GOL	B	407	-	-	0/4/4/4	0/0/0/0

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	406	HEM	C3B-C4B	-7.30	1.45	1.51
2	A	406	HEM	C3B-C4B	-5.92	1.46	1.51
2	A	406	HEM	C3D-C4D	-5.00	1.45	1.51
2	B	406	HEM	C2C-C1C	-4.36	1.44	1.52
2	A	406	HEM	C2C-C1C	-4.27	1.44	1.52
2	B	406	HEM	C3D-C4D	-3.93	1.46	1.51
2	A	406	HEM	C2D-C1D	-2.37	1.44	1.51
2	B	406	HEM	C2B-C1B	-2.13	1.44	1.51
2	B	406	HEM	C2A-C3A	-2.01	1.31	1.37
2	B	406	HEM	C2D-C1D	-2.01	1.45	1.51
2	B	406	HEM	C3B-CAB	2.02	1.55	1.51
2	A	406	HEM	FE-NC	2.14	2.04	1.95
2	B	406	HEM	FE-ND	2.21	2.09	1.97
2	A	406	HEM	C3B-CAB	2.34	1.55	1.51

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	406	HEM	CAA-CBA-CGA	-4.15	105.13	112.75
2	A	406	HEM	C3C-CAC-CBC	-3.54	119.02	124.46
2	B	406	HEM	C3C-CAC-CBC	-3.53	119.04	124.46
2	B	406	HEM	CBA-CAA-C2A	-3.51	106.24	112.53
2	B	406	HEM	CAA-CBA-CGA	-2.94	107.35	112.75
2	B	406	HEM	CAA-C2A-C3A	-2.04	123.17	129.00
2	B	406	HEM	CMA-C3A-C4A	-2.03	125.01	128.36
2	B	406	HEM	C2D-C3D-C4D	2.01	104.91	101.50
2	A	406	HEM	C2D-C3D-C4D	2.16	105.17	101.50
2	A	406	HEM	C3B-C4B-CHC	2.29	126.39	123.16
2	B	406	HEM	CMD-C2D-C3D	2.90	127.19	114.35
2	A	406	HEM	CMD-C2D-C3D	3.08	127.95	114.35
2	B	406	HEM	CAD-C3D-C2D	4.19	125.28	113.22
2	A	406	HEM	CAD-C3D-C2D	4.50	126.16	113.22
2	A	406	HEM	CAD-C3D-C4D	4.59	128.67	112.47
2	A	406	HEM	CMC-C2C-C3C	4.62	128.05	116.53
2	B	406	HEM	CMC-C2C-C3C	4.78	128.47	116.53
2	B	406	HEM	CMB-C2B-C3B	4.88	128.70	116.53
2	B	406	HEM	CAD-C3D-C4D	4.92	129.81	112.47
2	A	406	HEM	CMB-C2B-C3B	4.97	128.95	116.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.



3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	406	HEM	1	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 [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	380/441 (86%)	0.09	12 (3%) 51 50	27, 52, 101, 140	0
1	B	385/441 (87%)	0.08	4 (1%) 84 84	29, 52, 86, 133	1 (0%)
All	All	765/882 (86%)	0.09	16 (2%) 67 66	27, 52, 94, 140	1 (0%)

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	294	GLY	4.8
1	A	65	VAL	3.5
1	A	292	VAL	3.5
1	A	73	ARG	3.4
1	B	381	GLU	3.3
1	A	293	VAL	3.2
1	B	69	GLU	3.1
1	A	218	LEU	2.9
1	A	28	GLU	2.9
1	A	96	PHE	2.8
1	A	92	VAL	2.8
1	A	66	GLU	2.8
1	A	220	ASP	2.6
1	B	75	PRO	2.4
1	A	8	PHE	2.4
1	B	382	ASP	2.2

### 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
3	GOL	B	407	6/6	0.93	0.31	2.67	63,63,63,64	0
4	MG	A	410	1/1	0.82	0.24	2.51	53,53,53,53	0
4	MG	A	408	1/1	0.97	0.20	2.09	34,34,34,34	0
3	GOL	A	407	6/6	0.87	0.20	0.26	45,47,50,51	0
2	HEM	B	406	43/43	0.98	0.18	0.19	21,25,36,38	0
2	HEM	A	406	43/43	0.97	0.16	-0.43	22,26,37,39	0
4	MG	B	409	1/1	0.85	0.12	-1.37	48,48,48,48	0
4	MG	A	411	1/1	0.95	0.13	-	32,32,32,32	0
4	MG	A	409	1/1	0.87	0.24	-	43,43,43,43	0
4	MG	B	408	1/1	0.88	0.24	-	39,39,39,39	0

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

There are no such residues in this entry.