



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 12:14 PM GMT

PDB ID : 3LC4  
Title : Human Cytochrome P450 2E1 in Complex with Omega-Imidazolyl-DodecanoicAcid  
Authors : Scott, E.E.; Porubsky, P.R.  
Deposited on : 2010-01-09  
Resolution : 3.10 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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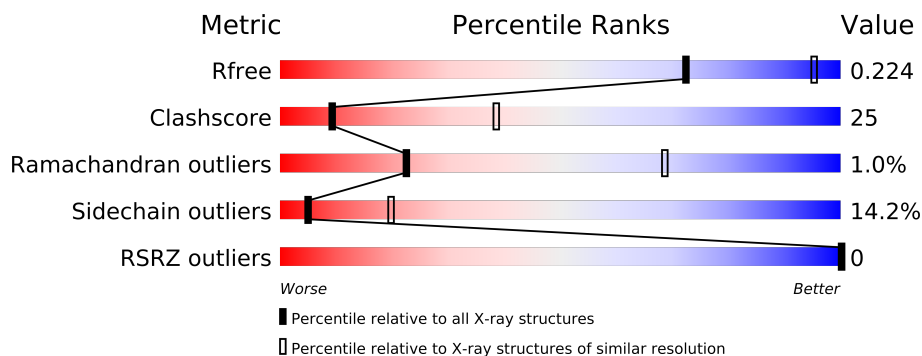
The following versions of software and data (see [references](#)) were used in the production of this report:

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 3.10 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	1007 (3.18-3.02)
Clashscore	79885	1078 (3.16-3.04)
Ramachandran outliers	78287	1044 (3.16-3.04)
Sidechain outliers	78261	1044 (3.16-3.04)
RSRZ outliers	66119	1008 (3.18-3.02)

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	476	
1	B	476	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7631 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 2E1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	460	Total	C	N	O	S	0	0	0
			3755	2431	643	663	18			
1	B	459	Total	C	N	O	S	0	0	0
			3747	2426	642	662	17			

There are 28 discrepancies between the modelled and reference sequences:

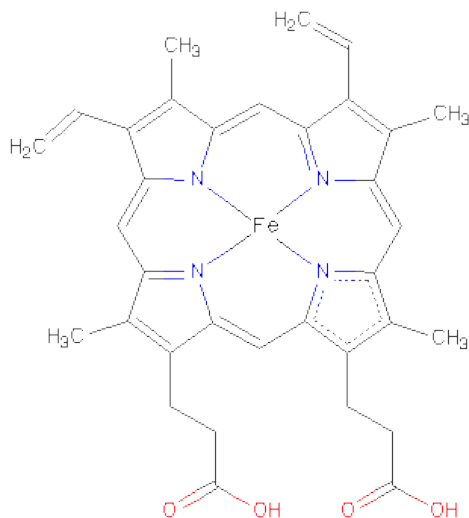
Chain	Residue	Modelled	Actual	Comment	Reference
A	22	MET	-	EXPRESSION TAG	UNP P05181
A	23	ALA	-	EXPRESSION TAG	UNP P05181
A	24	LYS	-	EXPRESSION TAG	UNP P05181
A	25	LYS	-	EXPRESSION TAG	UNP P05181
A	26	THR	-	EXPRESSION TAG	UNP P05181
A	27	SER	-	EXPRESSION TAG	UNP P05181
A	28	SER	-	EXPRESSION TAG	UNP P05181
A	29	LYS	-	EXPRESSION TAG	UNP P05181
A	30	GLY	-	EXPRESSION TAG	UNP P05181
A	31	LYS	-	EXPRESSION TAG	UNP P05181
A	494	HIS	-	EXPRESSION TAG	UNP P05181
A	495	HIS	-	EXPRESSION TAG	UNP P05181
A	496	HIS	-	EXPRESSION TAG	UNP P05181
A	497	HIS	-	EXPRESSION TAG	UNP P05181
B	22	MET	-	EXPRESSION TAG	UNP P05181
B	23	ALA	-	EXPRESSION TAG	UNP P05181
B	24	LYS	-	EXPRESSION TAG	UNP P05181
B	25	LYS	-	EXPRESSION TAG	UNP P05181
B	26	THR	-	EXPRESSION TAG	UNP P05181
B	27	SER	-	EXPRESSION TAG	UNP P05181
B	28	SER	-	EXPRESSION TAG	UNP P05181
B	29	LYS	-	EXPRESSION TAG	UNP P05181
B	30	GLY	-	EXPRESSION TAG	UNP P05181
B	31	LYS	-	EXPRESSION TAG	UNP P05181
B	494	HIS	-	EXPRESSION TAG	UNP P05181

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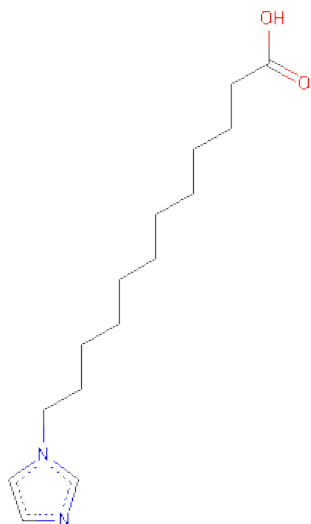
Chain	Residue	Modelled	Actual	Comment	Reference
B	495	HIS	-	EXPRESSION TAG	UNP P05181
B	496	HIS	-	EXPRESSION TAG	UNP P05181
B	497	HIS	-	EXPRESSION TAG	UNP P05181

- 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 12-(1H-IMIDAZOL-1-YL)DODECANOICACID (three-letter code: LC4) (formula:  $C_{15}H_{26}N_2O_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			19	15	2	2		
3	B	1	Total	C	N	O	0	0
			19	15	2	2		

- Molecule 4 is water.

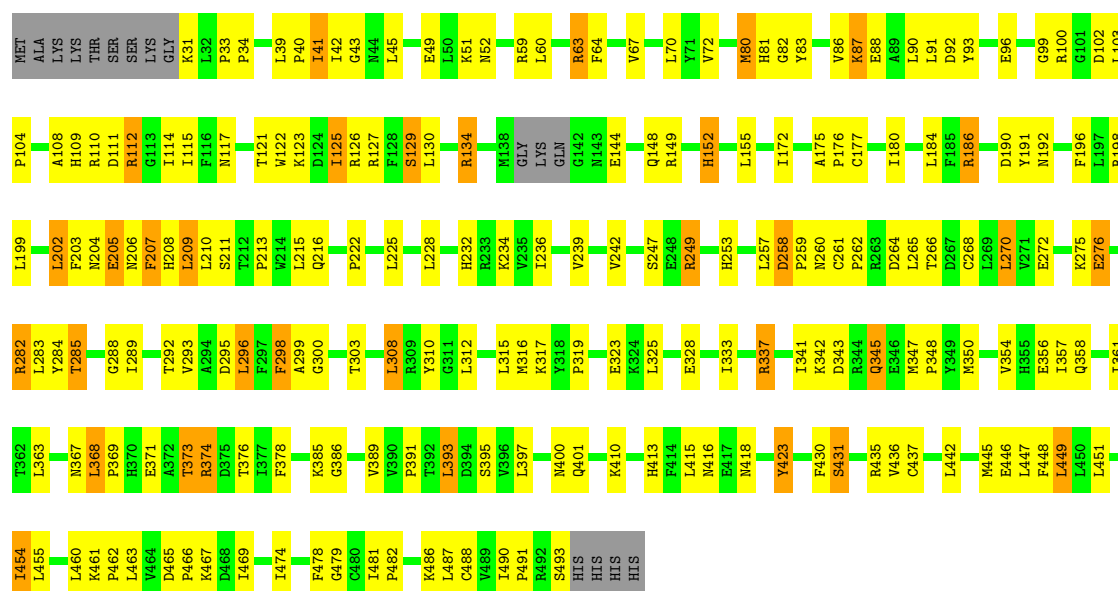
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	O	0	0
			2	2		
4	B	3	Total	O	0	0
			3	3		

### 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.

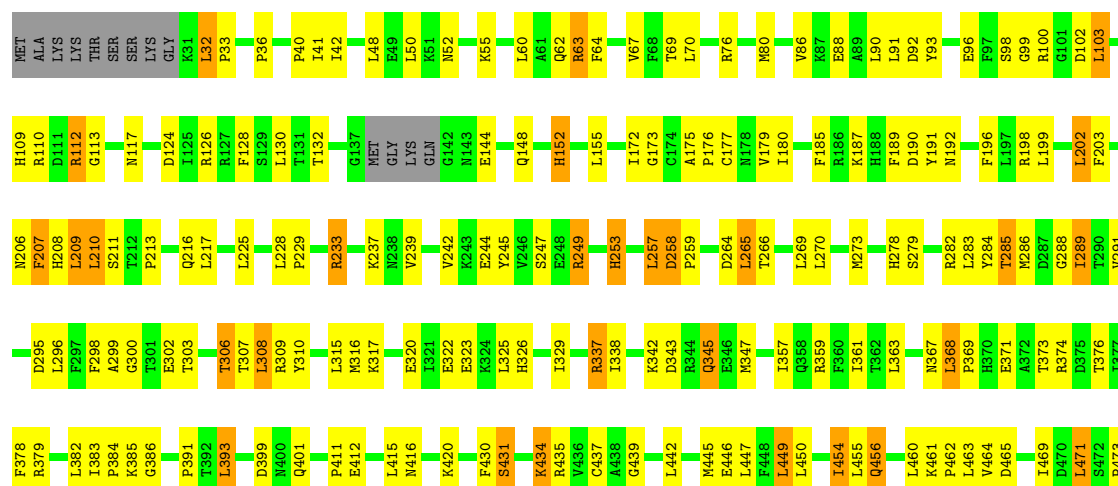
#### • Molecule 1: Cytochrome P450 2E1

Chain A:



#### • Molecule 1: Cytochrome P450 2E1

Chain B:



1474	
G479	
C480	
1481	
P482	
K486	
L487	
C488	
V489	
1490	
S493	
HIS	
HIS	
HIS	
HIS	

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	70.78Å 70.78Å 224.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.93 – 3.10 37.93 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.8 (37.93-3.10) 99.8 (37.93-3.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.19	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.29 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.198 , 0.270 0.190 , 0.224	Depositor DCC
$R_{free}$ test set	1018 reflections (5.41%)	DCC
Wilson B-factor (Å <sup>2</sup> )	52.7	Xtriage
Anisotropy	0.182	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 6.7	EDS
Estimated twinning fraction	0.460 for h,-k,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 19865 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	7631	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.83% 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, LC4

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	0.70	1/3859 (0.0%)	0.75	0/5226
1	B	0.70	0/3851	0.76	0/5216
All	All	0.70	1/7710 (0.0%)	0.75	0/10442

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	400	ASN	CG-OD1	5.19	1.35	1.24

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	3755	0	3756	189	0
1	B	3747	0	3747	181	0
2	A	43	0	30	11	0
2	B	43	0	30	11	0
3	A	19	0	25	8	0
3	B	19	0	25	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	2	0	0	0	0
4	B	3	0	0	0	0
All	All	7631	0	7613	378	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 25.

All (378) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:98:SER:HA	1:B:434:LYS:CE	1.37	1.51
1:B:98:SER:CA	1:B:434:LYS:HE2	1.60	1.30
1:B:98:SER:HA	1:B:434:LYS:NZ	1.51	1.26
1:A:40:PRO:O	1:A:41:ILE:HG12	1.43	1.15
1:A:310:TYR:HE1	1:A:482:PRO:HD3	1.14	1.08
1:B:229:PRO:HA	1:B:233:ARG:NH1	1.70	1.06
1:A:112:ARG:HG3	1:A:112:ARG:HH11	1.21	1.03
1:B:229:PRO:HA	1:B:233:ARG:HH12	1.15	1.02
1:B:229:PRO:CA	1:B:233:ARG:HH12	1.74	1.01
1:A:41:ILE:HG12	1:A:42:ILE:H	1.25	1.00
1:B:310:TYR:HE1	1:B:482:PRO:HD3	1.25	1.00
1:B:98:SER:CA	1:B:434:LYS:CE	2.28	0.98
1:B:343:ASP:HB3	1:B:347:MET:HE2	1.45	0.98
1:A:42:ILE:HG13	1:A:43:GLY:N	1.74	0.97
1:B:98:SER:HA	1:B:434:LYS:HE2	0.98	0.95
1:A:310:TYR:CE1	1:A:482:PRO:HD3	2.01	0.95
1:A:83:TYR:CZ	1:A:87:LYS:NZ	2.35	0.94
1:A:134:ARG:HH21	1:A:134:ARG:HB2	1.30	0.94
1:A:41:ILE:CG1	1:A:42:ILE:H	1.80	0.93
1:B:98:SER:CA	1:B:434:LYS:NZ	2.33	0.92
1:A:282:ARG:CZ	1:A:283:LEU:H	1.82	0.92
1:B:40:PRO:O	1:B:41:ILE:HG13	1.70	0.91
1:A:42:ILE:HG13	1:A:43:GLY:H	1.35	0.91
1:A:186:ARG:HH11	1:A:186:ARG:HG2	1.37	0.90
1:A:103:LEU:HD11	1:A:369:PRO:HG2	1.54	0.90
1:B:286:MET:HA	1:B:289:ILE:HD12	1.54	0.89
1:B:206:ASN:O	1:B:210:LEU:HB2	1.74	0.88
1:A:121:THR:O	1:A:125:ILE:HD11	1.73	0.88
1:A:41:ILE:CG1	1:A:42:ILE:N	2.37	0.86
1:B:310:TYR:CE1	1:B:482:PRO:HD3	2.11	0.86
1:B:98:SER:HA	1:B:434:LYS:HZ3	1.41	0.85
1:A:310:TYR:HE1	1:A:482:PRO:CD	1.90	0.85
1:B:302:GLU:O	1:B:306:THR:HG22	1.76	0.85

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:282:ARG:NH1	1:A:284:TYR:H	1.75	0.84
2:A:500:HEM:HBC2	2:A:500:HEM:CMC	2.09	0.83
1:A:83:TYR:CE2	1:A:87:LYS:NZ	2.47	0.82
1:B:316:MET:CE	1:B:462:PRO:HA	2.10	0.82
1:A:80:MET:CE	1:A:389:VAL:HG13	2.11	0.81
1:B:112:ARG:HG3	1:B:112:ARG:HH11	1.46	0.80
1:B:98:SER:CA	1:B:434:LYS:HZ3	1.91	0.80
1:A:198:ARG:O	1:A:202:LEU:HD22	1.81	0.80
1:A:282:ARG:HH12	1:A:284:TYR:H	1.28	0.80
1:A:316:MET:CE	1:A:462:PRO:HA	2.10	0.80
1:B:310:TYR:HE1	1:B:482:PRO:CD	1.94	0.79
1:A:410:LYS:HB2	1:A:413:HIS:CE1	2.17	0.79
1:A:461:LYS:HB3	1:A:488:CYS:HB2	1.66	0.78
1:A:121:THR:C	1:A:125:ILE:HD11	2.03	0.78
1:B:434:LYS:HZ2	1:B:435:ARG:HG3	1.49	0.77
1:A:39:LEU:HB2	1:A:42:ILE:HD11	1.66	0.77
1:B:300:GLY:HA2	2:B:500:HEM:HMC2	1.68	0.76
1:B:103:LEU:HD11	1:B:369:PRO:HG2	1.66	0.76
1:A:40:PRO:O	1:A:41:ILE:CG1	2.30	0.76
1:B:302:GLU:O	1:B:306:THR:CG2	2.34	0.76
1:B:112:ARG:CG	1:B:112:ARG:HH11	1.99	0.74
1:B:442:LEU:O	1:B:446:GLU:HB2	1.86	0.74
1:A:357:ILE:O	1:A:361:ILE:HG12	1.88	0.73
1:A:102:ASP:O	1:A:103:LEU:HD12	1.88	0.73
1:A:300:GLY:HA2	2:A:500:HEM:HMC2	1.70	0.73
1:A:266:THR:O	1:A:270:LEU:HD22	1.88	0.72
1:A:122:TRP:O	1:A:125:ILE:HD12	1.90	0.72
1:A:316:MET:HE1	1:A:462:PRO:HA	1.70	0.72
1:A:283:LEU:HD23	1:A:284:TYR:CE2	2.24	0.72
1:A:121:THR:O	1:A:125:ILE:CD1	2.37	0.72
1:B:99:GLY:HA3	1:B:371:GLU:HB3	1.72	0.72
1:B:110:ARG:O	1:B:112:ARG:NH1	2.23	0.72
1:B:98:SER:C	1:B:434:LYS:HZ3	1.94	0.71
1:A:276:GLU:HG2	1:A:276:GLU:O	1.90	0.71
1:A:350:MET:CE	1:A:451:LEU:HD23	2.20	0.71
2:B:500:HEM:CMC	2:B:500:HEM:HBC2	2.20	0.71
1:B:286:MET:HA	1:B:289:ILE:CD1	2.20	0.71
1:B:269:LEU:HD23	1:B:289:ILE:HG23	1.73	0.71
1:B:144:GLU:O	1:B:148:GLN:HG3	1.90	0.71
1:A:373:THR:O	1:A:385:LYS:HE3	1.91	0.70
1:A:206:ASN:O	1:A:210:LEU:HD12	1.91	0.70
1:A:310:TYR:CE1	1:A:482:PRO:CD	2.69	0.70

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:337:ARG:HH12	1:A:343:ASP:CG	1.95	0.69
1:B:310:TYR:CE1	1:B:482:PRO:HB3	2.27	0.69
1:A:442:LEU:O	1:A:446:GLU:HB2	1.92	0.69
1:A:282:ARG:NE	1:A:282:ARG:HA	2.07	0.69
1:B:343:ASP:CB	1:B:347:MET:HE2	2.21	0.69
1:B:41:ILE:HD12	1:B:42:ILE:HG23	1.73	0.69
1:A:123:LYS:HE2	1:A:127:ARG:HH22	1.58	0.68
1:B:98:SER:CB	1:B:434:LYS:HE2	2.23	0.68
1:B:198:ARG:O	1:B:202:LEU:HD12	1.93	0.68
1:B:203:PHE:HB3	1:B:302:GLU:HG2	1.75	0.68
1:A:350:MET:HE1	1:A:451:LEU:HD23	1.75	0.68
1:B:98:SER:N	1:B:434:LYS:HE2	2.10	0.67
1:B:415:LEU:O	1:B:416:ASN:CB	2.43	0.67
1:B:307:THR:HG21	1:B:447:LEU:HD21	1.76	0.67
2:A:500:HEM:HMC2	2:A:500:HEM:HBC2	1.76	0.66
1:B:310:TYR:CE1	1:B:482:PRO:CD	2.75	0.66
1:A:316:MET:CE	1:A:462:PRO:CA	2.73	0.66
2:B:500:HEM:HBC2	2:B:500:HEM:HMC2	1.78	0.66
1:A:41:ILE:HG13	1:A:42:ILE:N	2.09	0.66
1:B:228:LEU:C	1:B:233:ARG:HH22	1.99	0.66
1:B:450:LEU:O	1:B:454:ILE:HG12	1.95	0.66
1:A:110:ARG:O	1:A:112:ARG:NH1	2.29	0.65
1:B:357:ILE:O	1:B:361:ILE:HG12	1.96	0.65
1:B:316:MET:CE	1:B:462:PRO:CA	2.75	0.65
1:A:80:MET:HE1	1:A:389:VAL:HG13	1.78	0.65
1:A:232:HIS:O	1:A:236:ILE:HD12	1.97	0.65
1:B:363:LEU:O	1:B:479:GLY:HA2	1.97	0.65
1:B:373:THR:O	1:B:385:LYS:HE3	1.97	0.65
1:B:316:MET:HE2	1:B:462:PRO:CA	2.27	0.64
1:A:316:MET:HE3	1:A:462:PRO:CA	2.27	0.64
1:B:112:ARG:HD2	1:B:291:VAL:HG21	1.78	0.64
1:A:109:HIS:NE2	3:A:501:LC4:O17	2.30	0.64
1:B:285:THR:HG23	1:B:288:GLY:H	1.61	0.63
1:B:242:VAL:HG11	3:B:501:LC4:H3	1.80	0.63
1:A:186:ARG:HH11	1:A:186:ARG:CG	2.09	0.62
1:B:98:SER:HB2	1:B:373:THR:HG21	1.80	0.62
1:B:233:ARG:O	1:B:237:LYS:HG3	2.00	0.62
1:B:100:ARG:NH2	1:B:368:LEU:HB3	2.14	0.62
1:B:242:VAL:HB	3:B:501:LC4:O1	2.00	0.61
1:A:177:CYS:O	1:A:180:ILE:HG22	2.00	0.61
1:B:112:ARG:HG3	1:B:112:ARG:NH1	2.15	0.61
1:B:109:HIS:NE2	3:B:501:LC4:O17	2.33	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:245:TYR:CZ	1:B:249:ARG:CZ	2.83	0.61
1:B:98:SER:O	1:B:434:LYS:NZ	2.34	0.61
1:A:59:ARG:NH1	1:A:63:ARG:NH2	2.49	0.61
1:A:100:ARG:NH2	1:A:368:LEU:HB3	2.15	0.61
1:B:177:CYS:HG	1:B:196:PHE:HE1	1.50	0.60
1:B:239:VAL:HG13	3:B:501:LC4:O17	2.01	0.60
1:B:415:LEU:O	1:B:416:ASN:HB2	2.00	0.60
1:B:50:LEU:HD22	1:B:50:LEU:H	1.65	0.60
1:A:144:GLU:O	1:A:148:GLN:HG3	2.00	0.60
1:B:461:LYS:HB3	1:B:488:CYS:HB2	1.83	0.60
1:B:342:LYS:O	1:B:345:GLN:HG3	2.01	0.60
1:A:325:LEU:HD11	1:A:350:MET:HA	1.84	0.59
1:B:177:CYS:SG	1:B:196:PHE:HE1	2.26	0.59
1:A:184:LEU:HD12	1:A:293:VAL:HG13	1.84	0.59
1:A:172:ILE:HD12	1:A:308:LEU:HB3	1.85	0.59
1:A:198:ARG:O	1:A:202:LEU:CD2	2.51	0.58
1:A:310:TYR:CE1	1:A:482:PRO:HB3	2.37	0.58
1:B:295:ASP:O	1:B:299:ALA:CB	2.51	0.58
1:B:310:TYR:CE1	1:B:482:PRO:CB	2.86	0.58
1:A:312:LEU:HD21	1:A:454:ILE:CD1	2.33	0.58
1:A:39:LEU:HD22	1:A:42:ILE:HD11	1.84	0.58
1:A:285:THR:HG23	1:A:288:GLY:H	1.68	0.58
1:B:67:VAL:HG21	1:B:378:PHE:HE2	1.69	0.58
1:A:41:ILE:HG12	1:A:42:ILE:N	2.01	0.58
1:A:298:PHE:CD2	3:A:501:LC4:H3A	2.39	0.58
1:A:337:ARG:NH1	1:A:343:ASP:OD2	2.32	0.58
1:A:144:GLU:OE1	1:A:341:ILE:HG13	2.03	0.58
1:A:328:GLU:OE1	1:A:348:PRO:HD2	2.04	0.57
2:A:500:HEM:HMC2	2:A:500:HEM:CBC	2.34	0.57
1:A:39:LEU:CB	1:A:42:ILE:HD11	2.34	0.56
1:A:242:VAL:HB	3:A:501:LC4:O1	2.05	0.56
1:B:41:ILE:CD1	1:B:42:ILE:HG23	2.35	0.56
1:A:125:ILE:O	1:A:129:SER:OG	2.24	0.56
1:A:122:TRP:HA	1:A:125:ILE:CD1	2.36	0.56
1:B:415:LEU:O	1:B:420:LYS:O	2.24	0.56
1:B:273:MET:HG2	1:B:282:ARG:HH22	1.70	0.56
1:B:102:ASP:O	1:B:103:LEU:HD12	2.06	0.56
1:B:109:HIS:ND1	1:B:295:ASP:OD2	2.36	0.55
1:B:300:GLY:HA2	2:B:500:HEM:CMC	2.36	0.55
1:A:81:HIS:CD2	1:A:395:SER:HB3	2.41	0.55
1:A:206:ASN:C	1:A:210:LEU:HD12	2.26	0.55
1:A:109:HIS:ND1	1:A:295:ASP:OD2	2.40	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:239:VAL:O	3:A:501:LC4:O1	2.24	0.55
1:B:412:GLU:HA	1:B:415:LEU:HB3	1.89	0.55
1:B:67:VAL:HG21	1:B:378:PHE:CE2	2.42	0.55
1:B:295:ASP:O	1:B:299:ALA:HB2	2.06	0.54
1:A:445:MET:HG2	1:A:449:LEU:HD22	1.89	0.54
1:B:385:LYS:HG2	1:B:386:GLY:N	2.23	0.54
1:B:102:ASP:OD2	1:B:110:ARG:HD3	2.07	0.53
1:B:385:LYS:CG	1:B:386:GLY:N	2.71	0.53
1:B:229:PRO:N	1:B:233:ARG:HH22	2.07	0.53
1:A:52:ASN:C	1:A:52:ASN:OD1	2.47	0.53
1:A:317:LYS:HD2	1:A:469:ILE:HB	1.90	0.53
1:A:109:HIS:CE1	1:A:295:ASP:OD2	2.61	0.53
1:B:399:ASP:OD1	1:B:401:GLN:HB2	2.08	0.53
1:A:276:GLU:CD	1:A:282:ARG:CZ	2.77	0.53
1:B:298:PHE:CD2	3:B:501:LC4:H3A	2.44	0.53
1:A:208:HIS:ND1	1:A:209:LEU:HD13	2.24	0.53
1:B:32:LEU:H	1:B:32:LEU:HD12	1.72	0.53
1:A:316:MET:HE3	1:A:462:PRO:CB	2.38	0.53
1:A:104:PRO:HG2	1:A:222:PRO:HG3	1.91	0.53
1:A:350:MET:HE3	1:A:451:LEU:HD23	1.90	0.53
1:B:229:PRO:C	1:B:233:ARG:HH12	2.12	0.52
1:B:190:ASP:C	1:B:192:ASN:H	2.12	0.52
1:B:207:PHE:CD1	3:B:501:LC4:H8	2.45	0.52
1:A:374:ARG:O	1:A:376:THR:OG1	2.27	0.52
1:B:98:SER:C	1:B:434:LYS:NZ	2.60	0.52
1:B:286:MET:CA	1:B:289:ILE:HD12	2.34	0.52
1:A:225:LEU:HA	1:A:228:LEU:HD22	1.92	0.52
1:B:172:ILE:HD12	1:B:308:LEU:HB3	1.92	0.52
1:A:401:GLN:OE1	1:A:401:GLN:HA	2.10	0.51
1:A:80:MET:HE2	1:A:389:VAL:HG13	1.88	0.51
1:A:373:THR:O	1:A:385:LYS:CE	2.57	0.51
1:B:378:PHE:HB2	1:B:383:ILE:HD12	1.92	0.51
1:B:317:LYS:HD2	1:B:469:ILE:HB	1.92	0.51
1:B:239:VAL:O	3:B:501:LC4:O1	2.29	0.51
1:A:295:ASP:O	1:A:299:ALA:HB2	2.11	0.51
1:B:93:TYR:HB3	1:B:96:GLU:HB2	1.93	0.51
1:A:416:ASN:C	1:A:418:ASN:H	2.13	0.51
1:A:186:ARG:NH1	1:A:186:ARG:HG2	2.14	0.50
1:A:316:MET:HE3	1:A:462:PRO:HB3	1.93	0.50
1:B:317:LYS:HD3	1:B:471:LEU:HD22	1.93	0.50
1:A:100:ARG:HD3	1:A:369:PRO:O	2.12	0.50
1:B:329:ILE:HG21	1:B:456:GLN:HB2	1.94	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:42:ILE:CG1	1:A:43:GLY:N	2.62	0.50
1:A:368:LEU:HB2	2:A:500:HEM:HAA2	1.94	0.50
1:A:310:TYR:CE1	1:A:482:PRO:CB	2.95	0.50
1:B:245:TYR:CZ	1:B:249:ARG:NH2	2.79	0.50
1:B:378:PHE:CD2	1:B:379:ARG:HG3	2.47	0.50
1:B:316:MET:HE2	1:B:462:PRO:N	2.27	0.50
1:A:367:ASN:HA	1:A:393:LEU:HD22	1.94	0.49
1:B:257:LEU:O	1:B:257:LEU:HD13	2.11	0.49
1:B:373:THR:O	1:B:385:LYS:CE	2.59	0.49
1:A:39:LEU:HB2	1:A:42:ILE:CD1	2.39	0.49
1:B:310:TYR:CD1	1:B:482:PRO:HB3	2.47	0.49
1:A:354:VAL:O	1:A:358:GLN:HG3	2.12	0.49
1:B:216:GLN:NE2	1:B:216:GLN:HA	2.27	0.49
1:B:52:ASN:OD1	1:B:52:ASN:C	2.51	0.49
1:A:295:ASP:O	1:A:299:ALA:CB	2.61	0.49
1:B:437:CYS:HB2	2:B:500:HEM:NA	2.27	0.49
1:B:430:PHE:O	1:B:431:SER:CB	2.61	0.49
1:B:303:THR:HG22	3:B:501:LC4:H10A	1.95	0.48
1:B:412:GLU:HA	1:B:415:LEU:CB	2.42	0.48
1:A:63:ARG:HB3	1:A:64:PHE:CD2	2.48	0.48
1:B:63:ARG:HB3	1:B:64:PHE:CD2	2.48	0.48
1:A:416:ASN:C	1:A:418:ASN:N	2.67	0.48
1:A:112:ARG:O	1:A:117:ASN:HB2	2.13	0.48
1:B:177:CYS:SG	1:B:196:PHE:CE1	3.03	0.48
1:A:88:GLU:O	1:A:92:ASP:HB2	2.12	0.48
1:B:98:SER:OG	1:B:434:LYS:HE2	2.12	0.48
1:A:363:LEU:O	1:A:479:GLY:HA2	2.14	0.48
1:B:173:GLY:O	1:B:176:PRO:HD2	2.14	0.48
1:A:207:PHE:CD1	3:A:501:LC4:H8	2.49	0.48
1:B:217:LEU:HD23	1:B:225:LEU:HD21	1.96	0.48
1:B:266:THR:O	1:B:270:LEU:HD22	2.14	0.48
2:B:500:HEM:NA	3:B:501:LC4:N15	2.62	0.48
1:A:102:ASP:OD2	1:A:110:ARG:HD3	2.14	0.48
1:A:82:GLY:O	1:A:86:VAL:HG23	2.14	0.48
1:A:242:VAL:HG11	3:A:501:LC4:H3	1.96	0.48
1:A:114:ILE:HG22	2:A:500:HEM:O1D	2.14	0.47
1:A:416:ASN:O	1:A:418:ASN:N	2.47	0.47
1:A:282:ARG:NH1	1:A:283:LEU:H	2.10	0.47
1:B:307:THR:CG2	1:B:447:LEU:HD21	2.44	0.47
1:A:39:LEU:CD2	1:A:42:ILE:HD11	2.44	0.47
1:A:112:ARG:HG3	1:A:112:ARG:NH1	2.01	0.47
1:A:190:ASP:C	1:A:192:ASN:H	2.17	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:430:PHE:O	1:B:431:SER:HB3	2.14	0.47
1:B:253:HIS:CD2	1:B:266:THR:HB	2.50	0.47
1:A:465:ASP:C	1:A:467:LYS:H	2.18	0.47
1:A:59:ARG:HH12	1:A:63:ARG:NH2	2.12	0.47
1:B:435:ARG:O	2:B:500:HEM:HBA2	2.15	0.47
1:A:300:GLY:HA2	2:A:500:HEM:CMC	2.41	0.46
1:A:205:GLU:OE1	1:A:234:LYS:HE3	2.15	0.46
1:A:292:THR:O	1:A:296:LEU:HD12	2.15	0.46
1:A:448:PHE:CD2	1:A:449:LEU:HD13	2.50	0.46
1:B:152:HIS:ND1	1:B:152:HIS:C	2.68	0.46
1:B:177:CYS:O	1:B:180:ILE:HG22	2.16	0.46
1:B:80:MET:HB2	1:B:80:MET:HE2	1.61	0.46
1:A:96:GLU:OE2	1:A:96:GLU:N	2.48	0.46
1:B:445:MET:HG2	1:B:449:LEU:HD22	1.97	0.46
1:A:111:ASP:HA	1:A:117:ASN:HA	1.98	0.46
2:B:500:HEM:HMC2	2:B:500:HEM:CBC	2.43	0.46
1:A:216:GLN:HA	1:A:216:GLN:NE2	2.30	0.45
1:A:268:CYS:O	1:A:272:GLU:HG2	2.16	0.45
1:B:100:ARG:HD3	1:B:369:PRO:O	2.16	0.45
1:B:208:HIS:ND1	1:B:209:LEU:HD13	2.30	0.45
1:B:310:TYR:OH	1:B:473:PRO:HA	2.17	0.45
1:B:302:GLU:O	1:B:306:THR:HG23	2.15	0.45
1:B:283:LEU:HD23	1:B:284:TYR:CE2	2.52	0.45
1:B:434:LYS:NZ	1:B:435:ARG:HG3	2.26	0.45
1:A:208:HIS:HA	1:A:481:ILE:HD13	1.99	0.45
1:B:474:ILE:N	1:B:481:ILE:O	2.40	0.45
1:B:278:HIS:O	1:B:279:SER:C	2.55	0.45
1:A:134:ARG:HB2	1:A:134:ARG:NH2	2.13	0.45
1:B:110:ARG:O	1:B:112:ARG:HG3	2.17	0.45
1:B:132:THR:CG2	1:B:265:LEU:HD22	2.46	0.45
1:A:430:PHE:HB3	1:A:437:CYS:HB3	1.98	0.45
1:A:430:PHE:O	1:A:431:SER:CB	2.64	0.45
1:A:303:THR:HG22	3:A:501:LC4:H10A	1.99	0.45
1:A:298:PHE:C	1:A:298:PHE:CD1	2.91	0.44
1:A:122:TRP:HA	1:A:125:ILE:HD11	1.98	0.44
1:B:207:PHE:HD1	1:B:207:PHE:HA	1.69	0.44
1:B:33:PRO:HG2	1:B:69:THR:OG1	2.17	0.44
1:A:102:ASP:C	1:A:103:LEU:HD12	2.37	0.44
1:A:203:PHE:HE1	1:A:242:VAL:HG21	1.82	0.44
1:B:189:PHE:CD1	1:B:196:PHE:HB2	2.52	0.44
1:A:448:PHE:HD2	1:A:449:LEU:HD13	1.83	0.44
1:A:282:ARG:NH2	1:A:283:LEU:H	2.12	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:177:CYS:SG	1:A:196:PHE:HE1	2.40	0.44
1:B:175:ALA:O	1:B:179:VAL:HG23	2.18	0.44
1:A:343:ASP:O	1:A:347:MET:HG3	2.18	0.44
1:B:173:GLY:C	1:B:176:PRO:HD2	2.38	0.44
1:B:266:THR:O	1:B:270:LEU:CD2	2.66	0.44
1:A:126:ARG:NH2	1:A:436:VAL:O	2.50	0.44
1:B:86:VAL:HG13	1:B:391:PRO:HB2	1.98	0.44
1:A:312:LEU:CD2	1:A:454:ILE:HD11	2.48	0.44
1:B:439:GLY:HA3	2:B:500:HEM:C3C	2.53	0.44
1:A:437:CYS:HB2	2:A:500:HEM:NA	2.33	0.44
1:A:175:ALA:HB3	1:A:176:PRO:HD3	1.99	0.44
1:B:98:SER:OG	1:B:434:LYS:CD	2.66	0.44
1:A:373:THR:O	1:A:385:LYS:CD	2.66	0.44
1:A:385:LYS:CG	1:A:386:GLY:N	2.81	0.44
1:A:333:ILE:HD11	1:A:347:MET:HE2	2.00	0.44
1:B:245:TYR:CZ	1:B:249:ARG:NH1	2.86	0.43
1:B:258:ASP:HA	1:B:259:PRO:HD3	1.87	0.43
1:A:115:ILE:HG13	1:A:115:ILE:H	1.65	0.43
1:A:83:TYR:CZ	1:A:87:LYS:CE	3.02	0.43
1:B:113:GLY:HA3	1:B:291:VAL:HG12	2.00	0.43
1:A:257:LEU:HD22	1:A:270:LEU:HB3	2.00	0.43
1:B:316:MET:HB3	1:B:462:PRO:HG3	2.00	0.43
1:B:368:LEU:HD12	1:B:369:PRO:HD3	2.01	0.43
1:B:185:PHE:C	1:B:187:LYS:N	2.71	0.43
1:B:98:SER:OG	1:B:434:LYS:HD3	2.18	0.43
2:A:500:HEM:NA	3:A:501:LC4:N15	2.66	0.43
1:B:337:ARG:HH12	1:B:343:ASP:CG	2.22	0.43
1:A:342:LYS:O	1:A:345:GLN:HG3	2.18	0.43
1:A:260:ASN:O	1:A:262:PRO:HD3	2.18	0.43
1:B:209:LEU:HA	1:B:209:LEU:HD12	1.90	0.43
1:A:249:ARG:HD3	1:A:249:ARG:HA	1.52	0.43
1:B:374:ARG:O	1:B:376:THR:OG1	2.35	0.43
1:A:115:ILE:HA	2:A:500:HEM:HAD2	2.01	0.43
1:B:148:GLN:HB3	1:B:338:ILE:HD13	2.00	0.43
1:A:123:LYS:CE	1:A:127:ARG:HH22	2.29	0.43
1:A:51:LYS:HA	1:A:213:PRO:HG3	2.00	0.43
1:B:67:VAL:CG2	1:B:378:PHE:HE2	2.31	0.42
1:B:282:ARG:CZ	1:B:284:TYR:O	2.67	0.42
1:A:258:ASP:OD1	1:A:261:CYS:HB2	2.19	0.42
1:B:308:LEU:HD12	1:B:308:LEU:HA	1.79	0.42
1:A:310:TYR:CD1	1:A:482:PRO:HB3	2.54	0.42
1:A:356:GLU:OE2	1:A:413:HIS:HB2	2.18	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:350:MET:CE	1:A:354:VAL:HG23	2.49	0.42
1:B:253:HIS:NE2	1:B:264:ASP:OD1	2.52	0.42
1:B:490:ILE:H	1:B:490:ILE:HD13	1.84	0.42
1:B:88:GLU:O	1:B:92:ASP:HB2	2.18	0.42
1:A:285:THR:O	1:A:288:GLY:N	2.52	0.42
1:A:423:TYR:CD2	1:A:423:TYR:C	2.93	0.42
1:B:76:ARG:NH2	1:B:384:PRO:HB2	2.35	0.42
1:B:367:ASN:HA	1:B:393:LEU:HD22	2.01	0.42
1:B:295:ASP:O	1:B:299:ALA:HB3	2.18	0.42
1:B:378:PHE:CB	1:B:383:ILE:HD12	2.50	0.42
1:B:244:GLU:O	1:B:247:SER:HB3	2.20	0.42
1:A:207:PHE:CZ	1:A:479:GLY:HA3	2.55	0.42
1:A:122:TRP:CA	1:A:125:ILE:HD11	2.50	0.42
1:A:258:ASP:HA	1:A:259:PRO:HD3	1.77	0.42
1:B:112:ARG:O	1:B:117:ASN:HB2	2.19	0.42
1:A:253:HIS:NE2	1:A:264:ASP:OD1	2.46	0.42
1:A:177:CYS:SG	1:A:196:PHE:CE1	3.13	0.42
1:A:33:PRO:HA	1:A:34:PRO:HD3	1.91	0.42
1:A:282:ARG:NH1	1:A:284:TYR:N	2.55	0.41
1:A:253:HIS:CD2	1:A:266:THR:HB	2.55	0.41
1:A:385:LYS:HG2	1:A:386:GLY:N	2.34	0.41
1:A:152:HIS:C	1:A:152:HIS:ND1	2.73	0.41
1:A:41:ILE:CG1	1:A:42:ILE:HG23	2.50	0.41
1:A:435:ARG:O	2:A:500:HEM:HBA2	2.20	0.41
1:A:103:LEU:HD23	1:A:478:PHE:HE1	1.85	0.41
1:B:102:ASP:O	1:B:103:LEU:CD1	2.69	0.41
1:B:245:TYR:CE1	1:B:249:ARG:NH2	2.88	0.41
1:A:67:VAL:HG21	1:A:378:PHE:HE2	1.86	0.41
1:B:431:SER:CB	2:B:500:HEM:HBA1	2.50	0.41
1:A:341:ILE:HG13	1:A:341:ILE:H	1.60	0.41
1:A:474:ILE:N	1:A:481:ILE:O	2.42	0.41
1:A:93:TYR:HB3	1:A:96:GLU:HB2	2.02	0.41
1:A:99:GLY:C	1:A:371:GLU:H	2.24	0.41
1:B:303:THR:HB	2:B:500:HEM:CAB	2.51	0.41
1:B:50:LEU:CD2	1:B:50:LEU:H	2.32	0.41
1:A:284:TYR:HB3	1:A:289:ILE:HD11	2.03	0.41
1:B:128:PHE:CE2	1:B:269:LEU:HD12	2.56	0.41
1:A:59:ARG:HH12	1:A:63:ARG:HH22	1.69	0.41
1:A:144:GLU:CD	1:A:341:ILE:HG13	2.41	0.41
1:B:445:MET:O	1:B:449:LEU:HB2	2.20	0.41
1:A:149:ARG:O	1:A:152:HIS:HB3	2.20	0.41
1:B:316:MET:SD	1:B:487:LEU:HD23	2.60	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:322:GLU:HG2	1:B:326:HIS:NE2	2.36	0.40
1:A:312:LEU:HD21	1:A:454:ILE:HD11	2.04	0.40
1:B:306:THR:HB	1:B:309:ARG:NH1	2.36	0.40
1:B:316:MET:HE3	1:B:462:PRO:HA	1.95	0.40
1:B:50:LEU:HB2	1:B:213:PRO:HB3	2.04	0.40
1:A:317:LYS:O	1:A:319:PRO:HD3	2.21	0.40
1:B:337:ARG:NH1	1:B:343:ASP:OD2	2.47	0.40
1:A:410:LYS:O	1:A:413:HIS:ND1	2.55	0.40
1:B:411:PRO:O	1:B:415:LEU:HB2	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	456/476 (96%)	422 (92%)	27 (6%)	7 (2%)	15	57
1	B	455/476 (96%)	417 (92%)	36 (8%)	2 (0%)	43	84
All	All	911/952 (96%)	839 (92%)	63 (7%)	9 (1%)	22	68

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	275	LYS
1	A	491	PRO
1	A	431	SER
1	A	466	PRO
1	B	191	TYR
1	A	108	ALA
1	A	191	TYR
1	B	431	SER
1	A	391	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	415/428 (97%)	355 (86%)	60 (14%)	5	18
1	B	414/428 (97%)	356 (86%)	58 (14%)	5	21
All	All	829/856 (97%)	711 (86%)	118 (14%)	5	20

All (118) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	LYS
1	A	41	ILE
1	A	45	LEU
1	A	49	GLU
1	A	60	LEU
1	A	63	ARG
1	A	70	LEU
1	A	72	VAL
1	A	80	MET
1	A	87	LYS
1	A	90	LEU
1	A	91	LEU
1	A	112	ARG
1	A	125	ILE
1	A	129	SER
1	A	130	LEU
1	A	134	ARG
1	A	152	HIS
1	A	155	LEU
1	A	186	ARG
1	A	199	LEU
1	A	202	LEU
1	A	204	ASN
1	A	205	GLU
1	A	207	PHE
1	A	209	LEU
1	A	211	SER
1	A	215	LEU
1	A	247	SER

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Mol	Chain	Res	Type
1	A	249	ARG
1	A	258	ASP
1	A	265	LEU
1	A	270	LEU
1	A	276	GLU
1	A	282	ARG
1	A	285	THR
1	A	296	LEU
1	A	298	PHE
1	A	308	LEU
1	A	315	LEU
1	A	323	GLU
1	A	337	ARG
1	A	345	GLN
1	A	368	LEU
1	A	373	THR
1	A	374	ARG
1	A	393	LEU
1	A	397	LEU
1	A	415	LEU
1	A	423	TYR
1	A	447	LEU
1	A	449	LEU
1	A	454	ILE
1	A	455	LEU
1	A	460	LEU
1	A	463	LEU
1	A	486	LYS
1	A	487	LEU
1	A	490	ILE
1	A	493	SER
1	B	32	LEU
1	B	36	PRO
1	B	48	LEU
1	B	55	LYS
1	B	60	LEU
1	B	62	GLN
1	B	63	ARG
1	B	70	LEU
1	B	90	LEU
1	B	91	LEU
1	B	103	LEU

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Mol	Chain	Res	Type
1	B	112	ARG
1	B	124	ASP
1	B	126	ARG
1	B	130	LEU
1	B	152	HIS
1	B	155	LEU
1	B	199	LEU
1	B	202	LEU
1	B	207	PHE
1	B	209	LEU
1	B	210	LEU
1	B	211	SER
1	B	233	ARG
1	B	249	ARG
1	B	253	HIS
1	B	257	LEU
1	B	258	ASP
1	B	265	LEU
1	B	285	THR
1	B	289	ILE
1	B	296	LEU
1	B	306	THR
1	B	308	LEU
1	B	315	LEU
1	B	320	GLU
1	B	323	GLU
1	B	325	LEU
1	B	337	ARG
1	B	345	GLN
1	B	359	ARG
1	B	368	LEU
1	B	382	LEU
1	B	393	LEU
1	B	434	LYS
1	B	449	LEU
1	B	454	ILE
1	B	455	LEU
1	B	456	GLN
1	B	460	LEU
1	B	463	LEU
1	B	464	VAL
1	B	465	ASP

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Mol	Chain	Res	Type
1	B	471	LEU
1	B	486	LYS
1	B	487	LEU
1	B	490	ILE
1	B	493	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	ASN

### 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 ⓘ

4 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	500	1,3	49,50,50	2.36	14 (28%)	46,82,82	1.88	8 (17%)
3	LC4	A	501	2	19,19,19	0.84	0	21,21,21	1.13	3 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	HEM	B	500	1,3	49,50,50	2.22	14 (28%)	46,82,82	2.04	10 (21%)
3	LC4	B	501	2	19,19,19	0.77	0	21,21,21	1.18	2 (9%)

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	500	1,3	-	0/14/114/114	0/0/8/8
3	LC4	A	501	2	-	0/14/14/14	0/1/1/1
2	HEM	B	500	1,3	-	0/14/114/114	0/0/8/8
3	LC4	B	501	2	-	0/14/14/14	0/1/1/1

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	HEM	C3C-C2C	-6.44	1.32	1.43
2	A	500	HEM	C2B-C1B	6.37	1.46	1.44
2	B	500	HEM	C3C-C2C	-5.89	1.33	1.43
2	B	500	HEM	C3D-C2D	5.35	1.53	1.43
2	B	500	HEM	C3B-C2B	-5.28	1.34	1.43
2	A	500	HEM	C3B-C2B	-5.21	1.34	1.43
2	A	500	HEM	C3D-C2D	5.04	1.52	1.43
2	B	500	HEM	C2B-C1B	4.96	1.45	1.44
2	A	500	HEM	C3B-CAB	4.54	1.54	1.40
2	B	500	HEM	C3B-CAB	4.45	1.54	1.40
2	B	500	HEM	C3C-CAC	4.15	1.53	1.40
2	A	500	HEM	C3D-C4D	4.07	1.45	1.44
2	A	500	HEM	C3C-CAC	3.91	1.52	1.40
2	A	500	HEM	C4A-C3A	3.87	1.45	1.40
2	B	500	HEM	C4A-C3A	3.59	1.44	1.40
2	A	500	HEM	C2D-C1D	-3.33	1.43	1.44
2	B	500	HEM	FE-NC	3.13	2.09	1.97
2	B	500	HEM	C3D-C4D	2.97	1.45	1.44
2	A	500	HEM	CMC-C2C	2.44	1.55	1.47
2	A	500	HEM	FE-NA	2.43	2.02	1.92
2	A	500	HEM	CMD-C2D	2.32	1.54	1.47
2	B	500	HEM	CMC-C2C	2.30	1.54	1.47
2	B	500	HEM	CMB-C2B	2.30	1.54	1.47
2	A	500	HEM	CMB-C2B	2.28	1.54	1.47
2	B	500	HEM	FE-NA	2.28	2.02	1.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500	HEM	CMD-C2D	2.24	1.54	1.47
2	B	500	HEM	C2D-C1D	-2.21	1.44	1.44
2	A	500	HEM	FE-NC	2.19	2.06	1.97

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	500	HEM	C4D-ND-C1D	6.44	111.75	105.16
2	A	500	HEM	C4D-ND-C1D	6.15	111.46	105.16
2	B	500	HEM	C3B-C4B-NB	-4.87	110.52	114.00
2	A	500	HEM	C3B-C4B-NB	-4.57	110.73	114.00
2	A	500	HEM	CHD-C1D-ND	4.46	128.29	124.58
2	B	500	HEM	CHD-C1D-ND	4.42	128.25	124.58
2	B	500	HEM	CBD-CAD-C3D	-4.07	105.50	114.37
2	B	500	HEM	CHC-C4B-NB	3.71	127.67	124.58
2	B	500	HEM	C2D-C1D-ND	-3.58	108.70	112.93
2	A	500	HEM	C2D-C1D-ND	-3.57	108.71	112.93
2	A	500	HEM	CHC-C4B-NB	3.42	127.42	124.58
3	B	501	LC4	C14-C13-N12	2.70	108.77	106.37
2	B	500	HEM	C4A-CHB-C1B	-2.67	123.96	127.47
2	A	500	HEM	CMA-C3A-C4A	-2.60	124.62	128.62
2	A	500	HEM	C4A-CHB-C1B	-2.52	124.16	127.47
3	A	501	LC4	C14-C13-N12	2.51	108.60	106.37
2	B	500	HEM	O1D-CGD-CBD	-2.33	115.02	123.03
3	A	501	LC4	N15-C16-N12	-2.25	108.18	111.96
2	A	500	HEM	CAD-C3D-C4D	2.23	128.54	124.53
2	B	500	HEM	CHC-C1C-NC	2.21	126.66	124.73
3	B	501	LC4	C10-C11-N12	2.16	118.04	111.70
2	B	500	HEM	CHA-C4D-ND	2.04	127.12	124.31
3	A	501	LC4	O17-C2-O1	-2.03	118.12	123.30

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	460/476 (96%)	-0.21	0 100 100	20, 45, 71, 88	0
1	B	459/476 (96%)	-0.20	0 100 100	22, 44, 71, 88	0
All	All	919/952 (96%)	-0.21	0 100 100	20, 44, 71, 88	0

There are no RSRZ outliers to report.

### 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	LC4	B	501	19/19	0.30	1.85	51,52,61,61	0
3	LC4	A	501	19/19	0.29	1.62	49,51,58,59	0
2	HEM	B	500	43/43	0.22	0.44	26,30,42,43	0
2	HEM	A	500	43/43	0.20	0.14	19,24,38,39	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.