



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2014 – 08:31 AM GMT

PDB ID : 4B7D  
Title : PikC bound to the 10-DML analog with the 3-(N,N-dimethylamino)  
propanoate anchoring group  
Authors : Podust, L.M.  
Deposited on : 2012-08-17  
Resolution : 1.89 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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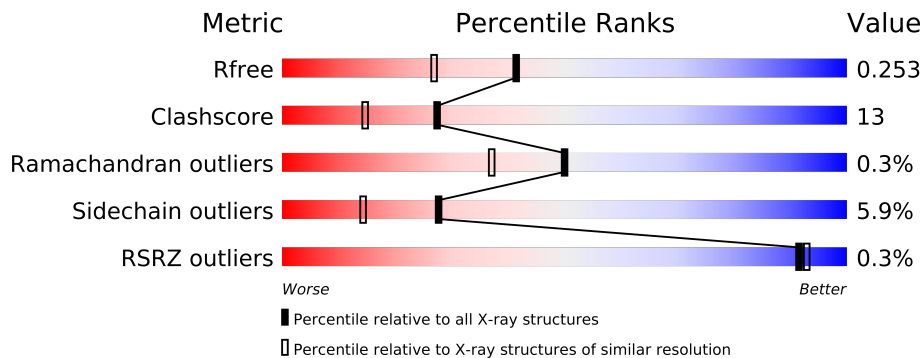
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 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 1.89 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))
$R_{free}$	66092	3684 (1.90-1.90)
Clashscore	79885	4465 (1.90-1.90)
Ramachandran outliers	78287	4413 (1.90-1.90)
Sidechain outliers	78261	4414 (1.90-1.90)
RSRZ outliers	66119	3686 (1.90-1.90)

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. 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	436	
1	B	436	

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	GOL	A	1406	-	X
2	GOL	B	1406	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6719 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 CYTOCHROME P450 HYDROXYLASE PIKC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	393	Total	C	N	O	S	0	1	0
			3038	1919	546	560	13			
1	B	393	Total	C	N	O	S	0	3	0
			3075	1939	554	569	13			

There are 40 discrepancies between the modelled and reference sequences:

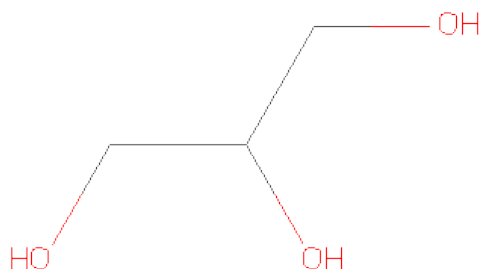
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	EXPRESSION TAG	UNP O87605
A	-18	GLY	-	EXPRESSION TAG	UNP O87605
A	-17	SER	-	EXPRESSION TAG	UNP O87605
A	-16	SER	-	EXPRESSION TAG	UNP O87605
A	-15	HIS	-	EXPRESSION TAG	UNP O87605
A	-14	HIS	-	EXPRESSION TAG	UNP O87605
A	-13	HIS	-	EXPRESSION TAG	UNP O87605
A	-12	HIS	-	EXPRESSION TAG	UNP O87605
A	-11	HIS	-	EXPRESSION TAG	UNP O87605
A	-10	HIS	-	EXPRESSION TAG	UNP O87605
A	-9	SER	-	EXPRESSION TAG	UNP O87605
A	-8	SER	-	EXPRESSION TAG	UNP O87605
A	-7	GLY	-	EXPRESSION TAG	UNP O87605
A	-6	LEU	-	EXPRESSION TAG	UNP O87605
A	-5	VAL	-	EXPRESSION TAG	UNP O87605
A	-4	PRO	-	EXPRESSION TAG	UNP O87605
A	-3	ARG	-	EXPRESSION TAG	UNP O87605
A	-2	GLY	-	EXPRESSION TAG	UNP O87605
A	-1	SER	-	EXPRESSION TAG	UNP O87605
A	0	HIS	-	EXPRESSION TAG	UNP O87605
B	-19	MET	-	EXPRESSION TAG	UNP O87605
B	-18	GLY	-	EXPRESSION TAG	UNP O87605
B	-17	SER	-	EXPRESSION TAG	UNP O87605
B	-16	SER	-	EXPRESSION TAG	UNP O87605
B	-15	HIS	-	EXPRESSION TAG	UNP O87605

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	HIS	-	EXPRESSION TAG	UNP O87605
B	-13	HIS	-	EXPRESSION TAG	UNP O87605
B	-12	HIS	-	EXPRESSION TAG	UNP O87605
B	-11	HIS	-	EXPRESSION TAG	UNP O87605
B	-10	HIS	-	EXPRESSION TAG	UNP O87605
B	-9	SER	-	EXPRESSION TAG	UNP O87605
B	-8	SER	-	EXPRESSION TAG	UNP O87605
B	-7	GLY	-	EXPRESSION TAG	UNP O87605
B	-6	LEU	-	EXPRESSION TAG	UNP O87605
B	-5	VAL	-	EXPRESSION TAG	UNP O87605
B	-4	PRO	-	EXPRESSION TAG	UNP O87605
B	-3	ARG	-	EXPRESSION TAG	UNP O87605
B	-2	GLY	-	EXPRESSION TAG	UNP O87605
B	-1	SER	-	EXPRESSION TAG	UNP O87605
B	0	HIS	-	EXPRESSION TAG	UNP O87605

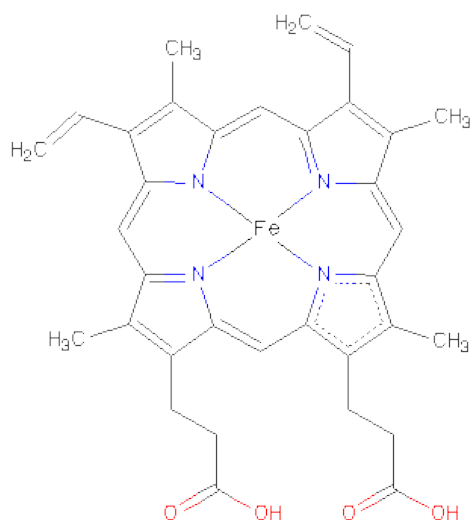
- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

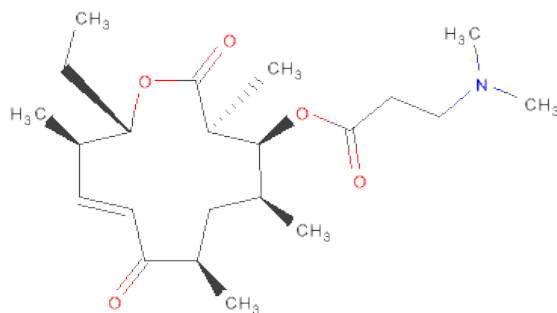
- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (for-

mula:  $C_{34}H_{32}FeN_4O_4$ ).



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

- Molecule 4 is [(3R,4S,5S,7R,9E,11R,12R)-12-ETHYL-3,5,7,11-TETRAMETHYL-2,8-BIS(OXIDANYLIDENE)-1-OXACYCLODODEC-9-EN-4-YL]3-(DIMETHYLAMINO)PROPANOATE (three-letter code: QLE) (formula:  $C_{22}H_{37}NO_5$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			28	22	1	5		
4	B	1	Total	C	N	O	0	0
			28	22	1	5		

- Molecule 5 is water.

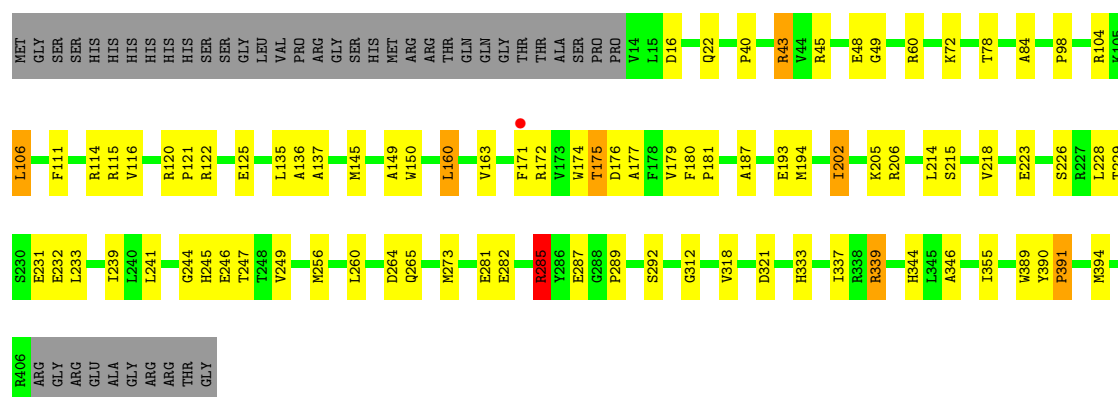
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	226	Total	O	0	0
			226	226		
5	B	220	Total	O	0	0
			220	220		

### 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.

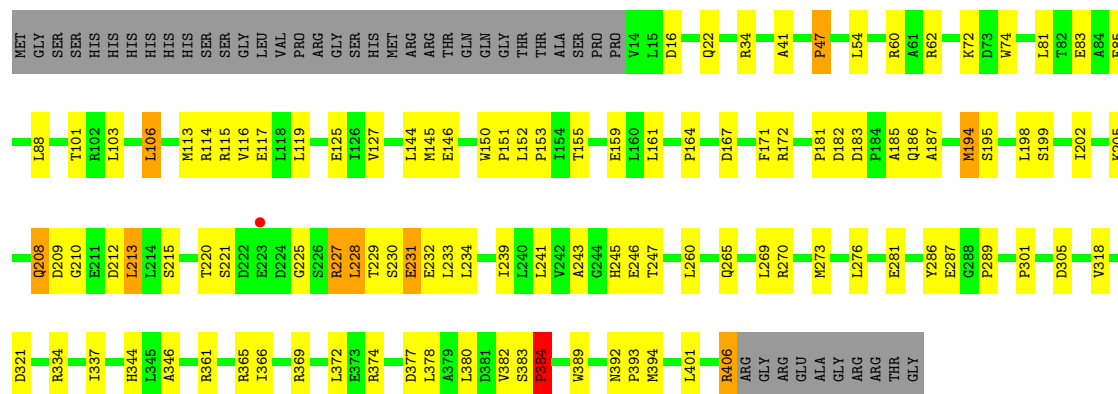
#### • Molecule 1: CYTOCHROME P450 HYDROXYLASE PIKC

Chain A: 



#### • Molecule 1: CYTOCHROME P450 HYDROXYLASE PIKC

Chain B: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	36.77Å 58.04Å 96.42Å 79.96° 79.52° 88.73°	Depositor
Resolution (Å)	93.37 – 1.89 93.37 – 1.89	Depositor EDS
% Data completeness (in resolution range)	93.9 (93.37-1.89) 93.9 (93.37-1.89)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.66 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.200 , 0.257 0.200 , 0.253	Depositor DCC
$R_{free}$ test set	2967 reflections (5.39%)	DCC
Wilson B-factor (Å <sup>2</sup> )	24.4	Xtriage
Anisotropy	0.758	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 30.1	EDS
Estimated twinning fraction	0.188 for h,-k,h-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 58035 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	6719	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.59% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities 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: GOL, QLE, 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	1.04	1/3109 (0.0%)	1.05	7/4244 (0.2%)
1	B	1.05	1/3146 (0.0%)	0.98	2/4292 (0.0%)
All	All	1.04	2/6255 (0.0%)	1.02	9/8536 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	287	GLU	CB-CG	6.42	1.64	1.52
1	B	125	GLU	CG-CD	5.13	1.59	1.51

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	285	ARG	NE-CZ-NH2	-17.89	111.36	120.30
1	A	285	ARG	NE-CZ-NH1	13.39	126.99	120.30
1	B	161	LEU	CB-CG-CD1	-6.05	100.71	111.00
1	A	16	ASP	CB-CG-OD1	5.91	123.62	118.30
1	A	160	LEU	CA-CB-CG	-5.60	102.42	115.30
1	A	285	ARG	CG-CD-NE	-5.44	100.38	111.80
1	A	285	ARG	CD-NE-CZ	5.24	130.93	123.60
1	B	16	ASP	CB-CG-OD1	5.19	122.97	118.30
1	A	273	MET	CG-SD-CE	-5.03	92.15	100.20

There are no chirality outliers.

There are no planarity outliers.

## 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	3038	0	2998	72	0
1	B	3075	0	3045	84	0
2	A	6	0	8	0	0
2	B	12	0	16	2	0
3	A	43	0	30	9	0
3	B	43	0	30	3	0
4	A	28	0	37	11	0
4	B	28	0	37	6	0
5	A	226	0	0	6	0
5	B	220	0	0	13	0
All	All	6719	0	6201	161	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 13.

All (161) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:264:ASP:HB2	5:A:2167:HOH:O	1.69	0.93
1:B:34:ARG:HD2	5:B:2022:HOH:O	1.69	0.93
1:A:175:THR:HG21	1:A:245:HIS:HE1	1.32	0.91
1:A:111:PHE:CE1	3:A:1407:HEM:HBC1	2.06	0.90
1:A:344:HIS:HD2	1:A:346:ALA:H	1.18	0.89
1:B:239:ILE:HD12	3:B:1407:HEM:HMD3	1.53	0.87
1:A:150:TRP:CZ2	1:A:172:ARG:HB2	2.12	0.83
1:A:282:GLU:OE1	1:A:285:ARG:HD3	1.78	0.81
1:B:406:ARG:C	5:B:2219:HOH:O	2.18	0.81
1:B:344:HIS:HD2	1:B:346:ALA:H	1.26	0.81
1:A:394:MET:HE2	4:A:1408:QLE:C21	2.10	0.80
1:B:301:PRO:HG3	5:B:2185:HOH:O	1.82	0.77
1:A:104:ARG:NH1	3:A:1407:HEM:O2D	2.18	0.75
1:A:394:MET:CE	4:A:1408:QLE:C21	2.67	0.73
1:A:43:ARG:HH11	1:A:43:ARG:HB3	1.54	0.73
1:A:111:PHE:CZ	3:A:1407:HEM:HBC1	2.24	0.72
1:A:394:MET:HE2	4:A:1408:QLE:H213	1.70	0.72

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:344:HIS:CD2	1:A:346:ALA:H	2.07	0.71
1:B:221:SER:O	1:B:225:GLY:HA2	1.90	0.71
1:A:394:MET:CE	4:A:1408:QLE:H213	2.23	0.69
1:B:22:GLN:HE22	1:B:389:TRP:H	1.39	0.67
1:A:163:VAL:HG11	1:A:171:PHE:HE2	1.59	0.67
1:B:229:THR:HB	1:B:232:GLU:HG3	1.77	0.66
1:B:144:LEU:HD23	1:B:401:LEU:HD23	1.78	0.65
1:A:256:MET:O	1:A:260:LEU:HG	1.97	0.65
1:A:22:GLN:HE22	1:A:389:TRP:H	1.46	0.64
1:B:152:LEU:HB3	1:B:153:PRO:HD3	1.80	0.63
1:A:175:THR:HG21	1:A:245:HIS:CE1	2.24	0.63
1:B:229:THR:HG22	1:B:230:SER:N	2.13	0.63
1:A:111:PHE:CE1	3:A:1407:HEM:CBC	2.81	0.62
1:B:273:MET:O	1:B:273:MET:HG3	2.00	0.62
1:B:247[A]:THR:HG21	4:B:1408:QLE:HA	1.79	0.62
1:B:227[A]:ARG:HB2	1:B:227[A]:ARG:HH11	1.66	0.61
1:A:394:MET:CE	4:A:1408:QLE:H211	2.30	0.61
1:B:228:LEU:HD12	1:B:232:GLU:HB2	1.82	0.60
1:B:227[A]:ARG:CB	1:B:227[A]:ARG:HH11	2.14	0.60
1:A:171:PHE:HD1	1:A:194:MET:CE	2.14	0.60
1:A:282:GLU:OE1	1:A:285:ARG:CD	2.49	0.59
1:A:205:LYS:HD2	1:A:215[A]:SER:OG	2.01	0.59
1:B:220:THR:HG23	1:B:227[A]:ARG:HH12	1.68	0.58
1:B:113:MET:O	1:B:117:GLU:HB2	2.03	0.58
1:A:40:PRO:HB2	1:A:60:ARG:HG2	1.85	0.58
1:A:163:VAL:HG11	1:A:171:PHE:CE2	2.39	0.58
1:B:60:ARG:NH2	1:B:305:ASP:HB2	2.19	0.57
1:B:85:GLU:HB3	4:B:1408:QLE:H163	1.85	0.57
1:B:334:ARG:HG3	1:B:334:ARG:HH11	1.70	0.56
1:B:146:GLU:OE2	1:B:172:ARG:NH2	2.35	0.56
1:A:181:PRO:HG3	1:A:187:ALA:HB2	1.87	0.56
1:B:210:GLY:CA	5:B:2140:HOH:O	2.54	0.55
1:B:183:ASP:OD2	1:B:185:ALA:HB3	2.06	0.55
1:B:60:ARG:HH22	1:B:305:ASP:HB2	1.71	0.55
1:B:164:PRO:HG2	1:B:167:ASP:OD2	2.06	0.55
1:B:213:LEU:HD12	1:B:213:LEU:O	2.07	0.55
1:A:116:VAL:HG12	5:A:2102:HOH:O	2.07	0.55
1:B:241:LEU:O	1:B:245:HIS:HB3	2.07	0.55
1:A:228:LEU:HD23	1:A:233:LEU:HD13	1.90	0.54
1:A:48:GLU:HG3	5:A:2040:HOH:O	2.05	0.54
1:B:88:LEU:HD21	1:B:195:SER:OG	2.07	0.54
1:B:406:ARG:HB3	1:B:406:ARG:CZ	2.35	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:43:ARG:HB3	1:A:43:ARG:NH1	2.21	0.53
1:A:163:VAL:CG1	1:A:171:PHE:HE2	2.20	0.53
1:A:145:MET:HA	1:A:149:ALA:HB3	1.91	0.53
1:A:171:PHE:HD1	1:A:194:MET:HE1	1.74	0.52
1:A:122:ARG:NH1	1:A:125:GLU:OE1	2.41	0.52
1:B:289:PRO:HG2	3:B:1407:HEM:HMB2	1.92	0.52
1:A:78:THR:HG23	1:A:312:GLY:HA3	1.92	0.52
1:B:227[A]:ARG:CB	1:B:227[A]:ARG:NH1	2.73	0.51
1:A:174:TRP:NE1	1:A:193:GLU:HG2	2.26	0.51
1:A:171:PHE:O	1:A:175:THR:HB	2.09	0.51
1:B:361:ARG:O	1:B:365:ARG:HG3	2.10	0.51
1:A:394:MET:HE1	4:A:1408:QLE:C21	2.41	0.51
1:B:182:ASP:HB2	1:B:186:GLN:OE1	2.10	0.51
1:A:333:HIS:HE1	5:A:2022:HOH:O	1.93	0.51
1:A:265:GLN:NE2	1:A:337:ILE:H	2.09	0.50
1:B:74:TRP:CD2	1:B:81:LEU:HD21	2.46	0.50
1:A:202:ILE:HG13	1:A:214:LEU:HD11	1.94	0.50
1:B:212:ASP:C	1:B:212:ASP:OD1	2.49	0.50
1:B:229:THR:CG2	1:B:230:SER:N	2.75	0.50
1:B:265:GLN:NE2	1:B:337:ILE:HG12	2.27	0.50
1:A:175:THR:CG2	1:A:246:GLU:OE1	2.60	0.49
1:A:244:GLY:HA2	3:A:1407:HEM:HMC2	1.93	0.49
1:A:228:LEU:CD2	1:A:233:LEU:HD13	2.42	0.49
1:B:208:GLN:HB2	5:B:2078:HOH:O	2.11	0.49
1:B:182:ASP:CB	1:B:186:GLN:OE1	2.60	0.49
1:B:181:PRO:HB3	1:B:187:ALA:HB2	1.94	0.49
3:A:1407:HEM:C2D	4:A:1408:QLE:H71C	2.47	0.49
1:B:171:PHE:HD1	1:B:194:MET:HE1	1.77	0.49
1:A:394:MET:HE1	4:A:1408:QLE:H211	1.93	0.49
1:B:155:THR:O	1:B:159:GLU:HG3	2.12	0.49
1:B:392:ASN:N	5:B:2218:HOH:O	2.45	0.49
1:A:318:VAL:HG12	1:A:321:ASP:H	1.78	0.48
4:B:1408:QLE:H192	4:B:1408:QLE:H9	1.69	0.48
1:A:106:LEU:CD2	1:A:228:LEU:HD13	2.43	0.48
1:B:183:ASP:OD1	1:B:186:GLN:HB2	2.14	0.48
1:B:394:MET:HE1	2:B:1406:GOL:H12	1.95	0.48
1:B:394:MET:CE	4:B:1408:QLE:H213	2.44	0.47
1:B:127:VAL:HG21	1:B:366:ILE:HG22	1.95	0.47
1:B:198:LEU:O	1:B:202:ILE:HG13	2.14	0.47
1:B:227[A]:ARG:HB3	1:B:227[A]:ARG:NH1	2.29	0.47
1:B:318:VAL:HG12	1:B:321:ASP:H	1.79	0.47
1:A:45:ARG:CZ	1:A:45:ARG:HB2	2.43	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:174:TRP:HE3	1:A:194:MET:HE2	1.80	0.47
1:A:355:ILE:HD11	3:A:1407:HEM:HMD2	1.96	0.47
1:B:243:ALA:HA	1:B:247[A]:THR:HG23	1.96	0.47
1:A:179:VAL:HG12	1:A:180:PHE:CZ	2.50	0.47
1:B:265:GLN:NE2	1:B:337:ILE:H	2.14	0.46
1:B:229:THR:HG22	1:B:231:GLU:H	1.80	0.46
1:B:269:LEU:HD11	1:B:276:LEU:HA	1.97	0.46
1:B:394:MET:CE	2:B:1406:GOL:H12	2.45	0.46
1:B:334:ARG:NH1	1:B:334:ARG:HG3	2.30	0.46
1:B:281:GLU:OE1	1:B:344:HIS:HE1	1.98	0.46
1:B:106:LEU:CD2	1:B:228:LEU:HD22	2.46	0.46
1:A:394:MET:HB3	1:A:394:MET:HE2	1.80	0.45
1:B:286:TYR:CD2	1:B:287:GLU:HG2	2.52	0.45
1:A:281:GLU:OE1	1:A:344:HIS:HE1	1.99	0.45
1:B:233:LEU:HD12	1:B:233:LEU:HA	1.85	0.45
1:A:98:PRO:HD2	5:A:2091:HOH:O	2.17	0.45
1:A:171:PHE:HD1	1:A:194:MET:HE2	1.81	0.45
3:A:1407:HEM:C3D	4:A:1408:QLE:H71C	2.52	0.45
1:A:202:ILE:HG23	1:A:218:VAL:HG22	1.99	0.45
1:B:205:LYS:HD2	1:B:215:SER:OG	2.17	0.45
1:A:120:ARG:HB3	1:A:121:PRO:HD3	1.98	0.45
1:B:210:GLY:HA3	5:B:2140:HOH:O	2.17	0.44
3:B:1407:HEM:HMB2	3:B:1407:HEM:HBB2	1.99	0.44
1:A:135:LEU:O	1:A:137:ALA:N	2.50	0.44
1:A:390:TYR:HA	1:A:391:PRO:HD3	1.91	0.44
1:B:145:MET:HE2	1:B:145:MET:HB2	1.89	0.44
1:B:41:ALA:HA	1:B:54:LEU:O	2.17	0.44
1:B:34:ARG:NH2	5:B:2023:HOH:O	2.51	0.44
1:A:229:THR:OG1	1:A:232:GLU:HG3	2.18	0.44
1:A:150:TRP:CE3	1:A:249:VAL:HG21	2.53	0.43
1:B:234:LEU:HD12	1:B:234:LEU:HA	1.74	0.43
1:B:270:ARG:NH1	5:B:2159:HOH:O	2.50	0.43
1:B:273:MET:HG2	1:B:369:ARG:CZ	2.48	0.43
1:B:119:LEU:HD23	5:B:2106:HOH:O	2.19	0.43
1:B:374:ARG:HD3	5:B:2112:HOH:O	2.18	0.42
1:A:285:ARG:HD2	1:A:339:ARG:HD2	2.01	0.42
1:A:84:ALA:HA	5:A:2037:HOH:O	2.19	0.42
1:B:245:HIS:CG	1:B:246:GLU:N	2.87	0.42
1:B:270:ARG:HH12	1:B:377:ASP:HA	1.85	0.42
1:A:45:ARG:HD3	1:A:49:GLY:HA2	2.01	0.42
4:A:1408:QLE:H43C	4:A:1408:QLE:H1	1.78	0.42
1:B:150:TRP:CE3	1:B:151:PRO:HG3	2.54	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:245:HIS:ND1	1:A:246:GLU:N	2.68	0.42
1:A:239:ILE:HD11	4:A:1408:QLE:H102	2.01	0.42
1:B:243:ALA:HB2	4:B:1408:QLE:H62C	2.02	0.42
1:B:103:LEU:O	1:B:106:LEU:HB2	2.21	0.41
1:B:394:MET:HB3	1:B:394:MET:HE2	1.72	0.41
1:B:62:ARG:HD3	5:B:2050:HOH:O	2.19	0.41
1:B:380:LEU:HD23	1:B:384:PRO:HD3	2.02	0.41
1:B:383[B]:SER:O	1:B:384:PRO:C	2.59	0.41
1:A:205:LYS:HD2	1:A:215[A]:SER:HG	1.84	0.41
1:A:177:ALA:O	1:A:181:PRO:HB3	2.20	0.41
1:B:270:ARG:CZ	5:B:2156:HOH:O	2.68	0.41
1:B:394:MET:HE2	4:B:1408:QLE:H213	2.03	0.41
1:A:241:LEU:HD23	1:A:241:LEU:HA	1.93	0.41
1:A:289:PRO:HG2	3:A:1407:HEM:HMB2	2.03	0.40
1:B:260:LEU:HD21	1:B:378:LEU:HG	2.03	0.40
1:B:47:PRO:HD2	1:B:393:PRO:HD3	2.02	0.40
1:A:355:ILE:HD13	1:A:355:ILE:HG21	1.92	0.40
1:A:292:SER:HB2	1:A:394:MET:HA	2.04	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	392/436 (90%)	374 (95%)	17 (4%)	1 (0%)	50	37
1	B	394/436 (90%)	372 (94%)	21 (5%)	1 (0%)	50	37
All	All	786/872 (90%)	746 (95%)	38 (5%)	2 (0%)	50	37

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	136	ALA
1	B	384	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	314/355 (88%)	297 (95%)	17 (5%)	31	17
1	B	321/355 (90%)	300 (94%)	21 (6%)	24	11
All	All	635/710 (89%)	597 (94%)	38 (6%)	28	13

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	ARG
1	A	72	LYS
1	A	106	LEU
1	A	114	ARG
1	A	115	ARG
1	A	160	LEU
1	A	175	THR
1	A	176	ASP
1	A	202	ILE
1	A	206	ARG
1	A	223	GLU
1	A	226	SER
1	A	231	GLU
1	A	247	THR
1	A	285	ARG
1	A	339	ARG
1	A	391	PRO
1	B	47	PRO
1	B	72	LYS
1	B	83	GLU
1	B	101	THR
1	B	106	LEU
1	B	114	ARG
1	B	115	ARG
1	B	116	VAL
1	B	194	MET
1	B	199	SER
1	B	208	GLN
1	B	209	ASP

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Mol	Chain	Res	Type
1	B	213	LEU
1	B	227[A]	ARG
1	B	227[B]	ARG
1	B	228	LEU
1	B	231	GLU
1	B	372	LEU
1	B	382	VAL
1	B	384	PRO
1	B	406	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	GLN
1	A	188	GLN
1	A	265	GLN
1	A	344	HIS
1	B	22	GLN
1	B	188	GLN
1	B	208	GLN
1	B	265	GLN
1	B	344	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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

7 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$
2	GOL	A	1406	-	5,5,5	0.65	0	5,5,5	0.91	0
3	HEM	A	1407	1	49,50,50	3.68	19 (38%)	46,82,82	2.47	10 (21%)
4	QLE	A	1408	-	28,28,28	1.47	2 (7%)	38,38,38	1.77	7 (18%)
2	GOL	B	1406	-	5,5,5	0.45	0	5,5,5	1.32	0
3	HEM	B	1407	1	49,50,50	3.84	19 (38%)	46,82,82	2.22	11 (23%)
4	QLE	B	1408	-	28,28,28	1.32	2 (7%)	38,38,38	1.95	9 (23%)
2	GOL	B	1409	-	5,5,5	0.75	0	5,5,5	1.10	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	GOL	A	1406	-	-	0/4/4/4	0/0/0/0
3	HEM	A	1407	1	-	0/14/114/114	0/0/8/8
4	QLE	A	1408	-	-	0/44/44/44	0/0/1/1
2	GOL	B	1406	-	-	0/4/4/4	0/0/0/0
3	HEM	B	1407	1	-	0/14/114/114	0/0/8/8
4	QLE	B	1408	-	-	0/44/44/44	0/0/1/1
2	GOL	B	1409	-	-	0/4/4/4	0/0/0/0

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1407	HEM	C3D-C4D	16.53	1.48	1.44
3	B	1407	HEM	C2B-C1B	15.26	1.48	1.44
3	B	1407	HEM	C3D-C4D	12.41	1.47	1.44
3	A	1407	HEM	C2D-C1D	11.87	1.47	1.44
3	B	1407	HEM	C2D-C1D	9.03	1.46	1.44
4	A	1408	QLE	O1-C8	5.79	1.47	1.34
3	B	1407	HEM	C3C-C2C	-5.52	1.34	1.43
3	B	1407	HEM	C4A-C3A	5.43	1.47	1.40
3	A	1407	HEM	C3C-C2C	-5.10	1.34	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1408	QLE	O1-C8	5.06	1.45	1.34
3	A	1407	HEM	FE-ND	4.81	2.15	1.97
3	B	1407	HEM	C3B-C2B	-4.77	1.35	1.43
3	B	1407	HEM	C3B-CAB	4.44	1.54	1.40
3	A	1407	HEM	C2B-C1B	4.39	1.45	1.44
3	A	1407	HEM	C3D-C2D	4.36	1.51	1.43
3	A	1407	HEM	FE-NC	4.21	2.13	1.97
3	B	1407	HEM	FE-ND	4.12	2.12	1.97
3	A	1407	HEM	C4A-C3A	3.97	1.45	1.40
3	B	1407	HEM	FE-NA	3.91	2.09	1.92
3	A	1407	HEM	C3B-CAB	3.90	1.52	1.40
3	B	1407	HEM	C3D-C2D	3.89	1.50	1.43
4	A	1408	QLE	O3-C12	3.80	1.45	1.34
3	B	1407	HEM	C3C-CAC	3.78	1.52	1.40
3	A	1407	HEM	C3B-C2B	-3.68	1.37	1.43
3	A	1407	HEM	C3C-CAC	3.66	1.51	1.40
3	A	1407	HEM	FE-NA	3.53	2.07	1.92
4	B	1408	QLE	O3-C12	3.51	1.45	1.34
3	A	1407	HEM	CMB-C2B	3.49	1.58	1.47
3	B	1407	HEM	FE-NB	3.27	2.09	1.97
3	A	1407	HEM	CHB-C1B	3.00	1.40	1.35
3	B	1407	HEM	FE-NC	2.85	2.08	1.97
3	A	1407	HEM	CMD-C2D	2.76	1.56	1.47
3	B	1407	HEM	CHA-C4D	2.69	1.39	1.35
3	B	1407	HEM	CMC-C2C	2.64	1.55	1.47
3	B	1407	HEM	CMB-C2B	2.60	1.55	1.47
3	A	1407	HEM	CMC-C2C	2.59	1.55	1.47
3	B	1407	HEM	CMA-C3A	2.58	1.57	1.51
3	B	1407	HEM	CMD-C2D	2.50	1.55	1.47
3	A	1407	HEM	CMA-C3A	2.36	1.56	1.51
3	B	1407	HEM	CHC-C1C	2.23	1.40	1.36
3	A	1407	HEM	FE-NB	2.21	2.05	1.97
3	A	1407	HEM	CAA-C2A	2.03	1.55	1.52

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1407	HEM	C3B-C4B-NB	-9.07	107.51	114.00
3	A	1407	HEM	C4D-ND-C1D	7.65	112.99	105.16
3	B	1407	HEM	C4D-ND-C1D	7.59	112.93	105.16
3	B	1407	HEM	C3B-C4B-NB	-6.79	109.14	114.00
4	B	1408	QLE	C13-C14-N	-6.18	104.79	113.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1408	QLE	C5-C3-C2	-5.53	100.50	110.62
3	A	1407	HEM	CBD-CAD-C3D	-5.51	102.35	114.37
4	A	1408	QLE	O5-C22-C20	-4.58	111.75	121.20
4	A	1408	QLE	C13-C14-N	-4.55	107.06	113.42
3	B	1407	HEM	C4C-NC-C1C	4.51	110.22	105.53
3	A	1407	HEM	C2D-C1D-ND	-4.40	107.74	112.93
3	B	1407	HEM	CBD-CAD-C3D	-4.09	105.45	114.37
3	B	1407	HEM	C2D-C1D-ND	-3.86	108.38	112.93
4	A	1408	QLE	C5-C3-C2	-3.78	103.70	110.62
4	B	1408	QLE	O1-C8-C9	3.59	119.97	111.64
3	A	1407	HEM	C1B-NB-C4B	3.59	108.83	105.16
3	A	1407	HEM	C4C-NC-C1C	3.54	109.21	105.53
4	B	1408	QLE	C4-C3-C2	3.46	118.36	110.05
3	B	1407	HEM	O1A-CGA-CBA	-3.34	111.55	123.03
4	A	1408	QLE	O3-C12-C13	3.25	118.67	111.56
3	A	1407	HEM	CHC-C4B-NB	3.05	127.12	124.58
4	B	1408	QLE	O5-C22-C20	-3.01	114.99	121.20
4	A	1408	QLE	O1-C8-C9	2.96	118.51	111.64
3	B	1407	HEM	C1B-NB-C4B	2.87	108.09	105.16
4	B	1408	QLE	O1-C8-O2	-2.75	118.35	123.83
3	A	1407	HEM	CBA-CAA-C2A	-2.74	107.86	112.69
4	B	1408	QLE	C2-C1-C22	-2.40	119.85	124.01
3	A	1407	HEM	CMA-C3A-C4A	-2.38	124.96	128.62
4	A	1408	QLE	O3-C12-O4	-2.36	117.32	123.65
4	A	1408	QLE	C15-N-C14	-2.19	101.75	110.76
3	B	1407	HEM	CMA-C3A-C4A	-2.17	125.29	128.62
4	B	1408	QLE	C3-C2-C1	2.12	133.23	126.47
4	B	1408	QLE	C10-C9-C11	-2.11	107.97	112.84
3	A	1407	HEM	CMB-C2B-C3B	2.08	131.07	126.16
3	B	1407	HEM	O2A-CGA-CBA	2.06	121.50	114.22
3	B	1407	HEM	C3A-C4A-NA	-2.02	107.89	109.41
3	B	1407	HEM	CAD-C3D-C4D	2.02	128.16	124.53

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, 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	393/436 (90%)	-0.31	1 (0%) 91 93	13, 28, 47, 55	0
1	B	393/436 (90%)	-0.23	1 (0%) 91 93	14, 29, 51, 68	0
All	All	786/872 (90%)	-0.27	2 (0%) 91 93	13, 29, 50, 68	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	223	GLU	2.7
1	A	171	PHE	2.1

### 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 ⓘ

There are no carbohydrates in this entry.

### 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, 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	GOL	B	1406	6/6	0.11	4.72	25,36,38,44	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	GOL	A	1406	6/6	0.11	3.33	20,31,37,39	0
2	GOL	B	1409	6/6	0.11	1.20	37,40,41,46	0
4	QLE	A	1408	28/28	0.12	1.16	21,31,35,36	0
4	QLE	B	1408	28/28	0.12	1.09	21,27,32,34	0
3	HEM	B	1407	43/43	0.08	-0.29	10,17,20,26	0
3	HEM	A	1407	43/43	0.08	-0.32	12,17,21,32	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.