



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:43 PM GMT

PDB ID : 4FXB  
Title : Crystal structure of CYP105N1 from *Streptomyces coelicolor*: a cytochrome P450 oxidase in the coelibactin siderophore biosynthetic pathway  
Authors : Hong, M.K.; Lim, Y.R.; Kim, J.K.; Kim, D.H.; Kang, L.W.  
Deposited on : 2012-07-03  
Resolution : 2.90 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

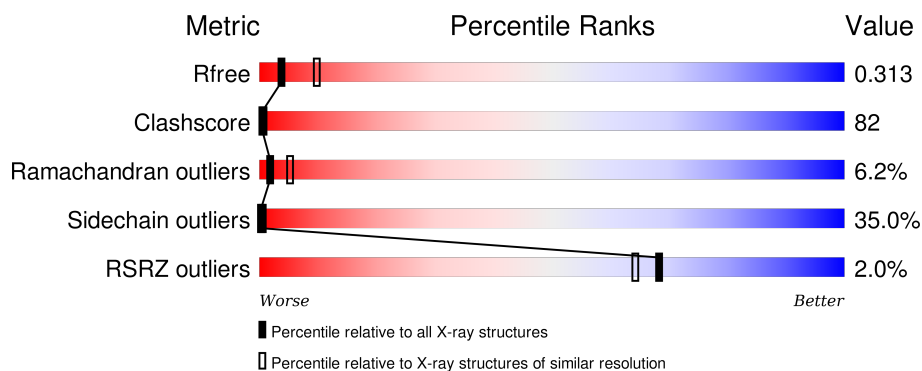
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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))
$R_{free}$	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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  $\leq 5\%$ . 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	Quality of chain
1	A	417	<div> <div>16%</div> <div>45%</div> <div>25%</div> <div>7%</div> <div>6%</div> </div>
1	B	417	<div> <div>17%</div> <div>42%</div> <div>23%</div> <div>6%</div> <div>11%</div> </div>

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
2	HEM	B	501	-	-	X	-

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6021 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.

- Molecule 1 is a protein called Putative cytochrome P450.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	390	Total	C	N	O	S	0	0	0
			3020	1886	553	572	9			
1	B	370	Total	C	N	O	S	0	0	0
			2858	1790	523	537	8			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	412	HIS	-	EXPRESSION TAG	UNP Q9EWP1
A	413	HIS	-	EXPRESSION TAG	UNP Q9EWP1
A	414	HIS	-	EXPRESSION TAG	UNP Q9EWP1
A	415	HIS	-	EXPRESSION TAG	UNP Q9EWP1
A	416	HIS	-	EXPRESSION TAG	UNP Q9EWP1
A	417	HIS	-	EXPRESSION TAG	UNP Q9EWP1
B	412	HIS	-	EXPRESSION TAG	UNP Q9EWP1
B	413	HIS	-	EXPRESSION TAG	UNP Q9EWP1
B	414	HIS	-	EXPRESSION TAG	UNP Q9EWP1
B	415	HIS	-	EXPRESSION TAG	UNP Q9EWP1
B	416	HIS	-	EXPRESSION TAG	UNP Q9EWP1
B	417	HIS	-	EXPRESSION TAG	UNP Q9EWP1

- 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		

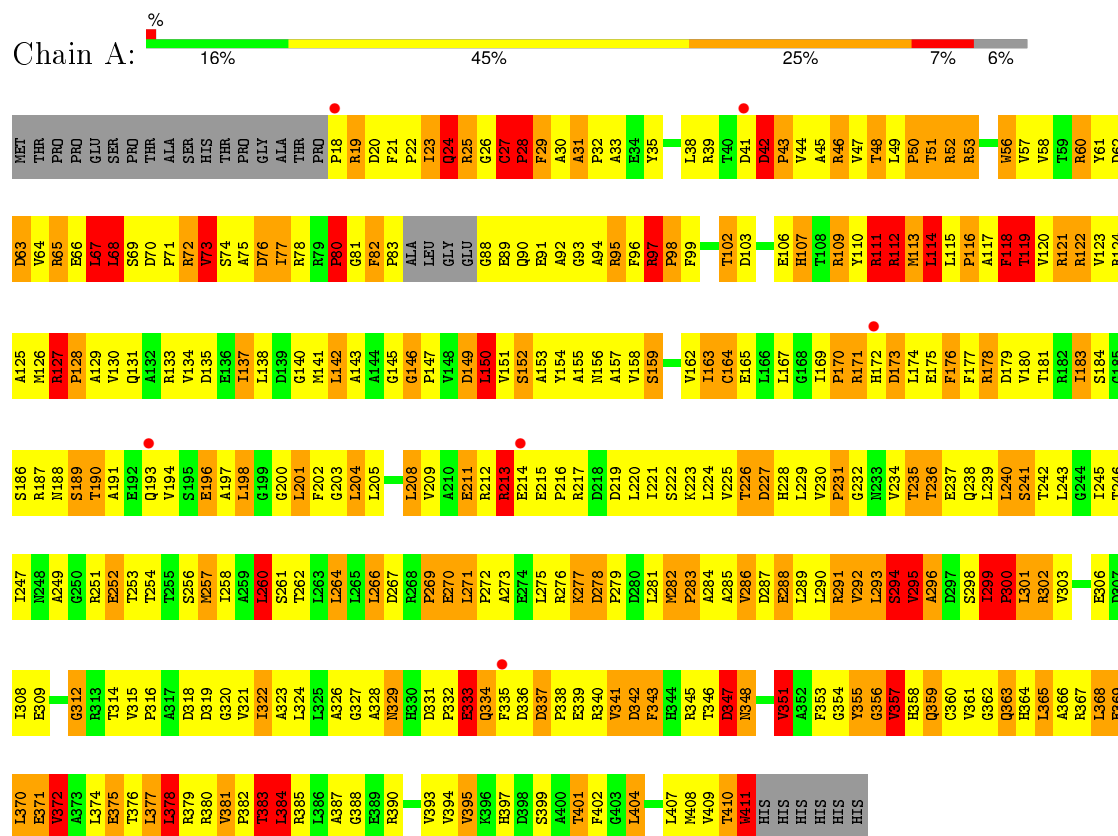
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	35	Total	O	0	0
			35	35		
3	B	22	Total	O	0	0
			22	22		

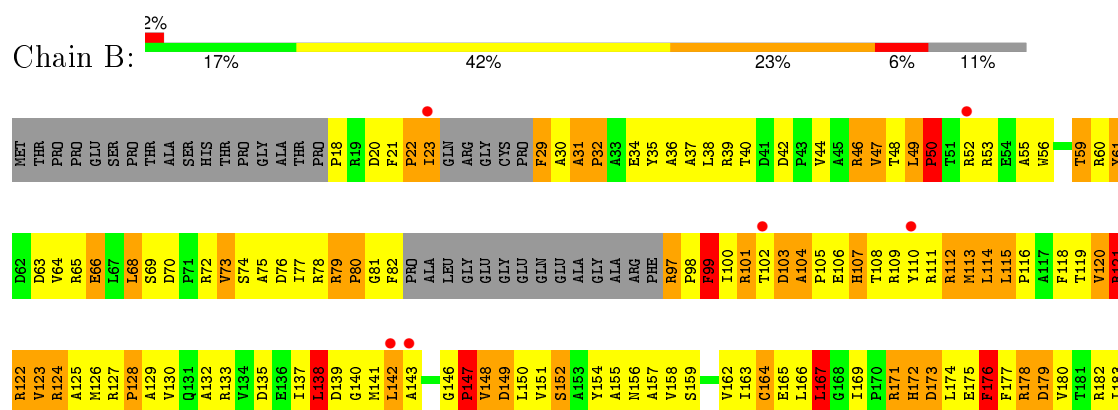
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: Putative cytochrome P450



#### • Molecule 1: Putative cytochrome P450





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	133.09Å 133.09Å 227.11Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.93 – 2.90 19.93 – 2.90	Depositor EDS
% Data completeness (in resolution range)	91.9 (19.93-2.90) 99.2 (19.93-2.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.53 (at 2.88Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.281 , 0.302 0.302 , 0.313	Depositor DCC
$R_{free}$ test set	1375 reflections (5.42%)	DCC
Wilson B-factor (Å <sup>2</sup> )	35.1	Xtriage
Anisotropy	0.211	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.20 , 47.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.35$ , $\langle L^2 \rangle = 0.18$	Xtriage
Outliers	0 of 91688 reflections	Xtriage
$F_o, F_c$ correlation	0.80	EDS
Total number of atoms	6021	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 4.83% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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



## 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	1.33	8/3076 (0.3%)	1.70	57/4186 (1.4%)
1	B	1.22	2/2905 (0.1%)	1.64	51/3951 (1.3%)
All	All	1.28	10/5981 (0.2%)	1.67	108/8137 (1.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	9
1	B	0	9
All	All	0	18

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	333	GLU	CG-CD	7.48	1.63	1.51
1	A	288	GLU	CD-OE1	6.29	1.32	1.25
1	A	56	TRP	CD2-CE2	6.21	1.48	1.41
1	B	99	PHE	CB-CG	-5.86	1.41	1.51
1	A	411	TRP	CD2-CE2	5.81	1.48	1.41
1	A	355	TYR	CG-CD1	5.68	1.46	1.39
1	A	118	PHE	CB-CG	-5.57	1.41	1.51
1	A	119	THR	CB-CG2	5.22	1.69	1.52
1	B	391	ASP	CB-CG	5.17	1.62	1.51
1	A	288	GLU	CD-OE2	5.07	1.31	1.25

All (108) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	186	SER	N-CA-C	13.04	146.20	111.00
1	A	53	ARG	NE-CZ-NH1	12.82	126.71	120.30
1	A	114	LEU	CA-CB-CG	11.17	140.99	115.30
1	B	186	SER	CB-CA-C	-10.91	89.36	110.10
1	A	53	ARG	NE-CZ-NH2	-10.82	114.89	120.30
1	B	303	VAL	CB-CA-C	10.64	131.62	111.40
1	B	112	ARG	NE-CZ-NH1	9.99	125.30	120.30
1	B	304	ALA	N-CA-CB	-9.64	96.61	110.10
1	A	68	LEU	CA-CB-CG	-9.38	93.74	115.30
1	A	114	LEU	N-CA-CB	-9.09	92.23	110.40
1	B	397	HIS	CB-CA-C	-8.81	92.77	110.40
1	B	302	ARG	NE-CZ-NH2	-8.62	115.99	120.30
1	A	98	PRO	N-CA-C	-8.42	90.21	112.10
1	A	240	LEU	CA-CB-CG	-8.26	96.30	115.30
1	A	276	ARG	NE-CZ-NH1	-8.24	116.18	120.30
1	A	127	ARG	NE-CZ-NH2	-8.10	116.25	120.30
1	A	97	ARG	N-CA-C	-8.07	89.22	111.00
1	A	368	LEU	CB-CG-CD1	-8.06	97.30	111.00
1	A	301	LEU	N-CA-C	-7.90	89.66	111.00
1	A	60	ARG	NE-CZ-NH2	7.89	124.24	120.30
1	B	99	PHE	CB-CA-C	-7.73	94.93	110.40
1	B	229	LEU	N-CA-C	7.67	131.71	111.00
1	A	291	ARG	NE-CZ-NH1	-7.59	116.50	120.30
1	A	63	ASP	CB-CG-OD2	7.54	125.08	118.30
1	A	337	ASP	CB-CG-OD1	7.52	125.07	118.30
1	A	357	VAL	CB-CA-C	-7.50	97.15	111.40
1	A	260	LEU	CB-CG-CD2	7.43	123.64	111.00
1	B	395	VAL	CB-CA-C	7.41	125.48	111.40
1	B	260	LEU	CA-CB-CG	-7.35	98.40	115.30
1	B	198	LEU	CB-CG-CD2	-7.30	98.60	111.00
1	B	245	ILE	CB-CA-C	-7.27	97.06	111.60
1	A	60	ARG	NE-CZ-NH1	-7.20	116.70	120.30
1	A	293	LEU	CB-CG-CD1	-7.14	98.87	111.00
1	B	167	LEU	CB-CG-CD2	7.13	123.12	111.00
1	B	66	GLU	CB-CA-C	-7.11	96.18	110.40
1	B	232	GLY	N-CA-C	-7.03	95.52	113.10
1	A	150	LEU	CA-CB-CG	6.97	131.34	115.30
1	A	275	LEU	CB-CG-CD2	-6.92	99.24	111.00
1	B	243	LEU	CA-CB-CG	-6.91	99.42	115.30
1	A	301	LEU	CB-CG-CD1	6.83	122.62	111.00
1	A	188	ASN	N-CA-C	6.76	129.24	111.00
1	B	289	LEU	CA-CB-CG	-6.74	99.79	115.30
1	A	365	LEU	CA-CB-CG	-6.68	99.94	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	367	ARG	NE-CZ-NH2	-6.61	116.99	120.30
1	B	286	VAL	CB-CA-C	-6.57	98.92	111.40
1	A	24	GLN	N-CA-C	-6.51	93.43	111.00
1	A	213	ARG	NE-CZ-NH1	6.51	123.56	120.30
1	B	245	ILE	CG1-CB-CG2	6.40	125.49	111.40
1	B	142	LEU	CA-CB-CG	6.34	129.89	115.30
1	A	384	LEU	CA-CB-CG	6.31	129.81	115.30
1	A	295	VAL	CB-CA-C	-6.31	99.42	111.40
1	B	299	ILE	N-CA-C	6.26	127.90	111.00
1	B	385	ARG	NE-CZ-NH2	-6.26	117.17	120.30
1	A	208	LEU	CB-CG-CD1	6.25	121.62	111.00
1	B	187	ARG	N-CA-C	-6.22	94.21	111.00
1	B	386	LEU	CA-CB-CG	-6.22	101.00	115.30
1	A	63	ASP	CB-CG-OD1	-6.21	112.72	118.30
1	B	337	ASP	N-CA-CB	6.11	121.59	110.60
1	B	115	LEU	CB-CG-CD1	-6.08	100.66	111.00
1	A	375	GLU	N-CA-CB	-6.07	99.68	110.60
1	B	378	LEU	CA-CB-CG	-6.01	101.47	115.30
1	A	257	MET	CG-SD-CE	5.99	109.79	100.20
1	A	260	LEU	CB-CG-CD1	-5.95	100.89	111.00
1	B	193	GLN	N-CA-CB	-5.93	99.92	110.60
1	A	112	ARG	CG-CD-NE	5.90	124.19	111.80
1	B	396	LYS	N-CA-C	-5.89	95.08	111.00
1	B	280	ASP	CB-CG-OD1	5.89	123.60	118.30
1	B	234	VAL	CB-CA-C	-5.84	100.30	111.40
1	A	68	LEU	CB-CG-CD1	-5.84	101.08	111.00
1	A	187	ARG	N-CA-C	5.81	126.69	111.00
1	B	61	TYR	CB-CG-CD1	5.77	124.46	121.00
1	B	192	GLU	CB-CA-C	-5.76	98.88	110.40
1	A	111	ARG	NE-CZ-NH2	5.75	123.18	120.30
1	B	365	LEU	CB-CG-CD2	-5.66	101.37	111.00
1	A	378	LEU	CA-CB-CG	-5.66	102.28	115.30
1	B	176	PHE	CB-CA-C	-5.66	99.09	110.40
1	A	383	THR	CA-C-N	-5.65	104.78	117.20
1	A	291	ARG	NE-CZ-NH2	5.61	123.11	120.30
1	A	236	THR	CA-CB-CG2	-5.56	104.62	112.40
1	A	25	ARG	N-CA-C	-5.52	96.09	111.00
1	A	318	ASP	CB-CG-OD1	-5.51	113.34	118.30
1	A	312	GLY	N-CA-C	5.50	126.86	113.10
1	B	286	VAL	CA-CB-CG1	-5.49	102.67	110.90
1	B	282	MET	CG-SD-CE	5.47	108.96	100.20
1	A	198	LEU	CB-CG-CD2	-5.40	101.82	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	115	LEU	CA-CB-CG	5.39	127.69	115.30
1	A	277	LYS	CB-CA-C	-5.37	99.66	110.40
1	A	167	LEU	CB-CG-CD2	-5.37	101.88	111.00
1	B	304	ALA	N-CA-C	5.35	125.45	111.00
1	B	290	LEU	CB-CG-CD2	-5.34	101.92	111.00
1	A	215	GLU	OE1-CD-OE2	-5.33	116.91	123.30
1	B	340	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	A	299	ILE	N-CA-C	-5.29	96.71	111.00
1	B	296	ALA	N-CA-C	-5.27	96.78	111.00
1	A	294	SER	CB-CA-C	5.22	120.02	110.10
1	A	343	PHE	CB-CA-C	-5.21	99.98	110.40
1	B	138	LEU	CB-CG-CD2	5.19	119.82	111.00
1	A	67	LEU	CB-CG-CD1	5.18	119.80	111.00
1	B	303	VAL	N-CA-C	-5.17	97.04	111.00
1	B	163	ILE	CG1-CB-CG2	-5.15	100.07	111.40
1	A	372	VAL	CB-CA-C	-5.13	101.64	111.40
1	B	112	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	A	276	ARG	NE-CZ-NH2	5.11	122.86	120.30
1	B	340	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	A	150	LEU	CB-CG-CD1	5.07	119.62	111.00
1	B	121	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	A	347	ASP	N-CA-C	5.02	124.54	111.00
1	B	369	GLU	CA-CB-CG	5.01	124.42	113.40

There are no chirality outliers.

All (18) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	170	PRO	Peptide
1	A	186	SER	Peptide
1	A	23	ILE	Peptide
1	A	27	CYS	Peptide
1	A	296	ALA	Peptide
1	A	383	THR	Peptide
1	A	401	THR	Peptide
1	A	80	PRO	Peptide
1	A	97	ARG	Peptide
1	B	104	ALA	Peptide
1	B	146	GLY	Peptide
1	B	186	SER	Peptide
1	B	193	GLN	Peptide
1	B	248	ASN	Peptide

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Mol	Chain	Res	Type	Group
1	B	279	PRO	Peptide
1	B	303	VAL	Peptide
1	B	318	ASP	Peptide
1	B	381	VAL	Peptide

## 5.2 Too-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 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	A	3020	0	3005	523	0
1	B	2858	0	2870	459	0
2	A	43	0	30	18	0
2	B	43	0	30	25	0
3	A	35	0	0	10	0
3	B	22	0	0	2	0
All	All	6021	0	5935	971	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 82.

All (971) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:LEU:HA	1:A:234:VAL:CB	1.07	1.52
1:A:24:GLN:HG2	1:A:33:ALA:CB	1.42	1.49
1:A:229:LEU:CA	1:A:234:VAL:CB	1.97	1.39
1:A:24:GLN:CG	1:A:33:ALA:HB1	1.57	1.33
1:A:80:PRO:O	1:A:301:LEU:HD13	1.28	1.33
1:B:172:HIS:CB	1:B:173:ASP:HB2	1.57	1.31
1:A:358:HIS:HB3	2:A:501:HEM:O1A	1.16	1.30
1:B:172:HIS:HB2	1:B:173:ASP:CB	1.64	1.25
1:A:235:THR:HG23	1:A:238:GLN:NE2	1.53	1.23
1:A:26:GLY:C	1:A:28:PRO:HD3	1.56	1.23
1:B:113:MET:SD	1:B:229:LEU:HD11	1.85	1.17
1:B:230:VAL:HG12	1:B:234:VAL:HG23	1.24	1.17
1:A:24:GLN:CG	1:A:33:ALA:CB	2.17	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:THR:HB	1:B:333:GLU:OE2	1.48	1.14
1:A:96:PHE:HD1	1:A:97:ARG:NH2	1.44	1.14
1:A:221:ILE:O	1:A:225:VAL:HG13	1.49	1.13
1:A:42:ASP:CB	1:A:45:ALA:HB2	1.79	1.12
1:A:19:ARG:HB2	1:A:47:VAL:HG22	1.25	1.12
1:B:231:PRO:HB3	1:B:232:GLY:HA3	1.33	1.10
1:B:23:ILE:HG23	1:B:32:PRO:HB3	1.12	1.09
1:A:97:ARG:HB2	1:A:97:ARG:NH1	1.69	1.08
1:A:31:ALA:H	1:A:32:PRO:CD	1.61	1.07
1:B:158:VAL:HG11	1:B:258:ILE:HD13	1.31	1.07
1:B:231:PRO:CB	1:B:232:GLY:HA3	1.78	1.07
1:B:137:ILE:O	1:B:141:MET:HG2	1.54	1.07
1:A:127:ARG:HB3	1:A:128:PRO:HD3	1.32	1.06
1:A:24:GLN:HB2	1:A:33:ALA:HB2	1.39	1.04
1:A:42:ASP:HB2	1:A:45:ALA:CB	1.88	1.04
1:A:96:PHE:CD1	1:A:97:ARG:NH2	2.25	1.03
1:A:358:HIS:CB	2:A:501:HEM:O1A	2.07	1.03
1:A:97:ARG:HB2	1:A:97:ARG:CZ	1.86	1.02
1:B:179:ASP:O	1:B:183:ILE:HG12	1.59	1.01
1:A:181:THR:CG2	1:A:251:ARG:HD3	1.90	1.01
1:A:31:ALA:N	1:A:32:PRO:CD	2.19	1.01
1:B:335:PHE:HE1	1:B:348:ASN:HB2	1.24	1.01
1:A:74:SER:HB2	1:A:103:ASP:HB3	1.40	1.00
1:B:23:ILE:CG2	1:B:32:PRO:HB3	1.91	1.00
1:A:179:ASP:O	1:A:183:ILE:HG13	1.61	1.00
1:B:335:PHE:HZ	1:B:346:THR:HB	1.23	0.99
1:A:96:PHE:O	1:A:98:PRO:HD3	1.61	0.99
1:B:230:VAL:HA	1:B:231:PRO:O	1.63	0.99
1:A:19:ARG:HB2	1:A:47:VAL:CG2	1.91	0.98
1:A:235:THR:CG2	1:A:238:GLN:NE2	2.25	0.98
2:A:501:HEM:HBA1	2:A:501:HEM:HHA	1.43	0.97
1:A:96:PHE:HD1	1:A:97:ARG:HH21	1.07	0.97
1:B:230:VAL:HG12	1:B:234:VAL:CG2	1.95	0.97
1:A:31:ALA:H	1:A:32:PRO:HD3	1.29	0.96
1:A:189:SER:HB3	1:A:190:THR:C	1.84	0.96
1:A:19:ARG:HG3	1:A:47:VAL:HA	1.45	0.96
1:A:335:PHE:CE1	1:A:345:ARG:HG2	1.99	0.95
1:A:42:ASP:HB2	1:A:45:ALA:HB2	0.96	0.95
1:B:369:GLU:O	1:B:373:ALA:HB2	1.65	0.95
1:B:335:PHE:CZ	1:B:346:THR:HB	2.02	0.94
1:B:212:ARG:NH1	1:B:217:ARG:NH2	2.15	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:GLN:HA	1:A:24:GLN:OE1	1.67	0.94
1:B:175:GLU:HA	1:B:178:ARG:HB2	1.47	0.93
1:A:74:SER:CB	1:A:103:ASP:HB3	1.97	0.93
1:B:82:PHE:CB	1:B:301:LEU:HD13	1.98	0.93
1:A:383:THR:OG1	1:A:385:ARG:NH2	2.01	0.93
1:A:189:SER:HA	1:A:194:VAL:HG23	1.50	0.93
1:A:89:GLU:HA	1:A:90:GLN:HE21	1.31	0.93
1:A:147:PRO:HA	1:A:410:THR:HG23	1.50	0.93
1:A:19:ARG:O	1:A:48:THR:OG1	1.84	0.93
1:A:368:LEU:O	1:A:372:VAL:HG22	1.69	0.92
1:A:97:ARG:HG2	1:A:245:ILE:HD11	1.51	0.92
1:A:117:ALA:O	1:A:122:ARG:HG2	1.68	0.92
1:A:43:PRO:HB3	1:A:60:ARG:HH21	1.33	0.92
1:B:385:ARG:O	1:B:409:VAL:HG12	1.70	0.92
1:A:19:ARG:CG	1:A:47:VAL:HA	1.99	0.92
1:A:80:PRO:O	1:A:301:LEU:CD1	2.18	0.92
1:B:253:THR:HG22	2:B:501:HEM:HBB2	1.51	0.91
1:A:113:MET:HG3	1:A:228:HIS:ND1	1.85	0.91
1:A:235:THR:HG23	1:A:238:GLN:HE21	1.33	0.91
1:A:270:GLU:O	1:A:273:ALA:HB3	1.70	0.91
1:B:22:PRO:C	1:B:23:ILE:HG12	1.91	0.90
1:A:354:GLY:HA3	1:A:359:GLN:HA	1.54	0.90
1:A:335:PHE:CZ	1:A:345:ARG:HG2	2.07	0.90
1:A:162:VAL:HG11	1:A:369:GLU:HG2	1.54	0.89
1:B:225:VAL:HG12	1:B:239:LEU:CD1	2.03	0.89
1:B:98:PRO:HD2	1:B:101:ARG:HB3	1.55	0.89
1:A:291:ARG:NH2	1:A:292:VAL:HG23	1.88	0.89
1:A:75:ALA:O	1:A:76:ASP:HB2	1.68	0.89
1:A:282:MET:HA	1:A:285:ALA:HB3	1.54	0.88
1:A:124:ARG:O	1:A:127:ARG:HB2	1.72	0.88
1:B:358:HIS:O	2:B:501:HEM:HAA1	1.73	0.88
1:A:229:LEU:HD23	1:A:229:LEU:C	1.93	0.88
1:A:138:LEU:O	1:A:142:LEU:HD12	1.74	0.88
1:A:223:LYS:NZ	1:A:227:ASP:OD1	2.07	0.88
1:A:21:PHE:HE1	1:A:50:PRO:CD	1.86	0.88
1:B:158:VAL:HG11	1:B:258:ILE:CD1	2.03	0.87
1:A:24:GLN:CB	1:A:33:ALA:HB2	2.02	0.87
1:B:363:GLN:HG3	1:B:364:HIS:N	1.85	0.87
1:A:189:SER:HB3	1:A:190:THR:CA	2.04	0.86
1:A:58:VAL:HG21	1:A:67:LEU:CD2	2.04	0.86
1:A:291:ARG:O	1:A:294:SER:HB3	1.75	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:PHE:O	1:A:83:PRO:C	2.11	0.86
1:A:82:PHE:O	1:A:83:PRO:O	1.95	0.85
1:B:23:ILE:HG23	1:B:32:PRO:CB	2.02	0.85
1:A:32:PRO:O	1:A:35:TYR:CD2	2.29	0.85
1:A:96:PHE:O	1:A:97:ARG:C	2.15	0.85
1:A:118:PHE:CZ	1:A:362:GLY:HA2	2.11	0.85
1:B:383:THR:C	1:B:384:LEU:HD13	1.97	0.85
1:A:180:VAL:O	1:A:184:SER:HB2	1.75	0.85
1:B:80:PRO:CB	1:B:303:VAL:HG23	2.07	0.84
1:B:296:ALA:C	1:B:298:SER:H	1.79	0.84
1:A:90:GLN:HB3	1:A:92:ALA:O	1.78	0.84
1:A:25:ARG:C	1:A:27:CYS:H	1.81	0.84
1:B:196:GLU:O	1:B:200:GLY:N	2.10	0.84
1:A:149:ASP:OD2	1:A:152:SER:HB3	1.77	0.83
1:A:240:LEU:H	1:A:240:LEU:HD12	1.39	0.83
1:A:335:PHE:CD1	1:A:345:ARG:HD3	2.13	0.83
1:B:243:LEU:N	1:B:243:LEU:CD1	2.41	0.83
1:A:264:LEU:O	1:A:264:LEU:HD12	1.78	0.83
1:B:231:PRO:CB	1:B:232:GLY:CA	2.56	0.83
1:A:26:GLY:O	1:A:28:PRO:HD3	1.79	0.83
1:A:367:ARG:O	1:A:371:GLU:HG2	1.79	0.83
1:A:96:PHE:O	1:A:98:PRO:CD	2.26	0.83
1:B:20:ASP:CB	1:B:50:PRO:HD3	2.07	0.83
1:A:70:ASP:HB3	1:A:73:VAL:CG2	2.09	0.82
1:B:224:LEU:O	1:B:229:LEU:HB2	1.80	0.81
1:B:76:ASP:HA	1:B:101:ARG:O	1.81	0.81
1:B:350:HIS:O	1:B:350:HIS:CG	2.32	0.81
1:A:229:LEU:HD23	1:A:229:LEU:O	1.78	0.81
1:A:58:VAL:HG21	1:A:67:LEU:HD22	1.60	0.81
1:A:19:ARG:H	1:A:19:ARG:HD2	1.44	0.81
1:B:231:PRO:HB3	1:B:232:GLY:CA	2.10	0.81
1:A:295:VAL:HG12	1:A:402:PHE:HD2	1.45	0.81
1:A:118:PHE:CE1	1:A:362:GLY:HA2	2.16	0.80
1:B:369:GLU:O	1:B:373:ALA:CB	2.28	0.80
1:A:31:ALA:N	1:A:32:PRO:HD2	1.97	0.80
1:B:107:HIS:ND1	1:B:107:HIS:C	2.34	0.80
1:A:21:PHE:HE1	1:A:50:PRO:HD2	1.44	0.80
1:B:260:LEU:HG	1:B:404:LEU:HD21	1.62	0.80
1:B:118:PHE:HE2	2:B:501:HEM:HBC2	1.47	0.79
1:A:41:ASP:O	1:A:43:PRO:HD3	1.83	0.79
1:B:335:PHE:CE1	1:B:348:ASN:HB2	2.15	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:MET:HG3	1:A:228:HIS:CE1	2.17	0.79
1:A:97:ARG:CB	1:A:97:ARG:NH1	2.46	0.79
1:A:164:CYS:SG	1:A:169:ILE:HB	2.23	0.79
1:B:119:THR:O	1:B:123:VAL:CG1	2.31	0.79
1:A:112:ARG:HH11	1:A:112:ARG:HB2	1.48	0.78
1:B:155:ALA:O	1:B:158:VAL:CG1	2.31	0.78
1:B:155:ALA:HA	1:B:158:VAL:HG12	1.65	0.78
1:B:18:PRO:HB3	1:B:48:THR:HG23	1.64	0.78
1:B:80:PRO:HA	1:B:303:VAL:CG2	2.13	0.78
1:B:158:VAL:CG1	1:B:258:ILE:HD13	2.13	0.78
1:A:138:LEU:HD23	1:A:141:MET:HG3	1.66	0.77
1:A:31:ALA:HB2	3:A:601:HOH:O	1.84	0.77
1:B:156:ASN:HA	1:B:255:THR:CG2	2.14	0.77
1:A:316:PRO:HB2	1:A:319:ASP:OD1	1.84	0.77
1:B:72:ARG:HH21	1:B:308:ILE:HA	1.48	0.77
1:A:112:ARG:HH11	1:A:112:ARG:CB	1.97	0.77
1:B:225:VAL:CG2	1:B:226:THR:N	2.47	0.77
1:B:229:LEU:HD23	1:B:234:VAL:HG11	1.66	0.77
1:A:68:LEU:HD23	1:A:355:TYR:O	1.85	0.77
1:B:158:VAL:CG1	1:B:258:ILE:CD1	2.63	0.77
1:B:76:ASP:CA	1:B:101:ARG:O	2.34	0.76
1:B:155:ALA:O	1:B:158:VAL:HG12	1.85	0.76
1:A:266:LEU:HD21	1:A:384:LEU:HD23	1.67	0.76
1:A:151:VAL:HA	1:A:155:ALA:HB3	1.66	0.76
1:B:230:VAL:HA	1:B:231:PRO:C	2.06	0.76
1:B:316:PRO:HD2	1:B:319:ASP:OD2	1.84	0.76
1:A:235:THR:O	1:A:238:GLN:N	2.17	0.76
1:B:243:LEU:HD13	1:B:243:LEU:H	1.51	0.76
1:B:97:ARG:N	1:B:98:PRO:HD3	2.01	0.76
1:A:117:ALA:O	1:A:122:ARG:HD2	1.85	0.76
1:B:76:ASP:N	1:B:101:ARG:O	2.18	0.75
1:A:229:LEU:HD12	1:A:239:LEU:HD22	1.68	0.75
1:B:120:VAL:O	1:B:124:ARG:HB2	1.85	0.75
1:B:204:LEU:O	1:B:208:LEU:HG	1.86	0.75
1:B:113:MET:CE	1:B:229:LEU:HD11	2.17	0.75
1:A:117:ALA:O	1:A:122:ARG:CG	2.34	0.75
1:A:333:GLU:N	1:B:121:ARG:HE	1.84	0.75
1:A:181:THR:HG22	1:A:251:ARG:HD3	1.67	0.75
1:B:194:VAL:CG1	1:B:195:SER:N	2.49	0.75
1:B:260:LEU:HD23	1:B:263:LEU:HD23	1.66	0.74
1:A:368:LEU:O	1:A:372:VAL:CG2	2.34	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:THR:OG1	1:A:238:GLN:HG3	1.87	0.74
1:B:35:TYR:O	1:B:38:LEU:HB2	1.85	0.74
1:B:82:PHE:CB	1:B:301:LEU:CD1	2.65	0.74
1:A:147:PRO:CA	1:A:410:THR:HG23	2.17	0.74
1:B:123:VAL:HB	1:B:365:LEU:HD12	1.69	0.74
1:B:98:PRO:HD2	1:B:101:ARG:CB	2.17	0.74
1:A:357:VAL:HG13	1:B:69:SER:OG	1.86	0.74
1:B:102:THR:O	1:B:107:HIS:HB3	1.87	0.74
1:B:363:GLN:CG	1:B:364:HIS:N	2.50	0.74
1:B:175:GLU:O	1:B:179:ASP:HB2	1.87	0.74
1:B:291:ARG:HH11	1:B:291:ARG:HG2	1.53	0.74
1:A:93:GLY:C	1:A:95:ARG:H	1.92	0.74
1:B:214:GLU:O	1:B:216:PRO:HD3	1.87	0.73
1:B:119:THR:O	1:B:123:VAL:HG13	1.87	0.73
1:A:362:GLY:HA3	2:A:501:HEM:C4C	2.24	0.73
1:B:386:LEU:HD12	1:B:386:LEU:N	2.04	0.73
1:B:263:LEU:HG	1:B:264:LEU:N	2.04	0.73
1:B:212:ARG:HH12	1:B:217:ARG:NH2	1.84	0.73
1:A:295:VAL:HG12	1:A:402:PHE:CD2	2.24	0.73
1:A:19:ARG:N	1:A:19:ARG:HD2	2.03	0.73
1:B:22:PRO:O	1:B:23:ILE:HG12	1.87	0.73
1:A:118:PHE:O	1:A:119:THR:O	2.06	0.72
1:A:147:PRO:HA	1:A:410:THR:CG2	2.19	0.72
2:A:501:HEM:CBA	2:A:501:HEM:HHA	2.17	0.72
1:A:53:ARG:HH22	1:A:82:PHE:HA	1.53	0.72
1:B:230:VAL:CA	1:B:231:PRO:O	2.35	0.72
1:B:383:THR:O	1:B:384:LEU:HD13	1.90	0.72
1:A:370:LEU:HD23	1:A:374:LEU:HD12	1.71	0.72
1:B:212:ARG:NH1	1:B:217:ARG:HH22	1.86	0.72
1:B:347:ASP:OD2	1:B:350:HIS:HB3	1.90	0.72
1:A:351:VAL:O	1:A:353:PHE:O	2.07	0.72
1:A:299:ILE:O	1:A:300:PRO:O	2.06	0.72
1:B:164:CYS:SG	1:B:169:ILE:HB	2.29	0.72
1:B:149:ASP:OD1	1:B:406:GLU:HB2	1.90	0.72
1:B:111:ARG:NH1	1:B:357:VAL:O	2.23	0.71
1:B:340:ARG:HG2	1:B:342:ASP:HB2	1.71	0.71
1:A:164:CYS:SG	1:A:174:LEU:HD22	2.30	0.71
1:B:300:PRO:HA	2:B:501:HEM:O1A	1.89	0.71
1:A:123:VAL:HG22	1:A:365:LEU:HD13	1.71	0.71
1:A:229:LEU:HD11	1:A:236:THR:HG22	1.72	0.71
1:A:229:LEU:CD2	1:A:229:LEU:C	2.59	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:GLU:HA	1:A:314:THR:HG22	1.71	0.71
1:A:117:ALA:O	1:A:122:ARG:CD	2.39	0.71
1:B:149:ASP:HB2	1:B:408:MET:HG3	1.71	0.70
1:B:381:VAL:CG1	1:B:384:LEU:HD11	2.20	0.70
1:B:80:PRO:HB3	1:B:303:VAL:CG2	2.21	0.70
1:A:24:GLN:CG	1:A:33:ALA:HB2	2.11	0.70
1:A:254:THR:HG22	2:A:501:HEM:CAB	2.21	0.70
1:B:78:ARG:HD2	1:B:303:VAL:HG11	1.72	0.70
1:B:148:VAL:O	1:B:408:MET:HB3	1.91	0.70
1:B:132:ALA:O	1:B:135:ASP:HB2	1.90	0.70
1:A:230:VAL:HB	1:A:231:PRO:HD3	1.73	0.70
1:B:34:GLU:O	1:B:37:ALA:HB3	1.91	0.70
1:A:374:LEU:O	1:A:378:LEU:HG	1.91	0.70
1:B:353:PHE:HE1	2:B:501:HEM:C3B	2.09	0.70
1:A:254:THR:O	1:A:257:MET:N	2.24	0.70
1:A:126:MET:HA	3:A:620:HOH:O	1.92	0.70
1:A:240:LEU:N	1:A:240:LEU:HD12	2.05	0.69
1:A:264:LEU:C	1:A:264:LEU:HD12	2.12	0.69
1:B:300:PRO:O	1:B:322:ILE:HG23	1.92	0.69
1:B:260:LEU:HD21	1:B:404:LEU:HD11	1.74	0.69
1:A:358:HIS:ND1	2:A:501:HEM:O1D	2.22	0.69
1:B:271:LEU:HA	1:B:274:GLU:OE2	1.92	0.69
1:A:25:ARG:NE	1:A:402:PHE:CE2	2.54	0.69
1:A:25:ARG:HD2	3:A:601:HOH:O	1.92	0.69
1:B:229:LEU:HB3	1:B:234:VAL:CG2	2.22	0.69
1:B:68:LEU:HD22	1:B:355:TYR:O	1.91	0.69
1:B:238:GLN:HA	1:B:241:SER:OG	1.92	0.69
1:B:107:HIS:HD1	1:B:107:HIS:C	1.96	0.69
1:B:231:PRO:HB2	1:B:232:GLY:HA3	1.72	0.69
1:B:167:LEU:CD1	1:B:167:LEU:N	2.56	0.69
1:B:18:PRO:O	1:B:48:THR:OG1	2.08	0.69
1:A:410:THR:C	1:A:411:TRP:CD1	2.66	0.69
1:B:278:ASP:OD2	1:B:280:ASP:HB2	1.92	0.69
1:A:21:PHE:CE1	1:A:50:PRO:HD2	2.27	0.68
1:B:149:ASP:HB2	1:B:408:MET:CG	2.22	0.68
1:A:173:ASP:OD1	3:A:626:HOH:O	2.10	0.68
1:A:286:VAL:HG23	1:A:370:LEU:CD2	2.22	0.68
1:A:19:ARG:HG2	1:A:48:THR:H	1.59	0.68
1:A:25:ARG:C	1:A:27:CYS:N	2.44	0.68
1:A:49:LEU:O	1:A:52:ARG:N	2.27	0.68
1:B:395:VAL:O	1:B:405:GLU:HG2	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:138:LEU:HD23	1:B:141:MET:HB2	1.74	0.68
1:B:304:ALA:HB2	1:B:315:VAL:CG1	2.24	0.68
1:A:65:ARG:NH1	1:A:355:TYR:CE2	2.61	0.68
1:B:259:ALA:HB1	1:B:404:LEU:HD23	1.76	0.68
1:A:43:PRO:CD	1:A:44:VAL:H	2.07	0.67
1:B:29:PHE:CD1	1:B:30:ALA:N	2.59	0.67
1:A:25:ARG:HH21	1:A:30:ALA:HA	1.59	0.67
1:B:156:ASN:HA	1:B:255:THR:HG21	1.75	0.67
1:A:164:CYS:HA	1:A:169:ILE:HD12	1.76	0.67
1:B:225:VAL:HG23	1:B:226:THR:N	2.08	0.67
1:B:195:SER:O	1:B:199:GLY:N	2.24	0.67
1:A:150:LEU:N	1:A:407:LEU:O	2.25	0.67
1:B:80:PRO:HB3	1:B:303:VAL:HG23	1.76	0.67
1:B:179:ASP:O	1:B:182:ARG:HB3	1.95	0.67
1:B:172:HIS:CA	1:B:173:ASP:HB2	2.25	0.67
1:A:62:ASP:HA	1:A:65:ARG:HG2	1.75	0.67
1:B:150:LEU:O	1:B:155:ALA:N	2.24	0.67
1:B:164:CYS:SG	1:B:177:PHE:CD1	2.89	0.66
1:A:25:ARG:O	1:A:27:CYS:N	2.27	0.66
1:B:99:PHE:HE2	1:B:110:TYR:CB	2.09	0.66
1:B:282:MET:O	1:B:285:ALA:HB3	1.95	0.66
1:A:363:GLN:HA	1:A:366:ALA:HB3	1.78	0.66
1:A:56:TRP:O	1:A:321:VAL:HA	1.95	0.66
1:A:89:GLU:HA	1:A:90:GLN:NE2	2.09	0.66
1:A:205:LEU:O	1:A:209:VAL:HG23	1.95	0.66
1:A:80:PRO:HA	1:A:301:LEU:HD22	1.76	0.66
1:B:296:ALA:C	1:B:298:SER:N	2.48	0.66
1:B:260:LEU:HG	1:B:404:LEU:CD2	2.25	0.66
1:A:18:PRO:N	1:A:19:ARG:HH11	1.94	0.66
1:B:18:PRO:HB3	1:B:48:THR:CG2	2.25	0.66
1:B:194:VAL:HG13	1:B:195:SER:N	2.10	0.66
1:A:27:CYS:N	1:A:28:PRO:HD3	1.95	0.66
1:B:80:PRO:CB	1:B:303:VAL:CG2	2.74	0.66
1:B:186:SER:OG	1:B:187:ARG:N	2.17	0.66
1:A:254:THR:HG22	2:A:501:HEM:HAB	1.78	0.65
1:B:358:HIS:O	2:B:501:HEM:CAA	2.44	0.65
1:B:383:THR:CG2	1:B:384:LEU:N	2.58	0.65
1:B:38:LEU:O	1:B:42:ASP:O	2.13	0.65
1:A:112:ARG:NH1	1:A:112:ARG:CB	2.59	0.65
1:B:295:VAL:HG13	1:B:295:VAL:O	1.95	0.65
1:A:18:PRO:CD	1:A:19:ARG:NH1	2.60	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:243:LEU:N	1:B:243:LEU:HD12	2.10	0.65
1:A:97:ARG:CB	1:A:97:ARG:CZ	2.70	0.65
1:B:296:ALA:O	1:B:297:ASP:HB3	1.96	0.65
1:B:76:ASP:HA	1:B:101:ARG:C	2.16	0.65
1:B:171:ARG:HA	1:B:174:LEU:HB2	1.77	0.65
1:A:387:ALA:N	1:A:408:MET:O	2.30	0.65
1:B:80:PRO:CA	1:B:303:VAL:CG2	2.75	0.65
1:A:281:LEU:O	1:A:282:MET:C	2.35	0.65
1:A:30:ALA:HB1	1:A:31:ALA:HB2	1.77	0.65
1:A:25:ARG:NH2	1:A:30:ALA:HA	2.11	0.64
1:A:21:PHE:CE1	1:A:50:PRO:CD	2.76	0.64
1:A:269:PRO:HA	1:A:272:PRO:HG2	1.80	0.64
1:B:155:ALA:CA	1:B:158:VAL:HG12	2.27	0.64
1:B:167:LEU:O	1:B:219:ASP:HB2	1.97	0.64
1:A:74:SER:HB3	1:A:103:ASP:HB3	1.80	0.64
1:A:385:ARG:HG2	3:A:604:HOH:O	1.97	0.64
1:A:96:PHE:O	1:A:98:PRO:N	2.31	0.64
1:A:96:PHE:CG	1:A:97:ARG:N	2.65	0.64
1:A:24:GLN:HB3	1:A:25:ARG:C	2.17	0.64
1:A:366:ALA:O	1:A:370:LEU:HB2	1.98	0.64
1:A:49:LEU:HG	1:A:82:PHE:HD2	1.63	0.64
1:A:72:ARG:NH1	1:B:104:ALA:HB3	2.13	0.64
1:B:271:LEU:O	1:B:274:GLU:HB2	1.98	0.64
1:B:343:PHE:HD1	1:B:343:PHE:N	1.95	0.64
1:B:243:LEU:N	1:B:243:LEU:HD13	2.11	0.63
1:B:343:PHE:N	1:B:343:PHE:CD1	2.66	0.63
1:B:80:PRO:HA	1:B:303:VAL:HG21	1.79	0.63
1:B:306:GLU:OE1	1:B:307:ASP:N	2.30	0.63
1:A:286:VAL:CG1	1:A:287:ASP:N	2.60	0.63
1:B:39:ARG:O	1:B:60:ARG:NH2	2.31	0.63
1:A:286:VAL:HG23	1:A:370:LEU:HD22	1.78	0.63
1:A:335:PHE:CE1	1:A:345:ARG:CG	2.80	0.63
1:B:269:PRO:O	1:B:272:PRO:HD2	1.98	0.63
1:A:130:VAL:O	1:A:134:VAL:HG23	1.98	0.63
1:A:257:MET:O	1:A:261:SER:OG	2.11	0.63
1:B:281:LEU:HD13	1:B:343:PHE:HD2	1.63	0.63
1:B:167:LEU:HD13	1:B:167:LEU:N	2.13	0.63
1:A:102:THR:HG21	1:A:106:GLU:HG2	1.80	0.63
1:A:332:PRO:C	1:B:121:ARG:HE	2.02	0.63
1:A:387:ALA:H	1:A:409:VAL:HA	1.63	0.63
1:A:111:ARG:O	1:A:114:LEU:HB3	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:205:LEU:O	1:B:208:LEU:N	2.32	0.63
1:A:44:VAL:HG12	1:A:56:TRP:CE3	2.35	0.62
1:B:99:PHE:HB2	1:B:245:ILE:HD13	1.81	0.62
1:B:149:ASP:C	1:B:149:ASP:OD2	2.37	0.62
1:B:107:HIS:NE2	1:B:357:VAL:HG11	2.13	0.62
1:B:133:ARG:O	1:B:137:ILE:HG13	1.97	0.62
1:B:335:PHE:CZ	1:B:346:THR:CB	2.79	0.62
1:A:147:PRO:HG3	1:A:410:THR:HG21	1.80	0.62
1:B:260:LEU:HD23	1:B:263:LEU:CD2	2.29	0.62
1:B:286:VAL:HG11	1:B:370:LEU:HB2	1.80	0.62
1:B:119:THR:O	1:B:123:VAL:HG12	1.99	0.62
1:A:390:ARG:O	1:A:393:VAL:HG12	1.99	0.62
1:A:291:ARG:HD3	1:A:348:ASN:ND2	2.15	0.62
1:B:118:PHE:CE2	2:B:501:HEM:HBC2	2.34	0.62
1:B:102:THR:O	1:B:107:HIS:CB	2.47	0.62
1:A:18:PRO:HD2	1:A:19:ARG:NH1	2.14	0.62
1:B:65:ARG:HG3	1:B:355:TYR:CD2	2.34	0.62
1:B:353:PHE:CE1	2:B:501:HEM:C2B	2.88	0.62
1:A:64:VAL:HG13	1:A:323:ALA:HB1	1.82	0.62
1:A:73:VAL:O	1:A:302:ARG:HB3	2.00	0.61
1:B:225:VAL:HG12	1:B:239:LEU:HD13	1.83	0.61
1:A:189:SER:HB3	1:A:190:THR:HA	1.81	0.61
1:A:25:ARG:HH21	1:A:25:ARG:HG2	1.64	0.61
1:A:70:ASP:HB3	1:A:73:VAL:HG21	1.81	0.61
1:B:110:TYR:O	1:B:113:MET:HB2	2.00	0.61
1:B:157:ALA:O	1:B:178:ARG:NH1	2.32	0.61
1:B:99:PHE:HE2	1:B:110:TYR:HB3	1.65	0.61
1:B:346:THR:C	1:B:348:ASN:H	2.02	0.61
1:A:131:GLN:OE1	1:A:372:VAL:HG12	2.01	0.61
1:B:155:ALA:HA	1:B:158:VAL:CG1	2.30	0.61
1:A:88:GLY:C	1:A:89:GLU:HG2	2.21	0.61
1:A:31:ALA:CB	3:A:601:HOH:O	2.46	0.61
1:B:340:ARG:CG	1:B:342:ASP:HB2	2.29	0.61
1:A:295:VAL:HG12	1:A:402:PHE:HB3	1.82	0.61
1:B:105:PRO:C	1:B:107:HIS:N	2.52	0.61
1:A:270:GLU:H	1:A:270:GLU:CD	2.02	0.61
1:B:149:ASP:OD2	1:B:152:SER:HB2	2.01	0.61
1:A:229:LEU:CB	1:A:234:VAL:CB	2.79	0.60
1:A:381:VAL:N	1:A:382:PRO:HD3	2.15	0.60
1:A:80:PRO:HD2	1:A:91:GLU:HG3	1.83	0.60
1:B:80:PRO:CA	1:B:303:VAL:HG23	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:301:LEU:HD23	1:A:302:ARG:C	2.21	0.60
1:B:225:VAL:HG12	1:B:239:LEU:HD11	1.83	0.60
1:A:173:ASP:N	1:A:173:ASP:OD1	2.33	0.60
1:A:184:SER:OG	1:A:198:LEU:CD1	2.50	0.60
1:B:72:ARG:NH2	1:B:308:ILE:HA	2.17	0.60
1:A:229:LEU:C	1:A:234:VAL:CB	2.68	0.60
1:A:97:ARG:HG2	1:A:245:ILE:CD1	2.27	0.60
1:B:155:ALA:O	1:B:158:VAL:HG13	1.99	0.60
1:A:127:ARG:CB	1:A:128:PRO:HD3	2.17	0.60
1:B:230:VAL:CG1	1:B:234:VAL:CG2	2.77	0.60
1:A:286:VAL:CG2	1:A:370:LEU:HB3	2.31	0.60
1:B:107:HIS:CG	1:B:108:THR:N	2.70	0.60
1:A:189:SER:HB3	1:A:191:ALA:N	2.16	0.60
1:B:151:VAL:O	1:B:156:ASN:HB2	2.00	0.60
1:B:271:LEU:HB2	1:B:272:PRO:HD3	1.82	0.60
1:B:335:PHE:HZ	1:B:346:THR:CB	2.06	0.59
1:A:74:SER:HB2	1:A:103:ASP:CB	2.23	0.59
1:A:181:THR:HG23	1:A:251:ARG:HD3	1.83	0.59
1:B:195:SER:O	1:B:198:LEU:HB3	2.02	0.59
1:A:213:ARG:CZ	1:A:230:VAL:HG22	2.32	0.59
1:A:249:ALA:HB3	2:A:501:HEM:CBC	2.33	0.59
1:A:371:GLU:O	1:A:375:GLU:HB2	2.01	0.59
1:A:370:LEU:HD23	1:A:374:LEU:CD1	2.31	0.59
1:B:225:VAL:HG22	1:B:226:THR:H	1.68	0.59
1:A:271:LEU:HD12	1:A:343:PHE:CE2	2.38	0.59
1:B:187:ARG:N	1:B:187:ARG:HD2	2.17	0.59
1:A:240:LEU:H	1:A:240:LEU:CD1	2.15	0.59
1:B:253:THR:CG2	2:B:501:HEM:HBB2	2.30	0.59
1:B:122:ARG:O	1:B:125:ALA:HB3	2.03	0.59
1:B:229:LEU:HB3	1:B:234:VAL:HG21	1.83	0.59
1:A:24:GLN:HG2	1:A:33:ALA:HB1	0.65	0.59
1:B:228:HIS:O	1:B:229:LEU:HD12	2.01	0.59
1:B:208:LEU:O	1:B:212:ARG:N	2.27	0.59
1:B:291:ARG:NH1	1:B:291:ARG:HG2	2.17	0.59
1:B:172:HIS:HB2	1:B:173:ASP:HB2	0.69	0.59
1:B:386:LEU:HD12	1:B:386:LEU:H	1.68	0.59
1:A:66:GLU:OE2	1:B:115:LEU:HD11	2.03	0.58
1:A:384:LEU:HA	1:A:410:THR:O	2.03	0.58
1:B:76:ASP:HB3	1:B:102:THR:HA	1.85	0.58
1:B:228:HIS:HB3	1:B:229:LEU:HD13	1.85	0.58
1:A:335:PHE:HD2	1:A:347:ASP:HB3	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:381:VAL:HG13	1:B:384:LEU:HD11	1.84	0.58
1:A:93:GLY:C	1:A:95:ARG:N	2.57	0.58
1:A:43:PRO:HB3	1:A:60:ARG:NH2	2.13	0.58
1:B:135:ASP:O	1:B:139:ASP:HB2	2.04	0.58
1:B:126:MET:CE	1:B:365:LEU:HD11	2.33	0.58
1:B:295:VAL:CG1	1:B:295:VAL:O	2.50	0.58
1:A:18:PRO:N	1:A:19:ARG:HD2	2.18	0.58
1:B:346:THR:O	1:B:348:ASN:N	2.21	0.58
1:B:289:LEU:O	1:B:293:LEU:HB2	2.04	0.58
1:A:286:VAL:CG2	1:A:370:LEU:HD22	2.34	0.58
1:A:103:ASP:OD1	1:A:103:ASP:N	2.33	0.58
1:A:326:ALA:O	1:A:329:ASN:N	2.36	0.58
1:B:303:VAL:HG22	1:B:319:ASP:O	2.03	0.58
1:B:78:ARG:HD2	1:B:303:VAL:CG1	2.32	0.58
1:A:24:GLN:N	1:A:25:ARG:HA	2.19	0.58
1:A:379:ARG:HG2	1:A:380:ARG:HG2	1.86	0.58
1:A:42:ASP:OD1	1:A:42:ASP:N	2.36	0.58
1:B:31:ALA:HB1	1:B:32:PRO:CD	2.34	0.58
1:A:53:ARG:NH1	1:A:91:GLU:OE2	2.37	0.57
1:A:18:PRO:CD	1:A:19:ARG:HH11	2.17	0.57
1:A:119:THR:HB	1:B:333:GLU:CD	2.23	0.57
1:B:205:LEU:O	1:B:206:GLY:C	2.42	0.57
1:A:387:ALA:N	1:A:409:VAL:HA	2.19	0.57
1:B:281:LEU:HD13	1:B:343:PHE:CD2	2.39	0.57
1:B:381:VAL:HG11	1:B:384:LEU:HD11	1.87	0.57
1:A:43:PRO:HG2	1:A:44:VAL:N	2.19	0.57
1:B:221:ILE:O	1:B:225:VAL:HG13	2.05	0.57
1:B:162:VAL:HG11	1:B:369:GLU:CD	2.25	0.57
1:A:113:MET:HA	1:A:228:HIS:CE1	2.40	0.57
1:B:211:GLU:O	1:B:214:GLU:N	2.35	0.57
1:B:250:GLY:CA	2:B:501:HEM:C2C	2.88	0.57
1:B:130:VAL:HG21	1:B:368:LEU:HD12	1.87	0.57
1:B:301:LEU:O	1:B:302:ARG:HG3	2.05	0.57
1:B:278:ASP:OD2	1:B:280:ASP:CB	2.52	0.57
1:A:27:CYS:O	1:A:29:PHE:O	2.24	0.56
1:A:249:ALA:HB1	2:A:501:HEM:C4C	2.39	0.56
1:A:97:ARG:HB3	1:A:98:PRO:CA	2.33	0.56
1:A:292:VAL:CG1	1:A:293:LEU:N	2.69	0.56
1:B:155:ALA:C	1:B:158:VAL:HG12	2.25	0.56
1:B:99:PHE:HZ	1:B:111:ARG:HA	1.70	0.56
1:B:118:PHE:CZ	1:B:166:LEU:HD21	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:278:ASP:C	1:B:280:ASP:H	2.09	0.56
1:A:252:GLU:OE1	1:A:401:THR:HG23	2.05	0.56
1:A:65:ARG:HB2	1:A:355:TYR:CD2	2.40	0.56
1:A:41:ASP:O	1:A:43:PRO:CD	2.54	0.56
1:B:29:PHE:CG	1:B:30:ALA:N	2.74	0.56
1:B:252:GLU:O	1:B:252:GLU:HG3	2.05	0.56
1:B:229:LEU:HB3	1:B:234:VAL:HG22	1.88	0.56
1:A:270:GLU:O	1:A:273:ALA:CB	2.47	0.56
1:A:286:VAL:HG21	1:A:370:LEU:HB3	1.87	0.55
1:A:381:VAL:CG2	1:A:381:VAL:O	2.54	0.55
2:A:501:HEM:HBA1	2:A:501:HEM:CHA	2.23	0.55
1:A:184:SER:OG	1:A:198:LEU:HD11	2.05	0.55
1:A:271:LEU:O	1:A:272:PRO:C	2.45	0.55
1:A:303:VAL:HA	1:A:319:ASP:O	2.07	0.55
1:B:281:LEU:O	1:B:285:ALA:HB2	2.06	0.55
1:A:133:ARG:O	1:A:137:ILE:HG23	2.07	0.55
1:A:24:GLN:N	1:A:25:ARG:CA	2.64	0.55
1:A:291:ARG:HD3	1:A:348:ASN:HD21	1.72	0.55
1:A:384:LEU:HB2	1:A:411:TRP:HD1	1.70	0.55
1:B:149:ASP:HA	1:B:408:MET:HA	1.88	0.55
1:A:230:VAL:CB	1:A:231:PRO:HD3	2.32	0.55
1:B:167:LEU:HD13	1:B:167:LEU:H	1.70	0.55
1:B:44:VAL:CG2	1:B:310:LEU:HD23	2.36	0.55
1:A:24:GLN:HB3	1:A:26:GLY:N	2.21	0.55
1:A:24:GLN:CB	1:A:33:ALA:CB	2.69	0.55
1:A:380:ARG:C	1:A:382:PRO:HD3	2.27	0.55
1:A:25:ARG:NE	1:A:402:PHE:CZ	2.74	0.55
1:A:266:LEU:HD21	1:A:384:LEU:CD2	2.36	0.55
1:B:199:GLY:O	1:B:200:GLY:C	2.44	0.55
1:A:301:LEU:HD21	1:A:320:GLY:HA2	1.89	0.55
1:A:74:SER:CB	1:A:103:ASP:CB	2.80	0.55
1:A:189:SER:CB	1:A:190:THR:CA	2.82	0.55
1:A:180:VAL:O	1:A:184:SER:CB	2.51	0.55
1:B:297:ASP:OD1	1:B:326:ALA:HB3	2.06	0.55
1:B:250:GLY:HA2	2:B:501:HEM:C2C	2.42	0.55
1:A:109:ARG:O	1:A:113:MET:HB2	2.07	0.55
1:A:236:THR:O	1:A:240:LEU:HD13	2.06	0.55
1:A:32:PRO:O	1:A:33:ALA:HB3	2.06	0.55
1:B:126:MET:O	1:B:127:ARG:C	2.43	0.55
1:A:43:PRO:CG	1:A:44:VAL:N	2.69	0.55
1:B:243:LEU:CD1	1:B:243:LEU:H	2.10	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:23:ILE:HD12	1:B:32:PRO:HG3	1.87	0.55
1:A:24:GLN:CB	1:A:25:ARG:CA	2.85	0.54
1:A:56:TRP:N	1:A:320:GLY:O	2.22	0.54
1:A:43:PRO:CG	1:A:44:VAL:H	2.19	0.54
1:B:78:ARG:O	1:B:79:ARG:HG3	2.07	0.54
1:A:286:VAL:CG1	1:A:287:ASP:H	2.20	0.54
1:A:150:LEU:HD21	1:A:262:THR:HG21	1.89	0.54
1:B:281:LEU:O	1:B:282:MET:C	2.45	0.54
1:A:282:MET:O	1:A:283:PRO:C	2.44	0.54
1:A:298:SER:C	1:A:299:ILE:O	2.41	0.54
1:A:97:ARG:CB	1:A:97:ARG:HH11	2.17	0.54
1:A:286:VAL:HG12	1:A:287:ASP:H	1.72	0.54
1:A:278:ASP:C	1:A:278:ASP:OD1	2.45	0.54
1:A:147:PRO:CB	1:A:410:THR:HG23	2.38	0.54
1:B:177:PHE:HA	1:B:180:VAL:HG22	1.90	0.54
1:B:383:THR:HG22	1:B:384:LEU:N	2.21	0.54
1:B:296:ALA:HB1	1:B:299:ILE:HG22	1.90	0.54
1:B:394:VAL:HG13	1:B:395:VAL:O	2.07	0.54
1:B:47:VAL:HG13	1:B:55:ALA:O	2.08	0.54
1:A:257:MET:SD	1:A:293:LEU:HD12	2.47	0.54
1:A:25:ARG:NH2	1:A:30:ALA:CA	2.71	0.54
1:B:230:VAL:HB	1:B:231:PRO:O	2.08	0.54
1:B:140:GLY:O	1:B:143:ALA:N	2.41	0.54
1:B:72:ARG:O	1:B:308:ILE:HD13	2.08	0.53
1:A:102:THR:HB	1:A:107:HIS:HB2	1.90	0.53
1:A:145:GLY:O	1:A:146:GLY:O	2.26	0.53
1:A:286:VAL:HG13	1:A:287:ASP:N	2.21	0.53
1:B:118:PHE:HB3	1:B:361:VAL:O	2.08	0.53
1:A:122:ARG:HA	3:A:621:HOH:O	2.07	0.53
1:A:242:THR:O	1:A:246:THR:N	2.39	0.53
1:B:225:VAL:CG2	1:B:226:THR:H	2.19	0.53
1:A:269:PRO:HG2	1:A:270:GLU:OE2	2.08	0.53
1:B:271:LEU:HD22	1:B:343:PHE:CE1	2.43	0.53
1:A:26:GLY:O	1:A:27:CYS:HB3	2.08	0.53
1:B:255:THR:O	1:B:256:SER:C	2.47	0.53
1:B:70:ASP:OD1	1:B:72:ARG:HG3	2.09	0.53
1:A:112:ARG:HB3	1:A:112:ARG:NH1	2.24	0.53
1:A:326:ALA:O	1:A:327:GLY:C	2.44	0.53
1:A:52:ARG:NH1	3:A:608:HOH:O	2.41	0.53
1:A:112:ARG:NH1	1:A:112:ARG:HB2	2.21	0.53
1:B:35:TYR:O	1:B:38:LEU:N	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:336:ASP:OD1	1:A:337:ASP:HB2	2.09	0.53
1:A:235:THR:OG1	1:A:235:THR:O	2.27	0.52
1:A:65:ARG:HB2	1:A:65:ARG:HH11	1.74	0.52
1:B:114:LEU:C	1:B:116:PRO:HD2	2.29	0.52
1:A:25:ARG:HG2	1:A:25:ARG:NH2	2.21	0.52
1:B:238:GLN:O	1:B:242:THR:HG23	2.09	0.52
1:B:242:THR:O	1:B:243:LEU:C	2.46	0.52
1:A:49:LEU:C	1:A:51:THR:H	2.13	0.52
1:B:165:GLU:HA	1:B:165:GLU:OE1	2.10	0.52
1:A:254:THR:CG2	2:A:501:HEM:HAB	2.39	0.52
1:A:19:ARG:CD	1:A:19:ARG:H	2.08	0.52
1:B:303:VAL:HG11	1:B:318:ASP:OD1	2.10	0.52
1:A:301:LEU:HD12	1:A:322:ILE:HG13	1.91	0.52
1:B:363:GLN:CG	1:B:364:HIS:H	2.22	0.52
1:A:118:PHE:CE1	1:A:362:GLY:CA	2.92	0.52
1:A:80:PRO:C	1:A:301:LEU:HD13	2.23	0.52
1:A:175:GLU:C	1:A:177:PHE:N	2.62	0.52
1:A:53:ARG:NH2	1:A:81:GLY:O	2.42	0.52
1:B:230:VAL:O	1:B:230:VAL:HG23	2.10	0.52
1:A:97:ARG:HB3	1:A:98:PRO:HA	1.92	0.52
1:B:361:VAL:CG2	2:B:501:HEM:HMD2	2.40	0.52
1:A:291:ARG:HH22	1:A:292:VAL:HG23	1.73	0.52
1:B:113:MET:CG	1:B:229:LEU:HD11	2.40	0.52
1:A:65:ARG:HB2	1:A:65:ARG:NH1	2.25	0.52
1:B:47:VAL:HG22	1:B:47:VAL:O	2.09	0.52
1:A:353:PHE:CE2	1:A:363:GLN:HB2	2.44	0.51
1:B:229:LEU:CD2	1:B:234:VAL:HG11	2.39	0.51
1:A:151:VAL:HA	1:A:155:ALA:CB	2.39	0.51
1:A:384:LEU:HB2	1:A:411:TRP:CD1	2.45	0.51
1:A:232:GLY:C	1:A:234:VAL:H	2.13	0.51
1:B:113:MET:SD	1:B:229:LEU:CD1	2.78	0.51
1:B:150:LEU:C	1:B:152:SER:N	2.61	0.51
1:A:24:GLN:H	1:A:25:ARG:HA	1.75	0.51
1:A:43:PRO:HG2	1:A:44:VAL:H	1.75	0.51
1:B:102:THR:HG22	1:B:103:ASP:H	1.75	0.51
1:B:148:VAL:O	1:B:408:MET:CB	2.58	0.51
1:A:257:MET:HB3	1:A:370:LEU:HD11	1.92	0.51
1:B:150:LEU:HB2	1:B:154:TYR:HB3	1.93	0.51
1:A:173:ASP:HB3	1:A:176:PHE:HD1	1.76	0.51
1:B:302:ARG:NH2	1:B:358:HIS:CB	2.74	0.51
1:A:63:ASP:O	1:A:67:LEU:HB3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:250:GLY:HA3	2:B:501:HEM:C3C	2.45	0.51
1:A:286:VAL:HG23	1:A:370:LEU:HD23	1.92	0.51
1:A:97:ARG:CG	1:A:97:ARG:HH11	2.23	0.51
1:A:239:LEU:O	1:A:242:THR:N	2.42	0.51
1:B:242:THR:O	1:B:245:ILE:HG13	2.10	0.51
1:A:189:SER:CB	1:A:190:THR:HA	2.41	0.51
1:A:147:PRO:CA	1:A:410:THR:CG2	2.84	0.51
1:A:122:ARG:O	1:A:125:ALA:HB3	2.11	0.51
1:B:350:HIS:O	1:B:350:HIS:ND1	2.44	0.51
1:A:140:GLY:O	1:A:143:ALA:N	2.44	0.51
1:A:90:GLN:HG3	1:A:92:ALA:H	1.77	0.50
1:B:105:PRO:C	1:B:107:HIS:H	2.14	0.50
1:A:19:ARG:CB	1:A:47:VAL:HA	2.41	0.50
1:A:61:TYR:HB3	1:A:333:GLU:OE2	2.11	0.50
1:A:24:GLN:HB3	1:A:25:ARG:CA	2.42	0.50
1:A:261:SER:HB3	1:A:289:LEU:HD13	1.93	0.50
1:A:300:PRO:O	1:A:322:ILE:HG23	2.11	0.50
1:B:159:SER:OG	1:B:255:THR:HG22	2.10	0.50
1:B:179:ASP:O	1:B:183:ILE:CG1	2.48	0.50
1:B:250:GLY:HA3	2:B:501:HEM:C2C	2.47	0.50
1:B:100:ILE:HD11	2:B:501:HEM:HAD2	1.94	0.50
1:B:381:VAL:O	1:B:381:VAL:HG13	2.09	0.50
1:B:102:THR:HB	1:B:106:GLU:HG2	1.94	0.50
1:B:223:LYS:HA	1:B:227:ASP:HB2	1.92	0.50
1:B:230:VAL:CG1	1:B:234:VAL:HG23	2.17	0.50
1:B:300:PRO:HG3	1:B:325:LEU:CD1	2.42	0.50
1:A:238:GLN:HA	1:A:241:SER:OG	2.11	0.50
1:B:304:ALA:CB	1:B:315:VAL:CG1	2.89	0.50
1:B:72:ARG:HB2	1:B:308:ILE:HG23	1.93	0.50
1:B:229:LEU:HD23	1:B:234:VAL:CG1	2.39	0.50
1:A:131:GLN:NE2	1:A:135:ASP:OD1	2.44	0.49
1:A:26:GLY:O	1:A:27:CYS:CB	2.59	0.49
1:A:370:LEU:O	1:A:374:LEU:HD12	2.11	0.49
1:B:118:PHE:HE2	2:B:501:HEM:CBC	2.23	0.49
1:B:353:PHE:CE1	2:B:501:HEM:C3B	2.96	0.49
1:A:94:ALA:O	1:A:95:ARG:C	2.50	0.49
1:A:354:GLY:C	1:A:359:GLN:HB2	2.33	0.49
1:A:62:ASP:C	1:B:112:ARG:HH22	2.15	0.49
1:B:221:ILE:CD1	1:B:243:LEU:HD21	2.42	0.49
1:B:118:PHE:HZ	1:B:166:LEU:HD21	1.76	0.49
1:A:355:TYR:HE1	1:B:355:TYR:HE1	1.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:PHE:CD2	1:A:21:PHE:O	2.66	0.49
1:A:200:GLY:O	1:A:203:GLY:N	2.46	0.49
1:B:107:HIS:ND1	1:B:108:THR:N	2.60	0.49
1:A:288:GLU:OE2	1:A:345:ARG:NH2	2.45	0.49
1:B:201:LEU:O	1:B:201:LEU:HD23	2.12	0.49
1:A:102:THR:HB	1:A:107:HIS:CB	2.43	0.49
1:A:293:LEU:O	1:A:294:SER:C	2.50	0.49
1:B:178:ARG:O	1:B:182:ARG:HB2	2.11	0.49
1:A:82:PHE:C	1:A:83:PRO:O	2.50	0.49
1:B:105:PRO:O	1:B:106:GLU:C	2.50	0.49
1:B:198:LEU:O	1:B:201:LEU:N	2.40	0.49
1:A:24:GLN:CB	1:A:25:ARG:HA	2.41	0.49
1:A:88:GLY:O	1:A:89:GLU:HG2	2.13	0.49
1:B:212:ARG:HH12	1:B:217:ARG:HH22	1.50	0.49
1:A:118:PHE:O	1:A:119:THR:C	2.49	0.49
1:A:289:LEU:O	1:A:290:LEU:C	2.51	0.49
1:B:102:THR:CG2	1:B:103:ASP:H	2.25	0.49
1:A:19:ARG:CD	1:A:19:ARG:N	2.69	0.49
1:A:162:VAL:HG21	1:A:369:GLU:OE1	2.12	0.49
1:B:194:VAL:HG12	1:B:195:SER:N	2.28	0.49
1:A:253:THR:O	1:A:256:SER:HB3	2.13	0.49
1:A:347:ASP:OD2	1:B:120:VAL:HG11	2.13	0.49
1:B:72:ARG:NE	1:B:307:ASP:O	2.41	0.49
1:B:73:VAL:O	1:B:73:VAL:CG1	2.60	0.49
1:B:353:PHE:HE1	2:B:501:HEM:C2B	2.29	0.48
1:B:72:ARG:HD2	1:B:306:GLU:HB3	1.94	0.48
1:B:49:LEU:O	1:B:52:ARG:N	2.46	0.48
1:A:281:LEU:O	1:A:284:ALA:N	2.47	0.48
1:B:356:GLY:C	1:B:358:HIS:N	2.65	0.48
1:B:118:PHE:CE2	2:B:501:HEM:CBC	2.96	0.48
1:A:240:LEU:O	1:A:241:SER:C	2.49	0.48
1:B:120:VAL:HG22	1:B:364:HIS:CE1	2.48	0.48
1:A:235:THR:CG2	1:A:238:GLN:CD	2.79	0.48
1:A:291:ARG:NH2	1:A:338:PRO:O	2.45	0.48
1:B:224:LEU:HD11	1:B:243:LEU:HD11	1.96	0.48
1:B:229:LEU:O	1:B:231:PRO:HB2	2.13	0.48
1:B:361:VAL:HG21	2:B:501:HEM:HMD2	1.94	0.48
1:A:172:HIS:C	1:A:174:LEU:H	2.16	0.48
1:A:278:ASP:OD1	1:A:278:ASP:O	2.31	0.48
1:A:301:LEU:HG	1:A:322:ILE:HG13	1.94	0.48
1:B:23:ILE:HD12	1:B:32:PRO:CG	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:300:PRO:O	1:B:322:ILE:CG2	2.60	0.48
1:B:341:VAL:CG1	1:B:343:PHE:HE1	2.27	0.48
1:A:361:VAL:HG13	2:A:501:HEM:HBD2	1.96	0.48
1:A:57:VAL:HG23	1:A:322:ILE:HD12	1.96	0.48
1:A:381:VAL:N	1:A:382:PRO:CD	2.76	0.48
1:B:80:PRO:CA	1:B:303:VAL:HG21	2.42	0.48
1:A:120:VAL:O	1:A:121:ARG:C	2.51	0.48
1:A:301:LEU:HA	1:A:322:ILE:HG23	1.96	0.48
1:A:18:PRO:CA	1:A:19:ARG:HH11	2.27	0.48
1:A:43:PRO:CD	1:A:44:VAL:N	2.72	0.47
1:B:353:PHE:CD1	2:B:501:HEM:C2B	3.02	0.47
1:B:166:LEU:HD22	2:B:501:HEM:HBC1	1.95	0.47
1:B:167:LEU:HA	1:B:220:LEU:HB3	1.96	0.47
1:B:147:PRO:O	1:B:147:PRO:HG2	2.14	0.47
1:A:257:MET:HG2	1:A:295:VAL:CG2	2.45	0.47
1:B:238:GLN:O	1:B:239:LEU:C	2.48	0.47
1:B:304:ALA:CB	1:B:315:VAL:HG12	2.43	0.47
1:B:326:ALA:O	1:B:327:GLY:C	2.52	0.47
1:A:62:ASP:OD1	1:A:65:ARG:HD2	2.14	0.47
1:A:282:MET:HA	1:A:285:ALA:CB	2.34	0.47
1:B:99:PHE:HE2	1:B:110:TYR:HB2	1.79	0.47
1:A:184:SER:OG	1:A:198:LEU:HD12	2.15	0.47
1:A:164:CYS:SG	1:A:169:ILE:CB	2.98	0.47
1:B:214:GLU:C	1:B:216:PRO:HD3	2.33	0.47
1:B:128:PRO:HB2	1:B:129:ALA:H	1.38	0.47
1:B:331:ASP:HA	1:B:332:PRO:HD2	1.51	0.47
1:B:36:ALA:O	1:B:40:THR:HG23	2.15	0.47
1:A:292:VAL:HG12	1:A:293:LEU:N	2.29	0.47
1:A:356:GLY:C	1:A:358:HIS:H	2.17	0.47
1:A:115:LEU:N	1:A:116:PRO:HD2	2.29	0.47
1:A:23:ILE:O	1:A:397:HIS:HE1	1.96	0.47
1:A:370:LEU:CD2	1:A:374:LEU:CD1	2.92	0.47
1:B:353:PHE:CZ	1:B:363:GLN:HA	2.49	0.47
1:B:278:ASP:HB3	1:B:281:LEU:HB2	1.97	0.47
1:A:64:VAL:HG21	1:A:328:ALA:HB2	1.97	0.47
1:A:156:ASN:O	1:A:159:SER:HB2	2.15	0.47
1:A:25:ARG:HE	1:A:402:PHE:HE2	1.46	0.47
1:A:385:ARG:C	1:A:409:VAL:HG12	2.36	0.47
1:A:21:PHE:C	1:A:21:PHE:CD2	2.89	0.47
1:B:383:THR:HG23	1:B:384:LEU:H	1.80	0.47
1:B:261:SER:HA	1:B:289:LEU:HD22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:372:VAL:O	1:B:376:THR:OG1	2.32	0.47
1:A:43:PRO:HD2	1:A:44:VAL:H	1.78	0.47
1:A:72:ARG:NH1	1:B:104:ALA:CB	2.78	0.47
1:A:21:PHE:HA	1:A:22:PRO:HD3	1.53	0.47
1:B:44:VAL:HG21	1:B:310:LEU:HD23	1.95	0.47
1:B:77:ILE:H	1:B:101:ARG:HE	1.63	0.46
1:B:21:PHE:CD2	1:B:50:PRO:HG2	2.50	0.46
1:A:194:VAL:O	1:A:197:ALA:N	2.48	0.46
1:A:383:THR:HG1	1:A:385:ARG:NH2	2.09	0.46
1:A:122:ARG:HE	1:A:122:ARG:HB2	1.66	0.46
1:A:225:VAL:HG23	1:A:226:THR:N	2.29	0.46
1:A:181:THR:CG2	1:A:251:ARG:CD	2.79	0.46
1:B:256:SER:OG	1:B:402:PHE:O	2.27	0.46
1:B:297:ASP:OD1	1:B:326:ALA:CB	2.64	0.46
1:B:359:GLN:C	1:B:359:GLN:OE1	2.53	0.46
1:A:211:GLU:HA	1:A:214:GLU:OE1	2.15	0.46
1:B:61:TYR:OH	1:B:349:HIS:HB2	2.15	0.46
1:A:301:LEU:HD23	1:A:302:ARG:O	2.15	0.46
1:A:179:ASP:O	1:A:183:ILE:CG1	2.48	0.46
1:A:62:ASP:HB2	1:A:333:GLU:OE1	2.16	0.46
1:B:304:ALA:HB2	1:B:315:VAL:HG11	1.94	0.46
1:B:278:ASP:C	1:B:280:ASP:N	2.68	0.46
1:A:370:LEU:HD21	1:A:374:LEU:HD11	1.98	0.46
1:A:42:ASP:O	1:A:45:ALA:N	2.49	0.46
1:A:19:ARG:HG2	1:A:48:THR:N	2.27	0.46
1:B:138:LEU:O	1:B:139:ASP:C	2.54	0.46
1:A:221:ILE:O	1:A:225:VAL:CG1	2.42	0.46
1:A:381:VAL:O	1:A:381:VAL:HG22	2.14	0.46
1:A:301:LEU:HD23	1:A:302:ARG:N	2.31	0.46
1:A:138:LEU:HA	1:A:141:MET:CG	2.46	0.46
1:B:375:GLU:OE2	1:B:379:ARG:NE	2.46	0.46
1:A:46:ARG:HG2	1:A:56:TRP:CZ2	2.50	0.46
1:B:102:THR:HG22	1:B:103:ASP:N	2.30	0.46
1:B:154:TYR:O	1:B:158:VAL:HG12	2.16	0.46
1:B:118:PHE:CD2	1:B:361:VAL:O	2.69	0.46
1:B:223:LYS:O	1:B:224:LEU:C	2.54	0.46
1:A:123:VAL:HG11	1:A:364:HIS:HB3	1.97	0.46
1:A:229:LEU:O	1:A:234:VAL:CB	2.63	0.45
1:A:257:MET:HB3	1:A:370:LEU:CD1	2.46	0.45
1:A:283:PRO:O	1:A:286:VAL:HG12	2.15	0.45
1:B:99:PHE:HZ	1:B:111:ARG:CA	2.29	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:158:VAL:HG13	1:B:258:ILE:CD1	2.45	0.45
1:B:383:THR:CG2	1:B:384:LEU:H	2.27	0.45
1:A:115:LEU:HD21	1:A:361:VAL:HB	1.98	0.45
1:A:261:SER:HB2	1:A:374:LEU:HD21	1.96	0.45
1:B:97:ARG:N	1:B:98:PRO:CD	2.76	0.45
1:A:177:PHE:C	1:A:179:ASP:N	2.70	0.45
1:A:377:LEU:HB3	1:A:378:LEU:HD23	1.99	0.45
1:A:378:LEU:HD23	1:A:378:LEU:N	2.32	0.45
1:A:121:ARG:HA	1:A:124:ARG:HE	1.81	0.45
1:A:117:ALA:HB1	1:A:220:LEU:HD13	1.97	0.45
1:A:67:LEU:HD12	1:A:67:LEU:O	2.16	0.45
1:B:315:VAL:HA	1:B:316:PRO:HD3	1.69	0.45
1:A:290:LEU:HD13	1:A:353:PHE:CE2	2.51	0.45
1:A:370:LEU:CD2	1:A:374:LEU:HD11	2.46	0.45
1:B:333:GLU:HG3	1:B:334:GLN:N	2.31	0.45
1:B:245:ILE:O	1:B:246:THR:C	2.55	0.45
1:B:159:SER:O	1:B:162:VAL:HG12	2.17	0.45
1:A:141:MET:HA	1:A:141:MET:CE	2.46	0.45
1:B:275:LEU:HD23	1:B:281:LEU:HB3	1.98	0.45
1:A:99:PHE:CD1	1:A:99:PHE:C	2.89	0.45
1:A:377:LEU:HA	1:A:377:LEU:HD22	1.71	0.45
1:B:230:VAL:CG2	1:B:230:VAL:O	2.65	0.45
1:B:46:ARG:HG3	1:B:56:TRP:CD2	2.52	0.45
1:A:177:PHE:C	1:A:179:ASP:H	2.19	0.45
1:A:65:ARG:NH1	1:A:355:TYR:CD2	2.85	0.45
1:B:38:LEU:O	1:B:42:ASP:C	2.55	0.45
1:B:271:LEU:O	1:B:274:GLU:N	2.49	0.45
1:B:147:PRO:O	1:B:147:PRO:CG	2.64	0.45
1:B:75:ALA:C	1:B:101:ARG:O	2.55	0.45
1:B:377:LEU:HD13	1:B:378:LEU:HG	1.99	0.45
1:B:270:GLU:O	1:B:274:GLU:N	2.49	0.45
1:A:340:ARG:C	1:A:342:ASP:H	2.20	0.45
1:B:149:ASP:CB	1:B:408:MET:CG	2.95	0.45
1:B:319:ASP:N	1:B:319:ASP:OD1	2.50	0.45
1:A:205:LEU:C	1:A:209:VAL:HG23	2.37	0.45
1:B:194:VAL:HG13	1:B:195:SER:CA	2.47	0.45
1:B:44:VAL:HG22	1:B:310:LEU:HD23	1.99	0.45
1:A:26:GLY:O	1:A:28:PRO:CD	2.57	0.45
1:B:149:ASP:CB	1:B:408:MET:HG2	2.47	0.45
1:A:150:LEU:HD13	1:A:154:TYR:HB3	2.00	0.45
1:A:279:PRO:O	1:A:282:MET:CE	2.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:ASP:HA	1:A:71:PRO:HD2	1.43	0.44
1:B:259:ALA:CB	1:B:404:LEU:HD23	2.44	0.44
1:A:151:VAL:CA	1:A:155:ALA:HB3	2.41	0.44
1:A:137:ILE:O	1:A:137:ILE:HD12	2.17	0.44
1:A:159:SER:O	1:A:163:ILE:HG13	2.17	0.44
1:A:204:LEU:O	1:A:208:LEU:HD13	2.17	0.44
1:A:235:THR:HG1	1:A:238:GLN:HG3	1.82	0.44
1:B:104:ALA:HA	1:B:105:PRO:HA	1.52	0.44
1:B:171:ARG:CA	1:B:174:LEU:HB2	2.47	0.44
1:A:181:THR:HG22	1:A:251:ARG:CD	2.43	0.44
1:B:65:ARG:HG3	1:B:355:TYR:CE2	2.52	0.44
1:A:153:ALA:O	1:A:157:ALA:HB2	2.17	0.44
1:B:261:SER:O	1:B:264:LEU:HB3	2.17	0.44
1:B:393:VAL:CG2	1:B:394:VAL:N	2.81	0.44
1:A:376:THR:O	1:A:377:LEU:C	2.55	0.44
1:B:101:ARG:HG3	1:B:102:THR:N	2.32	0.44
1:A:385:ARG:N	1:A:410:THR:O	2.49	0.44
1:A:142:LEU:HA	1:A:411:TRP:CH2	2.52	0.44
1:B:403:GLY:O	1:B:404:LEU:HD13	2.17	0.44
1:A:115:LEU:O	1:A:118:PHE:N	2.47	0.44
1:A:260:LEU:HD13	1:A:293:LEU:HD22	1.99	0.44
1:A:127:ARG:HB3	1:A:128:PRO:CD	2.23	0.44
1:A:133:ARG:NE	1:A:165:GLU:HB2	2.33	0.44
1:A:229:LEU:HG	1:A:234:VAL:CB	2.47	0.44
1:A:236:THR:HG23	1:A:236:THR:H	1.40	0.44
1:A:194:VAL:O	1:A:196:GLU:N	2.51	0.44
1:B:300:PRO:HG3	1:B:325:LEU:HD13	1.99	0.44
1:A:225:VAL:O	1:A:229:LEU:HB3	2.18	0.44
1:A:354:GLY:H	1:A:360:CYS:H	1.65	0.44
1:A:358:HIS:O	2:A:501:HEM:HBD1	2.18	0.44
1:B:149:ASP:OD2	1:B:150:LEU:N	2.51	0.44
1:A:190:THR:O	1:A:193:GLN:N	2.50	0.44
1:B:114:LEU:HD22	1:B:114:LEU:HA	1.70	0.44
1:B:360:CYS:HB2	2:B:501:HEM:C4A	2.51	0.44
1:A:19:ARG:HG3	1:A:47:VAL:CA	2.31	0.44
1:B:150:LEU:HB2	1:B:154:TYR:CB	2.48	0.44
1:A:212:ARG:O	1:A:216:PRO:HB3	2.18	0.44
1:B:116:PRO:CB	3:B:619:HOH:O	2.66	0.43
1:A:99:PHE:HA	1:A:102:THR:OG1	2.18	0.43
1:A:129:ALA:HB1	1:A:165:GLU:OE2	2.18	0.43
1:A:72:ARG:HH11	1:B:104:ALA:HB3	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:114:LEU:HD12	1:B:361:VAL:HG21	1.99	0.43
1:B:230:VAL:CB	1:B:231:PRO:O	2.65	0.43
1:B:217:ARG:CZ	1:B:217:ARG:HB2	2.47	0.43
1:B:303:VAL:HG13	1:B:318:ASP:HA	2.01	0.43
1:B:39:ARG:HG3	1:B:60:ARG:HA	2.00	0.43
1:B:235:THR:O	1:B:238:GLN:HB3	2.17	0.43
1:A:175:GLU:O	1:A:176:PHE:C	2.57	0.43
1:A:112:ARG:C	1:A:114:LEU:H	2.20	0.43
1:B:193:GLN:H	1:B:193:GLN:HG3	1.36	0.43
1:A:83:PRO:HB2	1:A:89:GLU:O	2.19	0.43
1:A:19:ARG:HB2	1:A:47:VAL:HA	2.01	0.43
1:A:115:LEU:O	1:A:116:PRO:C	2.57	0.43
1:A:371:GLU:O	1:A:372:VAL:C	2.57	0.43
1:A:301:LEU:HD21	1:A:320:GLY:CA	2.48	0.43
1:B:72:ARG:HB2	1:B:308:ILE:CG2	2.49	0.43
1:A:72:ARG:CB	3:A:602:HOH:O	2.67	0.43
1:B:245:ILE:HG13	1:B:245:ILE:H	1.59	0.43
1:A:360:CYS:HB2	2:A:501:HEM:C4A	2.54	0.43
2:B:501:HEM:CBA	2:B:501:HEM:CMA	2.97	0.43
1:B:46:ARG:HG2	1:B:55:ALA:O	2.18	0.43
1:B:63:ASP:O	1:B:66:GLU:HB2	2.18	0.43
1:B:176:PHE:O	1:B:180:VAL:HG13	2.19	0.43
1:B:64:VAL:HG13	1:B:323:ALA:HB1	1.99	0.43
1:B:138:LEU:CD2	1:B:141:MET:HB2	2.44	0.43
1:A:181:THR:HG23	1:A:251:ARG:HH11	1.84	0.43
1:B:211:GLU:C	1:B:213:ARG:N	2.72	0.43
1:A:25:ARG:O	1:A:26:GLY:C	2.56	0.42
1:A:25:ARG:NH1	1:A:27:CYS:O	2.51	0.42
1:A:377:LEU:HB3	1:A:378:LEU:CD2	2.48	0.42
1:B:35:TYR:HA	1:B:38:LEU:HD13	2.01	0.42
1:B:59:THR:HG23	1:B:324:LEU:HD12	2.00	0.42
1:A:249:ALA:HB3	2:A:501:HEM:HBC2	2.01	0.42
1:A:281:LEU:HA	1:A:281:LEU:HD23	1.76	0.42
1:A:53:ARG:HB2	1:A:53:ARG:HE	1.63	0.42
1:B:149:ASP:HB2	1:B:408:MET:HG2	1.99	0.42
1:B:302:ARG:HH22	1:B:358:HIS:CB	2.32	0.42
1:A:222:SER:O	1:A:223:LYS:C	2.57	0.42
1:A:282:MET:CA	1:A:285:ALA:HB3	2.37	0.42
1:A:356:GLY:O	1:A:358:HIS:N	2.52	0.42
1:B:346:THR:C	1:B:348:ASN:N	2.69	0.42
1:B:116:PRO:HB2	3:B:619:HOH:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:PHE:HE1	1:A:50:PRO:CG	2.31	0.42
1:A:149:ASP:O	1:A:153:ALA:HB3	2.19	0.42
1:A:315:VAL:HA	1:A:316:PRO:HD3	1.88	0.42
1:B:150:LEU:HD23	1:B:409:VAL:CG2	2.50	0.42
1:A:205:LEU:HA	1:A:205:LEU:HD23	1.91	0.42
1:B:174:LEU:HG	1:B:178:ARG:HD3	2.01	0.42
1:B:361:VAL:HG22	2:B:501:HEM:C2D	2.54	0.42
1:B:304:ALA:HB1	1:B:315:VAL:HG12	2.02	0.42
1:B:262:THR:O	1:B:263:LEU:C	2.55	0.42
1:B:269:PRO:C	1:B:272:PRO:HD2	2.39	0.42
1:B:179:ASP:O	1:B:183:ILE:N	2.49	0.42
1:B:212:ARG:NH1	1:B:217:ARG:HH21	2.06	0.42
1:B:56:TRP:NE1	1:B:319:ASP:OD2	2.52	0.42
1:A:49:LEU:O	1:A:51:THR:N	2.52	0.42
1:B:113:MET:SD	1:B:229:LEU:HD21	2.60	0.42
1:B:357:VAL:O	1:B:357:VAL:HG13	2.16	0.42
1:B:162:VAL:HG11	1:B:369:GLU:CG	2.49	0.42
1:B:46:ARG:HG3	1:B:56:TRP:CE2	2.55	0.42
1:B:275:LEU:C	1:B:278:ASP:H	2.22	0.42
1:B:282:MET:N	1:B:283:PRO:CD	2.83	0.42
1:A:296:ALA:HB2	2:A:501:HEM:HMB2	2.01	0.42
1:B:107:HIS:CE1	1:B:108:THR:HA	2.55	0.42
1:B:221:ILE:HA	1:B:224:LEU:HD12	2.02	0.42
1:A:70:ASP:O	1:A:73:VAL:HG23	2.19	0.42
1:B:377:LEU:HD22	1:B:377:LEU:O	2.20	0.42
1:B:175:GLU:O	1:B:179:ASP:N	2.52	0.42
1:A:147:PRO:CB	1:A:410:THR:CG2	2.98	0.42
1:B:46:ARG:HB2	1:B:56:TRP:CZ3	2.55	0.42
1:A:110:TYR:O	1:A:111:ARG:C	2.58	0.42
1:A:365:LEU:HD12	1:A:365:LEU:HA	1.34	0.42
1:A:164:CYS:SG	1:A:169:ILE:HD12	2.59	0.42
1:A:112:ARG:C	1:A:114:LEU:N	2.73	0.42
1:A:356:GLY:C	1:A:358:HIS:N	2.72	0.41
1:A:18:PRO:CG	1:A:19:ARG:NH1	2.83	0.41
1:B:138:LEU:CD1	1:B:377:LEU:HD23	2.50	0.41
1:A:335:PHE:CG	1:A:345:ARG:HD3	2.55	0.41
1:A:331:ASP:O	1:A:334:GLN:HB3	2.20	0.41
1:A:395:VAL:HA	1:A:404:LEU:HA	2.02	0.41
1:A:279:PRO:O	1:A:282:MET:HE2	2.19	0.41
1:B:162:VAL:HG11	1:B:369:GLU:HG2	2.02	0.41
1:A:299:ILE:HB	1:A:300:PRO:CD	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:ARG:HB2	3:A:602:HOH:O	2.20	0.41
1:B:107:HIS:NE2	1:B:357:VAL:CG1	2.83	0.41
1:A:154:TYR:O	1:A:157:ALA:HB3	2.19	0.41
1:A:205:LEU:O	1:A:209:VAL:N	2.39	0.41
1:A:28:PRO:HA	1:A:29:PHE:HA	1.68	0.41
1:B:118:PHE:HD2	1:B:362:GLY:HA2	1.85	0.41
1:A:219:ASP:H	1:A:222:SER:HB2	1.85	0.41
1:B:39:ARG:HG3	1:B:60:ARG:CA	2.50	0.41
1:A:379:ARG:O	1:A:382:PRO:HG3	2.21	0.41
1:A:96:PHE:CD1	1:A:97:ARG:CZ	3.00	0.41
1:A:202:PHE:HD2	1:A:240:LEU:HD23	1.86	0.41
1:A:27:CYS:C	1:A:29:PHE:O	2.58	0.41
1:A:376:THR:HA	1:A:379:ARG:HB3	2.01	0.41
1:B:385:ARG:HG2	1:B:385:ARG:H	1.67	0.41
1:B:171:ARG:HG3	1:B:171:ARG:H	1.71	0.41
1:B:115:LEU:N	1:B:116:PRO:CD	2.84	0.41
1:B:403:GLY:C	1:B:404:LEU:HD13	2.41	0.41
1:A:112:ARG:HH12	1:B:66:GLU:HG3	1.86	0.41
1:B:286:VAL:O	1:B:286:VAL:HG12	2.19	0.41
1:A:35:TYR:CE1	1:A:324:LEU:HD13	2.56	0.41
1:A:301:LEU:HD21	1:A:321:VAL:N	2.35	0.41
1:B:20:ASP:O	1:B:22:PRO:HD3	2.20	0.41
1:A:66:GLU:HB3	1:B:112:ARG:NH1	2.36	0.41
1:A:147:PRO:HB3	1:A:410:THR:HG23	2.01	0.41
1:A:149:ASP:OD2	1:A:152:SER:CB	2.59	0.41
1:B:282:MET:N	1:B:283:PRO:HD3	2.36	0.41
1:A:351:VAL:C	1:A:353:PHE:N	2.67	0.41
1:A:46:ARG:HG2	1:A:56:TRP:CE2	2.56	0.41
1:B:99:PHE:CE2	1:B:110:TYR:HB2	2.56	0.41
1:B:406:GLU:O	1:B:406:GLU:HG3	2.21	0.41
1:A:198:LEU:N	1:A:198:LEU:HD12	2.36	0.41
1:A:225:VAL:CG2	1:A:226:THR:N	2.83	0.41
1:A:29:PHE:CE2	1:A:264:LEU:HA	2.55	0.41
1:A:72:ARG:HH12	1:B:104:ALA:CB	2.33	0.41
1:B:192:GLU:C	1:B:194:VAL:H	2.23	0.41
1:A:174:LEU:O	1:A:178:ARG:N	2.39	0.41
1:B:395:VAL:CG2	1:B:396:LYS:N	2.83	0.41
1:B:49:LEU:HG	1:B:49:LEU:O	2.20	0.41
1:B:233:ASN:O	1:B:234:VAL:HG13	2.21	0.41
1:B:302:ARG:NH2	1:B:358:HIS:HB2	2.36	0.41
1:A:117:ALA:CB	1:A:220:LEU:HD13	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:387:ALA:H	1:A:408:MET:C	2.22	0.40
1:A:162:VAL:HG11	1:A:369:GLU:CG	2.38	0.40
1:B:177:PHE:HE2	1:B:247:ILE:HD13	1.86	0.40
1:B:368:LEU:HD22	1:B:368:LEU:HA	1.83	0.40
1:B:113:MET:CG	1:B:229:LEU:CD1	2.99	0.40
1:A:23:ILE:CB	1:A:24:GLN:O	2.69	0.40
1:A:24:GLN:CG	1:A:33:ALA:CA	2.95	0.40
1:A:296:ALA:HB2	2:A:501:HEM:CMB	2.51	0.40
1:A:375:GLU:HB3	1:A:376:THR:H	1.61	0.40
1:B:378:LEU:HA	1:B:378:LEU:HD23	1.94	0.40
1:B:81:GLY:O	1:B:82:PHE:CB	2.69	0.40
1:A:180:VAL:HG21	1:A:201:LEU:HD23	2.02	0.40
1:B:302:ARG:HH22	1:B:358:HIS:HB3	1.87	0.40
1:A:122:ARG:HG3	1:A:123:VAL:N	2.35	0.40
1:B:367:ARG:HB2	1:B:367:ARG:HH11	1.87	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	A	386/417 (93%)	261 (68%)	96 (25%)	29 (8%)	<b>1</b>	<b>3</b>
1	B	360/417 (86%)	232 (64%)	111 (31%)	17 (5%)	<b>3</b>	<b>11</b>
All	All	746/834 (89%)	493 (66%)	207 (28%)	46 (6%)	<b>2</b>	<b>5</b>

All (46) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	27	CYS
1	A	28	PRO
1	A	42	ASP

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Mol	Chain	Res	Type
1	A	50	PRO
1	A	76	ASP
1	A	97	ARG
1	A	119	THR
1	A	171	ARG
1	A	300	PRO
1	B	50	PRO
1	B	80	PRO
1	B	128	PRO
1	B	231	PRO
1	B	347	ASP
1	B	382	PRO
1	A	31	ALA
1	A	80	PRO
1	A	146	GLY
1	A	372	VAL
1	B	32	PRO
1	B	409	VAL
1	A	189	SER
1	A	356	GLY
1	B	194	VAL
1	A	116	PRO
1	B	22	PRO
1	B	31	ALA
1	B	332	PRO
1	B	351	VAL
1	A	269	PRO
1	A	341	VAL
1	A	357	VAL
1	A	388	GLY
1	B	147	PRO
1	A	170	PRO
1	A	312	GLY
1	A	351	VAL
1	B	215	GLU
1	A	82	PHE
1	A	283	PRO
1	B	206	GLY
1	A	73	VAL
1	A	77	ILE
1	A	299	ILE
1	B	283	PRO

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Mol	Chain	Res	Type
1	A	231	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	322/347 (93%)	209 (65%)	113 (35%)	0	0
1	B	306/347 (88%)	199 (65%)	107 (35%)	0	0
All	All	628/694 (90%)	408 (65%)	220 (35%)	0	0

All (220) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	ARG
1	A	20	ASP
1	A	24	GLN
1	A	28	PRO
1	A	29	PHE
1	A	38	LEU
1	A	39	ARG
1	A	42	ASP
1	A	43	PRO
1	A	46	ARG
1	A	48	THR
1	A	51	THR
1	A	52	ARG
1	A	65	ARG
1	A	67	LEU
1	A	68	LEU
1	A	69	SER
1	A	72	ARG
1	A	73	VAL
1	A	77	ILE
1	A	78	ARG
1	A	95	ARG

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Mol	Chain	Res	Type
1	A	97	ARG
1	A	102	THR
1	A	107	HIS
1	A	109	ARG
1	A	111	ARG
1	A	112	ARG
1	A	113	MET
1	A	114	LEU
1	A	118	PHE
1	A	121	ARG
1	A	122	ARG
1	A	127	ARG
1	A	128	PRO
1	A	137	ILE
1	A	142	LEU
1	A	149	ASP
1	A	150	LEU
1	A	152	SER
1	A	158	VAL
1	A	159	SER
1	A	163	ILE
1	A	164	CYS
1	A	171	ARG
1	A	173	ASP
1	A	176	PHE
1	A	178	ARG
1	A	183	ILE
1	A	190	THR
1	A	196	GLU
1	A	201	LEU
1	A	204	LEU
1	A	211	GLU
1	A	213	ARG
1	A	217	ARG
1	A	224	LEU
1	A	226	THR
1	A	227	ASP
1	A	235	THR
1	A	237	GLU
1	A	241	SER
1	A	243	LEU
1	A	247	ILE

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Mol	Chain	Res	Type
1	A	252	GLU
1	A	258	ILE
1	A	260	LEU
1	A	264	LEU
1	A	266	LEU
1	A	267	ASP
1	A	270	GLU
1	A	271	LEU
1	A	277	LYS
1	A	278	ASP
1	A	282	MET
1	A	286	VAL
1	A	292	VAL
1	A	294	SER
1	A	295	VAL
1	A	299	ILE
1	A	300	PRO
1	A	302	ARG
1	A	306	GLU
1	A	308	ILE
1	A	322	ILE
1	A	329	ASN
1	A	333	GLU
1	A	334	GLN
1	A	339	GLU
1	A	341	VAL
1	A	342	ASP
1	A	346	THR
1	A	347	ASP
1	A	348	ASN
1	A	351	VAL
1	A	357	VAL
1	A	359	GLN
1	A	363	GLN
1	A	369	GLU
1	A	370	LEU
1	A	371	GLU
1	A	372	VAL
1	A	377	LEU
1	A	378	LEU
1	A	381	VAL
1	A	383	THR

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Mol	Chain	Res	Type
1	A	384	LEU
1	A	394	VAL
1	A	395	VAL
1	A	399	SER
1	A	404	LEU
1	A	410	THR
1	A	411	TRP
1	B	23	ILE
1	B	29	PHE
1	B	46	ARG
1	B	47	VAL
1	B	49	LEU
1	B	50	PRO
1	B	53	ARG
1	B	59	THR
1	B	68	LEU
1	B	73	VAL
1	B	74	SER
1	B	79	ARG
1	B	97	ARG
1	B	99	PHE
1	B	101	ARG
1	B	103	ASP
1	B	107	HIS
1	B	109	ARG
1	B	113	MET
1	B	114	LEU
1	B	120	VAL
1	B	121	ARG
1	B	122	ARG
1	B	123	VAL
1	B	124	ARG
1	B	138	LEU
1	B	142	LEU
1	B	147	PRO
1	B	148	VAL
1	B	149	ASP
1	B	152	SER
1	B	164	CYS
1	B	167	LEU
1	B	171	ARG
1	B	172	HIS

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Mol	Chain	Res	Type
1	B	173	ASP
1	B	176	PHE
1	B	178	ARG
1	B	179	ASP
1	B	187	ARG
1	B	198	LEU
1	B	204	LEU
1	B	217	ARG
1	B	218	ASP
1	B	225	VAL
1	B	227	ASP
1	B	228	HIS
1	B	231	PRO
1	B	233	ASN
1	B	234	VAL
1	B	235	THR
1	B	245	ILE
1	B	246	THR
1	B	247	ILE
1	B	251	ARG
1	B	254	THR
1	B	255	THR
1	B	257	MET
1	B	263	LEU
1	B	267	ASP
1	B	270	GLU
1	B	276	ARG
1	B	278	ASP
1	B	280	ASP
1	B	281	LEU
1	B	290	LEU
1	B	294	SER
1	B	295	VAL
1	B	298	SER
1	B	299	ILE
1	B	303	VAL
1	B	308	ILE
1	B	313	ARG
1	B	314	THR
1	B	319	ASP
1	B	321	VAL
1	B	322	ILE

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Mol	Chain	Res	Type
1	B	333	GLU
1	B	337	ASP
1	B	339	GLU
1	B	340	ARG
1	B	345	ARG
1	B	347	ASP
1	B	351	VAL
1	B	355	TYR
1	B	357	VAL
1	B	359	GLN
1	B	365	LEU
1	B	367	ARG
1	B	368	LEU
1	B	371	GLU
1	B	375	GLU
1	B	376	THR
1	B	377	LEU
1	B	382	PRO
1	B	384	LEU
1	B	386	LEU
1	B	391	ASP
1	B	392	GLN
1	B	393	VAL
1	B	394	VAL
1	B	395	VAL
1	B	397	HIS
1	B	398	ASP
1	B	404	LEU
1	B	407	LEU
1	B	409	VAL

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

Mol	Chain	Res	Type
1	A	90	GLN
1	A	233	ASN
1	A	238	GLN
1	A	330	HIS
1	A	334	GLN
1	A	344	HIS
1	A	348	ASN
1	A	364	HIS

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Mol	Chain	Res	Type
1	A	397	HIS
1	B	233	ASN
1	B	330	HIS
1	B	364	HIS
1	B	392	GLN
1	B	397	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules 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	501	1	30,50,50	2.19	8 (26%)	24,82,82	2.31	9 (37%)
2	HEM	B	501	1	30,50,50	2.21	8 (26%)	24,82,82	2.31	9 (37%)

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	501	1	-	0/10/54/54	0/0/8/8
2	HEM	B	501	1	-	0/10/54/54	0/0/8/8

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	HEM	C3B-C4B	-7.24	1.45	1.51
2	A	501	HEM	C3B-C4B	-7.23	1.45	1.51
2	A	501	HEM	C3D-C4D	-5.04	1.45	1.51
2	B	501	HEM	C3D-C4D	-5.03	1.45	1.51
2	B	501	HEM	C2C-C1C	-3.81	1.45	1.52
2	A	501	HEM	C2C-C1C	-3.79	1.45	1.52
2	B	501	HEM	C2D-C1D	-2.06	1.45	1.51
2	A	501	HEM	C2D-C1D	-2.06	1.45	1.51
2	A	501	HEM	C4C-NC	2.14	1.38	1.36
2	A	501	HEM	FE-ND	2.14	2.08	1.97
2	B	501	HEM	FE-ND	2.19	2.09	1.97
2	B	501	HEM	C4C-NC	2.23	1.38	1.36
2	A	501	HEM	C1C-NC	2.24	1.38	1.36
2	B	501	HEM	C1C-NC	2.27	1.38	1.36
2	A	501	HEM	FE-NC	2.79	2.06	1.95
2	B	501	HEM	FE-NC	2.82	2.06	1.95

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	HEM	C3B-CAB-CBB	-2.90	120.01	124.46
2	B	501	HEM	C3C-CAC-CBC	-2.89	120.02	124.46
2	A	501	HEM	C3C-CAC-CBC	-2.89	120.02	124.46
2	A	501	HEM	C3B-CAB-CBB	-2.88	120.04	124.46
2	B	501	HEM	C3B-C4B-CHC	2.15	126.19	123.16
2	A	501	HEM	C3B-C4B-CHC	2.16	126.20	123.16
2	B	501	HEM	C2D-C3D-C4D	2.33	105.45	101.50
2	A	501	HEM	C2D-C3D-C4D	2.33	105.45	101.50
2	B	501	HEM	CMD-C2D-C3D	2.92	127.26	114.35
2	A	501	HEM	CMD-C2D-C3D	2.92	127.29	114.35
2	B	501	HEM	CMB-C2B-C3B	3.76	125.93	116.53
2	A	501	HEM	CMB-C2B-C3B	3.77	125.94	116.53
2	A	501	HEM	CMC-C2C-C3C	3.77	125.94	116.53
2	B	501	HEM	CMC-C2C-C3C	3.78	125.95	116.53
2	A	501	HEM	CAD-C3D-C4D	4.20	127.27	112.47
2	B	501	HEM	CAD-C3D-C4D	4.20	127.27	112.47
2	A	501	HEM	CAD-C3D-C2D	4.89	127.28	113.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	HEM	CAD-C3D-C2D	4.89	127.28	113.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 43 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	HEM	18	0
2	B	501	HEM	25	0

## 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 [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<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	390/417 (93%)	-0.06	6 (1%) 76 74	10, 40, 77, 114	0
1	B	370/417 (88%)	-0.02	9 (2%) 62 57	13, 45, 86, 125	0
All	All	760/834 (91%)	-0.04	15 (1%) 68 64	10, 43, 83, 125	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	172	HIS	4.4
1	A	214	GLU	3.8
1	A	193	GLN	3.6
1	B	23	ILE	3.1
1	B	52	ARG	2.6
1	A	41	ASP	2.6
1	B	193	GLN	2.5
1	B	228	HIS	2.3
1	B	142	LEU	2.2
1	B	143	ALA	2.2
1	B	102	THR	2.2
1	A	335	PHE	2.1
1	B	110	TYR	2.1
1	B	349	HIS	2.0
1	A	18	PRO	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 carbohydrates 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. 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	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	HEM	A	501	43/43	0.90	0.25	1.74	23,31,44,49	0
2	HEM	B	501	43/43	0.92	0.21	0.62	21,28,36,46	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.