



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 08:11 PM GMT

PDB ID : 3TNK  
Title : Crystal structure of mutant I87R in CYP158A2  
Authors : Zhao, B.; Waterman, M.R.  
Deposited on : 2011-09-01  
Resolution : 1.76 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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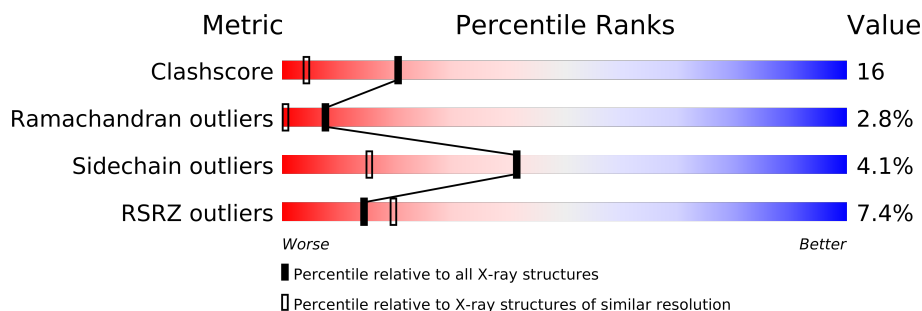
The following versions of software and data (see [references](#)) were used in the production of this report:

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 1.76 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	1304 (1.76-1.76)
Ramachandran outliers	78287	1288 (1.76-1.76)
Sidechain outliers	78261	1288 (1.76-1.76)
RSRZ outliers	66119	1135 (1.76-1.76)

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	407	
1	B	407	

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

Mol	Type	Chain	Res	Geometry	Electron density
3	SPM	B	432	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6842 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 Putative cytochrome P450.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	402	Total	C	N	O	S	0	0	0
			3112	1956	571	574	11			
1	B	402	Total	C	N	O	S	0	0	0
			3112	1956	571	574	11			

There are 8 discrepancies between the modelled and reference sequences:

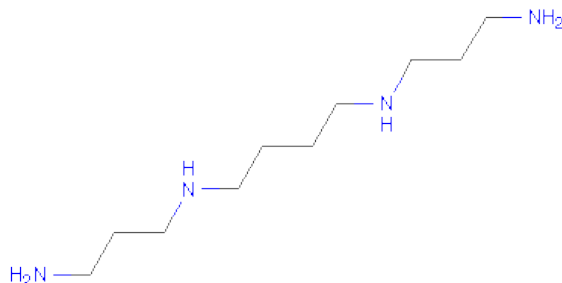
Chain	Residue	Modelled	Actual	Comment	Reference
A	87	ARG	ILE	ENGINEERED MUTATION	UNP Q9FCA6
A	405	HIS	-	EXPRESSION TAG	UNP Q9FCA6
A	406	HIS	-	EXPRESSION TAG	UNP Q9FCA6
A	407	HEM	-	EXPRESSION TAG	UNP Q9FCA6
B	87	ARG	ILE	ENGINEERED MUTATION	UNP Q9FCA6
B	405	HIS	-	EXPRESSION TAG	UNP Q9FCA6
B	406	HIS	-	EXPRESSION TAG	UNP Q9FCA6
B	407	HEM	-	EXPRESSION TAG	UNP Q9FCA6

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C<sub>34</sub>H<sub>32</sub>FeN<sub>4</sub>O<sub>4</sub>).



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 SPERMINE (three-letter code: SPM) (formula:  $C_{10}H_{26}N_4$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	N	0	0
			14	10	4		

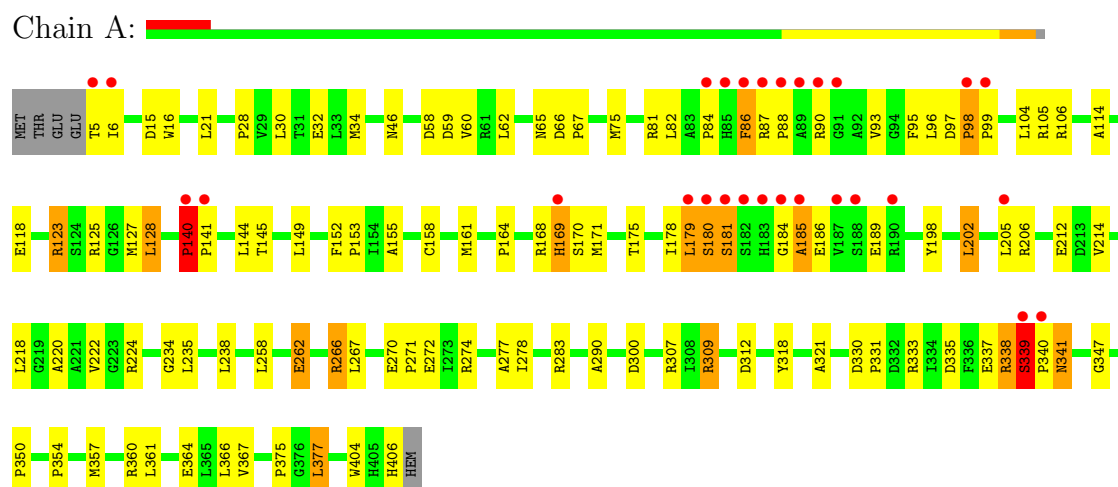
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	245	Total 245	O 245	0	0
4	B	273	Total 273	O 273	0	0

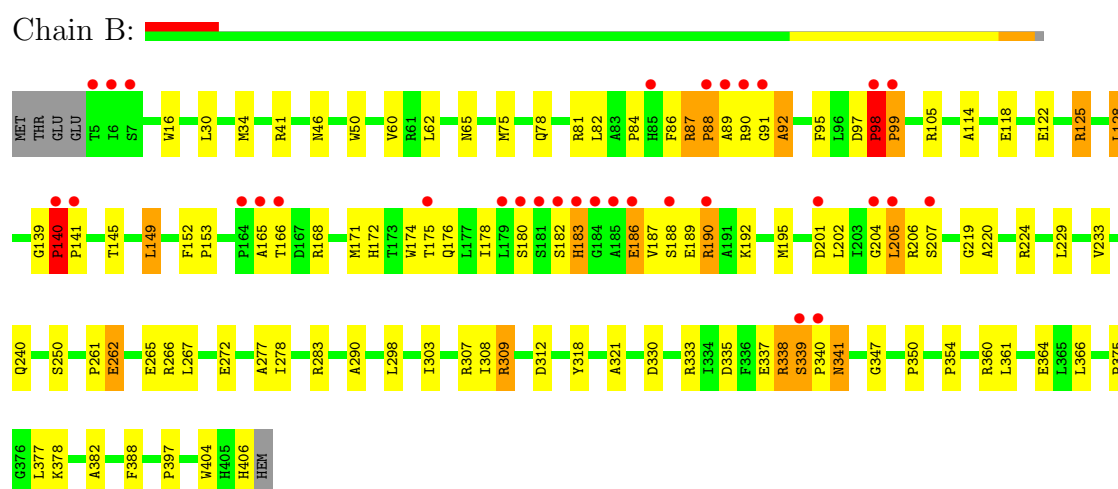
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: Putative cytochrome P450



#### • Molecule 1: Putative cytochrome P450



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	59.61Å 79.31Å 87.66Å 90.00° 94.08° 90.00°	Depositor
Resolution (Å)	30.00 – 1.76 47.57 – 1.76	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-1.76) 93.5 (47.57-1.76)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	0.17	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.54 (at 1.76Å)	Xtriage
Refinement program	CNS1.3	Depositor
R, $R_{free}$	0.222 , 0.268 0.226 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	11.3	Xtriage
Anisotropy	0.367	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 30.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 79247 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	6842	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.64% 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: HEM, SPM

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	0.29	0/3185	0.58	0/4339
1	B	0.29	0/3185	0.57	0/4339
All	All	0.29	0/6370	0.58	0/8678

There are no bond length outliers.

There are no bond angle outliers.

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	3112	0	3097	98	0
1	B	3112	0	3097	103	0
2	A	43	0	30	0	0
2	B	43	0	30	0	0
3	B	14	0	26	5	0
4	A	245	0	0	1	0
4	B	273	0	0	4	0
All	All	6842	0	6280	198	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 16.

All (198) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:339:SER:HB2	1:B:340:PRO:HD3	1.39	1.04
1:B:105:ARG:CZ	1:B:354:PRO:HG3	2.00	0.91
1:A:178:ILE:HG22	1:A:179:LEU:HG	1.53	0.91
1:B:378:LYS:HE3	3:B:432:SPM:HN5	1.40	0.87
1:A:105:ARG:CZ	1:A:354:PRO:HG3	2.05	0.84
1:B:378:LYS:CE	3:B:432:SPM:HN5	1.92	0.82
1:B:283:ARG:HD3	1:B:341:ASN:HD21	1.46	0.80
1:A:283:ARG:HD3	1:A:341:ASN:HD21	1.50	0.78
1:B:97:ASP:HB3	1:B:98:PRO:HD2	1.67	0.75
1:A:140:PRO:HG2	1:A:406:HIS:HB2	1.69	0.75
1:A:278:ILE:HD11	1:A:367:VAL:HG21	1.68	0.74
1:A:144:LEU:HG	1:A:149:LEU:HD13	1.68	0.74
1:B:175:THR:HG21	4:B:455:HOH:O	1.87	0.74
1:A:266:ARG:HH11	1:A:266:ARG:HG3	1.54	0.73
1:A:123:ARG:HA	1:A:123:ARG:HE	1.54	0.72
1:B:87:ARG:H	1:B:88:PRO:CD	2.02	0.72
1:B:220:ALA:HB1	1:B:224:ARG:HH22	1.55	0.72
1:B:78:GLN:NE2	1:B:81:ARG:HH12	1.88	0.71
1:B:171:MET:HE1	1:B:240:GLN:HG2	1.73	0.70
1:B:339:SER:HB2	1:B:340:PRO:CD	2.18	0.70
1:A:28:PRO:O	1:A:32:GLU:HG3	1.91	0.70
1:B:178:ILE:HD12	1:B:195:MET:HE3	1.75	0.69
1:B:87:ARG:H	1:B:88:PRO:HD2	1.56	0.69
1:B:140:PRO:CG	1:B:406:HIS:HB2	2.22	0.69
1:A:140:PRO:CG	1:A:406:HIS:HB2	2.24	0.67
1:B:339:SER:CB	1:B:340:PRO:HD3	2.22	0.67
1:A:97:ASP:C	1:A:99:PRO:HD2	2.15	0.66
1:B:75:MET:HE2	1:B:89:ALA:HB2	1.78	0.66
1:A:220:ALA:HB1	1:A:224:ARG:HH22	1.61	0.66
1:B:202:LEU:O	1:B:206:ARG:HG3	1.95	0.66
1:A:339:SER:CB	1:A:340:PRO:HD3	2.26	0.65
1:A:171:MET:O	1:A:175:THR:HG23	1.96	0.65
1:A:234:GLY:O	1:A:238:LEU:HD13	1.97	0.65
1:A:114:ALA:O	1:A:118:GLU:HG2	1.98	0.64
1:B:201:ASP:O	1:B:205:LEU:HD13	1.99	0.63
1:B:105:ARG:NH2	1:B:354:PRO:HG3	2.13	0.63
1:A:169:HIS:HD2	1:A:170:SER:H	1.46	0.63
1:B:171:MET:O	1:B:175:THR:HG23	1.99	0.63
1:A:81:ARG:NE	1:A:86:PHE:HB2	2.15	0.62
1:B:152:PHE:HB3	1:B:153:PRO:HD3	1.81	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:140:PRO:HB2	1:B:141:PRO:HD3	1.82	0.61
1:B:207:SER:HA	1:B:219:GLY:O	2.01	0.61
1:B:261:PRO:O	1:B:265:GLU:HG3	2.00	0.61
1:B:187:VAL:O	1:B:190:ARG:HG3	2.00	0.60
1:A:75:MET:HE1	1:A:90:ARG:HA	1.83	0.60
1:B:330:ASP:OD2	1:B:333:ARG:HD3	2.02	0.60
1:A:164:PRO:HD2	1:A:198:TYR:OH	2.02	0.60
1:A:98:PRO:HG3	4:A:651:HOH:O	2.02	0.59
1:A:339:SER:OG	1:A:340:PRO:HD3	2.02	0.59
1:A:105:ARG:NH2	1:A:354:PRO:HG3	2.17	0.58
1:B:87:ARG:N	1:B:88:PRO:CD	2.67	0.58
1:B:145:THR:HA	1:B:149:LEU:HB2	1.87	0.57
1:A:62:LEU:HD23	1:A:62:LEU:C	2.25	0.57
1:A:309:ARG:HD3	1:A:309:ARG:H	1.70	0.57
1:A:144:LEU:HG	1:A:149:LEU:CD1	2.35	0.56
1:B:75:MET:CE	1:B:89:ALA:HB2	2.34	0.56
1:A:274:ARG:O	1:A:278:ILE:HG12	2.05	0.56
1:B:140:PRO:CD	1:B:406:HIS:HB2	2.35	0.56
1:A:145:THR:HA	1:A:149:LEU:HB2	1.88	0.56
1:A:307:ARG:NH1	1:A:309:ARG:HG3	2.21	0.56
1:B:189:GLU:O	1:B:192:LYS:HG2	2.05	0.56
1:A:272:GLU:H	1:A:272:GLU:CD	2.09	0.56
1:B:318:TYR:CZ	1:B:347:GLY:HA2	2.41	0.55
1:A:206:ARG:HG3	1:A:206:ARG:HH21	1.71	0.55
1:B:60:VAL:HG21	1:B:321:ALA:HB2	1.89	0.55
1:B:307:ARG:NH1	1:B:309:ARG:HG3	2.21	0.55
1:A:46:ASN:ND2	1:A:84:PRO:HA	2.23	0.54
1:A:178:ILE:CG2	1:A:179:LEU:HG	2.33	0.54
1:B:303:ILE:HD12	1:B:308:ILE:HD12	1.88	0.54
1:B:65:ASN:HD22	1:B:350:PRO:HD3	1.73	0.54
1:B:140:PRO:HG2	1:B:406:HIS:HB2	1.88	0.54
1:A:169:HIS:CD2	1:A:170:SER:H	2.24	0.54
1:B:229:LEU:O	1:B:233:VAL:HG23	2.08	0.54
1:A:318:TYR:CZ	1:A:347:GLY:HA2	2.42	0.54
1:A:339:SER:HB2	1:A:340:PRO:HD3	1.89	0.53
1:B:87:ARG:HG2	1:B:88:PRO:HD3	1.91	0.53
1:B:309:ARG:H	1:B:309:ARG:HD3	1.74	0.53
1:A:140:PRO:HA	1:A:404:TRP:CE2	2.43	0.52
1:B:140:PRO:HA	1:B:404:TRP:CE2	2.44	0.52
1:B:378:LYS:NZ	3:B:432:SPM:HN5	2.06	0.52
1:A:258:LEU:HD21	1:A:377:LEU:HD13	1.91	0.52
1:B:62:LEU:HD23	1:B:62:LEU:C	2.30	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:86:PHE:HE1	1:B:95:PHE:HE2	1.57	0.52
1:B:267:LEU:HD21	1:B:277:ALA:CB	2.40	0.52
1:B:78:GLN:HE22	1:B:81:ARG:HH12	1.58	0.52
1:B:303:ILE:HD12	1:B:308:ILE:CD1	2.40	0.51
1:B:375:PRO:O	1:B:404:TRP:HB2	2.10	0.51
1:B:333:ARG:NH1	1:B:335:ASP:HB2	2.25	0.51
1:A:106:ARG:NH2	1:B:298:LEU:HB3	2.25	0.50
1:A:98:PRO:N	1:A:99:PRO:HD2	2.27	0.50
1:A:158:CYS:HB3	1:A:168:ARG:HD3	1.94	0.50
1:B:172:HIS:O	1:B:176:GLN:HG3	2.12	0.50
1:B:30:LEU:O	1:B:34:MET:HG3	2.12	0.49
1:A:128:LEU:HD11	1:A:366:LEU:HA	1.94	0.49
1:B:165:ALA:HA	1:B:168:ARG:HG3	1.94	0.49
1:B:202:LEU:HD21	1:B:206:ARG:CZ	2.43	0.49
1:A:16:TRP:CZ2	1:A:290:ALA:HA	2.48	0.49
1:A:140:PRO:HB2	1:A:141:PRO:HD3	1.94	0.49
1:A:169:HIS:CD2	1:A:170:SER:N	2.81	0.49
1:A:86:PHE:HE2	1:A:95:PHE:HZ	1.61	0.49
1:A:81:ARG:HD3	1:A:86:PHE:CD1	2.48	0.48
1:A:375:PRO:O	1:A:404:TRP:HB2	2.12	0.48
1:B:174:TRP:O	1:B:178:ILE:HG13	2.12	0.48
1:A:262:GLU:CD	1:A:262:GLU:H	2.10	0.48
1:B:46:ASN:ND2	1:B:84:PRO:HA	2.28	0.48
1:B:139:GLY:HA2	1:B:406:HIS:HD2	1.79	0.48
1:A:339:SER:CB	1:A:340:PRO:CD	2.91	0.48
1:B:205:LEU:C	1:B:206:ARG:HG2	2.34	0.48
1:A:205:LEU:C	1:A:205:LEU:HD13	2.34	0.48
1:A:114:ALA:HA	1:A:357:MET:HG2	1.96	0.48
1:B:378:LYS:HE3	3:B:432:SPM:N5	2.19	0.48
1:A:330:ASP:OD1	1:A:333:ARG:HD3	2.14	0.48
1:B:88:PRO:HB2	1:B:95:PHE:CE1	2.50	0.47
1:B:266:ARG:HB3	4:B:458:HOH:O	2.13	0.47
1:A:152:PHE:HB3	1:A:153:PRO:HD3	1.96	0.47
1:A:75:MET:CE	1:A:90:ARG:HA	2.45	0.47
1:A:164:PRO:HD3	1:A:202:LEU:HD11	1.96	0.47
1:B:220:ALA:HB1	1:B:224:ARG:NH2	2.25	0.47
1:B:97:ASP:C	1:B:99:PRO:HD2	2.36	0.47
1:B:382:ALA:N	3:B:432:SPM:H132	2.30	0.46
1:B:86:PHE:CE1	1:B:95:PHE:HE2	2.33	0.46
1:B:361:LEU:HD23	1:B:361:LEU:C	2.34	0.46
1:A:220:ALA:HB1	1:A:224:ARG:NH2	2.28	0.46
1:B:360:ARG:O	1:B:364:GLU:HG3	2.16	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:140:PRO:O	1:B:404:TRP:CZ3	2.69	0.46
1:A:5:THR:HG23	1:A:6:ILE:N	2.31	0.46
1:B:262:GLU:CD	1:B:262:GLU:H	2.12	0.46
1:A:123:ARG:HE	1:A:123:ARG:CA	2.27	0.46
1:A:65:ASN:HD22	1:A:350:PRO:HD3	1.80	0.46
1:B:171:MET:HA	1:B:171:MET:HE3	1.97	0.46
1:A:93:VAL:HA	1:A:96:LEU:HD12	1.98	0.46
1:B:180:SER:C	1:B:182:SER:H	2.19	0.46
1:B:140:PRO:HD3	1:B:406:HIS:CD2	2.51	0.45
1:A:360:ARG:O	1:A:364:GLU:HG3	2.16	0.45
1:B:204:GLY:C	1:B:206:ARG:H	2.19	0.45
1:A:106:ARG:HH22	1:B:298:LEU:HB3	1.80	0.45
1:B:272:GLU:H	1:B:272:GLU:CD	2.20	0.45
1:A:104:LEU:HG	1:A:235:LEU:HD22	1.96	0.45
1:A:97:ASP:HB3	1:A:98:PRO:HD2	1.97	0.45
1:A:206:ARG:NH2	1:A:206:ARG:HG3	2.31	0.45
1:A:185:ALA:O	1:A:189:GLU:HG3	2.16	0.45
1:B:309:ARG:NE	1:B:312:ASP:OD2	2.50	0.45
1:A:270:GLU:HG3	1:A:272:GLU:OE1	2.17	0.45
1:A:333:ARG:NH1	1:A:335:ASP:HB2	2.32	0.45
1:B:149:LEU:HG	1:B:250:SER:OG	2.17	0.45
1:A:180:SER:O	1:A:181:SER:HB3	2.17	0.45
1:A:66:ASP:HA	1:A:67:PRO:HD3	1.81	0.44
1:B:283:ARG:HD3	1:B:341:ASN:ND2	2.24	0.44
1:B:128:LEU:HD11	1:B:366:LEU:HA	1.99	0.44
1:B:171:MET:CE	1:B:240:GLN:HG2	2.45	0.43
1:A:127:MET:CE	1:A:155:ALA:HB1	2.48	0.43
1:B:16:TRP:CZ2	1:B:290:ALA:HA	2.53	0.43
1:A:300:ASP:OD2	1:A:307:ARG:NH2	2.51	0.43
1:B:91:GLY:O	1:B:92:ALA:O	2.37	0.43
1:A:99:PRO:HB3	1:B:99:PRO:HB3	2.00	0.43
1:B:114:ALA:O	1:B:118:GLU:HG2	2.19	0.43
1:A:267:LEU:HD21	1:A:277:ALA:CB	2.49	0.43
1:A:161:MET:HA	1:A:214:VAL:HB	2.01	0.42
1:B:182:SER:O	1:B:183:HIS:C	2.57	0.42
1:A:309:ARG:HD3	1:A:309:ARG:N	2.35	0.42
1:A:271:PRO:HD2	1:A:272:GLU:OE2	2.20	0.42
1:B:62:LEU:CD2	1:B:62:LEU:C	2.87	0.42
1:A:218:LEU:O	1:A:222:VAL:HG23	2.20	0.42
1:A:149:LEU:N	1:A:149:LEU:CD1	2.82	0.42
1:A:149:LEU:HD12	1:A:149:LEU:N	2.34	0.42
1:A:82:LEU:HD22	1:A:290:ALA:HB3	2.02	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:278:ILE:CD1	1:B:364:GLU:HA	2.50	0.42
1:A:87:ARG:HB3	1:A:87:ARG:HH11	1.85	0.42
1:A:198:TYR:HE2	1:A:202:LEU:HD12	1.84	0.42
1:A:309:ARG:NE	1:A:312:ASP:OD2	2.52	0.42
1:A:361:LEU:C	1:A:361:LEU:HD23	2.40	0.42
1:B:41:ARG:HD2	1:B:50:TRP:CE3	2.54	0.41
1:B:267:LEU:HG	4:B:458:HOH:O	2.20	0.41
1:B:337:GLU:O	1:B:338:ARG:C	2.59	0.41
1:A:114:ALA:CA	1:A:357:MET:HG2	2.50	0.41
1:B:171:MET:HA	1:B:171:MET:CE	2.51	0.41
1:B:267:LEU:N	4:B:458:HOH:O	2.53	0.41
1:A:60:VAL:HG21	1:A:321:ALA:HB2	2.03	0.41
1:A:266:ARG:HG3	1:A:266:ARG:NH1	2.27	0.41
1:B:339:SER:CB	1:B:340:PRO:CD	2.88	0.41
1:B:186:GLU:O	1:B:188:SER:N	2.42	0.41
1:A:123:ARG:HA	1:A:123:ARG:NE	2.29	0.41
1:B:89:ALA:O	1:B:90:ARG:C	2.59	0.41
1:A:81:ARG:CZ	1:A:86:PHE:HB2	2.50	0.41
1:A:58:ASP:OD1	1:A:59:ASP:N	2.54	0.41
1:B:86:PHE:CE1	1:B:95:PHE:CE2	3.08	0.41
1:A:30:LEU:O	1:A:34:MET:HG3	2.20	0.41
1:A:114:ALA:HA	1:A:357:MET:CG	2.50	0.41
1:B:82:LEU:HD22	1:B:290:ALA:HB3	2.03	0.41
1:B:388:PHE:HA	1:B:397:PRO:HA	2.03	0.41
1:B:309:ARG:HD3	1:B:309:ARG:N	2.36	0.40
1:B:46:ASN:CG	1:B:84:PRO:HA	2.41	0.40
1:A:283:ARG:HD3	1:A:341:ASN:ND2	2.26	0.40
1:A:330:ASP:N	1:A:331:PRO:CD	2.84	0.40
1:A:337:GLU:O	1:A:338:ARG:C	2.60	0.40
1:B:125:ARG:HD3	1:B:125:ARG:C	2.41	0.40
1:B:81:ARG:CZ	1:B:86:PHE:HB3	2.52	0.40
1:A:184:GLY:O	1:A:185:ALA:HB3	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	400/407 (98%)	380 (95%)	10 (2%)	10 (2%)	9	1
1	B	400/407 (98%)	373 (93%)	15 (4%)	12 (3%)	7	0
All	All	800/814 (98%)	753 (94%)	25 (3%)	22 (3%)	8	0

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	87	ARG
1	B	98	PRO
1	A	140	PRO
1	A	179	LEU
1	A	180	SER
1	A	339	SER
1	B	92	ALA
1	B	99	PRO
1	B	140	PRO
1	B	186	GLU
1	B	88	PRO
1	B	183	HIS
1	B	338	ARG
1	A	185	ALA
1	A	338	ARG
1	B	339	SER
1	A	181	SER
1	A	186	GLU
1	B	166	THR
1	B	205	LEU
1	A	98	PRO
1	A	88	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	332/336 (99%)	316 (95%)	16 (5%)	35	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	332/336 (99%)	321 (97%)	11 (3%)	50	22
All	All	664/672 (99%)	637 (96%)	27 (4%)	41	15

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	ASP
1	A	21	LEU
1	A	86	PHE
1	A	123	ARG
1	A	125	ARG
1	A	128	LEU
1	A	140	PRO
1	A	169	HIS
1	A	202	LEU
1	A	212	GLU
1	A	262	GLU
1	A	266	ARG
1	A	309	ARG
1	A	339	SER
1	A	341	ASN
1	A	377	LEU
1	B	98	PRO
1	B	122	GLU
1	B	125	ARG
1	B	128	LEU
1	B	140	PRO
1	B	149	LEU
1	B	190	ARG
1	B	262	GLU
1	B	309	ARG
1	B	341	ASN
1	B	377	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	GLN
1	A	46	ASN
1	A	65	ASN
1	A	169	HIS

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Mol	Chain	Res	Type
1	A	193	ASN
1	A	240	GLN
1	A	249	ASN
1	A	287	HIS
1	A	341	ASN
1	B	65	ASN
1	B	78	GLN
1	B	193	ASN
1	B	341	ASN
1	B	406	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 ⓘ

3 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	HEM	A	430	1	49,50,50	2.80	17 (34%)	46,82,82	1.41	6 (13%)
2	HEM	B	430	1	49,50,50	2.55	16 (32%)	46,82,82	1.44	6 (13%)
3	SPM	B	432	-	13,13,13	0.29	0	12,12,12	1.30	1 (8%)



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	430	1	-	0/14/114/114	0/0/8/8
2	HEM	B	430	1	-	0/14/114/114	0/0/8/8
3	SPM	B	432	-	-	0/11/11/11	0/0/0/0

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	430	HEM	C2B-C1B	10.04	1.47	1.44
2	B	430	HEM	C2B-C1B	7.38	1.46	1.44
2	B	430	HEM	C3D-C4D	5.63	1.46	1.44
2	A	430	HEM	C3D-C4D	5.42	1.45	1.44
2	A	430	HEM	C3C-C2C	-4.85	1.35	1.43
2	A	430	HEM	C3B-CAB	4.80	1.55	1.40
2	B	430	HEM	C3C-C2C	-4.74	1.35	1.43
2	B	430	HEM	C3C-CAC	4.71	1.55	1.40
2	A	430	HEM	C2D-C1D	4.69	1.45	1.44
2	A	430	HEM	C3C-CAC	4.62	1.54	1.40
2	B	430	HEM	C4A-C3A	4.53	1.45	1.40
2	B	430	HEM	C3B-C2B	-4.50	1.35	1.43
2	B	430	HEM	C3D-C2D	-4.49	1.35	1.43
2	A	430	HEM	CBB-CAB	4.48	1.55	1.28
2	B	430	HEM	CBC-CAC	4.37	1.54	1.28
2	A	430	HEM	CBC-CAC	4.37	1.54	1.28
2	A	430	HEM	C4A-C3A	4.35	1.45	1.40
2	A	430	HEM	C3D-C2D	-4.19	1.36	1.43
2	B	430	HEM	CBB-CAB	4.09	1.52	1.28
2	B	430	HEM	C3B-CAB	4.04	1.53	1.40
2	A	430	HEM	C3B-C2B	-3.59	1.37	1.43
2	A	430	HEM	CMC-C2C	2.82	1.56	1.47
2	B	430	HEM	CMC-C2C	2.82	1.56	1.47
2	A	430	HEM	FE-NA	2.79	2.04	1.92
2	B	430	HEM	FE-NA	2.69	2.04	1.92
2	A	430	HEM	CMB-C2B	2.67	1.55	1.47
2	B	430	HEM	CMB-C2B	2.45	1.55	1.47
2	B	430	HEM	CHA-C4D	2.41	1.39	1.35
2	B	430	HEM	CMD-C2D	2.38	1.54	1.47
2	A	430	HEM	CMD-C2D	2.29	1.54	1.47
2	A	430	HEM	CHA-C4D	2.15	1.38	1.35
2	B	430	HEM	C1A-C2A	2.11	1.47	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	430	HEM	O2A-CGA	-2.02	1.23	1.30

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	430	HEM	C3B-C4B-NB	-5.45	110.10	114.00
2	A	430	HEM	C3B-C4B-NB	-4.90	110.49	114.00
2	A	430	HEM	CBA-CAA-C2A	3.19	118.31	112.69
2	B	430	HEM	CBA-CAA-C2A	3.12	118.19	112.69
2	B	430	HEM	CMA-C3A-C4A	-2.98	124.04	128.62
2	A	430	HEM	CMA-C3A-C4A	-2.92	124.13	128.62
2	B	430	HEM	CBD-CAD-C3D	-2.84	108.18	114.37
2	A	430	HEM	CBD-CAD-C3D	-2.83	108.20	114.37
2	B	430	HEM	O1A-CGA-CBA	-2.34	114.99	123.03
2	A	430	HEM	C2D-C1D-ND	-2.24	110.28	112.93
2	A	430	HEM	O1A-CGA-CBA	-2.09	115.84	123.03
2	B	430	HEM	C2D-C1D-ND	-2.08	110.47	112.93
3	B	432	SPM	C7-C6-N5	-2.00	106.77	112.09

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	402/407 (98%)	0.47	28 (6%) 16 22	4, 14, 48, 95	0
1	B	402/407 (98%)	0.59	32 (7%) 12 17	3, 13, 48, 127	0
All	All	804/814 (98%)	0.53	60 (7%) 14 19	3, 13, 48, 127	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	184	GLY	21.2
1	B	183	HIS	21.1
1	B	185	ALA	20.6
1	A	179	LEU	15.9
1	B	182	SER	13.1
1	B	179	LEU	12.5
1	B	88	PRO	11.5
1	A	86	PHE	9.7
1	B	181	SER	8.3
1	B	339	SER	8.0
1	A	339	SER	7.8
1	A	88	PRO	7.2
1	B	89	ALA	6.8
1	A	87	ARG	6.6
1	A	181	SER	5.9
1	B	98	PRO	5.6
1	B	6	ILE	5.4
1	A	182	SER	5.2
1	A	183	HIS	5.1
1	A	90	ARG	5.0
1	A	99	PRO	5.0
1	B	166	THR	4.7
1	B	140	PRO	4.7
1	A	89	ALA	4.6

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Mol	Chain	Res	Type	RSRZ
1	B	205	LEU	4.3
1	A	85	HIS	4.2
1	A	140	PRO	4.2
1	B	90	ARG	4.1
1	B	5	THR	4.0
1	A	169	HIS	4.0
1	A	5	THR	3.9
1	B	186	GLU	3.9
1	A	91	GLY	3.9
1	A	180	SER	3.7
1	A	84	PRO	3.7
1	B	91	GLY	3.6
1	A	187	VAL	3.3
1	B	190	ARG	3.3
1	A	184	GLY	3.2
1	A	190	ARG	3.2
1	A	188	SER	3.0
1	B	141	PRO	2.9
1	B	164	PRO	2.9
1	B	85	HIS	2.9
1	A	141	PRO	2.9
1	A	340	PRO	2.9
1	A	98	PRO	2.8
1	B	180	SER	2.6
1	B	207	SER	2.6
1	A	185	ALA	2.4
1	B	99	PRO	2.4
1	B	7	SER	2.3
1	B	340	PRO	2.3
1	B	165	ALA	2.3
1	B	175	THR	2.3
1	A	205	LEU	2.1
1	B	188	SER	2.1
1	B	201	ASP	2.1
1	A	6	ILE	2.1
1	B	204	GLY	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
3	SPM	B	432	14/14	0.35	13.62	16,44,95,96	0
2	HEM	A	430	43/43	0.12	1.82	1,7,13,34	0
2	HEM	B	430	43/43	0.10	0.47	1,6,12,40	0

### 6.5 Other polymers ⓘ

There are no such residues in this entry.