

# Full wwPDB X-ray Structure Validation Report (i)

#### Dec 17, 2023 – 09:09 am GMT

PDB ID	:	4BY0
Title	:	Crystal structure of Trypanosoma cruzi CYP51 bound to the inhibitor (R)-N
		-(3-(1H-indol-3-yl)-1-oxo-1-(pyridin-4-ylamino)propan-2-yl)-3,3'- difluoro-(1,1
		'-biphenyl)-4-carboxamide
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		McKerrow, J.H.; Podust, L.M.; Roush, W.R.
Deposited on	:	2013-07-16
Resolution	:	3.10  Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org A user guide is available at https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7(2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36



# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $X\text{-}RAY\;DIFFRACTION$ 

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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
$R_{free}$	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Qu	ality of chain	
1	А	467	43%	44%	7% • 6%
1	В	467	42%	44%	9% 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:



Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	5 PS	А	1460	-	-	Х	-



## 2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 6834 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	А	441	Total 3389	C 2162	N 589	0 611	S 27	0	0	0
1	В	442	Total 3272	C 2077	N 570	O 598	S 27	0	0	0

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

Chain	Residue	Modelled	Actual	Comment	Reference
А	21	MET	-	expression tag	UNP Q5I4E1
А	22	ALA	-	expression tag	UNP Q5I4E1
А	23	LYS	-	expression tag	UNP Q5I4E1
А	24	LYS	-	expression tag	UNP Q5I4E1
А	25	THR	-	expression tag	UNP Q5I4E1
А	26	SER	-	expression tag	UNP Q5I4E1
А	27	SER	-	expression tag	UNP Q5I4E1
А	28	LYS	-	expression tag	UNP Q5I4E1
А	29	GLY	-	expression tag	UNP Q5I4E1
А	30	LYS	-	expression tag	UNP Q5I4E1
А	31	LEU	-	expression tag	UNP Q5I4E1
А	482	HIS	-	expression tag	UNP Q5I4E1
А	483	HIS	-	expression tag	UNP Q5I4E1
А	484	HIS	-	expression tag	UNP Q5I4E1
А	485	HIS	-	expression tag	UNP Q5I4E1
А	486	HIS	-	expression tag	UNP Q5I4E1
А	487	HIS	-	expression tag	UNP Q5I4E1
В	21	MET	-	expression tag	UNP Q5I4E1
В	22	ALA	-	expression tag	UNP Q5I4E1
В	23	LYS	-	expression tag	UNP Q5I4E1
В	24	LYS	-	expression tag	UNP Q5I4E1
В	25	THR	-	expression tag	UNP Q5I4E1
В	26	SER	-	expression tag	UNP Q5I4E1
В	27	SER	-	expression tag	UNP Q5I4E1
В	28	LYS	-	expression tag	UNP Q5I4E1

There are 34 discrepancies between the modelled and reference sequences:



Contentia								
Chain	Residue	Modelled	Actual	Comment	Reference			
В	29	GLY	-	expression tag	UNP Q5I4E1			
В	30	LYS	-	expression tag	UNP Q5I4E1			
В	31	LEU	-	expression tag	UNP Q5I4E1			
В	482	HIS	-	expression tag	UNP Q5I4E1			
В	483	HIS	-	expression tag	UNP Q5I4E1			
В	484	HIS	-	expression tag	UNP Q5I4E1			
В	485	HIS	-	expression tag	UNP Q5I4E1			
В	486	HIS	-	expression tag	UNP Q5I4E1			
В	487	HIS	-	expression tag	UNP Q5I4E1			

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



Mol	Chain	Residues		At	$\mathbf{oms}$			ZeroOcc	AltConf
2	А	1	Total 43	С 34	Fe 1	N 4	0 4	0	0
2	В	1	Total 43	C 34	Fe 1	N 4	0 4	0	0

• Molecule 3 is (R)-N-(3-(1H-indol-3-yl)-1-oxo-1-(pyridin-4-ylamino)propan-2-yl)-3,3'-difluoro -(1,1'-biphenyl)-4-carboxamide (three-letter code: 5PS) (formula:  $C_{29}H_{22}F_2N_4O_2$ ).





Mol	Chain	Residues		Ato	$\mathbf{ms}$			ZeroOcc	AltConf
3	Δ	1	Total	С	F	Ν	Ο	0	0
0	Л	I	37	29	2	4	2	0	0
2	В	1	Total	С	F	Ν	Ο	0	0
0	D	L	37	29	2	4	2	0	0

• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	8	Total O 8 8	0	0
4	В	5	Total O 5 5	0	0



# 3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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 14-ALPHA DEMETHYLASE





## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants	124.17Å 124.17Å 119.84Å	Deperitor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $120.00^{\circ}$	Depositor
$\mathbf{P}_{\text{assolution}}(\hat{\mathbf{A}})$	80.16 - 3.10	Depositor
Resolution (A)	80.04 - 3.10	EDS
% Data completeness	99.9 (80.16-3.10)	Depositor
(in resolution range)	99.9 (80.04-3.10)	EDS
R <sub>merge</sub>	0.16	Depositor
R <sub>sym</sub>	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.75 (at 3.13 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
D D.	0.232 , $0.297$	Depositor
$\Pi, \Pi_{free}$	0.228 , $0.298$	DCC
$R_{free}$ test set	1013 reflections $(5.12%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	85.9	Xtriage
Anisotropy	0.146	Xtriage
Bulk solvent $k_{sol}(e/A^3), B_{sol}(A^2)$	0.31 , $83.6$	EDS
L-test for twinning <sup>2</sup>	$< L >=0.49, < L^2>=0.32$	Xtriage
Estimated twinning fraction	0.027 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	6834	wwPDB-VP
Average B, all atoms $(Å^2)$	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.33% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 5 Model quality (i)

## 5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: HEM,  $5\mathrm{PS}$ 

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	
1VIOI	Unam	RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	А	0.61	0/3469	0.78	4/4710~(0.1%)
1	В	0.55	0/3350	0.73	0/4562
All	All	0.58	0/6819	0.75	4/9272~(0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	61	ARG	NE-CZ-NH1	8.11	124.36	120.30
1	А	222	PRO	N-CA-CB	6.54	111.14	103.30
1	А	470	LEU	CA-CB-CG	-5.24	103.25	115.30
1	А	449	ARG	N-CA-C	-5.10	97.23	111.00

There are no chirality outliers.

There are no planarity outliers.

#### 5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	3389	0	3249	255	0
1	В	3272	0	3007	350	0
2	А	43	0	30	13	0
2	В	43	0	30	16	0
3	А	37	0	22	9	0



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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes	
3	В	37	0	22	5	0	
4	А	8	0	0	0	0	
4	В	5	0	0	1	0	
All	All	6834	0	6360	620	0	

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 47.

All (620) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:35:TYR:CD1	1:B:36:PRO:HD2	1.53	1.42
1:A:59:CYS:O	1:A:63:LEU:CD1	1.78	1.29
1:B:326:PHE:O	1:B:441:ARG:NH2	1.66	1.26
1:B:110:PHE:O	1:B:233:ARG:NH2	1.63	1.26
1:A:363:VAL:HG23	1:A:378:ASP:O	1.33	1.25
1:A:366:GLU:OE2	1:A:373:VAL:HG11	1.23	1.25
1:A:449:ARG:NE	1:A:468:GLN:OE1	1.71	1.22
1:B:344:ARG:NH2	1:B:405:ASP:OD1	1.71	1.21
1:B:66:GLY:O	1:B:81:GLY:HA3	1.11	1.21
1:A:366:GLU:OE2	1:A:373:VAL:CG1	1.88	1.20
1:A:308:MET:CE	1:A:445:PHE:HB3	1.72	1.20
1:B:172:GLY:CA	1:B:297:THR:HG21	1.69	1.19
1:B:66:GLY:O	1:B:81:GLY:CA	1.91	1.19
1:B:89:PHE:HD2	1:B:90:PHE:CE1	1.62	1.16
1:B:89:PHE:HD2	1:B:90:PHE:CD1	1.62	1.16
1:A:110:PHE:O	1:A:233:ARG:NH2	1.78	1.16
1:A:147:GLN:OE1	1:A:330:LEU:HB2	1.43	1.15
1:B:89:PHE:CD2	1:B:90:PHE:CE1	2.34	1.15
1:B:33:PRO:HB2	1:B:63:LEU:HD22	1.30	1.12
1:A:308:MET:CE	1:A:445:PHE:CB	2.28	1.11
1:B:83:PRO:O	1:B:86:HIS:HB2	1.48	1.11
1:B:344:ARG:NH1	1:B:405:ASP:OD1	1.84	1.09
1:B:344:ARG:CZ	1:B:405:ASP:OD1	2.01	1.09
1:B:89:PHE:CD2	1:B:90:PHE:CD1	2.41	1.08
1:A:59:CYS:C	1:A:63:LEU:HD12	1.72	1.08
1:A:308:MET:HE1	1:A:445:PHE:HB3	1.36	1.07
1:B:111:GLY:O	1:B:114:VAL:HG23	1.54	1.07
1:B:172:GLY:HA2	1:B:297:THR:CG2	1.84	1.06
1:B:188:LEU:HD13	1:B:243:ILE:HD12	1.35	1.06
1:B:331:ASN:ND2	1:B:334:ASN:OD1	1.90	1.05



Atom-1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:277:SER:O	1:B:281:VAL:HG23	1.57	1.04
1:B:172:GLY:CA	1:B:297:THR:CG2	2.35	1.04
1:A:59:CYS:O	1:A:63:LEU:HD12	0.84	1.01
1:B:35:TYR:CD1	1:B:36:PRO:CD	2.43	1.01
1:B:344:ARG:HH22	1:B:405:ASP:CG	1.64	1.01
1:B:172:GLY:HA2	1:B:297:THR:HG21	1.40	1.00
1:B:215:MET:O	1:B:219:LEU:N	1.94	1.00
1:A:211:ALA:O	1:A:215:MET:N	1.94	1.00
1:B:420:HIS:ND1	2:B:1450:HEM:O1D	1.96	0.99
1:A:224:PRO:HB2	1:A:227:ALA:HB2	1.44	0.99
1:B:442:GLU:O	1:B:476:LYS:HB2	1.60	0.98
1:B:32:PRO:HB3	1:B:372:TYR:CD1	1.99	0.97
1:B:328:ALA:HB3	1:B:329:GLN:NE2	1.78	0.97
1:A:360:MET:SD	1:A:360:MET:N	2.38	0.96
1:B:360:MET:O	1:B:361:ARG:NH1	1.97	0.95
1:B:102:VAL:HG23	1:B:103:TYR:CD1	2.01	0.95
1:A:235:GLU:O	1:A:239:ILE:HG13	1.65	0.95
1:A:363:VAL:CG2	1:A:378:ASP:O	2.16	0.94
1:A:214:PHE:HB2	1:A:217:TRP:CZ3	2.02	0.93
1:B:361:ARG:HH22	2:B:1450:HEM:CGA	1.81	0.93
1:B:313:LYS:HA	1:B:316:LEU:HB3	1.50	0.93
1:B:172:GLY:N	1:B:297:THR:CG2	2.32	0.92
1:B:32:PRO:HA	1:B:372:TYR:CE1	2.04	0.92
1:B:33:PRO:CB	1:B:63:LEU:HD22	1.98	0.92
1:B:299:THR:O	1:B:303:SER:OG	1.87	0.92
1:B:147:GLN:O	1:B:151:ARG:N	2.03	0.91
1:A:308:MET:HE2	1:A:445:PHE:CB	1.98	0.91
1:B:139:PHE:HD2	1:B:332:TYR:HE2	1.16	0.91
1:A:48:PHE:O	1:A:52:PRO:HD3	1.69	0.91
1:A:449:ARG:CZ	1:A:468:GLN:OE1	2.20	0.89
1:A:211:ALA:C	1:A:215:MET:CB	2.40	0.89
1:B:277:SER:OG	1:B:280:GLU:HG3	1.72	0.89
1:B:32:PRO:HA	1:B:372:TYR:HE1	1.38	0.89
1:B:175:ILE:CD1	1:B:296:SER:HB2	2.03	0.89
1:B:361:ARG:NH2	2:B:1450:HEM:O1A	2.05	0.89
1:A:213:VAL:O	1:A:379:ILE:HD12	1.73	0.88
1:A:449:ARG:NH1	1:A:451:GLU:O	2.07	0.88
1:A:308:MET:CE	1:A:445:PHE:HB2	2.04	0.87
1:B:247:ARG:NH2	1:B:260:ASP:OD2	2.07	0.87
2:A:1450:HEM:C1A	3:A:1460:5PS:H2	2.10	0.86
1:A:339:MET:HE1	1:A:437:ALA:HB2	1.56	0.86



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:B:313:LYS:O	1:B:317:ASP:N	2.07	0.86
1:A:348:GLU:OE2	1:A:351:ARG:NH2	2.09	0.85
1:B:323:ILE:HA	1:B:326:PHE:CE2	2.10	0.85
1:B:86:HIS:CE1	1:B:413:ILE:HD13	2.10	0.85
1:A:465:THR:HB	1:A:468:GLN:HG3	1.57	0.85
1:A:211:ALA:HB1	1:A:215:MET:HA	1.59	0.85
1:A:143:VAL:HG21	1:A:332:TYR:HA	1.58	0.84
1:B:188:LEU:CD1	1:B:243:ILE:HD12	2.06	0.84
1:B:146:ILE:O	1:B:150:VAL:HG23	1.77	0.84
1:A:98:SER:OG	1:A:101:GLU:OE1	1.95	0.84
1:A:113:GLY:O	1:A:118:ALA:HB2	1.77	0.84
1:B:313:LYS:HD3	1:B:317:ASP:OD1	1.79	0.83
1:B:33:PRO:CB	1:B:63:LEU:CD2	2.57	0.83
1:B:420:HIS:ND1	2:B:1450:HEM:CGD	2.41	0.83
1:B:328:ALA:HB3	1:B:329:GLN:HE21	1.40	0.83
1:B:328:ALA:CB	1:B:329:GLN:NE2	2.42	0.83
1:B:115:ALA:O	1:B:123:MET:HG3	1.80	0.82
1:A:308:MET:HE2	1:A:445:PHE:HB3	1.60	0.81
1:B:139:PHE:HD2	1:B:332:TYR:CE2	1.97	0.81
1:B:35:TYR:CE1	1:B:36:PRO:HD2	2.15	0.81
1:B:90:PHE:CD2	1:B:417:ALA:HB3	2.16	0.81
1:B:33:PRO:HB3	1:B:63:LEU:HD23	1.63	0.80
1:B:441:ARG:O	1:B:476:LYS:HD3	1.81	0.80
1:A:113:GLY:HA2	1:A:117:ALA:O	1.80	0.80
1:B:86:HIS:NE2	1:B:413:ILE:HD13	1.97	0.79
1:B:33:PRO:HB2	1:B:63:LEU:CD2	2.13	0.79
1:B:89:PHE:CE2	1:B:90:PHE:CE1	2.69	0.79
1:B:172:GLY:HA2	1:B:297:THR:HG23	1.63	0.79
1:A:339:MET:CE	1:A:437:ALA:HB2	2.13	0.79
1:A:304:MET:O	1:A:308:MET:HG2	1.82	0.78
1:A:247:ARG:NH1	1:A:262:LEU:HD23	1.98	0.78
1:A:359:VAL:C	1:A:360:MET:SD	2.63	0.78
1:A:59:CYS:C	1:A:63:LEU:CD1	2.42	0.77
1:B:51:ASN:ND2	1:B:54:GLU:H	1.83	0.77
1:B:298:ILE:HD13	1:B:463:GLY:CA	2.15	0.77
1:B:313:LYS:CD	1:B:317:ASP:OD1	2.32	0.77
1:B:33:PRO:HB3	1:B:63:LEU:CD2	2.15	0.77
1:A:150:VAL:O	1:A:154:MET:HG3	1.84	0.77
1:B:339:MET:O	1:B:342:ALA:N	2.17	0.76
1:A:240:LEU:HD22	1:A:262:LEU:HD13	1.67	0.76
1:A:331:ASN:H	1:A:334:ASN:ND2	1.82	0.76



Atom-1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:316:LEU:O	1:B:316:LEU:HD12	1.86	0.76
1:B:214:PHE:C	1:B:216:PRO:HD2	2.05	0.76
1:B:175:ILE:HD13	1:B:296:SER:HB2	1.67	0.75
1:B:247:ARG:NH1	1:B:262:LEU:HD23	2.01	0.75
1:B:260:ASP:OD1	1:B:263:GLY:N	2.18	0.75
1:A:76:ARG:HB3	1:A:378:ASP:OD1	1.86	0.74
1:A:211:ALA:CB	1:A:215:MET:HA	2.17	0.74
1:B:191:ARG:HG2	1:B:191:ARG:HH11	1.52	0.74
1:B:348:GLU:OE1	1:B:401:ASP:O	2.04	0.74
1:B:366:GLU:HA	1:B:374:VAL:O	1.88	0.74
1:A:89:PHE:HD2	1:A:90:PHE:CE1	2.07	0.73
1:A:243:ILE:HG22	1:A:247:ARG:HG3	1.70	0.73
1:A:59:CYS:HA	1:A:63:LEU:HD11	1.70	0.73
1:B:314:LYS:HG3	1:B:315:TRP:H	1.54	0.73
1:B:323:ILE:HA	1:B:326:PHE:CD2	2.22	0.73
1:B:211:ALA:O	1:B:215:MET:CB	2.36	0.73
1:B:163:GLY:HA3	1:B:473:TYR:CE2	2.23	0.73
1:A:308:MET:HE2	1:A:445:PHE:HB2	1.67	0.72
1:A:262:LEU:O	1:A:266:LEU:HD13	1.89	0.72
1:B:174:MET:HA	1:B:177:ASN:HD22	1.55	0.72
1:B:319:LEU:HD12	1:B:319:LEU:O	1.89	0.72
1:A:319:LEU:O	1:A:322:GLU:HB3	1.90	0.72
2:A:1450:HEM:CHA	3:A:1460:5PS:H2	2.19	0.72
1:A:351:ARG:HD2	1:A:351:ARG:O	1.90	0.71
1:B:312:ASN:O	1:B:316:LEU:N	2.20	0.71
1:A:297:THR:O	1:A:301:SER:OG	2.08	0.71
1:B:60:LYS:O	1:B:63:LEU:O	2.07	0.71
1:A:306:HIS:O	1:A:312:ASN:ND2	2.18	0.71
1:B:32:PRO:CA	1:B:372:TYR:CE1	2.74	0.71
1:B:260:ASP:OD1	1:B:262:LEU:N	2.23	0.71
1:B:35:TYR:HD1	1:B:36:PRO:HD2	1.44	0.71
1:B:32:PRO:CB	1:B:372:TYR:CD1	2.73	0.71
1:B:98:SER:OG	1:B:101:GLU:OE1	2.05	0.71
1:A:147:GLN:OE1	1:A:330:LEU:CB	2.32	0.71
1:B:326:PHE:CE2	1:B:339:MET:HE2	2.26	0.70
1:A:59:CYS:CA	1:A:63:LEU:CD1	2.70	0.70
1:B:75:GLN:O	1:B:77:VAL:HG23	1.91	0.70
1:B:114:VAL:O	1:B:126:GLN:OE1	2.08	0.70
1:A:277:SER:OG	1:A:280:GLU:HG3	1.92	0.69
1:B:168:LEU:O	1:B:168:LEU:HD23	1.92	0.69
1:B:247:ARG:NH1	1:B:260:ASP:OD2	2.24	0.69



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:348:GLU:O	1:B:351:ARG:N	2.25	0.69
1:A:224:PRO:CB	1:A:227:ALA:HB2	2.20	0.69
1:B:442:GLU:O	1:B:476:LYS:CB	2.37	0.69
1:A:211:ALA:HB3	1:A:215:MET:CB	2.23	0.68
1:B:132:GLU:O	1:B:135:THR:HG23	1.93	0.68
1:A:59:CYS:CA	1:A:63:LEU:HD11	2.23	0.68
1:A:224:PRO:HB2	1:A:227:ALA:CB	2.21	0.68
1:B:247:ARG:HH21	1:B:258:THR:N	1.91	0.68
1:A:204:MET:HA	1:A:229:CYS:HB2	1.76	0.68
1:B:66:GLY:O	1:B:81:GLY:N	2.27	0.68
1:B:148:HIS:O	1:B:152:LYS:N	2.25	0.67
1:B:175:ILE:HD12	1:B:296:SER:HB2	1.75	0.67
1:A:401:ASP:OD1	1:A:403:GLU:N	2.25	0.67
1:B:262:LEU:O	1:B:266:LEU:HD22	1.94	0.67
1:A:52:PRO:O	1:A:56:MET:HG3	1.94	0.67
1:B:301:SER:O	1:B:305:LEU:HG	1.94	0.67
1:B:139:PHE:CD2	1:B:332:TYR:HE2	2.06	0.67
1:A:151:ARG:NH2	1:A:328:ALA:O	2.28	0.67
2:A:1450:HEM:HBC2	2:A:1450:HEM:HHD	1.77	0.67
1:B:326:PHE:HE2	1:B:339:MET:HE2	1.60	0.67
1:B:352:ARG:NH1	1:B:398:ARG:NH1	2.42	0.67
1:B:326:PHE:CE2	1:B:339:MET:CE	2.77	0.67
1:B:99:PRO:O	1:B:102:VAL:HG22	1.95	0.67
1:B:361:ARG:NH2	2:B:1450:HEM:CGA	2.52	0.67
1:A:343:GLU:OE1	1:A:433:LYS:NZ	2.28	0.66
1:B:306:HIS:ND1	1:B:400:TRP:CG	2.62	0.66
1:B:358:MET:HA	1:B:384:PRO:HD2	1.78	0.66
2:B:1450:HEM:C1A	3:B:1460:5PS:H2	2.31	0.66
1:B:111:GLY:C	1:B:114:VAL:HG23	2.15	0.66
1:B:325:GLU:OE1	1:B:325:GLU:HA	1.95	0.66
1:A:89:PHE:CD2	1:A:90:PHE:CE1	2.84	0.66
1:B:33:PRO:HD3	1:B:372:TYR:CE1	2.30	0.66
1:B:183:LEU:HD23	1:B:183:LEU:N	2.11	0.66
2:B:1450:HEM:HMC2	2:B:1450:HEM:HBC2	1.78	0.65
1:B:314:LYS:HG3	1:B:315:TRP:N	2.11	0.65
1:A:174:MET:O	1:A:178:THR:OG1	2.12	0.65
1:B:172:GLY:N	1:B:297:THR:HG21	2.00	0.65
1:B:229:CYS:O	1:B:232:ALA:N	2.28	0.65
1:B:59:CYS:O	1:B:63:LEU:HD12	1.96	0.65
1:A:341:PHE:O	1:A:344:ARG:HB2	1.96	0.65
1:A:348:GLU:HA	1:A:348:GLU:OE1	1.95	0.65



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:B:351:ARG:O	1:B:388:HIS:ND1	2.29	0.65
1:B:343:GLU:O	1:B:347:ARG:HB2	1.97	0.64
1:A:437:ALA:O	1:A:441:ARG:HB2	1.98	0.64
1:B:154:MET:O	1:B:158:TRP:N	2.30	0.64
1:B:394:PHE:CD2	1:B:404:ARG:HD3	2.33	0.64
1:B:443:TYR:CD1	1:B:475:ARG:HA	2.32	0.64
1:B:211:ALA:O	1:B:213:VAL:O	2.16	0.64
1:B:428:ALA:O	1:B:431:GLN:HB2	1.96	0.64
1:A:358:MET:HA	1:A:384:PRO:HD2	1.79	0.64
1:B:111:GLY:O	1:B:114:VAL:CG2	2.40	0.64
1:B:76:ARG:CB	1:B:378:ASP:OD1	2.45	0.64
1:B:260:ASP:OD1	1:B:262:LEU:HB3	1.97	0.64
1:A:247:ARG:HH12	1:A:262:LEU:HD23	1.62	0.63
1:B:348:GLU:OE2	1:B:351:ARG:NH2	2.32	0.63
1:B:351:ARG:HD2	1:B:351:ARG:C	2.18	0.63
1:A:351:ARG:HD2	1:A:351:ARG:C	2.18	0.63
1:A:211:ALA:O	1:A:215:MET:CA	2.46	0.63
1:B:375:PRO:HD2	1:B:378:ASP:OD2	1.98	0.63
1:A:136:ILE:HA	1:A:139:PHE:CD2	2.34	0.63
1:A:219:LEU:N	1:A:219:LEU:HD12	2.13	0.63
1:B:420:HIS:ND1	2:B:1450:HEM:O2D	2.32	0.63
1:A:305:LEU:HD13	1:A:453:PRO:HD2	1.81	0.63
1:B:135:THR:O	1:B:138:LYS:N	2.32	0.63
1:B:334:ASN:OD1	1:B:334:ASN:N	2.32	0.63
1:A:187:ASP:OD1	1:A:187:ASP:N	2.30	0.62
1:A:188:LEU:HD12	1:A:188:LEU:O	1.98	0.62
1:A:146:ILE:HG13	1:A:434:THR:HG21	1.82	0.62
1:B:215:MET:N	1:B:216:PRO:HD2	2.14	0.62
1:B:201:LEU:HD11	1:B:289:MET:HB3	1.81	0.62
1:B:298:ILE:HD13	1:B:463:GLY:HA3	1.80	0.62
1:B:293:GLN:O	1:B:297:THR:OG1	2.17	0.62
1:A:299:THR:O	1:A:303:SER:OG	2.17	0.61
1:A:272:ASP:OD1	1:A:273:GLY:N	2.33	0.61
1:B:88:ARG:O	1:B:92:PRO:HD3	1.99	0.61
1:A:86:HIS:O	1:A:89:PHE:N	2.32	0.61
2:B:1450:HEM:CHA	3:B:1460:5PS:H2	2.30	0.61
1:B:172:GLY:HA3	1:B:297:THR:HG21	1.75	0.61
1:A:213:VAL:O	1:A:379:ILE:CD1	2.47	0.60
1:B:172:GLY:CA	1:B:297:THR:HG23	2.27	0.60
1:A:229:CYS:O	1:A:232:ALA:N	2.35	0.60
1:A:425:GLN:O	1:A:429:LEU:HD12	2.01	0.60



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:B:394:PHE:HD2	1:B:404:ARG:HH11	1.48	0.60
1:A:158:TRP:HB3	1:A:473:TYR:CZ	2.36	0.60
1:A:363:VAL:HG12	1:A:365:ALA:O	2.01	0.60
1:B:44:HIS:CD2	1:B:55:PHE:HZ	2.19	0.60
1:B:247:ARG:CZ	1:B:260:ASP:OD2	2.49	0.60
1:A:229:CYS:SG	1:A:230:ARG:N	2.74	0.60
1:B:344:ARG:HD3	1:B:402:PRO:O	2.01	0.60
1:B:247:ARG:HH12	1:B:262:LEU:HD23	1.67	0.60
1:B:35:TYR:HB3	1:B:44:HIS:HE2	1.67	0.60
1:B:302:TRP:O	1:B:306:HIS:HD2	1.84	0.60
1:B:363:VAL:HG12	1:B:376:LYS:HA	1.82	0.60
1:B:467:ASN:C	1:B:467:ASN:HD22	2.05	0.60
1:A:51:ASN:C	1:A:51:ASN:HD22	2.06	0.59
1:A:152:LYS:O	1:A:156:GLU:HG3	2.01	0.59
2:A:1450:HEM:HMB2	2:A:1450:HEM:HBB2	1.83	0.59
2:B:1450:HEM:C4D	3:B:1460:5PS:H2	2.38	0.59
1:A:243:ILE:HG22	1:A:247:ARG:CG	2.32	0.59
1:B:51:ASN:C	1:B:51:ASN:HD22	2.05	0.59
1:B:291:ALA:O	1:B:295:THR:OG1	2.20	0.59
1:B:66:GLY:C	1:B:81:GLY:HA3	2.11	0.59
1:A:48:PHE:O	1:A:52:PRO:CD	2.48	0.59
1:B:94:ASN:OD1	1:B:94:ASN:N	2.29	0.59
1:B:168:LEU:HD23	1:B:168:LEU:C	2.23	0.59
1:B:328:ALA:CB	1:B:329:GLN:HE22	2.13	0.59
1:A:309:HIS:CE1	1:A:311:LYS:H	2.20	0.59
1:B:32:PRO:CA	1:B:372:TYR:CD1	2.85	0.58
1:B:110:PHE:O	1:B:114:VAL:HG21	2.03	0.58
1:A:146:ILE:HG22	1:A:182:CYS:SG	2.42	0.58
1:A:345:CYS:O	1:A:349:SER:OG	2.21	0.58
1:A:130:LEU:HD23	1:A:423:ILE:HD11	1.85	0.58
1:A:243:ILE:O	1:A:247:ARG:N	2.26	0.58
1:B:191:ARG:HG2	1:B:191:ARG:NH1	2.13	0.58
1:A:331:ASN:HD22	1:A:331:ASN:C	2.07	0.58
1:B:133:GLU:HG3	1:B:261:LEU:HD12	1.86	0.58
1:A:212:ALA:HA	1:A:215:MET:CB	2.33	0.57
1:B:101:GLU:O	1:B:104:THR:HG22	2.04	0.57
1:A:157:ASN:O	1:A:158:TRP:HD1	1.86	0.57
1:A:291:ALA:HB1	3:A:1460:5PS:H3	1.85	0.57
1:B:339:MET:HB3	1:B:342:ALA:HB3	1.85	0.57
1:B:306:HIS:CE1	1:B:400:TRP:CD1	2.92	0.57
1:B:175:ILE:HD13	1:B:296:SER:CB	2.35	0.57



Atom-1	Atom-2	Interatomic	Clash
		distance (Å)	overlap (Å)
1:B:394:PHE:HD2	1:B:404:ARG:HD3	1.69	0.57
1:A:211:ALA:CB	1:A:215:MET:CB	2.82	0.57
1:A:327:PRO:O	1:A:329:GLN:O	2.23	0.57
1:A:59:CYS:SG	1:A:70:ILE:HD11	2.45	0.57
1:A:141:ASN:O	1:A:144:PRO:HD2	2.05	0.56
1:A:210:PRO:HB3	1:A:460:MET:CE	2.35	0.56
1:A:385:LEU:O	1:A:389:HIS:ND1	2.33	0.56
1:B:434:THR:O	1:B:438:THR:OG1	2.23	0.56
1:A:59:CYS:HA	1:A:63:LEU:CD1	2.35	0.56
1:B:197:PHE:O	1:B:200:LEU:HB2	2.06	0.56
1:A:243:ILE:O	1:A:247:ARG:HG3	2.06	0.56
1:B:361:ARG:NH2	2:B:1450:HEM:O2A	2.31	0.56
1:A:89:PHE:HD2	1:A:90:PHE:CD1	2.24	0.56
1:B:244:ILE:O	1:B:248:GLU:N	2.36	0.56
1:B:316:LEU:HD12	1:B:316:LEU:C	2.26	0.56
1:B:429:LEU:N	1:B:429:LEU:HD23	2.21	0.56
1:A:205:GLU:OE2	1:A:293:GLN:NE2	2.38	0.56
1:B:193:ASN:C	1:B:193:ASN:HD22	2.10	0.56
1:A:465:THR:HB	1:A:468:GLN:CG	2.32	0.56
1:B:32:PRO:CB	1:B:372:TYR:CE1	2.89	0.55
2:A:1450:HEM:C4D	3:A:1460:5PS:H2	2.41	0.55
1:B:348:GLU:O	1:B:351:ARG:HB3	2.06	0.55
1:B:348:GLU:OE2	1:B:351:ARG:NE	2.38	0.55
1:A:358:MET:HE2	1:A:383:SER:HB2	1.89	0.55
1:A:243:ILE:HG22	1:A:247:ARG:CD	2.36	0.55
1:B:113:GLY:H	1:B:117:ALA:HB1	1.70	0.55
1:A:214:PHE:HD1	1:A:214:PHE:O	1.90	0.55
1:A:233:ARG:HH11	1:A:237:GLN:HE21	1.52	0.55
1:A:386:LEU:C	1:A:386:LEU:HD12	2.27	0.55
1:A:308:MET:HE3	1:A:445:PHE:HB2	1.85	0.55
1:B:237:GLN:NE2	1:B:279:HIS:ND1	2.55	0.55
1:B:162:GLU:HB3	1:B:474:THR:HG23	1.90	0.54
1:B:175:ILE:CD1	1:B:296:SER:CB	2.83	0.54
1:B:215:MET:N	1:B:216:PRO:CD	2.71	0.54
1:A:204:MET:O	1:A:207:SER:HB3	2.07	0.54
1:A:449:ARG:HH11	1:A:449:ARG:HG2	1.72	0.54
1:B:69:THR:HB	1:B:77:VAL:O	2.07	0.54
1:A:240:LEU:O	1:A:244:ILE:HG13	2.07	0.54
1:A:341:PHE:O	1:A:344:ARG:N	2.41	0.54
1:B:69:THR:HG22	1:B:78:THR:HG23	1.90	0.54
1:B:308:MET:SD	1:B:445:PHE:CB	2.96	0.54



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:166:ASN:C	1:A:166:ASN:HD22	2.10	0.54
1:A:211:ALA:O	1:A:215:MET:CB	2.55	0.54
1:A:212:ALA:N	1:A:215:MET:CB	2.70	0.54
1:A:229:CYS:O	1:A:232:ALA:HB3	2.08	0.54
1:A:428:ALA:O	1:A:432:VAL:HG23	2.07	0.54
1:B:32:PRO:HB3	1:B:372:TYR:CE1	2.41	0.54
1:B:170:ASP:N	1:B:170:ASP:OD1	2.41	0.54
1:B:103:TYR:CE2	3:B:1460:5PS:N4	2.74	0.53
1:B:136:ILE:HA	1:B:139:PHE:CE2	2.43	0.53
1:B:152:LYS:O	1:B:156:GLU:HG2	2.08	0.53
1:A:86:HIS:ND1	1:A:410:GLY:O	2.39	0.53
1:A:158:TRP:CZ2	1:A:165:ILE:HD13	2.43	0.53
1:B:88:ARG:CB	4:B:2004:HOH:O	2.56	0.53
1:B:315:TRP:HA	1:B:315:TRP:CE3	2.42	0.53
1:A:158:TRP:HB3	1:A:473:TYR:CE1	2.43	0.53
1:A:233:ARG:NH1	1:A:237:GLN:HE21	2.07	0.53
1:A:277:SER:O	1:A:280:GLU:N	2.40	0.53
1:B:171:CYS:C	1:B:297:THR:CG2	2.77	0.53
1:B:200:LEU:O	1:B:204:MET:HG3	2.09	0.53
1:B:44:HIS:HD2	1:B:55:PHE:HZ	1.56	0.53
1:B:361:ARG:NH1	1:B:361:ARG:HG2	2.24	0.53
1:A:210:PRO:HB3	1:A:460:MET:HE2	1.90	0.53
1:B:308:MET:SD	1:B:445:PHE:HB2	2.49	0.53
1:A:308:MET:HE3	1:A:445:PHE:CB	2.32	0.53
1:B:313:LYS:CA	1:B:316:LEU:HB3	2.33	0.53
1:B:53:LEU:HB2	1:B:385:LEU:HD21	1.90	0.52
1:A:223:LEU:O	1:A:225:GLN:N	2.38	0.52
1:B:104:THR:O	1:B:107:THR:OG1	2.27	0.52
1:A:76:ARG:CB	1:A:378:ASP:OD1	2.57	0.52
1:A:31:LEU:HD21	1:A:375:PRO:HG3	1.92	0.52
1:A:158:TRP:CE2	1:A:165:ILE:HD13	2.45	0.52
1:A:214:PHE:HB2	1:A:217:TRP:HZ3	1.69	0.52
1:B:344:ARG:HH12	1:B:404:ARG:C	2.12	0.52
1:A:85:GLU:OE1	1:A:370:GLY:N	2.43	0.52
1:A:366:GLU:OE2	1:A:373:VAL:HG13	1.98	0.52
1:A:266:LEU:N	1:A:266:LEU:HD12	2.25	0.51
1:B:342:ALA:O	1:B:346:VAL:HG23	2.10	0.51
1:B:412:PHE:CD1	1:B:412:PHE:C	2.83	0.51
1:B:413:ILE:HG13	1:B:413:ILE:O	2.11	0.51
1:B:32:PRO:HA	1:B:372:TYR:CD1	2.46	0.51
1:A:291:ALA:HB1	3:A:1460:5PS:C3	2.41	0.51



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:B:319:LEU:HD12	1:B:319:LEU:C	2.30	0.51
1:B:415:PHE:CD1	1:B:425:GLN:HB3	2.46	0.51
1:B:229:CYS:O	1:B:232:ALA:HB3	2.11	0.50
1:B:83:PRO:O	1:B:86:HIS:CB	2.40	0.50
1:B:163:GLY:CA	1:B:473:TYR:CE2	2.92	0.50
1:B:193:ASN:ND2	1:B:196:HIS:HB2	2.26	0.50
1:B:344:ARG:NH1	1:B:404:ARG:O	2.45	0.50
1:B:352:ARG:O	1:B:389:HIS:HE1	1.93	0.50
1:A:386:LEU:HD12	1:A:386:LEU:O	2.11	0.50
1:B:35:TYR:CG	1:B:36:PRO:CD	2.93	0.50
1:B:162:GLU:HA	1:B:473:TYR:O	2.10	0.50
1:B:233:ARG:NH1	1:B:282:CYS:SG	2.84	0.50
1:A:61:ARG:CB	1:A:61:ARG:HH11	2.25	0.50
1:A:416:GLY:N	2:A:1450:HEM:HMA3	2.27	0.50
1:B:362:MET:SD	1:B:363:VAL:N	2.84	0.50
1:A:32:PRO:HB3	1:A:67:VAL:O	2.11	0.50
1:A:332:TYR:CD1	1:A:332:TYR:C	2.85	0.50
1:B:68:PHE:CD1	1:B:68:PHE:N	2.78	0.50
1:B:449:ARG:NH1	1:B:451:GLU:HB2	2.27	0.50
1:A:309:HIS:ND1	1:A:310:PRO:N	2.60	0.50
1:B:224:PRO:O	1:B:227:ALA:HB3	2.11	0.50
1:A:205:GLU:O	1:A:208:LEU:N	2.43	0.50
1:B:110:PHE:C	1:B:114:VAL:HG21	2.32	0.50
1:B:139:PHE:HA	1:B:142:PHE:CG	2.46	0.50
1:B:214:PHE:CA	1:B:216:PRO:HD2	2.41	0.50
1:B:86:HIS:CE1	1:B:413:ILE:HG23	2.47	0.50
1:A:151:ARG:NH1	1:A:442:GLU:OE2	2.39	0.49
1:B:109:VAL:HG12	1:B:286:VAL:HG11	1.94	0.49
1:A:196:HIS:CE1	1:A:235:GLU:OE2	2.65	0.49
1:A:220:ARG:O	1:B:458:HIS:CD2	2.65	0.49
1:B:59:CYS:O	1:B:63:LEU:CD1	2.60	0.49
1:B:111:GLY:C	1:B:114:VAL:CG2	2.80	0.49
1:A:122:ARG:NH2	1:A:270:TYR:CE2	2.80	0.49
1:B:445:PHE:HA	1:B:472:LYS:O	2.13	0.49
1:B:175:ILE:HD12	1:B:297:THR:N	2.27	0.49
1:B:360:MET:C	1:B:361:ARG:HG2	2.32	0.49
1:A:211:ALA:CB	1:A:215:MET:CA	2.89	0.49
1:A:212:ALA:CA	1:A:215:MET:CB	2.91	0.49
1:A:330:LEU:HD22	1:A:334:ASN:HD22	1.78	0.49
1:B:90:PHE:CG	1:B:417:ALA:HB3	2.47	0.49
1:B:361:ARG:HG2	1:B:361:ARG:HH11	1.77	0.49



Atom 1	Atom 2	Interatomic	Clash		
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)		
1:A:146:ILE:HA	1:A:178:THR:HG22	1.95	0.49		
1:A:217:TRP:CD1	1:A:217:TRP:C	2.85	0.49		
1:A:399:LEU:HD12	1:A:400:TRP:N	2.27	0.49		
1:A:85:GLU:OE1	1:A:370:GLY:CA	2.61	0.48		
1:A:166:ASN:HD22	1:A:167:LEU:N	2.11	0.48		
1:A:215:MET:N	1:A:216:PRO:CD	2.75	0.48		
1:B:110:PHE:C	1:B:233:ARG:HH21	2.02	0.48		
1:B:147:GLN:HA	1:B:150:VAL:HB	1.96	0.48		
1:B:394:PHE:HB3	1:B:404:ARG:NH1	2.29	0.48		
1:A:147:GLN:CD	1:A:330:LEU:HB2	2.24	0.48		
1:B:33:PRO:HD2	1:B:67:VAL:O	2.14	0.48		
1:B:201:LEU:CD2	1:B:290:PHE:CD2	2.96	0.48		
1:B:351:ARG:O	1:B:388:HIS:HB3	2.13	0.48		
1:B:431:GLN:O	1:B:435:ILE:HG13	2.14	0.48		
1:B:174:MET:CA	1:B:177:ASN:HD22	2.21	0.48		
1:A:130:LEU:HD21	2:A:1450:HEM:HBC1	1.95	0.48		
1:A:214:PHE:HB2	1:A:217:TRP:CE3	2.45	0.48		
1:A:423:ILE:HD11	2:A:1450:HEM:HMD2	1.96	0.48		
1:B:315:TRP:HA	1:B:315:TRP:HE3	1.78	0.48		
1:B:319:LEU:HD12	1:B:323:ILE:HG23	1.96	0.48		
1:B:364:LYS:O	1:B:376:LYS:HD2	2.14	0.48		
1:B:359:VAL:C	1:B:360:MET:HE2	2.34	0.48		
1:A:219:LEU:N	1:A:219:LEU:CD1	2.77	0.48		
1:B:188:LEU:HA	1:B:243:ILE:CD1	2.44	0.48		
1:B:260:ASP:OD1	1:B:262:LEU:CA	2.61	0.48		
1:A:122:ARG:NH2	1:A:270:TYR:OH	2.46	0.48		
1:B:86:HIS:CE1	1:B:411:ALA:O	2.67	0.48		
1:B:70:ILE:O	1:B:77:VAL:HB	2.13	0.47		
1:B:90:PHE:CD1	1:B:90:PHE:N	2.82	0.47		
1:B:331:ASN:C	1:B:331:ASN:HD22	2.18	0.47		
1:A:214:PHE:CD1	1:A:214:PHE:C	2.86	0.47		
1:A:449:ARG:NH1	1:A:449:ARG:HG2	2.30	0.47		
1:B:109:VAL:HG13	1:B:204:MET:SD	2.54	0.47		
2:B:1450:HEM:HBC2	2:B:1450:HEM:CMC	2.41	0.47		
1:A:170:ASP:OD1	1:A:170:ASP:N	2.46	0.47		
1:B:308:MET:SD	1:B:445:PHE:HB3	2.54	0.47		
1:B:83:PRO:C	1:B:86:HIS:HB2	2.27	0.47		
1:B:260:ASP:OD1	1:B:262:LEU:CB	2.63	0.47		
1:A:166:ASN:OD1	1:A:466:LEU:HD11	2.15	0.47		
1:A:211:ALA:O	1:A:214:PHE:N	2.48	0.47		
1:B:166:ASN:C	1:B:166:ASN:HD22	2.18	0.47		



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:152:LYS:O	1:B:156:GLU:CG	2.63	0.47
1:A:238:LYS:O	1:A:242:GLU:HG3	2.14	0.47
1:A:344:ARG:NH1	1:A:405:ASP:OD1	2.45	0.47
1:B:139:PHE:CD2	1:B:332:TYR:CE2	2.89	0.47
1:B:306:HIS:ND1	1:B:400:TRP:CD1	2.82	0.47
1:B:359:VAL:CA	1:B:360:MET:HE2	2.45	0.47
3:A:1460:5PS:O2	3:A:1460:5PS:H4	2.14	0.46
1:B:345:CYS:O	1:B:349:SER:OG	2.24	0.46
1:A:215:MET:N	1:A:216:PRO:HD3	2.30	0.46
1:A:214:PHE:C	1:A:216:PRO:CD	2.84	0.46
1:A:277:SER:O	1:A:279:HIS:N	2.48	0.46
1:A:44:HIS:HD2	1:A:70:ILE:HG13	1.80	0.46
1:A:260:ASP:OD1	1:A:260:ASP:N	2.48	0.46
1:A:315:TRP:CE2	1:A:402:PRO:HD2	2.51	0.46
1:B:171:CYS:C	1:B:297:THR:HG23	2.36	0.46
1:B:412:PHE:CE1	1:B:414:GLY:N	2.81	0.46
1:A:425:GLN:HG3	1:A:426:LYS:N	2.30	0.46
1:A:61:ARG:HH11	1:A:61:ARG:HB2	1.81	0.46
1:A:157:ASN:C	1:A:158:TRP:CD1	2.89	0.46
1:B:313:LYS:HD2	1:B:317:ASP:OD1	2.13	0.46
1:B:44:HIS:HD2	1:B:55:PHE:CZ	2.34	0.46
1:A:44:HIS:HB2	1:A:71:SER:O	2.16	0.46
1:A:200:LEU:HD23	1:A:200:LEU:HA	1.77	0.46
1:B:394:PHE:HD2	1:B:404:ARG:NH1	2.13	0.46
1:B:396:ASN:ND2	1:B:399:LEU:HB2	2.31	0.46
1:B:466:LEU:HD12	1:B:466:LEU:O	2.16	0.46
1:A:90:PHE:O	1:A:91:SER:CB	2.64	0.45
1:A:449:ARG:CD	1:A:468:GLN:OE1	2.60	0.45
1:B:44:HIS:ND1	1:B:44:HIS:N	2.64	0.45
1:A:68:PHE:CD1	1:A:68:PHE:N	2.83	0.45
1:A:92:PRO:HG2	1:A:97:LEU:HD12	1.98	0.45
1:A:99:PRO:HB2	1:A:103:TYR:CD2	2.51	0.45
1:A:409:ASP:OD1	1:A:409:ASP:N	2.49	0.45
1:B:183:LEU:N	1:B:183:LEU:CD2	2.78	0.45
1:A:154:MET:O	1:A:158:TRP:N	2.45	0.45
1:B:96:ILE:O	1:B:364:LYS:HB2	2.16	0.45
1:A:162:GLU:HA	1:A:473:TYR:O	2.16	0.45
1:B:86:HIS:CE1	1:B:413:ILE:CD1	2.94	0.45
1:A:233:ARG:NH1	1:A:237:GLN:NE2	2.65	0.45
1:B:52:PRO:O	1:B:55:PHE:HB3	2.16	0.45
1:B:120:TYR:N	1:B:121:PRO:CD	2.80	0.45



Atom 1	Atom 2	Interatomic	Clash		
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)		
1:A:360:MET:HG3	1:A:381:ALA:HB2	1.98	0.45		
1:A:315:TRP:HA	1:A:315:TRP:CE3	2.51	0.45		
1:B:327:PRO:C	1:B:441:ARG:HH12	2.18	0.45		
1:B:344:ARG:CD	1:B:402:PRO:O	2.65	0.45		
1:A:106:MET:HE2	1:A:110:PHE:CZ	2.52	0.45		
1:A:201:LEU:HD11	1:A:289:MET:HB3	1.99	0.45		
1:A:83:PRO:HA	1:A:86:HIS:CE1	2.51	0.45		
1:A:233:ARG:NH1	1:A:282:CYS:SG	2.90	0.45		
1:B:360:MET:O	1:B:361:ARG:HG2	2.17	0.45		
1:A:153:PHE:CD1	1:A:153:PHE:C	2.91	0.44		
1:B:326:PHE:C	1:B:441:ARG:HH22	2.13	0.44		
1:B:389:HIS:HA	1:B:397:PRO:HB3	1.98	0.44		
1:A:470:LEU:O	1:A:471:VAL:HG23	2.18	0.44		
1:B:193:ASN:HD21	1:B:196:HIS:HB2	1.81	0.44		
1:B:352:ARG:HH11	1:B:398:ARG:NH1	2.14	0.44		
1:A:32:PRO:HA	1:A:372:TYR:CD1	2.52	0.44		
1:B:51:ASN:HD22	1:B:53:LEU:N	2.15	0.44		
1:B:113:GLY:N	1:B:117:ALA:CB	2.80	0.44		
1:B:302:TRP:HA	1:B:305:LEU:HD12	1.98	0.44		
1:A:115:ALA:O	1:A:123:MET:HG3	2.17	0.44		
1:A:72:ILE:HD13	1:A:72:ILE:HA	1.82	0.44		
1:A:214:PHE:CB	1:A:217:TRP:CZ3	2.88	0.44		
1:B:56:MET:HB2	1:B:386:LEU:HD13	2.00	0.44		
1:B:90:PHE:HD2	1:B:417:ALA:O	2.01	0.44		
1:B:319:LEU:HD11	1:B:323:ILE:CG2	2.47	0.44		
1:A:143:VAL:CG2	1:A:332:TYR:HA	2.39	0.44		
1:A:196:HIS:HE1	1:A:235:GLU:OE2	2.01	0.44		
1:B:237:GLN:HG3	1:B:282:CYS:SG	2.58	0.44		
1:A:110:PHE:C	1:A:233:ARG:HH21	1.96	0.44		
1:B:107:THR:HG22	1:B:117:ALA:HB2	2.00	0.44		
1:B:107:THR:CG2	1:B:117:ALA:HB2	2.48	0.44		
1:B:148:HIS:C	1:B:148:HIS:CD2	2.90	0.44		
1:B:424:GLY:HA3	2:B:1450:HEM:C4C	2.53	0.44		
2:B:1450:HEM:HBB2	2:B:1450:HEM:HMB2	2.00	0.44		
1:B:86:HIS:NE2	1:B:413:ILE:CD1	2.77	0.44		
1:B:323:ILE:CA	1:B:326:PHE:CD2	2.99	0.44		
1:A:60:LYS:HG3	1:A:66:GLY:HA3	1.99	0.43		
1:B:192:LEU:HA	1:B:192:LEU:HD12	1.74	0.43		
1:A:469:CYS:O	1:A:471:VAL:HG23	2.18	0.43		
1:B:102:VAL:HG23	1:B:103:TYR:N	2.33	0.43		
1:A:248:GLU:OE1	1:A:248:GLU:HA	2.18	0.43		



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:A:291:ALA:O	1:A:295:THR:OG1	2.36	0.43
1:A:398:ARG:HD2	1:A:398:ARG:HA	1.75	0.43
1:A:307:LEU:HD23	1:A:307:LEU:HA	1.87	0.43
1:A:352:ARG:HH12	1:A:398:ARG:CZ	2.31	0.43
1:B:146:ILE:C	1:B:150:VAL:HG23	2.38	0.43
1:B:186:GLU:O	1:B:190:LYS:N	2.32	0.43
1:B:277:SER:HG	1:B:280:GLU:HG3	1.82	0.43
1:B:69:THR:HA	1:B:78:THR:HA	2.01	0.43
1:B:330:LEU:HD22	1:B:334:ASN:HB2	2.01	0.43
1:B:193:ASN:O	1:B:196:HIS:HB3	2.18	0.43
2:A:1450:HEM:C1A	3:A:1460:5PS:C2	2.91	0.43
1:A:121:PRO:O	1:A:125:GLU:HG3	2.19	0.43
1:A:130:LEU:HD21	2:A:1450:HEM:CBC	2.49	0.43
1:A:157:ASN:N	1:A:157:ASN:ND2	2.67	0.43
1:B:166:ASN:HD22	1:B:169:GLU:H	1.66	0.43
1:B:360:MET:N	1:B:360:MET:CE	2.82	0.43
1:A:277:SER:HG	1:A:280:GLU:HG3	1.84	0.42
1:B:328:ALA:HB1	1:B:329:GLN:HE22	1.81	0.42
1:B:358:MET:HE2	1:B:358:MET:HB3	1.69	0.42
1:A:393:ALA:HB2	1:A:408:VAL:HG23	2.01	0.42
1:B:162:GLU:CB	1:B:474:THR:HG23	2.49	0.42
1:B:166:ASN:ND2	1:B:169:GLU:H	2.17	0.42
1:B:323:ILE:O	1:B:326:PHE:CD2	2.73	0.42
1:B:330:LEU:HD23	1:B:330:LEU:HA	1.91	0.42
1:B:344:ARG:NH1	1:B:404:ARG:C	2.72	0.42
1:A:358:MET:HE3	1:A:358:MET:HB3	1.88	0.42
1:B:139:PHE:CD1	1:B:139:PHE:N	2.83	0.42
1:B:329:GLN:NE2	1:B:329:GLN:N	2.67	0.42
1:A:166:ASN:OD1	1:A:466:LEU:CD1	2.67	0.42
1:A:351:ARG:C	1:A:351:ARG:CD	2.85	0.42
1:B:69:THR:HG22	1:B:78:THR:OG1	2.19	0.42
1:B:292:GLY:O	1:B:296:SER:OG	2.22	0.42
1:A:214:PHE:O	1:A:214:PHE:CD1	2.70	0.42
1:A:295:THR:HB	2:A:1450:HEM:CAB	2.49	0.42
1:B:127:LEU:O	1:B:130:LEU:N	2.52	0.42
1:B:201:LEU:HD22	1:B:290:PHE:CD2	2.55	0.42
1:B:233:ARG:HH12	1:B:282:CYS:HB3	1.84	0.42
1:B:421:LYS:O	1:B:422:CYS:C	2.54	0.42
1:B:166:ASN:C	1:B:166:ASN:ND2	2.72	0.42
1:B:383:SER:HA	1:B:384:PRO:HD2	1.92	0.42
1:A:293:GLN:HG3	1:A:294:HIS:N	2.34	0.42



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:A:298:ILE:HD12	1:A:461:VAL:HG12	2.02	0.42
1:A:359:VAL:O	1:A:381:ALA:HA	2.19	0.42
1:B:295:THR:HB	2:B:1450:HEM:CAB	2.50	0.42
1:B:363:VAL:CG1	1:B:376:LYS:HA	2.47	0.42
1:A:100:ARG:HA	1:A:116:TYR:HB3	2.01	0.42
1:A:439:ALA:O	1:A:443:TYR:HB2	2.20	0.42
3:A:1460:5PS:O2	3:A:1460:5PS:C4	2.67	0.42
1:B:89:PHE:HE2	1:B:90:PHE:CZ	2.37	0.42
1:B:306:HIS:HE1	1:B:352:ARG:HE	1.66	0.42
1:B:329:GLN:N	1:B:329:GLN:CD	2.73	0.42
1:B:348:GLU:OE1	1:B:401:ASP:C	2.58	0.42
1:A:61:ARG:HH11	1:A:61:ARG:CG	2.32	0.41
1:B:51:ASN:HD21	1:B:53:LEU:HB3	1.85	0.41
1:B:394:PHE:CD2	1:B:404:ARG:NH1	2.85	0.41
1:B:443:TYR:CE1	1:B:475:ARG:HB2	2.56	0.41
1:B:33:PRO:HD3	1:B:372:TYR:HE1	1.84	0.41
1:B:118:ALA:HB1	1:B:122:ARG:HG2	2.03	0.41
1:B:384:PRO:O	1:B:388:HIS:CD2	2.73	0.41
1:A:188:LEU:HD12	1:A:188:LEU:C	2.41	0.41
1:A:334:ASN:HA	1:A:338:GLU:HB2	2.00	0.41
1:B:326:PHE:C	1:B:441:ARG:NH2	2.62	0.41
1:A:101:GLU:O	1:A:104:THR:HG22	2.20	0.41
1:A:120:TYR:N	1:A:121:PRO:HD2	2.36	0.41
1:A:339:MET:HE3	1:A:437:ALA:HB2	1.99	0.41
1:B:113:GLY:CA	1:B:117:ALA:HB3	2.51	0.41
1:A:278:LEU:HA	1:A:281:VAL:HB	2.03	0.41
1:A:331:ASN:ND2	1:A:334:ASN:ND2	2.69	0.41
1:A:418:GLY:O	1:A:419:VAL:C	2.57	0.41
1:B:86:HIS:CE1	1:B:413:ILE:CG2	3.04	0.41
1:B:211:ALA:O	1:B:215:MET:N	2.53	0.41
1:B:298:ILE:HD12	1:B:461:VAL:HG12	2.03	0.41
1:A:75:GLN:HG2	1:A:217:TRP:CZ3	2.55	0.41
1:B:51:ASN:ND2	1:B:53:LEU:N	2.69	0.41
1:B:315:TRP:NE1	1:B:402:PRO:HD2	2.35	0.41
1:B:394:PHE:CB	1:B:404:ARG:NH1	2.84	0.41
1:A:136:ILE:HA	1:A:139:PHE:CE2	2.56	0.41
1:A:330:LEU:HD23	1:A:330:LEU:HA	1.79	0.41
1:B:147:GLN:O	1:B:151:ARG:HB2	2.21	0.41
1:B:298:ILE:HD13	1:B:463:GLY:HA2	2.02	0.41
1:B:398:ARG:HA	1:B:398:ARG:HD2	1.89	0.41
2:B:1450:HEM:C1A	3:B:1460:5PS:C2	3.02	0.41



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:453:PRO:HB3	1:A:468:GLN:HB2	2.03	0.41
2:A:1450:HEM:C4D	3:A:1460:5PS:C2	3.04	0.41
1:B:89:PHE:CE2	1:B:90:PHE:CZ	3.09	0.41
1:A:320:HIS:O	1:A:324:ASP:N	2.55	0.40
1:B:183:LEU:O	1:B:184:PHE:CD1 2.74		0.40
1:A:270:TYR:OH	1:A:280:GLU:OE1	2.35	0.40
1:A:295:THR:HG22	1:A:355:PRO:HB2	2.03	0.40
1:A:331:ASN:H	1:A:334:ASN:HD22	1.65	0.40
1:A:423:ILE:CD1	2:A:1450:HEM:HMD2	2.51	0.40
1:B:102:VAL:HG23	1:B:103:TYR:HD1	1.74	0.40
1:B:467:ASN:C	1:B:467:ASN:ND2	2.73	0.40
1:A:168:LEU:HA	1:A:168:LEU:HD12	1.84	0.40
1:A:277:SER:O	1:A:278:LEU:C	2.59	0.40
1:A:348:GLU:HG2	1:A:401:ASP:O	2.22	0.40
1:B:473:TYR:CD1	1:B:473:TYR:C	2.94	0.40
1:B:361:ARG:O	1:B:380:ILE:HG22	2.22	0.40

There are no symmetry-related clashes.

### 5.3 Torsion angles (i)

#### 5.3.1 Protein backbone (i)

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	А	437/467~(94%)	414 (95%)	21~(5%)	2~(0%)	29 64
1	В	438/467~(94%)	427 (98%)	9(2%)	2 (0%)	29 64
All	All	875/934~(94%)	841 (96%)	30~(3%)	4 (0%)	29 64

All (4) Ramachandran outliers are listed below:

А	91	SER
А	278	LEU
	A A	A         91           A         278



 $Continued \ from \ previous \ page...$ 

Mol	Chain	Res	Type
1	В	222	PRO
1	В	339	MET

#### 5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentile		es	
1	А	343/408~(84%)	289~(84%)	54 (16%)		2	11	
1	В	314/408~(77%)	253 (81%)	61 (19%)		1	6	
All	All	657/816~(80%)	542 (82%)	115~(18%)		2	8	

All (115) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	38	THR
1	А	39	VAL
1	А	51	ASN
1	А	61	ARG
1	А	63	LEU
1	А	65	SER
1	А	68	PHE
1	А	87	SER
1	А	88	ARG
1	А	90	PHE
1	А	104	THR
1	А	138	LYS
1	А	146	ILE
1	А	162	GLU
1	А	166	ASN
1	А	170	ASP
1	A	178	THR
1	A	188	LEU
1	А	192	LEU
1	А	197	PHE
1	А	203	LYS



Mol	Chain	Res	Type
1	А	205	GLU
1	А	213	VAL
1	А	214	PHE
1	А	217	TRP
1	А	230	ARG
1	А	251	GLU
1	А	274	THR
1	А	278	LEU
1	А	282	CYS
1	А	301	SER
1	А	303	SER
1	А	321	LYS
1	А	331	ASN
1	А	332	TYR
1	Α	336	MET
1	А	349	SER
1	А	352	ARG
1	А	353	ASP
1	А	360	MET
1	А	366	GLU
1	А	378	ASP
1	А	386	LEU
1	А	390	ASP
1	А	391	GLU
1	А	403	GLU
1	А	406	GLU
1	А	409	ASP
1	А	442	GLU
1	А	444	ASP
1	А	446	GLN
1	А	459	THR
1	A	467	ASN
1	А	470	LEU
1	В	34	VAL
1	В	39	VAL
1	В	44	HIS
1	В	51	ASN
1	В	53	LEU
1	В	63	LEU
1	В	86	HIS
1	В	94	ASN
1	В	106	MET



Mol	Chain	Res	Type
1	В	107	THR
1	В	122	ARG
1	В	139	PHE
1	В	154	MET
1	В	156	GLU
1	В	166	ASN
1	В	170	ASP
1	В	183	LEU
1	В	191	ARG
1	В	193	ASN
1	В	199	GLN
1	В	203	LYS
1	В	205	GLU
1	В	229	CYS
1	В	231	GLU
1	В	233	ARG
1	В	242	GLU
1	В	266	LEU
1	В	274	THR
1	В	290	PHE
1	В	295	THR
1	В	296	SER
1	В	297	THR
1	В	303	SER
1	В	304	MET
1	В	307	LEU
1	В	314	LYS
1	В	316	LEU
1	В	319	LEU
1	В	320	HIS
1	В	321	LYS
1	В	323	ILE
1	В	325	GLU
1	В	331	ASN
1	B	333	ASP
1	В	334	ASN
1	В	336	MET
1	В	339	MET
1	B	348	GLU
1	В	356	LEU
1	В	360	MET
1	В	361	ARG



Mol	Chain	Res	Type
1	В	366	GLU
1	В	402	PRO
1	В	438	THR
1	В	449	ARG
1	В	458	HIS
1	В	459	THR
1	В	460	MET
1	В	466	LEU
1	В	467	ASN
1	В	474	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	51	ASN
1	А	166	ASN
1	А	196	HIS
1	А	237	GLN
1	А	294	HIS
1	А	306	HIS
1	А	331	ASN
1	А	334	ASN
1	В	51	ASN
1	В	148	HIS
1	В	166	ASN
1	В	193	ASN
1	В	237	GLN
1	В	293	GLN
1	В	329	GLN
1	В	331	ASN
1	В	431	GLN
1	В	458	HIS
1	В	467	ASN

#### 5.3.3 RNA (i)

There are no RNA molecules in this entry.



#### 5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

#### 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

#### 5.6 Ligand geometry (i)

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).

Mal	Type	Chain	Dec	Tinle	Bo	ond leng	$_{\rm sths}$	B	Bond ang	gles
	туре	Chain	nes		Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	HEM	В	1450	3,1	41,50,50	1.43	6 (14%)	45,82,82	2.20	14 (31%)
3	5PS	А	1460	2	40,41,41	1.39	4 (10%)	53,57,57	1.43	7 (13%)
2	HEM	А	1450	3,1	41,50,50	1.49	7 (17%)	45,82,82	2.20	13 (28%)
3	5PS	В	1460	2	40,41,41	1.41	4 (10%)	53,57,57	1.58	9 (16%)

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	В	1450	3,1	-	4/12/54/54	-
3	5 PS	А	1460	2	-	0/23/24/24	0/5/5/5
2	HEM	А	1450	3,1	-	0/12/54/54	-
3	5 PS	В	1460	2	-	0/23/24/24	0/5/5/5

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	В	1460	5PS	C9-C20	6.10	1.47	1.38



Mol	Chain	Res	Type	Atoms	Ζ	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
3	А	1460	$5\mathrm{PS}$	C9-C20	6.08	1.47	1.38
2	В	1450	HEM	C1B-NB	-4.54	1.32	1.40
2	А	1450	HEM	C4B-NB	-3.78	1.31	1.38
2	А	1450	HEM	C1D-ND	-3.55	1.31	1.38
2	А	1450	HEM	C1B-NB	-3.43	1.34	1.40
3	В	1460	5PS	C5-N2	-3.33	1.34	1.41
2	В	1450	HEM	C4D-ND	-3.09	1.35	1.40
3	А	1460	5PS	C5-N2	-3.04	1.35	1.41
2	В	1450	HEM	C4B-NB	-2.92	1.32	1.38
3	А	1460	$5\mathrm{PS}$	C25-C24	-2.79	1.37	1.41
2	А	1450	HEM	C4D-ND	-2.61	1.35	1.40
2	В	1450	HEM	C1D-ND	-2.48	1.33	1.38
3	В	1460	5PS	C28-C29	-2.34	1.37	1.42
2	А	1450	HEM	C3C-C2C	-2.25	1.37	1.40
2	А	1450	HEM	FE-ND	-2.24	1.85	1.96
2	А	1450	HEM	FE-NB	2.09	2.07	1.96
2	В	1450	HEM	FE-NB	2.09	2.07	1.96
2	В	1450	HEM	C4D-C3D	2.07	1.48	1.45
3	A	1460	5PS	C28-C29	-2.03	1.38	1.42
3	В	1460	5PS	C25-C24	-2.02	1.38	1.41

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	А	1450	HEM	C1B-NB-C4B	5.53	110.79	105.07
2	В	1450	HEM	C1B-NB-C4B	5.29	110.53	105.07
2	В	1450	HEM	CHC-C4B-NB	5.23	130.12	124.43
2	А	1450	HEM	CHD-C1D-ND	5.21	130.09	124.43
2	А	1450	HEM	CHC-C4B-NB	5.16	130.03	124.43
2	В	1450	HEM	CAD-C3D-C4D	5.09	133.55	124.66
2	В	1450	HEM	CHD-C1D-ND	5.00	129.87	124.43
2	А	1450	HEM	CHA-C4D-ND	4.17	129.54	124.38
2	В	1450	HEM	CHD-C1D-C2D	-3.97	118.77	124.98
3	В	1460	5PS	C22-C21-C7	-3.97	105.67	113.45
2	А	1450	HEM	CBA-CAA-C2A	-3.77	106.19	112.62
3	А	1460	5PS	C22-C21-C7	-3.75	106.11	113.45
3	В	1460	5PS	C28-C29-C24	3.48	122.79	118.17
3	В	1460	5PS	C19-C20-C9	-3.48	119.82	123.53
2	A	1450	HEM	CHD-C1D-C2D	-3.42	119.63	124.98
3	A	1460	5PS	C19-C20-C9	-3.37	119.93	123.53
2	A	1450	HEM	CHA-C4D-C3D	-3.33	119.08	125.33
3	A	1460	5PS	$C\overline{28}-C29-C24$	3.20	122.41	118.17



Mol	Chain	$\mathbf{Res}$	Type	Atoms	$\mathbf{Z}$	$Observed(^{o})$	$Ideal(^{o})$
3	В	1460	5PS	O1-C8-C9	-3.12	115.30	121.01
2	А	1450	HEM	CAD-CBD-CGD	-3.06	107.02	113.60
3	В	1460	5PS	C9-C8-N3	3.03	122.41	116.80
2	В	1450	HEM	C4B-C3B-C2B	-2.96	104.77	107.11
2	В	1450	HEM	CBD-CAD-C3D	2.85	120.54	112.63
2	А	1450	HEM	CAD-C3D-C4D	2.82	129.58	124.66
3	В	1460	5PS	C5-N2-C6	-2.82	120.65	127.40
2	А	1450	HEM	C4B-CHC-C1C	2.78	126.23	122.56
2	А	1450	HEM	CBD-CAD-C3D	2.76	120.31	112.63
3	А	1460	5PS	O2-C6-C7	-2.75	114.67	120.45
3	А	1460	5PS	C9-C8-N3	2.71	121.82	116.80
3	В	1460	5PS	C10-C9-C20	2.70	119.74	116.67
2	В	1450	HEM	CAD-C3D-C2D	-2.69	122.87	127.88
2	В	1450	HEM	O2D-CGD-O1D	-2.67	116.64	123.30
2	В	1450	HEM	O2D-CGD-CBD	2.65	122.56	114.03
3	В	1460	5PS	C27-C28-C29	-2.62	117.26	120.89
2	А	1450	HEM	CHB-C1B-NB	2.59	127.58	124.38
2	А	1450	HEM	O2D-CGD-CBD	2.36	121.60	114.03
3	А	1460	5PS	C5-N2-C6	-2.36	121.76	127.40
2	В	1450	HEM	O2A-CGA-CBA	2.34	121.55	114.03
2	В	1450	HEM	C4D-C3D-C2D	-2.33	103.50	106.90
2	В	1450	HEM	CBA-CAA-C2A	-2.31	108.69	112.62
3	В	1460	5PS	C11-C12-C19	2.21	121.29	118.16
3	А	1460	5PS	C27-C28-C29	-2.17	117.88	120.89
2	В	1450	HEM	CHC-C4B-C3B	-2.02	121.47	124.57

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There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	В	1450	HEM	C4D-C3D-CAD-CBD
2	В	1450	HEM	C2D-C3D-CAD-CBD
2	В	1450	HEM	CAD-CBD-CGD-O1D
2	В	1450	HEM	CAD-CBD-CGD-O2D

There are no ring outliers.

4 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	В	1450	HEM	16	0
3	А	1460	5PS	9	0



	3	1	1 5		
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	А	1450	HEM	13	0
3	В	1460	5PS	5	0

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The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and sufficient the outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.















## 5.7 Other polymers (i)

There are no such residues in this entry.

## 5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



## 6 Fit of model and data (i)

## 6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median,  $95^{th}$  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	< <b>RSRZ</b> >	# RSRZ > 2		$OWAB(Å^2)$	Q<0.9
1	А	441/467~(94%)	-0.48	1 (0%) 95 90		43, 70, 99, 121	0
1	В	442/467~(94%)	-0.34	1 (0%) 95 90		59, 91, 120, 135	0
All	All	883/934 (94%)	-0.41	2 (0%) 95 90		43, 79, 116, 135	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	436	LEU	2.0
1	А	373	VAL	2.0

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

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

### 6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

### 6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median,  $95^{th}$  percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-factors}(\mathbf{A}^2)$	Q<0.9
3	5PS	В	1460	37/37	0.93	0.34	69,74,95,109	0
3	5PS	А	1460	37/37	0.94	0.26	54,63,78,100	0
2	HEM	В	1450	43/43	0.97	0.25	61,70,80,80	0



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Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q < 0.9
2	HEM	А	1450	43/43	0.98	0.20	40,48,55,60	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.











## 6.5 Other polymers (i)

There are no such residues in this entry.

