



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 26, 2014 – 10:55 PM GMT

PDB ID : 2BZ9  
Title : LIGAND-FREE STRUCTURE OF STEROL 14ALPHA-DEMETHYLASE  
FROM MYCOBACTERIUM TUBERCULOSIS IN P2(1) SPACE GROUP  
Authors : Yermalitskaya, L.V.; Waterman, M.R.; Podust, L.M.  
Deposited on : 2005-08-12  
Resolution : 2.21 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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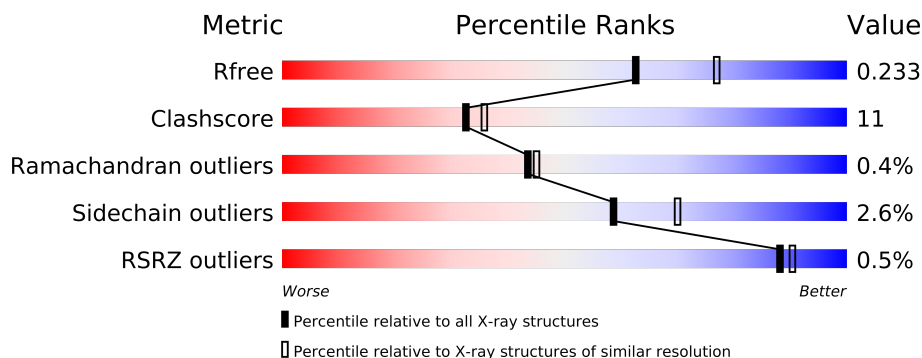
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.21 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	3340 (2.24-2.20)
Clashscore	79885	4208 (2.24-2.20)
Ramachandran outliers	78287	4135 (2.24-2.20)
Sidechain outliers	78261	4136 (2.24-2.20)
RSRZ outliers	66119	3341 (2.24-2.20)

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	455	
1	B	455	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7118 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.

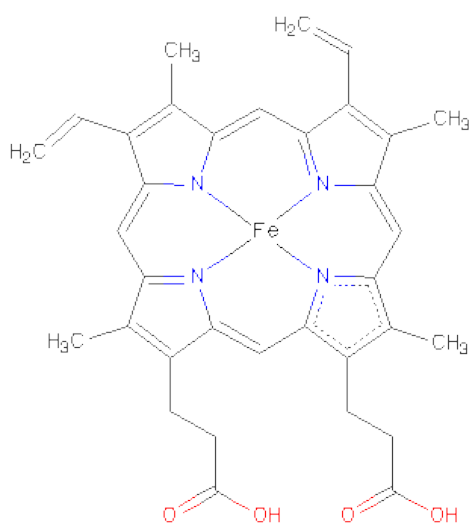
- Molecule 1 is a protein called STEROL 14ALPHA-DEMETHYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	430	Total	C	N	O	S	0	0	1
			3394	2146	612	620	16			
1	B	433	Total	C	N	O	S	0	0	1
			3422	2162	618	625	17			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	37	LEU	CYS	ENGINEERED MUTATION	UNP P0A512
A	442	ALA	CYS	ENGINEERED MUTATION	UNP P0A512
B	37	LEU	CYS	ENGINEERED MUTATION	UNP P0A512
B	442	ALA	CYS	ENGINEERED MUTATION	UNP P0A512

- 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 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

- Molecule 3 is water.

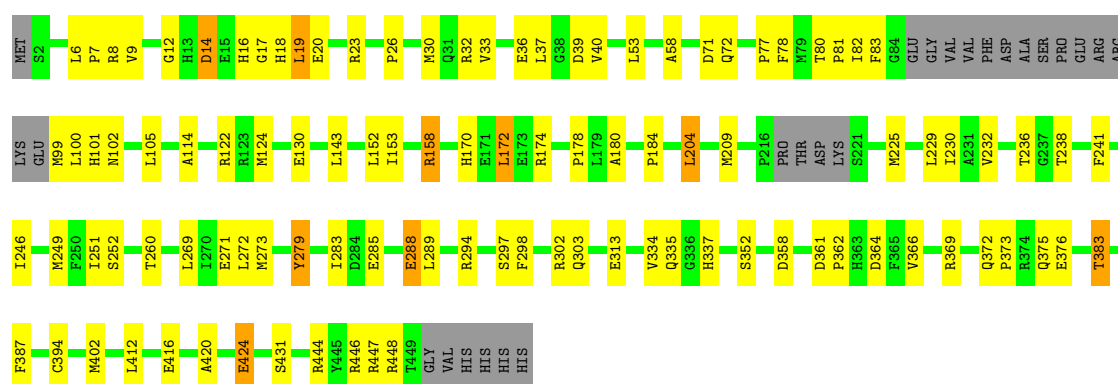
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	102	Total 102	O 102	0	0
3	B	114	Total 114	O 114	0	0

### 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.

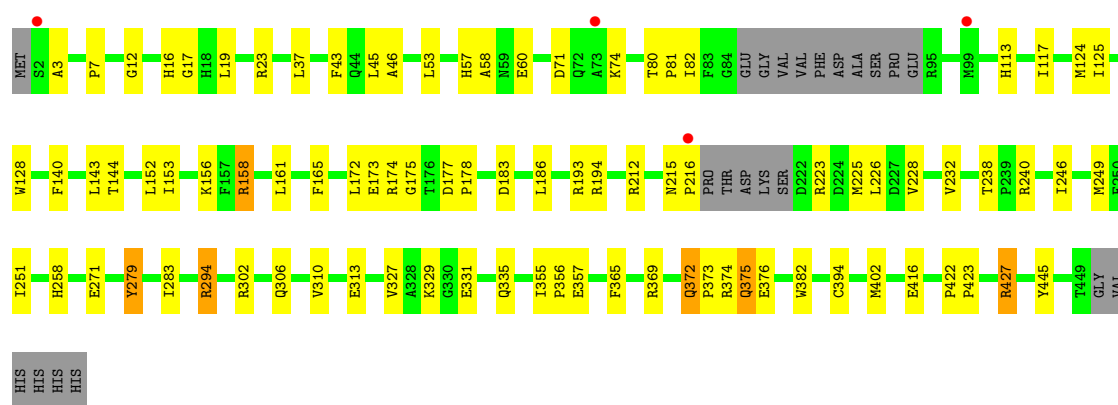
#### • Molecule 1: STEROL 14ALPHA-DEMETHYLASE

Chain A:



#### • Molecule 1: STEROL 14ALPHA-DEMETHYLASE

Chain B:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	38.91Å 110.34Å 99.63Å 90.00° 90.67° 90.00°	Depositor
Resolution (Å)	36.97 – 2.21 36.97 – 2.21	Depositor EDS
% Data completeness (in resolution range)	92.4 (36.97-2.21) 89.6 (36.97-2.21)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.12 (at 2.20Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.215 , 0.275 0.204 , 0.233	Depositor DCC
$R_{free}$ test set	3925 reflections (11.14%)	DCC
Wilson B-factor (Å <sup>2</sup> )	19.0	Xtriage
Anisotropy	0.339	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 35.9	EDS
Estimated twinning fraction	0.358 for h,-k,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 40855 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	7118	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.53% 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

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	0.36	0/3472	0.59	0/4697
1	B	0.36	0/3500	0.60	0/4733
All	All	0.36	0/6972	0.59	0/9430

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	3394	0	3299	81	0
1	B	3422	0	3327	73	0
2	A	43	0	30	3	0
2	B	43	0	30	2	0
3	A	102	0	0	6	0
3	B	114	0	0	10	0
All	All	7118	0	6686	154	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 11.

All (154) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:420:ALA:HA	1:A:444:ARG:HH21	1.08	1.11
1:B:294:ARG:HE	1:B:294:ARG:HA	1.31	0.95
1:B:80:THR:HB	1:B:81:PRO:HD3	1.60	0.83
1:A:9:VAL:HB	1:A:33:VAL:HG22	1.62	0.80
1:A:82:ILE:HG23	1:A:172:LEU:HG	1.66	0.78
1:A:236:THR:OG1	1:A:238:THR:HG22	1.83	0.78
1:A:420:ALA:HA	1:A:444:ARG:NH2	1.93	0.77
1:A:19:LEU:HD21	1:A:178:PRO:HB2	1.67	0.76
1:B:19:LEU:HD12	1:B:46:ALA:HB2	1.68	0.76
1:A:12:GLY:O	1:A:17:GLY:HA2	1.86	0.75
1:A:285:GLU:O	1:A:289:LEU:HD13	1.88	0.73
1:B:369:ARG:HA	1:B:374:ARG:HD3	1.69	0.72
1:A:416:GLU:HG3	1:A:448:ARG:HG2	1.70	0.71
1:A:294:ARG:HD2	1:A:298:PHE:CE2	2.27	0.70
1:B:82:ILE:HG23	1:B:172:LEU:HG	1.73	0.69
1:B:427:ARG:HB2	1:B:427:ARG:HH11	1.56	0.69
1:B:246:ILE:HA	1:B:249:MET:HE3	1.74	0.69
1:B:172:LEU:HD21	1:B:251:ILE:HD13	1.74	0.68
1:A:80:THR:HB	1:A:81:PRO:HD3	1.75	0.67
1:B:71:ASP:HB2	1:B:329:LYS:HD2	1.75	0.67
1:B:240:ARG:HG3	1:B:240:ARG:HH11	1.57	0.67
1:B:216:PRO:HD3	3:B:2060:HOH:O	1.93	0.66
1:B:294:ARG:HE	1:B:294:ARG:CA	2.02	0.66
1:B:60:GLU:HG3	1:B:382:TRP:CE2	2.30	0.66
1:A:229:LEU:O	1:A:232:VAL:HG22	1.97	0.65
1:A:303:GLN:HG3	3:A:2065:HOH:O	1.95	0.65
1:A:39:ASP:HB2	1:A:335:GLN:HE22	1.62	0.65
1:A:172:LEU:HD21	1:A:251:ILE:HD13	1.80	0.63
1:B:124:MET:HG3	1:B:143:LEU:HD13	1.83	0.60
1:B:294:ARG:NE	1:B:294:ARG:HA	2.11	0.59
1:A:313:GLU:HA	1:A:313:GLU:OE1	2.02	0.59
1:B:240:ARG:HG3	1:B:240:ARG:NH1	2.18	0.59
1:A:124:MET:HG3	1:A:143:LEU:HD13	1.85	0.58
1:B:372:GLN:CB	1:B:373:PRO:HD3	2.33	0.58
1:A:14:ASP:HB2	1:A:20:GLU:OE1	2.03	0.58
1:A:20:GLU:CD	1:A:20:GLU:H	2.08	0.56
1:B:140:PHE:O	1:B:144:THR:HG23	2.04	0.56
1:B:372:GLN:O	1:B:375:GLN:OE1	2.23	0.56
1:B:153:ILE:HG23	1:B:225:MET:HB3	1.87	0.56
1:A:372:GLN:HB3	1:A:373:PRO:HD3	1.88	0.55
1:A:302:ARG:HH11	1:A:302:ARG:HG3	1.73	0.54
1:B:302:ARG:HH11	1:B:302:ARG:HG3	1.72	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:7:PRO:O	1:B:37:LEU:HD13	2.07	0.54
1:B:156:LYS:HD2	1:B:212:ARG:NH2	2.23	0.54
1:B:240:ARG:NH1	3:B:2062:HOH:O	2.41	0.53
1:B:125:ILE:HG22	1:B:128:TRP:CE2	2.44	0.53
1:B:394:CYS:HB2	2:B:1449:HEM:NA	2.24	0.52
1:B:174:ARG:HB3	1:B:193:ARG:NH2	2.25	0.52
1:A:114:ALA:HB1	1:A:297:SER:HA	1.91	0.52
1:A:83:PHE:CE1	1:A:252:SER:HA	2.44	0.52
1:A:8:ARG:HE	1:A:18:HIS:HE1	1.57	0.52
1:A:361:ASP:HB3	1:A:364:ASP:OD2	2.10	0.52
1:B:271:GLU:HA	1:B:271:GLU:OE1	2.10	0.52
1:A:204:LEU:HD23	3:A:2045:HOH:O	2.09	0.51
1:B:173:GLU:OE2	1:B:258:HIS:ND1	2.39	0.51
1:A:424:GLU:H	1:A:424:GLU:CD	2.14	0.51
1:B:23:ARG:HG2	1:B:178:PRO:HG2	1.92	0.51
1:A:269:LEU:O	1:A:273:MET:HG3	2.11	0.50
1:A:53:LEU:HB3	1:A:58:ALA:HB1	1.92	0.50
1:A:32:ARG:O	1:A:36:GLU:HG3	2.12	0.50
1:A:232:VAL:HG21	1:A:241:PHE:CE2	2.47	0.49
1:B:427:ARG:CB	1:B:427:ARG:HH11	2.24	0.49
1:A:170:HIS:O	1:A:174:ARG:HG2	2.12	0.49
1:B:375:GLN:HG2	3:B:2091:HOH:O	2.12	0.49
1:A:447:ARG:HG2	1:A:447:ARG:HH11	1.76	0.49
1:A:16:HIS:HB2	1:A:20:GLU:OE2	2.13	0.49
1:A:209:MET:HG2	1:A:230:ILE:HD11	1.95	0.48
1:A:394:CYS:HB2	2:A:1449:HEM:NA	2.28	0.48
1:A:232:VAL:HG21	1:A:241:PHE:CD2	2.48	0.48
1:A:236:THR:HG1	1:A:238:THR:HG22	1.76	0.48
1:A:412:LEU:O	1:A:448:ARG:HD2	2.13	0.48
1:B:240:ARG:CZ	3:B:2062:HOH:O	2.60	0.48
1:B:372:GLN:HB2	1:B:373:PRO:HD3	1.95	0.48
1:B:279:TYR:HE1	1:B:283:ILE:HD11	1.79	0.47
1:B:369:ARG:O	1:B:376:GLU:HG3	2.14	0.47
1:B:57:HIS:HD2	1:B:335:GLN:NE2	2.12	0.47
1:B:313:GLU:OE1	1:B:313:GLU:HA	2.15	0.47
1:A:153:ILE:HG23	1:A:225:MET:HB3	1.97	0.46
1:B:16:HIS:HB3	1:B:46:ALA:HB2	1.97	0.46
1:B:374:ARG:O	1:B:375:GLN:C	2.54	0.46
1:A:246:ILE:HA	1:A:249:MET:HE3	1.96	0.46
1:B:113:HIS:O	1:B:117:ILE:HG13	2.16	0.46
1:B:12:GLY:O	1:B:17:GLY:HA2	2.15	0.46
1:B:19:LEU:HD21	1:B:178:PRO:HB2	1.98	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:369:ARG:HG3	1:A:376:GLU:OE1	2.16	0.46
1:B:53:LEU:HB3	1:B:58:ALA:HB1	1.97	0.45
1:A:78:PHE:HB3	1:A:180:ALA:CB	2.47	0.45
1:A:288:GLU:HG3	1:A:289:LEU:N	2.31	0.45
1:B:369:ARG:HA	1:B:374:ARG:CD	2.41	0.45
1:A:249:MET:O	1:A:252:SER:HB3	2.17	0.45
1:B:158:ARG:C	1:B:158:ARG:HD3	2.37	0.45
1:A:23:ARG:O	1:A:431:SER:HA	2.17	0.45
1:B:43:PHE:CE1	1:B:45:LEU:HD13	2.51	0.45
1:A:447:ARG:HG2	1:A:447:ARG:NH1	2.31	0.45
1:A:71:ASP:OD2	1:A:72:GLN:N	2.50	0.45
1:B:161:LEU:HD22	1:B:165:PHE:CD2	2.51	0.45
1:B:175:GLY:HA3	1:B:194:ARG:HB2	1.98	0.44
1:A:402:MET:SD	1:A:402:MET:C	2.95	0.44
1:A:130:GLU:HB3	3:A:2028:HOH:O	2.18	0.44
1:A:361:ASP:N	1:A:362:PRO:CD	2.80	0.44
1:B:228:VAL:O	1:B:232:VAL:HG23	2.18	0.44
1:B:416:GLU:O	1:B:445:TYR:HA	2.17	0.44
1:B:356:PRO:HG2	1:B:357:GLU:OE2	2.17	0.44
1:A:272:LEU:HD22	1:A:279:TYR:HA	2.00	0.44
1:A:130:GLU:OE2	1:A:446:ARG:NH1	2.51	0.44
1:A:375:GLN:HG2	3:A:2079:HOH:O	2.17	0.44
1:A:26:PRO:O	1:A:30:MET:HG3	2.18	0.43
1:A:288:GLU:HG3	1:A:289:LEU:HD12	2.01	0.43
1:A:352:SER:O	1:A:383:THR:HG22	2.18	0.43
1:B:310:VAL:HG13	1:B:365:PHE:HZ	1.82	0.43
1:B:3:ALA:N	3:B:2001:HOH:O	2.51	0.43
1:A:283:ILE:CD1	1:A:412:LEU:HB3	2.48	0.43
1:A:302:ARG:NH1	1:A:302:ARG:HG3	2.34	0.43
1:A:424:GLU:N	1:A:424:GLU:OE1	2.47	0.43
1:A:209:MET:SD	1:A:246:ILE:HD12	2.58	0.43
1:B:258:HIS:HE1	3:B:2046:HOH:O	2.00	0.43
1:A:77:PRO:HB2	1:A:184:PRO:HG3	2.01	0.43
1:B:372:GLN:CB	1:B:373:PRO:CD	2.97	0.43
1:B:74:LYS:HG3	1:B:327:VAL:HG21	2.01	0.42
1:A:99:MET:N	1:A:102:ASN:ND2	2.66	0.42
1:B:355:ILE:HA	1:B:356:PRO:HD2	1.82	0.42
1:A:158:ARG:HD3	1:A:158:ARG:C	2.40	0.42
1:A:40:VAL:HB	3:A:2008:HOH:O	2.19	0.42
1:A:294:ARG:HD2	1:A:298:PHE:CD2	2.55	0.42
1:A:39:ASP:HB2	1:A:335:GLN:NE2	2.32	0.42
1:A:101:HIS:CD2	1:A:105:LEU:HB2	2.55	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:212:ARG:NH1	1:B:226:LEU:HB3	2.34	0.42
1:A:366:VAL:O	1:A:369:ARG:HB2	2.20	0.42
1:B:422:PRO:HA	1:B:423:PRO:HD3	1.86	0.42
1:B:43:PHE:HE1	1:B:45:LEU:HD13	1.84	0.42
1:A:7:PRO:HB2	1:A:37:LEU:HD22	2.02	0.42
1:A:9:VAL:CB	1:A:33:VAL:HG22	2.43	0.41
1:B:302:ARG:HG3	1:B:302:ARG:NH1	2.34	0.41
1:B:117:ILE:HD12	1:B:402:MET:SD	2.60	0.41
1:B:177:ASP:HB2	3:B:2051:HOH:O	2.20	0.41
1:B:394:CYS:HB2	2:B:1449:HEM:C4A	2.55	0.41
1:A:53:LEU:HD22	1:A:334:VAL:HG11	2.02	0.41
1:B:306:GLN:HA	1:B:306:GLN:NE2	2.34	0.41
1:B:372:GLN:O	1:B:375:GLN:HG3	2.21	0.41
1:A:358:ASP:OD2	1:A:383:THR:HG21	2.20	0.41
1:B:357:GLU:CD	1:B:357:GLU:H	2.23	0.41
1:A:6:LEU:HD22	1:A:337:HIS:HB3	2.02	0.41
1:A:14:ASP:HB3	1:A:20:GLU:HG2	2.02	0.41
1:A:387:PHE:CE1	2:A:1449:HEM:HBB2	2.56	0.41
1:B:306:GLN:O	1:B:310:VAL:HG23	2.21	0.41
1:A:271:GLU:OE1	1:A:271:GLU:HA	2.21	0.41
1:B:215:ASN:HA	3:B:2060:HOH:O	2.19	0.40
1:A:20:GLU:CD	1:A:20:GLU:N	2.74	0.40
1:A:369:ARG:HG2	1:A:376:GLU:HB2	2.02	0.40
1:B:183:ASP:HB3	1:B:186:LEU:CD2	2.51	0.40
1:A:122:ARG:HG2	3:A:2026:HOH:O	2.20	0.40
1:A:260:THR:HB	2:A:1449:HEM:C3B	2.57	0.40
1:B:37:LEU:HD21	3:B:2004:HOH:O	2.21	0.40
1:B:174:ARG:HD3	3:B:2052:HOH:O	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	424/455 (93%)	405 (96%)	18 (4%)	1 (0%)	56 62

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	427/455 (94%)	409 (96%)	16 (4%)	2 (0%)	38	38
All	All	851/910 (94%)	814 (96%)	34 (4%)	3 (0%)	43	45

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	372	GLN
1	A	14	ASP
1	B	375	GLN

### 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	348/377 (92%)	338 (97%)	10 (3%)	55	66
1	B	351/377 (93%)	343 (98%)	8 (2%)	63	74
All	All	699/754 (93%)	681 (97%)	18 (3%)	59	70

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	LEU
1	A	100	LEU
1	A	152	LEU
1	A	158	ARG
1	A	172	LEU
1	A	204	LEU
1	A	279	TYR
1	A	288	GLU
1	A	383	THR
1	A	424	GLU
1	B	152	LEU
1	B	158	ARG
1	B	223	ARG
1	B	238	THR
1	B	279	TYR

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Mol	Chain	Res	Type
1	B	294	ARG
1	B	331	GLU
1	B	427	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	GLN
1	A	72	GLN
1	A	101	HIS
1	A	102	ASN
1	A	303	GLN
1	A	306	GLN
1	A	335	GLN
1	A	372	GLN
1	A	403	GLN
1	B	57	HIS
1	B	275	HIS
1	B	303	GLN
1	B	306	GLN
1	B	337	HIS
1	B	375	GLN
1	B	403	GLN
1	B	436	GLN

### 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

2 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	1449	1,3	49,50,50	2.59	14 (28%)	46,82,82	1.36	6 (13%)
2	HEM	B	1449	1,3	49,50,50	2.78	18 (36%)	46,82,82	1.37	6 (13%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	A	1449	1,3	-	0/14/114/114	0/0/8/8
2	HEM	B	1449	1,3	-	0/14/114/114	0/0/8/8

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1449	HEM	C2D-C1D	9.56	1.46	1.44
2	B	1449	HEM	C2D-C1D	7.53	1.46	1.44
2	B	1449	HEM	C3D-C4D	6.42	1.46	1.44
2	B	1449	HEM	C3C-C2C	-5.58	1.34	1.43
2	B	1449	HEM	C2B-C1B	5.51	1.45	1.44
2	A	1449	HEM	C3C-C2C	-5.20	1.34	1.43
2	B	1449	HEM	C3C-CAC	5.04	1.56	1.40
2	B	1449	HEM	C4A-C3A	4.95	1.46	1.40
2	A	1449	HEM	C3C-CAC	4.84	1.55	1.40
2	A	1449	HEM	C4A-C3A	4.72	1.46	1.40
2	B	1449	HEM	C3B-CAB	4.72	1.55	1.40
2	A	1449	HEM	C3B-CAB	4.71	1.55	1.40
2	B	1449	HEM	CBC-CAC	4.43	1.54	1.28
2	A	1449	HEM	CBC-CAC	4.33	1.54	1.28
2	B	1449	HEM	CBB-CAB	4.33	1.54	1.28
2	A	1449	HEM	CBB-CAB	4.33	1.54	1.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1449	HEM	C3D-C2D	-4.20	1.36	1.43
2	A	1449	HEM	C3D-C2D	-3.92	1.36	1.43
2	B	1449	HEM	C3B-C2B	-3.79	1.37	1.43
2	A	1449	HEM	C3B-C2B	-3.60	1.37	1.43
2	A	1449	HEM	CMC-C2C	2.81	1.56	1.47
2	B	1449	HEM	CMC-C2C	2.81	1.56	1.47
2	A	1449	HEM	FE-NA	2.71	2.04	1.92
2	A	1449	HEM	CMD-C2D	2.64	1.55	1.47
2	B	1449	HEM	FE-NA	2.61	2.03	1.92
2	B	1449	HEM	CMD-C2D	2.53	1.55	1.47
2	B	1449	HEM	CAD-CBD	2.27	1.58	1.52
2	B	1449	HEM	CHA-C4D	2.25	1.39	1.35
2	A	1449	HEM	CAD-CBD	2.23	1.58	1.52
2	A	1449	HEM	CHA-C4D	2.14	1.38	1.35
2	B	1449	HEM	CAA-C2A	2.05	1.55	1.52
2	B	1449	HEM	C1A-C2A	2.05	1.47	1.43

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1449	HEM	C3B-C4B-NB	-5.48	110.08	114.00
2	B	1449	HEM	C3B-C4B-NB	-5.31	110.20	114.00
2	B	1449	HEM	CBD-CAD-C3D	-3.13	107.55	114.37
2	A	1449	HEM	CBD-CAD-C3D	-2.77	108.34	114.37
2	A	1449	HEM	C2D-C1D-ND	-2.71	109.73	112.93
2	A	1449	HEM	CMA-C3A-C4A	-2.60	124.63	128.62
2	B	1449	HEM	CMA-C3A-C4A	-2.58	124.65	128.62
2	B	1449	HEM	C2D-C1D-ND	-2.41	110.08	112.93
2	A	1449	HEM	CHD-C4C-NC	-2.41	122.64	124.73
2	B	1449	HEM	CHD-C4C-NC	-2.39	122.66	124.73
2	B	1449	HEM	O1A-CGA-CBA	-2.21	115.42	123.03
2	A	1449	HEM	O1A-CGA-CBA	-2.06	115.94	123.03

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	430/455 (94%)	0.04	0 <span>100</span> <span>100</span>	10, 21, 35, 48	0
1	B	433/455 (95%)	0.07	4 (0%) <span>81</span> <span>83</span>	11, 21, 38, 61	0
All	All	863/910 (94%)	0.06	4 (0%) <span>88</span> <span>90</span>	10, 21, 36, 61	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	73	ALA	3.4
1	B	99	MET	3.3
1	B	216	PRO	2.7
1	B	2	SER	2.2

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

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

### 6.3 Carbohydrates

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( $\text{\AA}^2$ )	Q<0.9
2	HEM	B	1449	43/43	0.15	0.48	13,20,30,34	0
2	HEM	A	1449	43/43	0.14	0.35	11,17,30,33	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.