



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:32 PM GMT

PDB ID : 3TYW  
Title : Crystal Structure of CYP105N1 from Streptomyces coelicolor A3(2)  
Authors : Zhao, B.; Waterman, M.R.  
Deposited on : 2011-09-26  
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

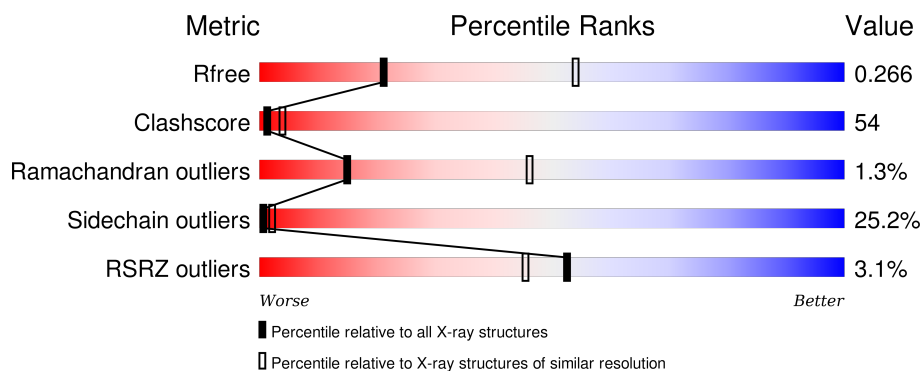
# 1 Overall quality at a glance

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>2%</div> <div>40% 41% 14% 5%</div> </div>
1	B	417	<div> <div>%</div> <div>38% 43% 14% • 5%</div> </div>
1	C	417	<div> <div>5%</div> <div>34% 44% 17% • 5%</div> </div>
1	D	417	<div> <div>4%</div> <div>32% 48% 15% • •</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12633 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	397	Total	C	N	O	S	0	0	0
			3084	1927	567	581	9			
1	B	397	Total	C	N	O	S	0	0	0
			3084	1927	567	581	9			
1	C	398	Total	C	N	O	S	0	0	0
			3094	1933	570	582	9			
1	D	399	Total	C	N	O	S	0	0	0
			3104	1939	573	583	9			

There are 24 discrepancies between the modelled and reference sequences:

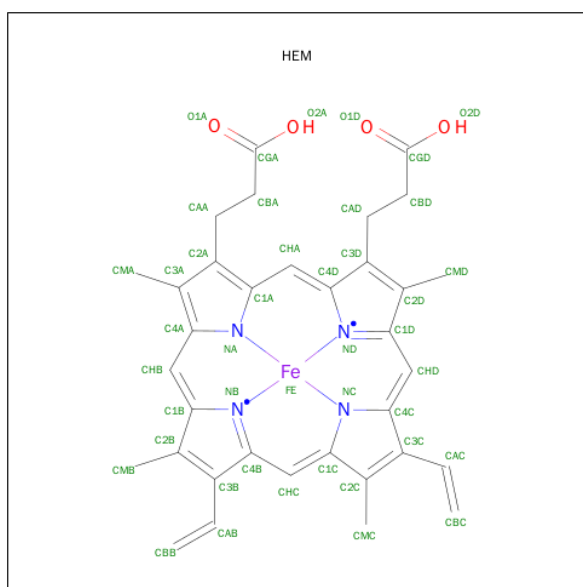
Chain	Residue	Modelled	Actual	Comment	Reference
A	412	HIS	-	EXPRESSION TAG	UNP Q9EWP1
A	413	HIS	-	EXPRESSION TAG	UNP Q9EWP1
A	414	HIS	-	EXPRESSION TAG	UNP Q9EWP1
A	415	HIS	-	EXPRESSION TAG	UNP Q9EWP1
A	416	HIS	-	EXPRESSION TAG	UNP Q9EWP1
A	417	HIS	-	EXPRESSION TAG	UNP Q9EWP1
B	412	HIS	-	EXPRESSION TAG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

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Chain	Residue	Modelled	Actual	Comment	Reference
D	415	HIS	-	EXPRESSION TAG	UNP Q9EWP1
D	416	HIS	-	EXPRESSION TAG	UNP Q9EWP1
D	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 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	22	Total O 22 22	0	0
3	B	23	Total O 23 23	0	0
3	C	30	Total O 30 30	0	0

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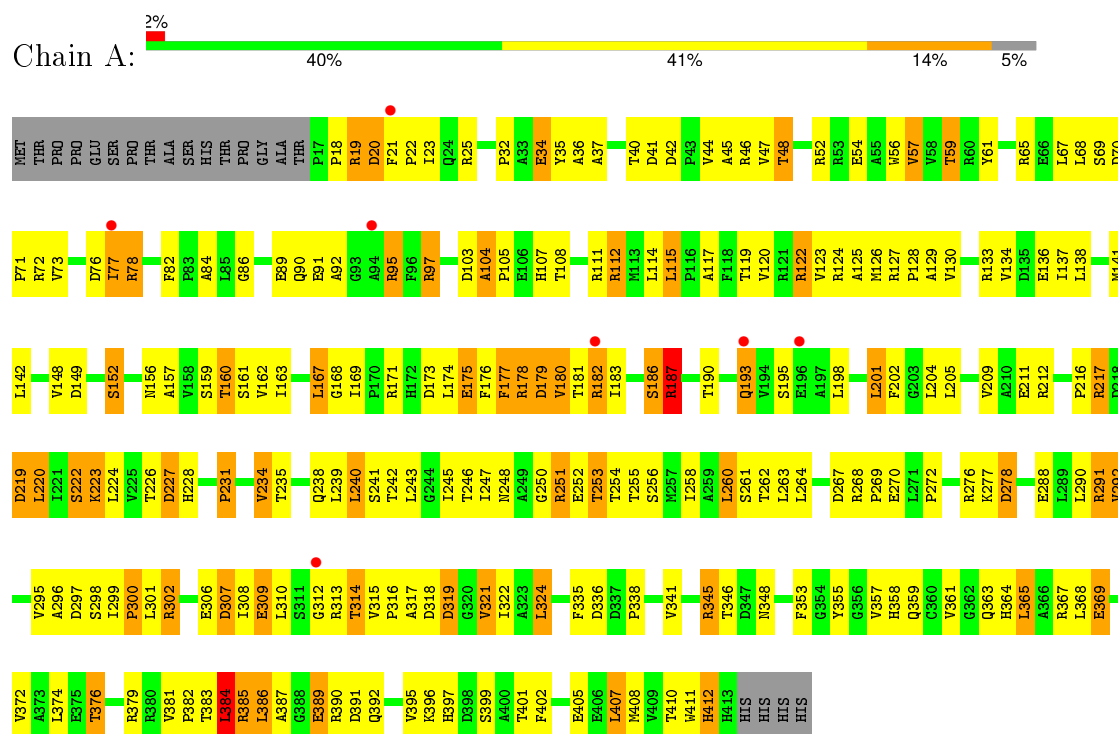
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	20	Total	O	0	0
			20	20		

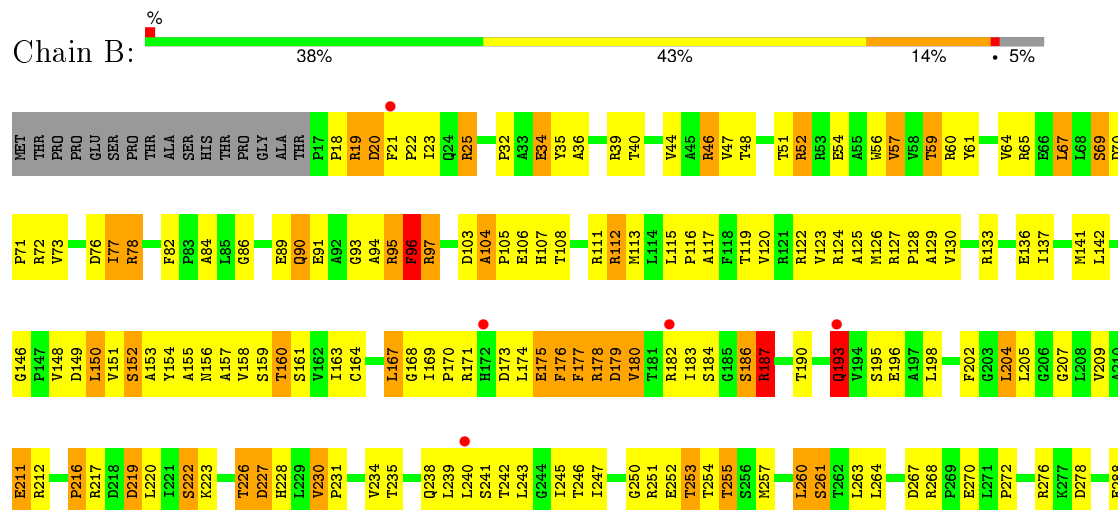
### 3 Residue-property plots [i](#)

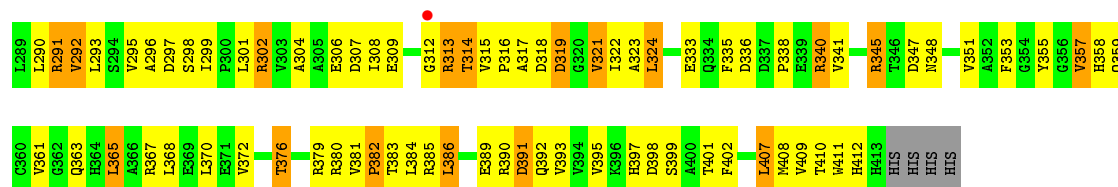
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ( $\text{RSRZ} > 2$ ). 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

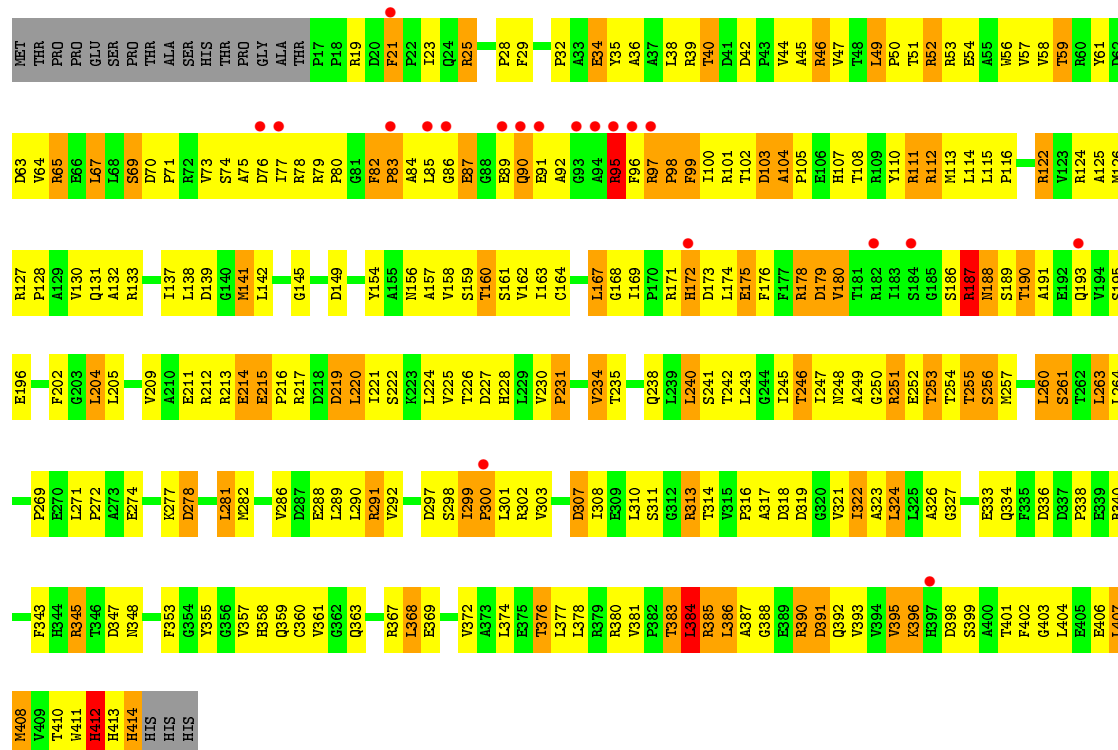


#### • Molecule 1: Putative cytochrome P450

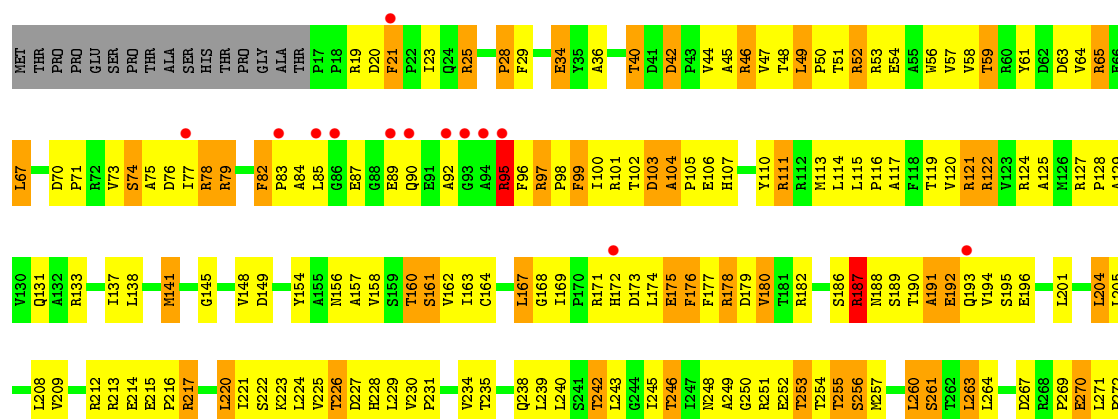


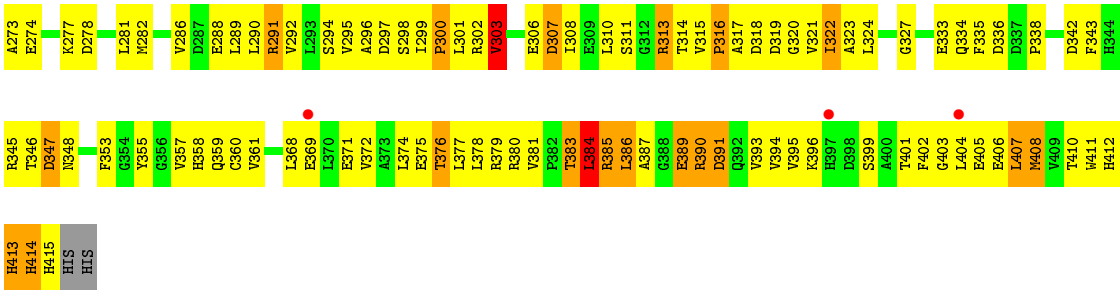


• Molecule 1: Putative cytochrome P450



• Molecule 1: Putative cytochrome P450







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	134.54Å 134.54Å 230.58Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.90 29.79 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.7 (30.00-2.90) 99.5 (29.79-2.90)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.12 (at 2.90Å)	Xtriage
Refinement program	CNS1.3	Depositor
R, $R_{free}$	0.282 , 0.300 0.255 , 0.266	Depositor DCC
$R_{free}$ test set	2646 reflections (5.37%)	DCC
Wilson B-factor (Å <sup>2</sup> )	74.4	Xtriage
Anisotropy	0.258	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 49.0	EDS
Estimated twinning fraction	0.480 for h,-h-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 52020 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	12633	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.11% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: HEM

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.76	2/3144 (0.1%)	0.89	3/4280 (0.1%)
1	B	0.75	2/3144 (0.1%)	0.87	1/4280 (0.0%)
1	C	0.78	2/3155 (0.1%)	0.91	4/4295 (0.1%)
1	D	0.79	3/3166 (0.1%)	0.91	5/4310 (0.1%)
All	All	0.77	9/12609 (0.1%)	0.90	13/17165 (0.1%)

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	B	0	1
1	C	0	1
All	All	0	2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	95	ARG	CZ-NH2	16.36	1.54	1.33
1	D	95	ARG	CZ-NH2	15.61	1.53	1.33
1	D	95	ARG	CZ-NH1	13.58	1.50	1.33
1	C	95	ARG	CZ-NH1	10.69	1.47	1.33
1	B	193	GLN	CG-CD	10.02	1.74	1.51
1	A	193	GLN	CD-NE2	8.41	1.53	1.32
1	D	303	VAL	CB-CG1	-7.84	1.36	1.52
1	B	193	GLN	CD-NE2	7.09	1.50	1.32
1	A	193	GLN	CD-OE1	6.38	1.38	1.24

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	95	ARG	NE-CZ-NH2	7.74	124.17	120.30
1	A	384	LEU	CA-CB-CG	7.08	131.59	115.30
1	B	230	VAL	C-N-CD	-6.62	106.03	120.60
1	D	384	LEU	CA-CB-CG	6.49	130.23	115.30
1	C	384	LEU	CA-CB-CG	5.67	128.34	115.30
1	C	299	ILE	C-N-CD	5.51	139.97	128.40
1	D	95	ARG	NH1-CZ-NH2	-5.48	113.38	119.40
1	C	278	ASP	C-N-CD	5.33	139.60	128.40
1	C	21	PHE	C-N-CD	5.26	139.45	128.40
1	D	278	ASP	C-N-CD	5.10	139.11	128.40
1	A	115	LEU	C-N-CD	5.05	139.01	128.40
1	D	21	PHE	C-N-CD	5.04	138.98	128.40
1	A	278	ASP	C-N-CD	5.02	138.93	128.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	94	ALA	Peptide
1	C	412	HIS	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	3084	0	3078	283	11
1	B	3084	0	3079	268	16
1	C	3094	0	3083	397	20
1	D	3104	0	3093	420	15
2	A	43	0	30	5	0
2	B	43	0	30	4	0
2	C	43	0	30	4	0
2	D	43	0	30	6	0
3	A	22	0	0	3	0
3	B	23	0	0	4	0
3	C	30	0	0	4	0
3	D	20	0	0	4	0
All	All	12633	0	12453	1352	31

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 54.

All (1352) 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:190:THR:CG2	1:A:193:GLN:HB2	1.30	1.57
1:A:190:THR:HG21	1:A:193:GLN:CB	1.42	1.49
1:C:171:ARG:HD2	1:C:172:HIS:CE1	1.49	1.45
1:C:107:HIS:NE2	1:C:358:HIS:CD2	1.84	1.45
1:A:190:THR:CG2	1:A:193:GLN:CB	1.92	1.40
1:C:92:ALA:O	1:C:95:ARG:HD3	1.17	1.31
1:C:234:VAL:HG12	1:C:238:GLN:NE2	1.46	1.30
1:D:107:HIS:NE2	1:D:358:HIS:CD2	1.97	1.30
1:C:104:ALA:HB1	1:C:105:PRO:CD	1.62	1.29
1:B:65:ARG:NH1	1:B:355:TYR:CZ	2.01	1.29
1:C:374:LEU:O	1:C:378:LEU:CD1	1.81	1.27
1:B:136:GLU:OE2	1:B:171:ARG:NH1	1.68	1.25
1:C:291:ARG:NH2	1:C:338:PRO:O	1.68	1.25
1:C:234:VAL:CG1	1:C:238:GLN:HE21	1.50	1.22
1:C:299:ILE:HD11	1:C:401:THR:CG2	1.71	1.21
1:C:107:HIS:CD2	1:C:358:HIS:HE2	1.59	1.21
1:D:133:ARG:NH1	1:D:161:SER:O	1.74	1.20
1:D:77:ILE:HA	1:D:82:PHE:CD2	1.76	1.19
1:D:98:PRO:HB3	1:D:245:ILE:CD1	1.71	1.19
1:C:74:SER:OG	1:C:103:ASP:OD2	1.60	1.19
1:B:341:VAL:O	3:B:602:HOH:O	1.63	1.17
1:D:302:ARG:NH2	1:D:358:HIS:ND1	1.93	1.16
1:C:299:ILE:HD11	1:C:401:THR:HG22	1.19	1.16
1:D:98:PRO:CB	1:D:245:ILE:CD1	2.24	1.16
1:A:169:ILE:HD13	1:A:178:ARG:CD	1.74	1.16
1:D:386:LEU:HD23	1:D:408:MET:O	1.41	1.16
1:C:104:ALA:CB	1:C:105:PRO:HD2	1.76	1.15
1:D:49:LEU:CD1	1:D:84:ALA:O	1.94	1.15
1:C:77:ILE:HA	1:C:82:PHE:CD2	1.80	1.15
1:D:92:ALA:O	1:D:95:ARG:CD	1.96	1.13
1:D:107:HIS:NE2	1:D:358:HIS:HD2	1.39	1.13
1:A:383:THR:HG21	1:A:412:HIS:HB2	1.22	1.13
1:D:57:VAL:CG2	1:D:322:ILE:HD12	1.78	1.13
1:C:392:GLN:O	3:C:606:HOH:O	1.67	1.12
1:C:77:ILE:O	1:C:90:GLN:NE2	1.80	1.12
1:C:191:ALA:O	3:C:603:HOH:O	1.66	1.11
1:A:169:ILE:HD13	1:A:178:ARG:HD3	1.25	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:104:ALA:HB1	1:D:105:PRO:HD2	1.29	1.10
1:C:299:ILE:CD1	1:C:401:THR:HG22	1.81	1.09
1:A:190:THR:CG2	1:A:193:GLN:HB3	1.83	1.08
1:C:92:ALA:O	1:C:95:ARG:CD	2.01	1.08
1:D:98:PRO:HB3	1:D:245:ILE:HD11	1.32	1.08
1:A:190:THR:HG22	1:A:193:GLN:CB	1.79	1.08
1:B:383:THR:HG21	1:B:412:HIS:HB2	1.33	1.07
1:C:303:VAL:HG13	1:C:319:ASP:O	1.52	1.07
1:C:171:ARG:CD	1:C:172:HIS:CE1	2.38	1.07
1:D:301:LEU:HD23	1:D:322:ILE:HG23	1.11	1.07
1:C:374:LEU:O	1:C:378:LEU:HD12	1.46	1.06
1:C:372:VAL:O	1:C:376:THR:HG23	1.53	1.06
1:D:250:GLY:HA3	2:D:501:HEM:HBC2	1.29	1.06
1:A:288:GLU:OE1	1:A:291:ARG:NH1	1.89	1.06
1:D:216:PRO:O	1:D:217:ARG:NH1	1.89	1.06
1:D:98:PRO:CB	1:D:245:ILE:HD13	1.85	1.05
1:B:251:ARG:O	1:B:255:THR:HG23	1.57	1.04
1:C:303:VAL:CG1	1:C:319:ASP:O	2.04	1.04
1:A:302:ARG:HH11	1:A:302:ARG:HG3	1.18	1.04
1:A:381:VAL:HG12	1:A:384:LEU:HB2	1.39	1.04
1:A:190:THR:HG21	1:A:193:GLN:HB3	1.35	1.04
1:B:250:GLY:HA3	2:B:501:HEM:HBC2	1.38	1.04
1:D:386:LEU:HD21	1:D:408:MET:SD	1.98	1.03
1:D:74:SER:HB3	1:D:103:ASP:OD2	1.58	1.03
1:C:171:ARG:HD2	1:C:172:HIS:ND1	1.73	1.03
1:C:98:PRO:CB	1:C:245:ILE:HD13	1.89	1.03
1:B:288:GLU:OE1	1:B:291:ARG:NH1	1.91	1.03
1:C:113:MET:SD	1:C:228:HIS:ND1	2.30	1.03
1:C:99:PHE:HD2	1:C:110:TYR:HB2	1.20	1.03
1:C:386:LEU:HD23	1:C:408:MET:O	1.59	1.02
1:C:301:LEU:HD23	1:C:322:ILE:HG23	1.39	1.02
1:C:174:LEU:HD13	1:C:204:LEU:HD21	1.07	1.02
1:C:107:HIS:CD2	1:C:358:HIS:NE2	2.26	1.02
1:C:104:ALA:HB1	1:C:105:PRO:HD2	1.04	1.02
1:D:77:ILE:HA	1:D:82:PHE:CE2	1.95	1.02
1:D:190:THR:OG1	1:D:193:GLN:N	1.90	1.02
1:C:99:PHE:HD2	1:C:110:TYR:CB	1.73	1.01
1:D:301:LEU:CD2	1:D:322:ILE:HG23	1.89	1.01
1:C:250:GLY:HA3	2:C:501:HEM:HBC2	1.37	1.01
1:C:174:LEU:CD1	1:C:204:LEU:HD21	1.91	1.00
1:D:176:PHE:O	1:D:180:VAL:HG23	1.61	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:169:ILE:HD13	1:B:178:ARG:HD3	1.43	0.99
1:C:75:ALA:O	1:C:101:ARG:O	1.81	0.99
1:A:18:PRO:HG2	1:A:54:GLU:OE2	1.61	0.99
1:D:251:ARG:O	1:D:255:THR:HG23	1.62	0.98
1:D:78:ARG:HH11	1:D:78:ARG:HG3	1.28	0.98
1:D:386:LEU:CD2	1:D:408:MET:O	2.12	0.97
1:D:121:ARG:HG2	1:D:121:ARG:HH11	1.28	0.97
1:D:217:ARG:HA	1:D:217:ARG:CZ	1.93	0.97
1:B:104:ALA:HB1	1:B:105:PRO:HD2	1.43	0.97
1:A:250:GLY:HA3	2:A:501:HEM:HBC2	1.45	0.97
1:B:21:PHE:HB3	1:B:22:PRO:HD3	1.45	0.96
1:C:84:ALA:HB1	1:C:89:GLU:OE1	1.63	0.96
1:C:49:LEU:CD1	1:C:84:ALA:O	2.14	0.96
1:C:77:ILE:HA	1:C:82:PHE:CE2	2.00	0.96
1:A:291:ARG:NH2	1:A:338:PRO:O	2.00	0.95
1:C:107:HIS:NE2	1:C:358:HIS:NE2	2.12	0.95
1:B:34:GLU:N	1:B:34:GLU:OE2	2.00	0.95
1:D:92:ALA:O	1:D:95:ARG:HD2	1.64	0.95
1:C:282:MET:O	1:C:286:VAL:HG23	1.66	0.95
1:C:171:ARG:HD2	1:C:172:HIS:HE1	1.14	0.95
1:D:190:THR:HG21	1:D:193:GLN:HB2	1.49	0.94
1:A:190:THR:HG23	1:A:193:GLN:HB2	1.48	0.94
1:D:52:ARG:HH11	1:D:52:ARG:HG3	1.32	0.94
1:B:372:VAL:O	1:B:376:THR:OG1	1.86	0.94
1:D:98:PRO:HB2	1:D:245:ILE:HD13	1.50	0.93
1:A:372:VAL:O	1:A:376:THR:OG1	1.86	0.93
1:A:104:ALA:HB1	1:A:105:PRO:HD2	1.48	0.93
1:D:267:ASP:OD2	1:D:390:ARG:NH2	2.01	0.93
1:C:98:PRO:HB2	1:C:245:ILE:HD13	1.50	0.93
1:D:75:ALA:CB	1:D:358:HIS:HE1	1.81	0.93
1:D:190:THR:CB	1:D:193:GLN:HB2	1.99	0.93
1:D:57:VAL:HG22	1:D:322:ILE:HD12	1.49	0.93
1:A:381:VAL:CG1	1:A:384:LEU:HB2	1.98	0.93
1:B:65:ARG:NH1	1:B:355:TYR:CE1	2.34	0.93
1:A:169:ILE:CD1	1:A:178:ARG:CD	2.47	0.93
1:C:257:MET:O	1:C:261:SER:OG	1.87	0.93
1:A:21:PHE:HB3	1:A:22:PRO:HD3	1.51	0.92
1:D:173:ASP:HB3	1:D:174:LEU:CD2	2.00	0.92
1:D:303:VAL:HG13	1:D:320:GLY:HA2	1.48	0.92
1:B:169:ILE:HD13	1:B:178:ARG:CD	1.99	0.92
1:D:131:GLN:OE1	1:D:376:THR:HG21	1.69	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:234:VAL:CG1	1:C:238:GLN:NE2	2.21	0.92
1:D:383:THR:OG1	1:D:413:HIS:HB3	1.70	0.92
1:D:336:ASP:O	1:D:345:ARG:NH2	2.03	0.92
1:A:175:GLU:OE2	1:A:179:ASP:OD2	1.89	0.91
1:B:222:SER:O	1:B:226:THR:OG1	1.88	0.91
1:D:92:ALA:O	1:D:95:ARG:HD3	1.67	0.91
1:D:104:ALA:HB1	1:D:105:PRO:CD	2.01	0.90
1:B:219:ASP:OD1	1:B:222:SER:HB3	1.71	0.90
1:D:313:ARG:HG2	1:D:313:ARG:HH11	1.36	0.90
1:C:156:ASN:O	1:C:160:THR:OG1	1.89	0.90
1:D:395:VAL:HG12	1:D:396:LYS:H	1.36	0.90
1:D:76:ASP:OD1	1:D:78:ARG:NH1	2.05	0.90
1:D:190:THR:HG23	1:D:191:ALA:H	1.35	0.90
1:C:75:ALA:CB	1:C:358:HIS:HE1	1.85	0.89
1:A:104:ALA:HB1	1:A:105:PRO:CD	2.03	0.89
1:B:257:MET:O	1:B:261:SER:OG	1.88	0.89
1:D:257:MET:O	1:D:261:SER:OG	1.88	0.89
1:D:190:THR:CG2	1:D:193:GLN:HB2	2.03	0.89
1:D:107:HIS:CE1	1:D:358:HIS:CD2	2.60	0.89
1:C:133:ARG:NH1	1:C:161:SER:O	2.06	0.89
1:A:173:ASP:C	1:A:174:LEU:HD23	1.93	0.89
1:A:205:LEU:O	1:A:209:VAL:HG23	1.73	0.89
1:B:90:GLN:NE2	1:B:90:GLN:O	2.05	0.89
1:B:302:ARG:HH11	1:B:302:ARG:HG3	1.38	0.89
1:C:395:VAL:HG12	1:C:396:LYS:H	1.35	0.89
1:A:169:ILE:CD1	1:A:178:ARG:HD3	2.01	0.88
1:D:49:LEU:HD12	1:D:84:ALA:O	1.73	0.88
1:B:73:VAL:CG2	1:B:308:ILE:CD1	2.51	0.88
1:C:393:VAL:CG1	1:C:407:LEU:HD21	2.04	0.88
1:C:99:PHE:CD2	1:C:110:TYR:CB	2.57	0.87
1:C:234:VAL:HG12	1:C:238:GLN:HE21	0.72	0.87
1:C:98:PRO:HB3	1:C:245:ILE:HD13	1.55	0.87
1:D:385:ARG:HG3	1:D:386:LEU:N	1.88	0.86
1:A:219:ASP:OD1	1:A:222:SER:HB2	1.75	0.86
1:C:50:PRO:HG3	1:C:85:LEU:O	1.75	0.86
1:B:104:ALA:HB1	1:B:105:PRO:CD	2.06	0.86
1:D:263:LEU:HD12	1:D:404:LEU:HD11	1.54	0.86
1:C:49:LEU:HD13	1:C:84:ALA:O	1.74	0.86
1:B:123:VAL:HG22	1:B:365:LEU:HD12	1.58	0.86
1:A:217:ARG:HH11	1:A:217:ARG:HG3	1.39	0.86
1:C:107:HIS:NE2	1:C:358:HIS:HD2	1.37	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:171:ARG:CD	1:C:172:HIS:HE1	1.81	0.85
1:D:257:MET:CE	1:D:290:LEU:HD23	2.06	0.85
1:C:154:TYR:O	1:C:158:VAL:HG23	1.77	0.85
1:A:379:ARG:NH1	1:B:276:ARG:O	2.09	0.85
1:B:212:ARG:O	1:B:216:PRO:HB3	1.75	0.85
1:A:251:ARG:O	1:A:255:THR:HG23	1.75	0.85
1:C:381:VAL:HG12	1:C:384:LEU:HB2	1.59	0.85
1:C:98:PRO:CB	1:C:245:ILE:CD1	2.55	0.84
1:D:102:THR:O	1:D:107:HIS:HB2	1.76	0.84
1:B:217:ARG:O	1:B:222:SER:OG	1.95	0.84
1:C:77:ILE:HA	1:C:82:PHE:HD2	1.37	0.84
1:C:171:ARG:O	1:C:174:LEU:O	1.95	0.84
1:D:98:PRO:HB2	1:D:245:ILE:CD1	2.01	0.84
1:A:223:LYS:O	1:A:227:ASP:HB2	1.78	0.84
1:A:77:ILE:CG2	1:A:97:ARG:HG2	2.08	0.84
1:C:169:ILE:CD1	1:C:178:ARG:HD2	2.07	0.84
1:C:98:PRO:HB3	1:C:245:ILE:CD1	2.07	0.84
1:A:169:ILE:HD13	1:A:178:ARG:HD2	1.57	0.84
1:D:107:HIS:CE1	1:D:358:HIS:HD2	1.96	0.84
1:D:173:ASP:C	1:D:174:LEU:HD23	1.98	0.84
1:D:107:HIS:CD2	1:D:358:HIS:HE2	1.95	0.84
1:C:217:ARG:O	1:C:219:ASP:OD1	1.94	0.84
1:B:205:LEU:O	1:B:209:VAL:HG23	1.79	0.83
1:A:174:LEU:CD1	1:A:204:LEU:HD21	2.06	0.83
1:C:313:ARG:HG2	1:C:313:ARG:HH11	1.40	0.83
1:D:84:ALA:HB1	1:D:89:GLU:HB2	1.60	0.83
1:C:374:LEU:O	1:C:378:LEU:HD13	1.76	0.83
1:C:297:ASP:OD2	1:C:326:ALA:HB3	1.79	0.83
1:D:385:ARG:HG3	1:D:386:LEU:H	1.44	0.83
1:C:99:PHE:CE1	1:C:100:ILE:HG13	2.13	0.83
1:D:394:VAL:HG12	1:D:405:GLU:HB2	1.59	0.82
1:C:95:ARG:CZ	1:C:97:ARG:HD3	2.09	0.82
1:D:75:ALA:HB2	1:D:358:HIS:HE1	1.43	0.82
1:D:381:VAL:HG12	1:D:384:LEU:HB2	1.61	0.82
1:D:190:THR:OG1	1:D:192:GLU:HG3	1.79	0.82
1:C:297:ASP:OD2	1:C:326:ALA:CB	2.28	0.82
1:D:99:PHE:HB3	1:D:110:TYR:HD2	1.45	0.82
1:D:77:ILE:HG21	1:D:97:ARG:HG2	1.61	0.82
1:C:408:MET:HE3	1:C:408:MET:N	1.95	0.82
1:D:158:VAL:O	1:D:162:VAL:HG23	1.79	0.82
1:C:386:LEU:HD21	1:C:408:MET:SD	2.19	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:107:HIS:CE1	1:C:358:HIS:CD2	2.67	0.81
1:D:98:PRO:HB3	1:D:245:ILE:HD13	1.51	0.81
1:B:291:ARG:NH2	1:B:338:PRO:O	2.14	0.81
1:C:363:GLN:OE1	1:C:367:ARG:NH1	2.13	0.81
1:C:251:ARG:O	1:C:255:THR:HG23	1.80	0.81
1:C:368:LEU:O	1:C:368:LEU:HD12	1.79	0.81
1:A:92:ALA:HA	1:A:95:ARG:CG	2.10	0.81
1:A:212:ARG:O	1:A:216:PRO:HB3	1.79	0.81
1:D:234:VAL:HG13	1:D:238:GLN:HE21	1.45	0.81
1:D:175:GLU:OE1	3:D:612:HOH:O	1.98	0.81
1:A:73:VAL:HG23	1:A:308:ILE:CD1	2.11	0.80
1:A:239:LEU:O	1:A:239:LEU:HD23	1.81	0.80
1:D:238:GLN:O	1:D:242:THR:HG23	1.82	0.80
1:C:176:PHE:O	1:C:180:VAL:HG23	1.82	0.80
1:B:239:LEU:HD23	1:B:239:LEU:O	1.81	0.80
1:C:175:GLU:O	1:C:179:ASP:HB2	1.82	0.80
1:D:154:TYR:O	1:D:158:VAL:HG23	1.80	0.80
1:B:107:HIS:NE2	1:B:358:HIS:CD2	2.49	0.80
1:A:190:THR:HG21	1:A:193:GLN:CG	2.12	0.80
1:D:205:LEU:O	1:D:209:VAL:HG23	1.82	0.80
1:D:121:ARG:HG2	1:D:121:ARG:NH1	1.96	0.79
1:A:368:LEU:O	1:A:368:LEU:HD12	1.83	0.79
1:D:99:PHE:HB3	1:D:110:TYR:CD2	2.16	0.79
1:B:242:THR:O	1:B:246:THR:HG23	1.82	0.79
1:D:408:MET:SD	1:D:408:MET:N	2.55	0.79
1:D:57:VAL:HG23	1:D:322:ILE:HD12	1.64	0.79
1:B:173:ASP:C	1:B:174:LEU:HD23	2.02	0.79
1:D:74:SER:CB	1:D:103:ASP:OD2	2.30	0.79
1:D:257:MET:HE1	1:D:290:LEU:HD23	1.64	0.79
1:D:234:VAL:CG1	1:D:238:GLN:HB3	2.12	0.79
1:C:190:THR:HG22	1:C:193:GLN:H	1.48	0.79
1:D:171:ARG:HG3	1:D:172:HIS:N	1.95	0.79
1:C:190:THR:CG2	1:C:193:GLN:HB2	2.12	0.79
1:C:190:THR:HB	1:C:193:GLN:HB2	1.65	0.79
1:C:254:THR:HG21	1:C:369:GLU:OE2	1.83	0.79
1:C:299:ILE:CD1	1:C:401:THR:CG2	2.49	0.79
1:C:110:TYR:O	1:C:113:MET:HB3	1.82	0.79
1:C:158:VAL:O	1:C:162:VAL:HG23	1.82	0.79
1:D:44:VAL:HG21	1:D:313:ARG:HB2	1.65	0.79
1:A:268:ARG:HB3	1:A:270:GLU:OE2	1.83	0.79
1:A:190:THR:HG22	1:A:193:GLN:HB2	1.44	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:340:ARG:NH1	3:B:621:HOH:O	2.14	0.78
1:D:379:ARG:HH11	1:D:379:ARG:HG2	1.48	0.78
1:C:99:PHE:HB3	1:C:110:TYR:CD2	2.18	0.78
1:C:138:LEU:CD2	1:C:141:MET:CE	2.62	0.78
1:C:378:LEU:H	1:C:378:LEU:HD12	1.48	0.78
1:C:131:GLN:OE1	1:C:376:THR:HG21	1.84	0.78
1:A:73:VAL:CG2	1:A:308:ILE:CD1	2.61	0.78
1:D:46:ARG:HH21	1:D:54:GLU:CB	1.97	0.78
1:D:168:GLY:O	1:D:212:ARG:NH2	2.17	0.78
1:D:414:HIS:O	1:D:415:HIS:HB2	1.84	0.78
1:B:73:VAL:HG23	1:B:308:ILE:CD1	2.13	0.78
1:A:381:VAL:HG12	1:A:384:LEU:CB	2.14	0.78
1:C:260:LEU:HD11	1:C:402:PHE:HE1	1.49	0.78
1:A:107:HIS:NE2	1:A:358:HIS:CD2	2.52	0.78
1:B:302:ARG:HG3	1:B:302:ARG:NH1	1.98	0.78
1:D:46:ARG:HH21	1:D:54:GLU:HB2	1.48	0.78
1:D:347:ASP:OD1	3:D:601:HOH:O	2.01	0.78
1:B:316:PRO:O	1:B:319:ASP:HB2	1.83	0.78
1:D:394:VAL:HG12	1:D:405:GLU:CB	2.14	0.77
1:B:93:GLY:O	1:B:95:ARG:HA	1.83	0.77
1:D:78:ARG:HG3	1:D:78:ARG:NH1	1.99	0.77
1:B:253:THR:HG23	1:B:401:THR:HG21	1.67	0.77
1:C:107:HIS:CE1	1:C:358:HIS:HD2	2.03	0.77
1:D:111:ARG:NH1	1:D:359:GLN:O	2.15	0.77
1:A:111:ARG:NH1	1:A:359:GLN:O	2.15	0.77
1:A:76:ASP:OD1	1:A:78:ARG:HG3	1.84	0.77
1:D:190:THR:HG21	1:D:193:GLN:CB	2.14	0.77
1:D:167:LEU:HD23	1:D:221:ILE:HG13	1.67	0.77
1:C:138:LEU:CD2	1:C:141:MET:HE3	2.14	0.76
1:B:111:ARG:NH1	1:B:359:GLN:O	2.17	0.76
1:A:242:THR:O	1:A:246:THR:HG23	1.86	0.76
1:A:202:PHE:HD1	1:A:240:LEU:HD12	1.49	0.76
1:B:65:ARG:O	1:B:69:SER:HB2	1.84	0.76
1:C:248:ASN:OD1	3:C:604:HOH:O	2.03	0.76
1:C:99:PHE:CD2	1:C:110:TYR:HB3	2.20	0.76
1:A:277:LYS:HE2	1:B:380:ARG:NH2	2.00	0.76
1:C:234:VAL:HG12	1:C:238:GLN:HB3	1.68	0.76
1:B:383:THR:HG21	1:B:412:HIS:CB	2.14	0.76
1:A:77:ILE:O	1:A:90:GLN:NE2	2.19	0.76
1:C:188:ASN:O	1:C:189:SER:OG	2.03	0.76
1:D:395:VAL:HG12	1:D:396:LYS:N	2.00	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:264:LEU:O	1:B:264:LEU:HD12	1.84	0.76
1:D:97:ARG:HG3	1:D:98:PRO:HD2	1.67	0.75
1:C:49:LEU:HB2	1:C:53:ARG:O	1.86	0.75
1:D:381:VAL:CG1	1:D:384:LEU:HB2	2.16	0.75
1:C:383:THR:HG21	1:C:412:HIS:O	1.84	0.75
1:D:138:LEU:HD23	1:D:141:MET:CE	2.16	0.75
1:A:179:ASP:O	1:A:183:ILE:HD12	1.86	0.75
1:C:174:LEU:HD13	1:C:204:LEU:CD2	2.03	0.75
1:A:253:THR:HG23	1:A:401:THR:HG21	1.67	0.75
1:B:65:ARG:NH1	1:B:355:TYR:CE2	2.40	0.75
1:C:303:VAL:HG12	1:C:319:ASP:O	1.85	0.75
1:B:78:ARG:HB2	1:B:78:ARG:HH11	1.51	0.74
1:D:302:ARG:HH21	1:D:358:HIS:CG	2.05	0.74
1:A:242:THR:HA	1:A:245:ILE:HD12	1.69	0.74
1:C:385:ARG:HG3	1:C:386:LEU:N	2.02	0.74
1:A:78:ARG:HH11	1:A:78:ARG:CB	1.99	0.74
1:A:92:ALA:HA	1:A:95:ARG:HD3	1.68	0.74
1:C:99:PHE:CD2	1:C:110:TYR:HB2	2.12	0.74
1:B:149:ASP:OD1	1:B:152:SER:OG	2.05	0.74
1:C:99:PHE:HB3	1:C:110:TYR:HD2	1.53	0.74
1:B:242:THR:HA	1:B:245:ILE:HD12	1.70	0.74
1:D:410:THR:HG22	1:D:411:TRP:N	2.02	0.74
1:A:368:LEU:O	1:A:372:VAL:HG23	1.87	0.74
1:D:156:ASN:O	1:D:160:THR:OG1	2.04	0.74
1:C:75:ALA:CB	1:C:358:HIS:CE1	2.69	0.74
1:A:149:ASP:OD1	1:A:152:SER:OG	2.06	0.74
1:D:75:ALA:CB	1:D:358:HIS:CE1	2.69	0.74
1:C:133:ARG:HD3	1:C:161:SER:OG	1.87	0.74
1:A:216:PRO:HB2	1:A:222:SER:OG	1.88	0.74
1:A:258:ILE:O	1:A:262:THR:OG1	2.03	0.74
1:D:122:ARG:NH1	1:D:122:ARG:HG2	2.02	0.73
1:D:75:ALA:O	1:D:101:ARG:O	2.07	0.73
1:D:107:HIS:NE2	1:D:358:HIS:NE2	2.34	0.73
1:D:234:VAL:CG1	1:D:238:GLN:HE21	2.01	0.73
1:D:235:THR:H	1:D:238:GLN:NE2	1.86	0.73
1:D:76:ASP:HB3	1:D:79:ARG:HG3	1.71	0.73
1:D:44:VAL:HG11	1:D:315:VAL:HG12	1.68	0.73
1:C:393:VAL:CG1	1:C:407:LEU:CD2	2.66	0.73
1:A:107:HIS:CD2	1:A:358:HIS:NE2	2.57	0.73
1:A:302:ARG:HG3	1:A:302:ARG:NH1	1.93	0.73
1:C:395:VAL:HG12	1:C:396:LYS:N	2.02	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:18:PRO:HG3	1:B:54:GLU:OE2	1.88	0.72
1:B:163:ILE:HG22	1:B:167:LEU:HD12	1.70	0.72
1:C:387:ALA:HB2	1:C:410:THR:OG1	1.89	0.72
1:D:251:ARG:O	1:D:255:THR:CG2	2.38	0.72
1:C:313:ARG:HG2	1:C:313:ARG:NH1	1.99	0.72
1:C:95:ARG:HD3	1:C:97:ARG:HG2	1.70	0.72
1:D:368:LEU:O	1:D:372:VAL:HG23	1.90	0.72
1:B:133:ARG:HD3	1:B:161:SER:OG	1.89	0.72
1:D:317:ALA:O	1:D:318:ASP:HB2	1.89	0.72
1:D:124:ARG:HG3	1:D:124:ARG:HH11	1.53	0.72
1:C:381:VAL:CG1	1:C:384:LEU:HB2	2.18	0.72
1:C:107:HIS:HD2	1:C:358:HIS:HE2	1.35	0.72
1:D:107:HIS:CD2	1:D:358:HIS:NE2	2.57	0.72
1:D:122:ARG:HG2	1:D:122:ARG:HH11	1.52	0.72
1:D:49:LEU:HD13	1:D:84:ALA:O	1.90	0.72
1:C:225:VAL:O	1:C:230:VAL:HG23	1.89	0.72
1:B:368:LEU:O	1:B:372:VAL:HG23	1.90	0.71
1:A:92:ALA:O	1:A:95:ARG:HG3	1.90	0.71
1:A:190:THR:HG22	1:A:193:GLN:H	1.55	0.71
1:C:86:GLY:N	1:C:89:GLU:OE2	2.23	0.71
1:D:217:ARG:HH11	1:D:217:ARG:HG2	1.54	0.71
1:B:253:THR:HB	2:B:501:HEM:HBB2	1.72	0.71
1:D:190:THR:HG23	1:D:191:ALA:N	2.05	0.71
1:C:32:PRO:HG2	1:C:35:TYR:CD1	2.25	0.71
1:D:190:THR:HG1	1:D:193:GLN:H	1.36	0.71
1:A:341:VAL:O	3:A:605:HOH:O	2.08	0.71
1:A:159:SER:CB	1:A:255:THR:HG22	2.19	0.71
1:B:126:MET:O	1:B:130:VAL:HG23	1.91	0.71
1:C:104:ALA:HB1	1:C:105:PRO:HD3	1.71	0.71
1:B:73:VAL:HG22	1:B:308:ILE:CD1	2.19	0.71
1:D:301:LEU:HD23	1:D:322:ILE:CG2	2.07	0.71
1:A:383:THR:CG2	1:A:412:HIS:HB2	2.14	0.71
1:C:190:THR:CB	1:C:193:GLN:HB2	2.20	0.71
1:A:190:THR:HG21	1:A:193:GLN:HB2	1.08	0.71
1:C:95:ARG:NE	1:C:97:ARG:HD3	2.06	0.71
1:D:75:ALA:HB2	1:D:358:HIS:CE1	2.26	0.71
1:C:368:LEU:HD12	1:C:372:VAL:HG23	1.72	0.71
1:B:168:GLY:O	1:B:212:ARG:NH2	2.24	0.71
1:B:76:ASP:OD1	1:B:78:ARG:HG3	1.90	0.71
1:A:368:LEU:HD12	1:A:372:VAL:HG23	1.73	0.71
1:A:217:ARG:NH1	1:A:217:ARG:HG3	2.02	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:SER:HB2	1:A:255:THR:HG22	1.73	0.70
1:C:125:ALA:O	1:C:128:PRO:HD2	1.90	0.70
1:D:375:GLU:OE2	1:D:376:THR:HG22	1.91	0.70
1:D:42:ASP:OD1	1:D:42:ASP:N	2.24	0.70
1:C:253:THR:HG23	1:C:401:THR:HG21	1.72	0.70
1:A:276:ARG:O	1:B:379:ARG:NH1	2.24	0.70
1:D:303:VAL:HG13	1:D:320:GLY:CA	2.22	0.70
1:D:313:ARG:HG2	1:D:313:ARG:NH1	1.99	0.70
1:C:99:PHE:CD1	1:C:100:ILE:HG13	2.26	0.70
1:D:77:ILE:HA	1:D:82:PHE:HD2	1.50	0.69
1:C:149:ASP:OD2	1:C:407:LEU:N	2.25	0.69
1:D:98:PRO:CB	1:D:245:ILE:HD11	2.08	0.69
1:A:156:ASN:O	1:A:160:THR:OG1	2.10	0.69
1:D:23:ILE:HD13	1:D:34:GLU:HG3	1.75	0.69
1:C:299:ILE:HD11	1:C:401:THR:HG23	1.70	0.69
1:D:412:HIS:O	1:D:413:HIS:HB2	1.93	0.69
1:A:174:LEU:HD12	1:A:204:LEU:HD21	1.72	0.69
1:A:163:ILE:HG22	1:A:167:LEU:HD12	1.74	0.69
1:B:383:THR:HG21	1:B:412:HIS:H	1.58	0.69
1:B:268:ARG:HB3	1:B:270:GLU:OE2	1.92	0.69
1:C:75:ALA:HB3	1:C:358:HIS:HE1	1.58	0.69
1:B:357:VAL:HG12	3:D:609:HOH:O	1.91	0.69
1:D:186:SER:O	1:D:187:ARG:HB2	1.93	0.69
1:D:372:VAL:O	1:D:376:THR:HG23	1.93	0.69
1:D:413:HIS:CG	1:D:414:HIS:H	2.11	0.69
1:B:78:ARG:CB	1:B:78:ARG:HH11	2.06	0.69
1:A:125:ALA:O	1:A:128:PRO:HD2	1.93	0.68
1:D:110:TYR:HD1	1:D:113:MET:CE	2.06	0.68
1:B:410:THR:HG22	1:B:411:TRP:N	2.09	0.68
1:C:297:ASP:O	1:C:300:PRO:HD3	1.93	0.68
1:B:363:GLN:O	1:B:367:ARG:HG3	1.93	0.68
1:D:302:ARG:NH2	1:D:358:HIS:CG	2.60	0.68
1:A:383:THR:HG21	1:A:412:HIS:H	1.59	0.68
1:C:234:VAL:HG12	1:C:238:GLN:CB	2.24	0.68
1:D:51:THR:O	1:D:52:ARG:HB2	1.94	0.68
1:A:92:ALA:HA	1:A:95:ARG:CD	2.23	0.68
1:C:190:THR:HG21	1:C:193:GLN:CG	2.24	0.68
1:C:99:PHE:CB	1:C:110:TYR:HD2	2.07	0.67
1:D:264:LEU:HD23	1:D:289:LEU:CD2	2.23	0.67
1:C:76:ASP:HB3	1:C:79:ARG:HG3	1.76	0.67
1:C:307:ASP:OD2	1:C:307:ASP:N	2.26	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:254:THR:HG21	1:D:369:GLU:OE2	1.95	0.67
1:D:413:HIS:O	1:D:414:HIS:ND1	2.28	0.67
1:D:217:ARG:HA	1:D:217:ARG:NE	2.09	0.67
1:A:171:ARG:O	1:A:175:GLU:HB2	1.95	0.67
1:A:20:ASP:N	1:A:20:ASP:OD2	2.19	0.67
1:D:138:LEU:CD2	1:D:141:MET:CE	2.73	0.67
1:A:129:ALA:O	1:A:133:ARG:HG3	1.95	0.67
1:A:133:ARG:O	1:A:137:ILE:HG13	1.95	0.67
1:A:78:ARG:HH11	1:A:78:ARG:HB2	1.60	0.67
1:A:241:SER:O	1:A:245:ILE:HG13	1.94	0.66
1:C:163:ILE:O	1:C:167:LEU:HB2	1.95	0.66
1:C:45:ALA:HB3	1:C:57:VAL:CG1	2.25	0.66
1:C:216:PRO:HB2	1:C:222:SER:OG	1.95	0.66
1:A:301:LEU:HD23	1:A:322:ILE:HG12	1.77	0.66
1:A:71:PRO:HB2	1:C:71:PRO:HB3	1.78	0.66
1:B:383:THR:CG2	1:B:412:HIS:HB2	2.20	0.66
1:C:393:VAL:HG11	1:C:407:LEU:HD21	1.75	0.66
1:D:65:ARG:HD2	1:D:355:TYR:CE1	2.30	0.66
1:B:21:PHE:CB	1:B:22:PRO:HD3	2.21	0.66
1:D:110:TYR:O	1:D:113:MET:HB3	1.96	0.66
1:D:163:ILE:O	1:D:167:LEU:HB2	1.96	0.66
1:B:44:VAL:HB	1:B:313:ARG:HG3	1.76	0.66
1:C:253:THR:HB	2:C:501:HEM:HBB2	1.78	0.66
1:D:52:ARG:NH1	1:D:52:ARG:HG3	1.95	0.66
1:B:142:LEU:HD23	1:B:411:TRP:NE1	2.11	0.66
1:B:108:THR:O	1:B:112:ARG:HB2	1.96	0.66
1:D:84:ALA:HB1	1:D:89:GLU:CB	2.26	0.65
1:A:235:THR:H	1:A:238:GLN:HE21	1.44	0.65
1:C:50:PRO:CG	1:C:85:LEU:O	2.44	0.65
1:D:253:THR:HB	2:D:501:HEM:HBB2	1.78	0.65
1:A:228:HIS:C	1:A:231:PRO:HD2	2.17	0.65
1:C:89:GLU:O	1:C:92:ALA:HB3	1.96	0.65
1:B:136:GLU:CD	1:B:171:ARG:NH1	2.49	0.65
1:C:384:LEU:HD13	1:C:385:ARG:N	2.11	0.65
1:D:138:LEU:HD23	1:D:141:MET:HE3	1.78	0.65
1:C:219:ASP:N	1:C:219:ASP:OD1	2.29	0.65
1:C:169:ILE:HD12	1:C:178:ARG:HD2	1.77	0.65
1:C:383:THR:OG1	1:C:413:HIS:O	2.13	0.65
1:B:239:LEU:C	1:B:239:LEU:HD23	2.16	0.65
1:D:173:ASP:HB3	1:D:174:LEU:HD21	1.76	0.65
1:D:138:LEU:HD23	1:D:141:MET:HE2	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:THR:O	1:A:190:THR:HG22	1.97	0.65
1:B:136:GLU:CD	1:B:171:ARG:HH11	1.99	0.65
1:C:173:ASP:O	1:C:174:LEU:HD23	1.97	0.65
1:A:387:ALA:HB2	1:A:410:THR:OG1	1.97	0.65
1:B:20:ASP:HA	1:B:48:THR:O	1.97	0.65
1:C:234:VAL:CG1	1:C:238:GLN:HB3	2.26	0.64
1:C:169:ILE:HD12	1:C:178:ARG:CD	2.27	0.64
1:D:84:ALA:HB1	1:D:89:GLU:OE1	1.97	0.64
1:D:394:VAL:CG1	1:D:405:GLU:HB3	2.28	0.64
1:D:99:PHE:CD2	1:D:110:TYR:HB2	2.31	0.64
1:C:390:ARG:O	1:C:391:ASP:HB2	1.98	0.64
1:A:84:ALA:HB1	1:A:89:GLU:HB3	1.79	0.64
1:B:52:ARG:HG3	1:B:52:ARG:NH1	2.13	0.64
1:C:102:THR:O	1:C:107:HIS:HB2	1.97	0.64
1:D:414:HIS:O	1:D:415:HIS:CB	2.45	0.64
1:D:230:VAL:N	1:D:231:PRO:HD2	2.13	0.64
1:A:190:THR:HG22	1:A:193:GLN:N	2.13	0.64
1:D:46:ARG:NH2	1:D:54:GLU:CB	2.61	0.64
1:B:234:VAL:HG13	1:B:238:GLN:HE21	1.62	0.64
1:B:156:ASN:O	1:B:160:THR:OG1	2.15	0.64
1:D:286:VAL:HG21	1:D:371:GLU:HB2	1.80	0.64
1:A:335:PHE:HB2	1:A:338:PRO:HB3	1.80	0.64
1:C:393:VAL:HG13	1:C:407:LEU:CD2	2.28	0.64
1:C:378:LEU:N	1:C:378:LEU:HD12	2.13	0.64
1:C:167:LEU:HD23	1:C:221:ILE:HG13	1.79	0.64
1:D:302:ARG:HH11	1:D:302:ARG:HG3	1.63	0.63
1:B:159:SER:O	1:B:163:ILE:HG13	1.98	0.63
1:D:52:ARG:HH11	1:D:52:ARG:CG	2.10	0.63
1:A:173:ASP:O	1:A:174:LEU:HD23	1.97	0.63
1:D:307:ASP:OD2	1:D:307:ASP:N	2.21	0.63
1:B:383:THR:CG2	1:B:412:HIS:H	2.11	0.63
1:C:145:GLY:HA2	1:C:411:TRP:CZ2	2.33	0.63
1:C:336:ASP:O	1:C:345:ARG:NH2	2.31	0.63
1:A:163:ILE:O	1:A:167:LEU:HB2	1.97	0.63
1:B:390:ARG:NH1	1:B:393:VAL:HG21	2.13	0.63
1:B:113:MET:HG3	1:B:228:HIS:CE1	2.33	0.63
1:A:73:VAL:HG23	1:A:308:ILE:HD13	1.80	0.63
1:A:77:ILE:HA	1:A:82:PHE:CD2	2.34	0.63
1:D:175:GLU:O	1:D:179:ASP:N	2.30	0.63
1:D:59:THR:HG22	1:D:327:GLY:HA3	1.79	0.63
1:A:70:ASP:OD1	1:A:72:ARG:N	2.27	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:386:LEU:CD2	1:D:408:MET:SD	2.84	0.63
1:D:190:THR:CG2	1:D:191:ALA:H	2.05	0.63
1:C:264:LEU:HD23	1:C:289:LEU:CD2	2.29	0.63
1:A:86:GLY:HA3	1:A:89:GLU:OE2	1.98	0.63
1:D:63:ASP:O	1:D:67:LEU:HB2	1.98	0.63
1:C:169:ILE:HD13	1:C:178:ARG:HD2	1.80	0.62
1:C:248:ASN:OD1	1:C:249:ALA:N	2.32	0.62
1:A:169:ILE:CD1	1:A:178:ARG:HD2	2.24	0.62
1:A:190:THR:HG22	1:A:193:GLN:CA	2.28	0.62
1:C:169:ILE:CD1	1:C:178:ARG:CD	2.76	0.62
1:D:104:ALA:CB	1:D:105:PRO:HD2	2.19	0.62
1:A:235:THR:H	1:A:238:GLN:NE2	1.96	0.62
1:B:149:ASP:HA	1:B:407:LEU:O	2.00	0.62
1:D:61:TYR:CE1	1:D:334:GLN:HG3	2.34	0.62
1:C:396:LYS:HE2	1:C:399:SER:HB2	1.81	0.62
1:D:133:ARG:HH12	1:D:164:CYS:HB2	1.62	0.62
1:B:159:SER:CB	1:B:255:THR:HG22	2.29	0.62
1:C:110:TYR:HD1	1:C:113:MET:CE	2.10	0.62
1:C:241:SER:O	1:C:245:ILE:HG13	1.99	0.62
1:D:222:SER:O	1:D:226:THR:OG1	2.16	0.62
1:D:291:ARG:HG3	1:D:292:VAL:N	2.14	0.62
1:A:169:ILE:HG21	1:A:178:ARG:HD3	1.82	0.62
1:A:202:PHE:CD1	1:A:240:LEU:HD12	2.33	0.62
1:C:32:PRO:HG2	1:C:35:TYR:CE1	2.35	0.62
1:B:86:GLY:HA3	1:B:89:GLU:HG3	1.82	0.62
1:A:108:THR:O	1:A:112:ARG:HB2	2.00	0.62
1:D:57:VAL:CG2	1:D:322:ILE:CD1	2.69	0.61
1:C:122:ARG:HG2	1:C:122:ARG:HH11	1.64	0.61
1:D:110:TYR:HD1	1:D:113:MET:HE2	1.65	0.61
1:A:71:PRO:CB	1:C:71:PRO:HB3	2.30	0.61
1:D:149:ASP:OD2	1:D:407:LEU:N	2.28	0.61
1:B:125:ALA:O	1:B:128:PRO:HD2	2.00	0.61
1:C:234:VAL:HA	1:C:238:GLN:NE2	2.16	0.61
1:D:190:THR:HB	1:D:193:GLN:HB2	1.82	0.61
1:A:21:PHE:CB	1:A:22:PRO:HD3	2.29	0.61
1:D:396:LYS:HD2	1:D:399:SER:HB2	1.82	0.61
1:B:18:PRO:O	1:B:48:THR:OG1	2.15	0.61
1:D:73:VAL:CG2	1:D:308:ILE:CD1	2.78	0.61
1:C:386:LEU:CD2	1:C:408:MET:O	2.44	0.61
1:D:190:THR:HG23	1:D:194:VAL:HG23	1.81	0.61
1:D:182:ARG:HE	1:D:251:ARG:HD3	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:107:HIS:CD2	1:B:358:HIS:NE2	2.69	0.61
1:D:410:THR:HG22	1:D:411:TRP:H	1.64	0.61
1:B:223:LYS:O	1:B:227:ASP:HB2	2.00	0.61
1:C:316:PRO:HG2	1:C:319:ASP:CG	2.20	0.61
1:D:46:ARG:NH2	1:D:54:GLU:HB3	2.16	0.61
1:B:230:VAL:CB	1:B:231:PRO:HD3	2.29	0.61
1:C:297:ASP:OD2	1:C:326:ALA:HB2	2.00	0.61
1:C:406:GLU:O	1:C:407:LEU:HD23	2.00	0.61
1:A:295:VAL:HG13	1:A:402:PHE:O	2.00	0.61
1:B:217:ARG:HG2	1:B:217:ARG:HH11	1.65	0.61
1:A:335:PHE:O	1:A:338:PRO:HD3	1.99	0.61
1:A:149:ASP:HA	1:A:407:LEU:O	2.01	0.61
1:C:52:ARG:HH11	1:C:52:ARG:CG	2.14	0.61
1:A:92:ALA:HA	1:A:95:ARG:HG3	1.82	0.61
1:A:176:PHE:O	1:A:180:VAL:CG2	2.49	0.61
1:B:301:LEU:CD2	1:B:322:ILE:HG12	2.30	0.61
1:B:73:VAL:HG23	1:B:308:ILE:HD13	1.82	0.61
1:C:138:LEU:HD23	1:C:141:MET:CE	2.31	0.60
1:A:410:THR:HG22	1:A:411:TRP:H	1.66	0.60
1:C:44:VAL:O	1:C:44:VAL:HG12	2.00	0.60
1:C:235:THR:H	1:C:238:GLN:NE2	2.00	0.60
1:A:92:ALA:C	1:A:95:ARG:HG3	2.21	0.60
1:C:138:LEU:CD2	1:C:141:MET:HE2	2.29	0.60
1:D:145:GLY:HA2	1:D:411:TRP:CZ2	2.37	0.60
1:D:138:LEU:CD2	1:D:141:MET:HE2	2.31	0.60
1:B:73:VAL:HG22	1:B:308:ILE:HD12	1.84	0.60
1:A:202:PHE:HD1	1:A:240:LEU:CD1	2.12	0.60
1:C:95:ARG:NH2	1:C:96:PHE:O	2.33	0.60
1:C:291:ARG:HG3	1:C:292:VAL:N	2.15	0.60
1:A:383:THR:HG21	1:A:412:HIS:CB	2.14	0.60
1:A:264:LEU:O	1:A:264:LEU:HD12	2.00	0.60
1:D:250:GLY:CA	2:D:501:HEM:HBC2	2.18	0.60
1:D:234:VAL:HG13	1:D:238:GLN:NE2	2.16	0.60
1:C:190:THR:HG21	1:C:193:GLN:HG2	1.84	0.60
1:C:205:LEU:O	1:C:209:VAL:HG23	2.01	0.60
1:D:21:PHE:HB2	1:D:47:VAL:CG2	2.31	0.60
1:B:253:THR:CG2	1:B:401:THR:HG21	2.32	0.60
1:A:95:ARG:CZ	1:A:95:ARG:HB2	2.30	0.60
1:B:390:ARG:HH11	1:B:393:VAL:HG21	1.67	0.60
1:C:75:ALA:HB2	1:C:358:HIS:HE1	1.64	0.60
1:D:82:PHE:HD1	1:D:83:PRO:N	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:95:ARG:NE	1:D:96:PHE:O	2.33	0.60
1:C:82:PHE:CD1	1:C:83:PRO:HD2	2.36	0.60
1:A:239:LEU:C	1:A:239:LEU:HD23	2.22	0.60
1:D:316:PRO:O	1:D:319:ASP:HB2	2.01	0.60
1:B:190:THR:HG22	1:B:193:GLN:CB	2.32	0.60
1:D:264:LEU:HD23	1:D:289:LEU:HD21	1.82	0.60
1:D:394:VAL:CG1	1:D:405:GLU:CB	2.80	0.60
1:C:111:ARG:NH2	1:C:359:GLN:O	2.34	0.60
1:C:299:ILE:HD12	1:C:401:THR:HG22	1.79	0.60
1:B:291:ARG:HG3	1:B:292:VAL:N	2.16	0.60
1:D:190:THR:HG1	1:D:192:GLU:HG3	1.66	0.60
1:A:162:VAL:HG11	1:A:369:GLU:HG3	1.83	0.60
1:A:159:SER:O	1:A:163:ILE:HG13	2.02	0.60
1:C:95:ARG:CD	1:C:97:ARG:HD3	2.31	0.59
1:B:173:ASP:O	1:B:174:LEU:HD23	2.00	0.59
1:B:115:LEU:HD23	1:B:361:VAL:HG13	1.84	0.59
1:C:113:MET:SD	1:C:228:HIS:CE1	2.95	0.59
1:D:77:ILE:CA	1:D:82:PHE:CD2	2.70	0.59
1:D:290:LEU:HD13	1:D:353:PHE:CE2	2.37	0.59
1:D:302:ARG:HH11	1:D:302:ARG:CG	2.15	0.59
1:D:178:ARG:NH1	1:D:178:ARG:HG2	2.17	0.59
1:B:78:ARG:HD3	1:B:97:ARG:HE	1.66	0.59
1:A:301:LEU:CD2	1:A:322:ILE:HG12	2.31	0.59
1:D:189:SER:C	1:D:190:THR:HG22	2.23	0.59
1:B:123:VAL:CG2	1:B:365:LEU:HD12	2.31	0.59
1:A:316:PRO:O	1:A:319:ASP:HB2	2.02	0.59
1:C:63:ASP:O	1:C:67:LEU:HB2	2.02	0.59
1:C:238:GLN:O	1:C:242:THR:HG23	2.02	0.59
1:C:316:PRO:O	1:C:319:ASP:HB2	2.01	0.59
1:D:174:LEU:CD1	1:D:204:LEU:HD21	2.32	0.59
1:C:77:ILE:CA	1:C:82:PHE:HD2	2.13	0.59
1:A:59:THR:HG23	1:A:324:LEU:HD23	1.84	0.59
1:D:49:LEU:HD11	1:D:84:ALA:O	1.96	0.59
1:D:84:ALA:CB	1:D:89:GLU:HB2	2.30	0.59
1:D:122:ARG:HH11	1:D:122:ARG:CG	2.16	0.59
1:C:234:VAL:HA	1:C:238:GLN:HE22	1.67	0.59
1:A:336:ASP:O	1:A:345:ARG:NH2	2.35	0.59
1:B:243:LEU:O	1:B:247:ILE:HG13	2.03	0.59
1:B:111:ARG:HD2	2:B:501:HEM:O2D	2.02	0.59
1:B:20:ASP:N	1:B:20:ASP:OD2	2.24	0.59
1:C:209:VAL:HG13	1:C:225:VAL:CG2	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:307:ASP:N	1:A:307:ASP:OD2	2.35	0.59
1:B:117:ALA:O	1:B:122:ARG:HD3	2.03	0.59
1:C:77:ILE:HD12	1:C:82:PHE:CE2	2.37	0.59
1:A:381:VAL:O	1:A:381:VAL:HG12	2.02	0.59
1:A:182:ARG:HH22	1:A:248:ASN:HD21	1.51	0.59
1:B:368:LEU:O	1:B:368:LEU:HD12	2.03	0.58
1:C:263:LEU:HD12	1:C:404:LEU:HD11	1.84	0.58
1:B:52:ARG:HH11	1:B:52:ARG:CG	2.16	0.58
1:D:21:PHE:HB2	1:D:47:VAL:HB	1.85	0.58
1:B:52:ARG:HG3	1:B:52:ARG:HH11	1.68	0.58
1:C:92:ALA:O	1:C:97:ARG:HG2	2.03	0.58
1:B:235:THR:H	1:B:238:GLN:HE21	1.51	0.58
1:D:291:ARG:O	1:D:294:SER:OG	2.21	0.58
1:B:190:THR:O	1:B:190:THR:HG22	2.03	0.58
1:C:281:LEU:HD13	1:C:343:PHE:HB3	1.86	0.58
1:D:95:ARG:HD3	1:D:95:ARG:O	2.03	0.58
1:C:368:LEU:C	1:C:368:LEU:HD12	2.24	0.58
1:D:253:THR:HG23	1:D:401:THR:HG21	1.84	0.58
1:C:301:LEU:O	1:C:302:ARG:HG2	2.03	0.58
1:B:202:PHE:HD1	1:B:240:LEU:HD12	1.68	0.58
1:A:389:GLU:OE2	1:A:390:ARG:N	2.36	0.58
1:D:260:LEU:HD11	1:D:402:PHE:HE1	1.68	0.58
1:A:103:ASP:O	1:A:104:ALA:HB3	2.04	0.58
1:A:309:GLU:O	1:A:310:LEU:HD23	2.04	0.58
1:A:220:LEU:CD2	1:A:224:LEU:HG	2.33	0.58
1:C:82:PHE:HD1	1:C:83:PRO:N	2.02	0.58
1:D:242:THR:O	1:D:246:THR:HG23	2.03	0.58
1:D:307:ASP:HB3	1:D:316:PRO:HA	1.86	0.58
1:C:167:LEU:O	1:C:221:ILE:HG13	2.04	0.58
1:D:248:ASN:OD1	1:D:249:ALA:N	2.37	0.58
1:C:36:ALA:O	1:C:40:THR:OG1	2.22	0.58
1:D:178:ARG:HG2	1:D:178:ARG:HH11	1.69	0.58
1:C:76:ASP:OD1	1:C:78:ARG:HD2	2.03	0.58
1:D:173:ASP:HB3	1:D:174:LEU:HD23	1.86	0.58
1:C:99:PHE:CD1	1:C:100:ILE:N	2.71	0.57
1:D:234:VAL:HG13	1:D:238:GLN:HB3	1.86	0.57
1:D:149:ASP:HA	1:D:407:LEU:O	2.04	0.57
1:B:230:VAL:HB	1:B:231:PRO:HD3	1.84	0.57
1:A:176:PHE:O	1:A:180:VAL:HG22	2.04	0.57
1:D:76:ASP:O	1:D:82:PHE:CD2	2.57	0.57
1:B:73:VAL:CG2	1:B:308:ILE:HD13	2.33	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:99:PHE:CB	1:D:110:TYR:HD2	2.14	0.57
1:B:190:THR:CG2	1:B:193:GLN:CB	2.83	0.57
1:D:121:ARG:CG	1:D:121:ARG:HH11	2.08	0.57
1:B:234:VAL:CG1	1:B:238:GLN:HB2	2.34	0.57
1:B:390:ARG:O	1:B:391:ASP:OD2	2.22	0.57
1:B:70:ASP:OD1	1:B:72:ARG:N	2.32	0.57
1:C:75:ALA:HB2	1:C:358:HIS:CE1	2.38	0.57
1:C:408:MET:O	1:C:408:MET:HG2	2.04	0.57
1:A:92:ALA:CA	1:A:95:ARG:HG3	2.34	0.57
1:C:23:ILE:HD13	1:C:34:GLU:HG3	1.85	0.57
1:B:207:GLY:O	1:B:211:GLU:HB2	2.04	0.57
1:D:251:ARG:NH1	1:D:251:ARG:HG2	2.19	0.57
1:D:379:ARG:NH1	1:D:379:ARG:HG2	2.17	0.57
1:C:65:ARG:O	1:C:69:SER:OG	2.23	0.57
1:A:104:ALA:CB	1:A:105:PRO:HD2	2.29	0.57
1:C:171:ARG:CD	1:C:172:HIS:ND1	2.59	0.57
1:A:381:VAL:HG11	1:A:384:LEU:HB2	1.86	0.57
1:A:174:LEU:N	1:A:174:LEU:HD23	2.20	0.57
1:B:104:ALA:CB	1:B:105:PRO:HD2	2.26	0.57
1:A:65:ARG:O	1:A:69:SER:CB	2.53	0.57
1:D:75:ALA:HB3	1:D:358:HIS:HE1	1.69	0.57
1:B:103:ASP:O	1:B:104:ALA:HB3	2.05	0.57
1:A:410:THR:HG22	1:A:411:TRP:N	2.19	0.57
1:A:65:ARG:O	1:A:69:SER:HB3	2.05	0.57
1:B:260:LEU:HD11	1:B:402:PHE:CE1	2.39	0.57
1:C:227:ASP:C	1:C:228:HIS:HD2	2.08	0.56
1:A:368:LEU:HD12	1:A:372:VAL:CG2	2.35	0.56
1:A:21:PHE:O	1:A:23:ILE:CG1	2.53	0.56
1:D:282:MET:O	1:D:286:VAL:HG23	2.05	0.56
1:C:317:ALA:O	1:C:318:ASP:HB2	2.04	0.56
1:A:186:SER:O	1:A:187:ARG:HB2	2.05	0.56
1:B:150:LEU:HD12	1:B:409:VAL:HG21	1.86	0.56
1:B:163:ILE:O	1:B:167:LEU:HB2	2.04	0.56
1:D:297:ASP:O	1:D:299:ILE:N	2.35	0.56
1:A:300:PRO:HB3	2:A:501:HEM:O1A	2.06	0.56
1:D:99:PHE:HD1	1:D:99:PHE:H	1.54	0.56
1:C:73:VAL:HG22	1:C:308:ILE:CD1	2.35	0.56
1:C:103:ASP:O	1:C:104:ALA:HB3	2.05	0.56
1:B:383:THR:O	1:B:383:THR:HG22	2.04	0.56
1:C:138:LEU:HD23	1:C:141:MET:HE3	1.87	0.56
1:B:129:ALA:O	1:B:133:ARG:HG3	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:175:GLU:HA	1:C:178:ARG:HB2	1.88	0.56
1:A:288:GLU:OE2	1:A:345:ARG:HG3	2.04	0.56
1:A:44:VAL:HG12	1:A:44:VAL:O	2.06	0.56
1:C:61:TYR:CE1	1:C:334:GLN:HG3	2.41	0.56
1:D:301:LEU:CD2	1:D:322:ILE:CG2	2.74	0.56
1:A:383:THR:CG2	1:A:412:HIS:H	2.18	0.56
1:A:21:PHE:O	1:A:23:ILE:HG12	2.05	0.56
1:D:257:MET:HE1	1:D:290:LEU:HA	1.87	0.56
1:A:222:SER:O	1:A:226:THR:OG1	2.24	0.56
1:D:167:LEU:CD2	1:D:221:ILE:HG13	2.35	0.56
1:C:84:ALA:HB1	1:C:89:GLU:HB2	1.86	0.56
1:C:159:SER:CB	1:C:255:THR:HG22	2.35	0.56
1:C:209:VAL:HG13	1:C:225:VAL:HG22	1.87	0.56
1:C:45:ALA:O	1:C:57:VAL:HG12	2.06	0.56
1:A:382:PRO:HB2	1:B:382:PRO:HB2	1.88	0.56
1:B:56:TRP:O	1:B:321:VAL:HA	2.06	0.56
1:C:99:PHE:CE1	1:C:100:ILE:CG1	2.87	0.56
1:A:104:ALA:CB	1:A:105:PRO:CD	2.81	0.56
1:C:138:LEU:HD22	1:C:141:MET:HE3	1.86	0.56
1:A:46:ARG:HB2	1:A:56:TRP:CZ3	2.39	0.56
1:C:137:ILE:HD13	1:C:157:ALA:CB	2.36	0.56
1:D:76:ASP:O	1:D:82:PHE:HD2	1.89	0.55
1:B:288:GLU:OE2	1:B:345:ARG:HD2	2.06	0.55
1:A:78:ARG:HH11	1:A:78:ARG:CG	2.19	0.55
1:D:124:ARG:HG3	1:D:124:ARG:NH1	2.21	0.55
1:D:25:ARG:HD3	1:D:402:PHE:CD2	2.41	0.55
1:C:98:PRO:HB3	1:C:245:ILE:HD11	1.86	0.55
1:B:179:ASP:O	1:B:183:ILE:HD12	2.06	0.55
1:B:104:ALA:CB	1:B:105:PRO:CD	2.82	0.55
1:B:171:ARG:O	1:B:175:GLU:HB2	2.07	0.55
1:D:296:ALA:O	1:D:299:ILE:HG12	2.06	0.55
1:D:173:ASP:HB3	1:D:174:LEU:CG	2.36	0.55
1:C:261:SER:O	1:C:264:LEU:HB3	2.06	0.55
1:C:297:ASP:OD1	1:C:298:SER:N	2.39	0.55
1:A:253:THR:HB	2:A:501:HEM:HBB2	1.88	0.55
1:D:261:SER:HB3	1:D:289:LEU:HD13	1.87	0.55
1:C:57:VAL:HG22	1:C:324:LEU:HD22	1.88	0.55
1:C:21:PHE:HB2	1:C:47:VAL:HB	1.89	0.55
1:A:301:LEU:HD23	1:A:322:ILE:HG23	1.86	0.55
1:C:227:ASP:HB3	1:C:228:HIS:HD2	1.72	0.55
1:B:234:VAL:HG13	1:B:238:GLN:NE2	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:ARG:NH2	1:A:248:ASN:ND2	2.55	0.55
1:D:260:LEU:O	1:D:260:LEU:HD23	2.06	0.55
1:D:174:LEU:HD13	1:D:204:LEU:HD21	1.88	0.55
1:C:168:GLY:O	1:C:212:ARG:NH2	2.39	0.55
1:C:132:ALA:HA	3:C:624:HOH:O	2.07	0.55
1:A:32:PRO:HG2	1:A:35:TYR:CE1	2.42	0.55
1:B:174:LEU:HD13	1:B:204:LEU:HD11	1.88	0.55
1:D:169:ILE:HD13	1:D:208:LEU:CD1	2.37	0.55
1:B:133:ARG:O	1:B:137:ILE:HG13	2.07	0.55
1:A:70:ASP:OD1	1:A:71:PRO:HD2	2.06	0.55
1:B:368:LEU:HD12	1:B:372:VAL:HG23	1.89	0.55
1:A:123:VAL:HG22	1:A:365:LEU:HD12	1.89	0.55
1:C:188:ASN:OD1	1:C:188:ASN:N	2.38	0.55
1:A:130:VAL:O	1:A:134:VAL:HG23	2.07	0.55
1:C:56:TRP:NE1	1:C:316:PRO:HD2	2.22	0.54
1:C:386:LEU:HD23	1:C:387:ALA:H	1.73	0.54
1:B:73:VAL:HG23	1:B:308:ILE:HD11	1.86	0.54
1:C:149:ASP:CG	1:C:406:GLU:HG2	2.27	0.54
1:C:159:SER:HB2	1:C:255:THR:HG22	1.88	0.54
1:D:212:ARG:O	1:D:216:PRO:HB3	2.07	0.54
1:A:73:VAL:CG1	1:A:302:ARG:HB3	2.38	0.54
1:B:217:ARG:CG	1:B:217:ARG:HH11	2.20	0.54
1:B:59:THR:HG23	1:B:324:LEU:HD23	1.90	0.54
1:A:56:TRP:HE1	1:A:316:PRO:HD2	1.71	0.54
1:C:59:THR:HG22	1:C:327:GLY:HA3	1.89	0.54
1:C:299:ILE:H	1:C:300:PRO:HD3	1.72	0.54
1:D:173:ASP:O	1:D:174:LEU:HD23	2.06	0.54
1:B:36:ALA:O	1:B:40:THR:HG23	2.06	0.54
1:A:73:VAL:HG23	1:A:308:ILE:HD11	1.86	0.54
1:B:115:LEU:N	1:B:116:PRO:HD2	2.21	0.54
1:C:73:VAL:CG2	1:C:308:ILE:HD13	2.38	0.54
1:A:256:SER:O	1:A:260:LEU:HB2	2.08	0.54
1:B:64:VAL:HG13	1:B:323:ALA:HB1	1.90	0.54
1:D:217:ARG:NH1	1:D:217:ARG:HG2	2.22	0.54
1:B:21:PHE:O	1:B:23:ILE:HG12	2.08	0.54
1:A:136:GLU:OE2	1:A:171:ARG:NH1	2.41	0.54
1:B:177:PHE:O	1:B:180:VAL:HG23	2.08	0.54
1:A:126:MET:O	1:A:130:VAL:HG23	2.08	0.54
1:C:139:ASP:OD1	1:C:380:ARG:NH1	2.38	0.54
1:D:103:ASP:O	1:D:104:ALA:HB3	2.08	0.54
1:A:296:ALA:HB1	1:A:299:ILE:HG12	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:234:VAL:HG13	1:B:238:GLN:CB	2.38	0.54
1:D:227:ASP:HB3	1:D:228:HIS:CD2	2.43	0.53
1:C:57:VAL:CG2	1:C:324:LEU:HD21	2.39	0.53
1:C:65:ARG:HD2	1:C:355:TYR:CE1	2.44	0.53
1:C:142:LEU:HA	1:C:411:TRP:CZ2	2.44	0.53
1:B:21:PHE:O	1:B:23:ILE:CG1	2.56	0.53
1:D:390:ARG:O	1:D:391:ASP:HB2	2.09	0.53
1:B:234:VAL:HG12	1:B:235:THR:O	2.08	0.53
1:C:126:MET:O	1:C:130:VAL:HG23	2.09	0.53
1:C:361:VAL:HG23	2:C:501:HEM:HBD2	1.90	0.53
1:D:251:ARG:HH11	1:D:251:ARG:CG	2.20	0.53
1:A:77:ILE:HG23	1:A:97:ARG:HG2	1.88	0.53
1:D:234:VAL:CG1	1:D:238:GLN:CB	2.85	0.53
1:B:301:LEU:HD23	1:B:322:ILE:HG23	1.90	0.53
1:C:21:PHE:CD2	1:C:21:PHE:C	2.80	0.53
1:D:44:VAL:CG2	1:D:313:ARG:HB2	2.35	0.53
1:C:313:ARG:CG	1:C:313:ARG:HH11	2.15	0.53
1:D:229:LEU:HD12	1:D:234:VAL:O	2.09	0.53
1:B:386:LEU:HD23	1:B:408:MET:O	2.09	0.53
1:C:227:ASP:C	1:C:228:HIS:CD2	2.81	0.53
1:C:25:ARG:HD3	1:C:402:PHE:CD2	2.43	0.53
1:D:21:PHE:CD2	1:D:21:PHE:C	2.82	0.53
1:A:138:LEU:O	1:A:142:LEU:HB2	2.08	0.53
1:D:410:THR:CG2	1:D:411:TRP:N	2.71	0.53
1:B:235:THR:H	1:B:238:GLN:NE2	2.06	0.53
1:B:390:ARG:O	1:B:391:ASP:CG	2.47	0.53
1:C:46:ARG:NH2	1:C:54:GLU:HB3	2.23	0.53
1:D:104:ALA:CB	1:D:105:PRO:CD	2.81	0.53
1:C:368:LEU:HD12	1:C:372:VAL:CG2	2.39	0.53
1:C:149:ASP:HA	1:C:407:LEU:O	2.09	0.53
1:D:149:ASP:OD1	1:D:406:GLU:HG2	2.09	0.53
1:D:260:LEU:HD11	1:D:402:PHE:CE1	2.43	0.53
1:D:374:LEU:O	1:D:378:LEU:HG	2.08	0.53
1:C:410:THR:HG22	1:C:411:TRP:N	2.25	0.52
1:C:167:LEU:HD11	1:C:247:ILE:HD11	1.91	0.52
1:A:73:VAL:HG22	1:A:308:ILE:CD1	2.39	0.52
1:B:336:ASP:O	1:B:345:ARG:NH2	2.42	0.52
1:D:138:LEU:HD13	1:D:380:ARG:HG3	1.92	0.52
1:C:190:THR:CG2	1:C:193:GLN:CB	2.86	0.52
1:B:190:THR:CG2	1:B:193:GLN:HB2	2.39	0.52
1:C:172:HIS:O	1:C:173:ASP:C	2.48	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:242:THR:O	1:C:246:THR:HG23	2.09	0.52
1:C:57:VAL:O	1:C:57:VAL:HG13	2.09	0.52
1:A:56:TRP:HB2	1:A:321:VAL:HG13	1.92	0.52
1:D:82:PHE:CD1	1:D:83:PRO:CD	2.92	0.52
1:D:95:ARG:HE	1:D:95:ARG:C	2.13	0.52
1:D:381:VAL:HG12	1:D:384:LEU:CB	2.37	0.52
1:B:21:PHE:HB3	1:B:22:PRO:CD	2.31	0.52
1:B:302:ARG:HH11	1:B:302:ARG:CG	2.15	0.52
1:A:389:GLU:HB3	1:A:392:GLN:HG3	1.91	0.52
1:C:301:LEU:CD2	1:C:322:ILE:HG23	2.27	0.52
1:D:395:VAL:CG1	1:D:396:LYS:H	2.16	0.52
1:B:410:THR:CG2	1:B:411:TRP:N	2.72	0.52
1:B:190:THR:CG2	1:B:193:GLN:HB3	2.39	0.52
1:B:71:PRO:HB3	1:D:71:PRO:HB3	1.91	0.52
1:C:368:LEU:O	1:C:372:VAL:HG23	2.10	0.52
1:D:256:SER:OG	1:D:403:GLY:CA	2.58	0.52
1:B:315:VAL:O	1:B:315:VAL:HG23	2.09	0.52
1:A:317:ALA:O	1:A:318:ASP:HB2	2.08	0.52
1:D:44:VAL:HG23	1:D:313:ARG:HG3	1.90	0.52
1:B:137:ILE:HD13	1:B:157:ALA:HB1	1.92	0.52
1:B:39:ARG:O	1:B:60:ARG:NE	2.33	0.52
1:C:91:GLU:HG2	1:C:91:GLU:O	2.07	0.52
1:B:183:ILE:O	1:B:187:ARG:HD3	2.10	0.52
1:C:299:ILE:N	1:C:300:PRO:HD3	2.24	0.52
1:A:133:ARG:NH1	1:A:161:SER:O	2.43	0.52
1:C:353:PHE:HB3	1:C:360:CYS:HB3	1.92	0.52
1:A:312:GLY:HA3	3:A:616:HOH:O	2.10	0.52
1:C:368:LEU:CD1	1:C:372:VAL:CG2	2.88	0.52
1:C:386:LEU:HD23	1:C:387:ALA:N	2.25	0.52
1:D:176:PHE:O	1:D:180:VAL:CG2	2.46	0.52
1:A:117:ALA:O	1:A:122:ARG:HD2	2.10	0.52
1:D:182:ARG:HE	1:D:251:ARG:CD	2.23	0.52
1:D:261:SER:O	1:D:264:LEU:HB3	2.10	0.52
1:B:268:ARG:O	1:B:272:PRO:HD2	2.10	0.52
1:D:302:ARG:NH2	1:D:358:HIS:CB	2.73	0.51
1:D:377:LEU:O	1:D:377:LEU:HD12	2.10	0.51
1:B:51:THR:O	1:B:52:ARG:HB2	2.10	0.51
1:B:21:PHE:CB	1:B:22:PRO:CD	2.89	0.51
1:C:251:ARG:NH1	1:C:251:ARG:HG2	2.25	0.51
1:A:177:PHE:O	1:A:180:VAL:HG23	2.09	0.51
1:D:95:ARG:CZ	1:D:97:ARG:HH11	2.23	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:99:PHE:CB	1:C:110:TYR:CD2	2.88	0.51
1:D:138:LEU:CD1	1:D:380:ARG:HG3	2.40	0.51
1:A:238:GLN:O	1:A:241:SER:OG	2.26	0.51
1:D:124:ARG:HH11	1:D:124:ARG:CG	2.22	0.51
1:A:122:ARG:HH11	1:A:122:ARG:HG3	1.74	0.51
1:B:288:GLU:OE2	1:B:345:ARG:HG3	2.11	0.51
1:D:227:ASP:C	1:D:228:HIS:CD2	2.84	0.51
1:D:77:ILE:HD12	1:D:82:PHE:CE2	2.46	0.51
1:D:256:SER:O	1:D:260:LEU:HB2	2.11	0.51
1:B:44:VAL:HG12	1:B:44:VAL:O	2.11	0.51
1:D:256:SER:OG	1:D:403:GLY:HA2	2.10	0.51
1:B:46:ARG:NH1	1:B:56:TRP:NE1	2.59	0.51
1:D:220:LEU:HD22	1:D:220:LEU:O	2.10	0.51
1:C:234:VAL:CA	1:C:238:GLN:NE2	2.74	0.51
1:C:84:ALA:CB	1:C:89:GLU:OE1	2.50	0.51
1:D:78:ARG:HH11	1:D:78:ARG:CG	2.10	0.51
1:D:99:PHE:CE1	1:D:100:ILE:HG13	2.46	0.51
1:C:260:LEU:HD11	1:C:402:PHE:CE1	2.37	0.51
1:B:57:VAL:HG22	1:B:324:LEU:HD11	1.93	0.51
1:A:315:VAL:O	1:A:315:VAL:HG23	2.11	0.51
1:B:381:VAL:O	1:B:381:VAL:HG12	2.10	0.51
1:B:120:VAL:O	1:B:124:ARG:HB2	2.11	0.51
1:D:96:PHE:HD1	1:D:96:PHE:N	2.08	0.50
1:D:175:GLU:O	1:D:179:ASP:HB2	2.11	0.50
1:D:208:LEU:O	1:D:212:ARG:HG2	2.11	0.50
1:A:57:VAL:HG23	1:A:322:ILE:HB	1.93	0.50
1:D:138:LEU:CD2	1:D:141:MET:HE3	2.37	0.50
1:A:137:ILE:HD13	1:A:157:ALA:HB1	1.94	0.50
1:B:347:ASP:OD1	3:B:610:HOH:O	2.18	0.50
1:C:49:LEU:HD11	1:C:84:ALA:O	2.07	0.50
1:B:169:ILE:HD13	1:B:178:ARG:HD2	1.88	0.50
1:B:395:VAL:HG23	1:B:395:VAL:O	2.10	0.50
1:B:77:ILE:HG13	1:B:77:ILE:O	2.11	0.50
1:B:73:VAL:CG2	1:B:308:ILE:HD11	2.34	0.50
1:C:395:VAL:O	1:C:396:LYS:HG2	2.11	0.50
1:B:390:ARG:HH11	1:B:393:VAL:CG2	2.24	0.50
1:C:52:ARG:NH1	1:C:52:ARG:CG	2.74	0.50
1:D:133:ARG:HH11	1:D:161:SER:C	2.11	0.50
1:D:361:VAL:HG23	2:D:501:HEM:HBD2	1.94	0.50
1:D:52:ARG:N	1:D:52:ARG:HD2	2.26	0.50
1:D:413:HIS:CG	1:D:414:HIS:N	2.79	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:260:LEU:O	1:C:260:LEU:HD23	2.11	0.50
1:B:296:ALA:O	1:B:299:ILE:HG12	2.11	0.50
1:A:365:LEU:O	1:A:369:GLU:HB2	2.10	0.50
1:A:107:HIS:CD2	1:A:358:HIS:CD2	3.00	0.50
1:B:234:VAL:HG13	1:B:238:GLN:HB2	1.94	0.50
1:D:271:LEU:O	1:D:274:GLU:HB2	2.11	0.50
1:C:95:ARG:CD	1:C:97:ARG:HG2	2.40	0.50
1:C:98:PRO:HB2	1:C:245:ILE:CD1	2.28	0.50
1:C:77:ILE:HD12	1:C:82:PHE:CD2	2.47	0.50
1:D:99:PHE:N	1:D:99:PHE:CD1	2.79	0.50
1:D:34:GLU:H	1:D:34:GLU:CD	2.14	0.50
1:A:182:ARG:NH2	1:A:248:ASN:HD21	2.10	0.50
1:D:78:ARG:O	1:D:90:GLN:NE2	2.45	0.50
1:B:241:SER:O	1:B:245:ILE:HD12	2.12	0.50
1:C:149:ASP:OD2	1:C:406:GLU:HG2	2.12	0.49
1:B:93:GLY:C	1:B:95:ARG:HA	2.32	0.49
1:B:161:SER:O	1:B:164:CYS:HB2	2.11	0.49
1:C:52:ARG:NH1	1:C:52:ARG:HG3	2.26	0.49
1:B:193:GLN:HG3	1:B:196:GLU:HB3	1.94	0.49
1:A:353:PHE:CD1	1:A:363:GLN:HB3	2.46	0.49
1:D:50:PRO:HG3	1:D:85:LEU:O	2.12	0.49
1:C:408:MET:CE	1:C:408:MET:N	2.71	0.49
1:B:123:VAL:HG13	1:B:368:LEU:HD23	1.94	0.49
1:A:379:ARG:O	1:B:276:ARG:HD3	2.13	0.49
1:D:46:ARG:NH2	1:D:54:GLU:HB2	2.21	0.49
1:C:51:THR:O	1:C:52:ARG:HB2	2.10	0.49
1:A:395:VAL:HG23	1:A:395:VAL:O	2.12	0.49
1:C:169:ILE:HG21	1:C:178:ARG:HD3	1.92	0.49
1:C:299:ILE:N	1:C:300:PRO:CD	2.75	0.49
1:D:120:VAL:O	1:D:124:ARG:HB2	2.12	0.49
1:B:96:PHE:CD1	1:B:96:PHE:C	2.85	0.49
1:C:368:LEU:CD1	1:C:372:VAL:HG23	2.42	0.49
1:A:23:ILE:HD13	1:A:34:GLU:HG3	1.94	0.49
1:B:333:GLU:OE1	1:D:119:THR:HG21	2.13	0.49
1:A:68:LEU:CD2	1:A:302:ARG:NE	2.75	0.49
1:B:317:ALA:O	1:B:318:ASP:HB2	2.12	0.49
1:D:209:VAL:HG13	1:D:225:VAL:CG2	2.43	0.49
1:C:220:LEU:HD22	1:C:224:LEU:HG	1.94	0.49
1:C:21:PHE:CE1	1:C:322:ILE:HD13	2.48	0.49
1:B:290:LEU:HD13	1:B:353:PHE:HE2	1.77	0.49
1:C:57:VAL:CG2	1:C:324:LEU:CD2	2.90	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:21:PHE:HB2	1:C:47:VAL:CG2	2.43	0.49
1:A:34:GLU:H	1:A:34:GLU:CD	2.16	0.49
1:B:230:VAL:N	1:B:231:PRO:CD	2.76	0.49
1:A:65:ARG:HA	1:A:355:TYR:HD1	1.77	0.49
1:C:251:ARG:CG	1:C:251:ARG:HH11	2.26	0.49
1:D:96:PHE:CD1	1:D:96:PHE:N	2.78	0.48
1:A:177:PHE:CD2	1:A:177:PHE:C	2.85	0.48
1:B:56:TRP:HB2	1:B:321:VAL:HG13	1.93	0.48
1:A:120:VAL:HG11	1:C:347:ASP:OD2	2.12	0.48
1:D:299:ILE:N	1:D:300:PRO:CD	2.76	0.48
1:B:217:ARG:CG	1:B:217:ARG:NH1	2.74	0.48
1:C:190:THR:HG22	1:C:193:GLN:N	2.24	0.48
1:C:214:GLU:OE2	1:C:215:GLU:N	2.46	0.48
1:D:117:ALA:HA	1:D:122:ARG:HE	1.79	0.48
1:C:23:ILE:HG21	1:C:34:GLU:HG3	1.95	0.48
1:D:95:ARG:CZ	1:D:97:ARG:NH1	2.77	0.48
1:C:99:PHE:HD1	1:C:100:ILE:H	1.62	0.48
1:D:177:PHE:HD1	1:D:204:LEU:CD1	2.26	0.48
1:A:123:VAL:CG1	1:A:368:LEU:HD23	2.43	0.48
1:D:196:GLU:HA	1:D:196:GLU:OE1	2.14	0.48
1:D:269:PRO:O	1:D:272:PRO:HG2	2.13	0.48
1:C:113:MET:HG3	1:C:228:HIS:CE1	2.48	0.48
1:C:288:GLU:HA	1:C:288:GLU:OE2	2.14	0.48
1:D:20:ASP:HA	1:D:48:THR:HB	1.95	0.48
1:C:110:TYR:HD1	1:C:113:MET:HE1	1.78	0.48
1:B:21:PHE:CD2	1:B:21:PHE:C	2.84	0.48
1:B:390:ARG:HG3	1:B:391:ASP:N	2.27	0.48
1:B:176:PHE:O	1:B:180:VAL:HG22	2.13	0.48
1:D:302:ARG:CG	1:D:302:ARG:NH1	2.74	0.48
1:C:82:PHE:C	1:C:82:PHE:HD1	2.17	0.48
1:C:228:HIS:C	1:C:231:PRO:HD2	2.33	0.48
1:B:77:ILE:HD12	1:B:82:PHE:CE1	2.49	0.48
1:D:125:ALA:O	1:D:128:PRO:HD2	2.13	0.48
1:C:86:GLY:H	1:C:89:GLU:CD	2.17	0.48
1:D:95:ARG:CZ	1:D:96:PHE:O	2.62	0.48
1:A:78:ARG:CG	1:A:78:ARG:NH1	2.76	0.48
1:A:112:ARG:NH2	1:C:70:ASP:OD2	2.34	0.48
1:C:301:LEU:O	1:C:302:ARG:CG	2.61	0.48
1:A:133:ARG:HG2	1:A:171:ARG:NH2	2.29	0.48
1:D:73:VAL:HG23	1:D:308:ILE:CD1	2.44	0.48
1:D:271:LEU:HB3	1:D:343:PHE:HE2	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:408:MET:CE	1:C:408:MET:H	2.27	0.48
1:B:234:VAL:CG1	1:B:238:GLN:CB	2.92	0.48
1:B:304:ALA:O	1:B:318:ASP:N	2.34	0.48
1:A:201:LEU:HD23	1:A:201:LEU:O	2.13	0.48
1:B:389:GLU:HB3	1:B:392:GLN:HG3	1.96	0.48
1:B:335:PHE:O	1:B:338:PRO:HD3	2.13	0.47
1:C:386:LEU:HD22	1:C:388:GLY:H	1.77	0.47
1:A:167:LEU:HD21	1:A:243:LEU:HD22	1.96	0.47
1:C:353:PHE:HB3	1:C:360:CYS:CB	2.44	0.47
1:B:301:LEU:HD23	1:B:322:ILE:HG12	1.96	0.47
1:B:312:GLY:HA3	3:B:605:HOH:O	2.14	0.47
1:B:309:GLU:HG3	1:B:314:THR:HB	1.96	0.47
1:D:385:ARG:CG	1:D:386:LEU:N	2.70	0.47
1:A:21:PHE:C	1:A:21:PHE:CD2	2.85	0.47
1:A:21:PHE:CB	1:A:22:PRO:CD	2.92	0.47
1:B:107:HIS:NE2	1:B:358:HIS:NE2	2.62	0.47
1:C:21:PHE:HB2	1:C:47:VAL:CB	2.44	0.47
1:D:316:PRO:HG2	1:D:319:ASP:CG	2.35	0.47
1:A:389:GLU:CB	1:A:392:GLN:HG3	2.44	0.47
1:D:209:VAL:HG13	1:D:225:VAL:HG22	1.96	0.47
1:B:260:LEU:HD11	1:B:402:PHE:HE1	1.79	0.47
1:A:119:THR:OG1	1:C:333:GLU:OE1	2.21	0.47
1:C:245:ILE:O	1:C:248:ASN:OD1	2.32	0.47
1:D:77:ILE:CA	1:D:82:PHE:CE2	2.83	0.47
1:D:173:ASP:HB3	1:D:174:LEU:HG	1.96	0.47
1:A:21:PHE:HB3	1:A:22:PRO:CD	2.34	0.47
1:D:99:PHE:N	1:D:99:PHE:HD1	2.13	0.47
1:C:35:TYR:HA	1:C:38:LEU:HB2	1.97	0.47
1:A:57:VAL:HG22	1:A:324:LEU:CD1	2.44	0.47
1:B:170:PRO:HD2	1:B:174:LEU:HD12	1.97	0.47
1:A:174:LEU:HD13	1:A:204:LEU:HD21	1.96	0.47
1:A:92:ALA:CA	1:A:95:ARG:CG	2.87	0.47
1:A:364:HIS:HB2	3:A:601:HOH:O	2.14	0.47
1:C:76:ASP:O	1:C:82:PHE:CD2	2.67	0.47
1:C:301:LEU:C	1:C:302:ARG:CG	2.83	0.47
1:B:290:LEU:HD13	1:B:353:PHE:CE2	2.50	0.47
1:A:78:ARG:HD3	1:A:97:ARG:HE	1.80	0.47
1:C:190:THR:HG21	1:C:193:GLN:HB2	1.96	0.47
1:D:384:LEU:HD13	1:D:385:ARG:N	2.30	0.47
1:A:291:ARG:HG3	1:A:292:VAL:N	2.30	0.47
1:D:234:VAL:HA	1:D:238:GLN:NE2	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:202:PHE:HD1	1:C:240:LEU:CD1	2.28	0.47
1:D:21:PHE:HB2	1:D:47:VAL:CB	2.44	0.47
1:A:112:ARG:HH12	1:C:308:ILE:HG23	1.80	0.47
1:C:347:ASP:OD1	1:C:347:ASP:N	2.45	0.47
1:B:361:VAL:HG23	2:B:501:HEM:HBD2	1.97	0.47
1:A:260:LEU:HD11	1:A:402:PHE:CE1	2.49	0.47
1:D:64:VAL:HG13	1:D:323:ALA:HB1	1.96	0.47
1:D:384:LEU:C	1:D:384:LEU:CD1	2.83	0.46
1:B:163:ILE:CG2	1:B:167:LEU:HD12	2.42	0.46
1:A:361:VAL:HG12	1:A:361:VAL:O	2.15	0.46
1:C:122:ARG:HG2	1:C:122:ARG:NH1	2.29	0.46
1:C:402:PHE:CD1	1:C:402:PHE:C	2.88	0.46
1:B:146:GLY:O	1:B:148:VAL:HG23	2.15	0.46
1:D:34:GLU:OE1	1:D:34:GLU:N	2.47	0.46
1:D:97:ARG:HD2	1:D:97:ARG:HA	1.66	0.46
1:D:190:THR:OG1	1:D:193:GLN:HB2	2.15	0.46
1:D:251:ARG:HH11	1:D:251:ARG:HG2	1.80	0.46
1:C:42:ASP:OD1	1:C:45:ALA:HA	2.14	0.46
1:C:57:VAL:HG22	1:C:324:LEU:CD2	2.45	0.46
1:B:77:ILE:HA	1:B:82:PHE:CD2	2.51	0.46
1:A:386:LEU:HD23	1:A:408:MET:O	2.15	0.46
1:C:414:HIS:ND1	1:C:414:HIS:N	2.62	0.46
1:B:174:LEU:N	1:B:174:LEU:HD23	2.29	0.46
1:B:167:LEU:HD21	1:B:243:LEU:HD22	1.97	0.46
1:A:302:ARG:CG	1:A:302:ARG:NH1	2.70	0.46
1:A:149:ASP:OD2	1:A:407:LEU:O	2.34	0.46
1:C:67:LEU:O	1:C:67:LEU:HD22	2.15	0.46
1:A:61:TYR:C	1:A:61:TYR:CD1	2.89	0.46
1:D:82:PHE:C	1:D:82:PHE:CD1	2.87	0.46
1:C:110:TYR:CD1	1:C:113:MET:HE1	2.50	0.46
1:D:353:PHE:HB3	1:D:360:CYS:HB3	1.97	0.46
1:A:77:ILE:O	1:A:77:ILE:HG13	2.15	0.46
1:B:84:ALA:HB1	1:B:89:GLU:HB2	1.97	0.46
1:C:87:GLU:N	1:C:87:GLU:CD	2.69	0.46
1:C:97:ARG:HB3	1:C:98:PRO:HD2	1.97	0.46
1:D:164:CYS:SG	1:D:178:ARG:HD3	2.55	0.46
1:D:82:PHE:CD1	1:D:83:PRO:N	2.81	0.46
1:C:82:PHE:C	1:C:82:PHE:CD1	2.87	0.46
1:C:390:ARG:O	1:C:391:ASP:CB	2.62	0.46
1:A:382:PRO:CB	1:B:382:PRO:HB2	2.45	0.46
1:D:271:LEU:HB3	1:D:343:PHE:CE2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:84:ALA:CB	1:C:89:GLU:HB2	2.46	0.46
1:A:57:VAL:HG22	1:A:324:LEU:HD11	1.97	0.46
1:B:67:LEU:O	1:B:67:LEU:HD22	2.15	0.46
1:D:301:LEU:O	1:D:302:ARG:HG2	2.16	0.46
1:D:82:PHE:C	1:D:82:PHE:HD1	2.19	0.46
1:C:368:LEU:HD11	1:C:372:VAL:HG21	1.98	0.46
1:A:368:LEU:CD1	1:A:372:VAL:CG2	2.94	0.46
1:D:414:HIS:O	1:D:414:HIS:CD2	2.68	0.46
1:B:149:ASP:O	1:B:153:ALA:CB	2.63	0.46
1:B:149:ASP:O	1:B:153:ALA:HB3	2.16	0.46
1:C:73:VAL:CG2	1:C:308:ILE:CD1	2.94	0.46
1:C:234:VAL:CB	1:C:238:GLN:HE21	2.20	0.46
1:D:129:ALA:O	1:D:133:ARG:HG3	2.16	0.46
1:B:335:PHE:HB2	1:B:338:PRO:HB3	1.96	0.46
1:C:21:PHE:HB2	1:C:47:VAL:HG21	1.98	0.46
1:B:177:PHE:CD2	1:B:177:PHE:C	2.88	0.46
1:C:174:LEU:CD1	1:C:204:LEU:CD2	2.80	0.45
1:C:384:LEU:C	1:C:384:LEU:CD1	2.84	0.45
1:C:257:MET:CE	1:C:290:LEU:HD23	2.45	0.45
1:B:257:MET:HE2	1:B:295:VAL:HG23	1.99	0.45
1:C:133:ARG:HH12	1:C:164:CYS:HB2	1.81	0.45
1:D:263:LEU:O	1:D:263:LEU:HD23	2.15	0.45
1:D:110:TYR:CD1	1:D:113:MET:CE	2.94	0.45
1:D:229:LEU:HD22	1:D:239:LEU:HD13	1.98	0.45
1:D:73:VAL:HG22	1:D:308:ILE:CD1	2.45	0.45
1:C:100:ILE:O	1:C:100:ILE:HG22	2.15	0.45
1:D:189:SER:O	1:D:190:THR:HG22	2.17	0.45
1:B:21:PHE:HB2	1:B:47:VAL:HG21	1.97	0.45
1:C:137:ILE:HD13	1:C:157:ALA:HB1	1.99	0.45
1:A:36:ALA:O	1:A:40:THR:HG23	2.16	0.45
1:D:301:LEU:C	1:D:302:ARG:CG	2.85	0.45
1:A:384:LEU:C	1:A:384:LEU:CD1	2.85	0.45
1:D:110:TYR:CD1	1:D:113:MET:HE1	2.52	0.45
1:D:124:ARG:NH1	1:D:124:ARG:CG	2.75	0.45
1:C:73:VAL:HG22	1:C:308:ILE:HD13	1.96	0.45
1:B:390:ARG:O	1:B:391:ASP:CB	2.64	0.45
1:D:87:GLU:N	1:D:87:GLU:CD	2.70	0.45
1:D:74:SER:CA	1:D:103:ASP:OD2	2.65	0.45
1:B:175:GLU:O	1:B:179:ASP:HB2	2.16	0.45
1:A:384:LEU:C	1:A:384:LEU:HD13	2.37	0.45
1:D:234:VAL:HG12	1:D:238:GLN:CB	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:77:ILE:CA	1:D:82:PHE:HD2	2.23	0.45
1:B:182:ARG:HD3	1:B:247:ILE:HG21	1.98	0.45
1:B:96:PHE:O	1:B:96:PHE:CD1	2.70	0.45
1:A:181:THR:HG21	1:A:201:LEU:HB2	1.97	0.45
1:B:95:ARG:O	1:B:96:PHE:CD2	2.69	0.45
1:A:19:ARG:O	1:A:47:VAL:HA	2.16	0.45
1:B:198:LEU:O	1:B:202:PHE:HD2	2.00	0.45
1:B:174:LEU:CD1	1:B:204:LEU:HD21	2.47	0.45
1:D:78:ARG:NH2	3:D:606:HOH:O	2.50	0.45
1:B:73:VAL:CG1	1:B:302:ARG:HB3	2.47	0.45
1:C:353:PHE:CD1	1:C:363:GLN:HB3	2.52	0.45
1:D:21:PHE:O	1:D:23:ILE:HG13	2.16	0.45
1:D:393:VAL:CG1	1:D:407:LEU:CD2	2.95	0.45
1:D:36:ALA:O	1:D:40:THR:OG1	2.33	0.45
1:C:172:HIS:N	1:C:172:HIS:ND1	2.64	0.45
1:C:378:LEU:H	1:C:378:LEU:CD1	2.25	0.45
1:A:123:VAL:HG13	1:A:368:LEU:HD23	1.99	0.45
1:D:342:ASP:O	1:D:345:ARG:HG3	2.16	0.45
1:D:157:ALA:O	1:D:161:SER:HB2	2.17	0.45
1:D:111:ARG:HD2	2:D:501:HEM:O2D	2.17	0.45
1:A:34:GLU:CD	1:A:34:GLU:N	2.70	0.45
1:A:168:GLY:O	1:A:212:ARG:NH2	2.50	0.45
1:A:37:ALA:O	1:A:41:ASP:HB2	2.17	0.45
1:C:300:PRO:HB3	2:C:501:HEM:O1A	2.17	0.45
1:D:49:LEU:HB2	1:D:53:ARG:O	2.16	0.45
1:C:411:TRP:O	1:C:412:HIS:CG	2.70	0.45
1:D:99:PHE:CD2	1:D:110:TYR:CB	2.99	0.45
1:A:396:LYS:HG3	1:A:405:GLU:HB2	1.99	0.45
1:D:299:ILE:HD11	1:D:401:THR:HG22	1.99	0.44
1:C:110:TYR:CD1	1:C:113:MET:CE	2.97	0.44
1:D:225:VAL:O	1:D:230:VAL:HG23	2.17	0.44
1:D:95:ARG:NH2	1:D:96:PHE:O	2.50	0.44
1:A:23:ILE:HG21	1:A:34:GLU:CG	2.48	0.44
1:D:257:MET:HE3	1:D:290:LEU:HD23	1.96	0.44
1:C:25:ARG:HG3	1:C:402:PHE:CE2	2.52	0.44
1:C:234:VAL:HG12	1:C:238:GLN:CD	2.27	0.44
1:C:383:THR:HG21	1:C:412:HIS:C	2.37	0.44
1:D:227:ASP:CB	1:D:228:HIS:HD2	2.29	0.44
1:D:300:PRO:HG2	1:D:300:PRO:O	2.18	0.44
1:C:264:LEU:HD23	1:C:289:LEU:HD21	1.99	0.44
1:D:395:VAL:CG1	1:D:396:LYS:N	2.72	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:379:ARG:NH1	1:D:379:ARG:CG	2.75	0.44
1:B:95:ARG:O	1:B:96:PHE:CG	2.71	0.44
1:D:21:PHE:HB2	1:D:47:VAL:HG21	1.99	0.44
1:B:390:ARG:NH1	1:B:393:VAL:CG2	2.78	0.44
1:A:21:PHE:O	1:A:23:ILE:HG13	2.17	0.44
1:C:256:SER:O	1:C:260:LEU:HB2	2.18	0.44
1:A:177:PHE:O	1:A:177:PHE:HD2	2.01	0.44
1:C:82:PHE:CD1	1:C:83:PRO:CD	3.00	0.44
1:A:299:ILE:HD11	1:A:401:THR:HG22	1.98	0.44
1:D:46:ARG:HH21	1:D:54:GLU:HB3	1.74	0.44
1:D:385:ARG:CG	1:D:386:LEU:H	2.23	0.44
1:A:361:VAL:HG23	2:A:501:HEM:HBD2	2.00	0.44
1:A:239:LEU:CD2	1:A:239:LEU:C	2.85	0.44
1:B:60:ARG:O	1:B:64:VAL:HG23	2.18	0.44
1:D:220:LEU:HD22	1:D:224:LEU:HG	1.99	0.44
1:B:25:ARG:HD2	1:B:32:PRO:HD3	2.00	0.44
1:C:316:PRO:HG2	1:C:319:ASP:OD1	2.18	0.44
1:D:154:TYR:CE1	1:D:377:LEU:HD22	2.53	0.44
1:B:107:HIS:CD2	1:B:358:HIS:CD2	3.06	0.44
1:C:271:LEU:O	1:C:274:GLU:HB2	2.18	0.44
1:D:281:LEU:HA	1:D:281:LEU:HD23	1.82	0.44
1:B:169:ILE:CD1	1:B:178:ARG:CD	2.85	0.44
1:C:149:ASP:OD2	1:C:407:LEU:O	2.36	0.44
1:A:182:ARG:HA	1:A:182:ARG:HD2	1.76	0.44
1:A:220:LEU:HD23	1:A:224:LEU:HG	2.00	0.44
1:B:70:ASP:OD1	1:B:71:PRO:CD	2.66	0.44
1:D:297:ASP:OD1	1:D:298:SER:N	2.51	0.43
1:C:28:PRO:HG2	1:C:29:PHE:CD1	2.53	0.43
1:D:407:LEU:HD22	1:D:407:LEU:HA	1.73	0.43
1:C:65:ARG:CD	1:C:355:TYR:CE1	3.01	0.43
1:D:302:ARG:HH21	1:D:358:HIS:CB	2.31	0.43
1:D:299:ILE:H	1:D:300:PRO:CD	2.30	0.43
1:B:19:ARG:O	1:B:48:THR:N	2.41	0.43
1:C:70:ASP:OD1	1:C:71:PRO:CD	2.66	0.43
1:C:115:LEU:N	1:C:116:PRO:HD2	2.33	0.43
1:D:82:PHE:CD1	1:D:83:PRO:HD2	2.53	0.43
1:C:385:ARG:HG3	1:C:386:LEU:H	1.81	0.43
1:C:154:TYR:CE1	1:C:377:LEU:HD22	2.52	0.43
1:C:190:THR:HG21	1:C:193:GLN:CB	2.47	0.43
1:A:70:ASP:OD1	1:A:71:PRO:CD	2.67	0.43
1:A:363:GLN:O	1:A:367:ARG:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:92:ALA:O	1:C:95:ARG:CG	2.64	0.43
1:D:190:THR:O	1:D:191:ALA:CB	2.67	0.43
1:D:113:MET:SD	1:D:228:HIS:ND1	2.91	0.43
1:C:138:LEU:HA	1:C:138:LEU:HD23	1.73	0.43
1:A:46:ARG:HD3	1:A:56:TRP:CH2	2.53	0.43
1:B:151:VAL:HA	1:B:155:ALA:HB3	2.01	0.43
1:A:313:ARG:H	1:A:313:ARG:HG2	1.66	0.43
1:A:111:ARG:HD2	2:A:501:HEM:O2D	2.17	0.43
1:C:29:PHE:CD2	1:C:264:LEU:HD13	2.52	0.43
1:A:76:ASP:O	1:A:82:PHE:HD2	2.01	0.43
1:D:115:LEU:N	1:D:116:PRO:HD2	2.33	0.43
1:D:174:LEU:C	1:D:176:PHE:H	2.20	0.43
1:A:175:GLU:CD	1:A:179:ASP:OD2	2.54	0.43
1:D:227:ASP:HB3	1:D:228:HIS:HD2	1.84	0.43
1:C:75:ALA:O	1:C:101:ARG:C	2.53	0.43
1:B:96:PHE:C	1:B:97:ARG:HG3	2.38	0.43
1:C:64:VAL:HG13	1:C:323:ALA:HB1	2.01	0.43
1:D:75:ALA:N	1:D:103:ASP:OD2	2.51	0.43
1:C:412:HIS:ND1	1:C:412:HIS:N	2.64	0.43
1:A:368:LEU:C	1:A:368:LEU:HD12	2.33	0.43
1:D:73:VAL:CG2	1:D:308:ILE:HD13	2.49	0.43
1:B:57:VAL:HG23	1:B:322:ILE:HB	2.00	0.43
1:D:70:ASP:OD1	1:D:71:PRO:CD	2.67	0.43
1:C:269:PRO:O	1:C:272:PRO:HD2	2.19	0.43
1:B:148:VAL:HG12	1:B:149:ASP:H	1.84	0.43
1:D:61:TYR:CD1	1:D:334:GLN:HG3	2.53	0.43
1:A:353:PHE:CE1	1:A:363:GLN:HA	2.54	0.43
1:B:32:PRO:HG2	1:B:35:TYR:CE1	2.54	0.43
1:C:174:LEU:O	1:C:175:GLU:CB	2.66	0.42
1:C:303:VAL:HG13	1:C:319:ASP:C	2.30	0.42
1:C:407:LEU:HD22	1:C:407:LEU:HA	1.72	0.42
1:D:243:LEU:HD23	1:D:243:LEU:HA	1.83	0.42
1:C:108:THR:O	1:C:112:ARG:HB2	2.19	0.42
1:C:227:ASP:HB3	1:C:228:HIS:CD2	2.53	0.42
1:A:177:PHE:C	1:A:177:PHE:HD2	2.23	0.42
1:A:56:TRP:NE1	1:A:316:PRO:HD2	2.34	0.42
1:D:269:PRO:O	1:D:272:PRO:HD2	2.19	0.42
1:C:310:LEU:O	1:C:311:SER:HB2	2.18	0.42
1:B:186:SER:O	1:B:187:ARG:HB2	2.18	0.42
1:B:182:ARG:HE	1:B:251:ARG:HE	1.66	0.42
1:A:142:LEU:HD23	1:A:411:TRP:NE1	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:306:GLU:O	1:D:308:ILE:HG13	2.18	0.42
1:D:301:LEU:C	1:D:302:ARG:HG3	2.39	0.42
1:A:217:ARG:CG	1:A:217:ARG:HH11	2.18	0.42
1:B:190:THR:HG22	1:B:193:GLN:HB3	1.97	0.42
1:A:42:ASP:CG	1:A:45:ALA:HB2	2.39	0.42
1:B:361:VAL:HG12	1:B:361:VAL:O	2.20	0.42
1:A:107:HIS:NE2	1:A:358:HIS:NE2	2.62	0.42
1:A:19:ARG:O	1:A:48:THR:N	2.49	0.42
1:C:169:ILE:HD13	1:C:178:ARG:CD	2.44	0.42
1:B:368:LEU:HD12	1:B:372:VAL:CG2	2.50	0.42
1:C:251:ARG:HG2	1:C:251:ARG:HH11	1.83	0.42
1:D:42:ASP:HB2	1:D:45:ALA:HB2	2.01	0.42
1:D:25:ARG:H	1:D:25:ARG:HG2	1.60	0.42
1:B:71:PRO:CB	1:D:71:PRO:HB3	2.49	0.42
1:B:296:ALA:HB1	1:B:299:ILE:HG12	2.00	0.42
1:A:201:LEU:HD23	1:A:201:LEU:C	2.39	0.42
1:C:25:ARG:H	1:C:25:ARG:HG2	1.56	0.42
1:D:307:ASP:N	1:D:317:ALA:HB2	2.35	0.42
1:B:57:VAL:HG22	1:B:324:LEU:CD1	2.50	0.42
1:B:25:ARG:H	1:B:25:ARG:HG2	1.60	0.42
1:B:65:ARG:HA	1:B:355:TYR:HD1	1.84	0.42
1:C:113:MET:CG	1:C:228:HIS:CE1	3.03	0.42
1:D:380:ARG:HD2	1:D:415:HIS:CE1	2.54	0.42
1:D:413:HIS:O	1:D:414:HIS:CG	2.72	0.42
1:A:253:THR:CG2	1:A:401:THR:HG21	2.44	0.42
1:B:154:TYR:O	1:B:158:VAL:HG23	2.19	0.42
1:D:174:LEU:HD12	1:D:204:LEU:HD21	2.00	0.42
1:A:115:LEU:HD23	1:A:361:VAL:HG13	2.02	0.42
1:B:239:LEU:CD2	1:B:239:LEU:C	2.85	0.42
1:D:230:VAL:N	1:D:231:PRO:CD	2.80	0.42
1:A:309:GLU:HG2	1:A:314:THR:HB	2.02	0.42
1:B:61:TYR:C	1:B:61:TYR:CD1	2.94	0.42
1:D:386:LEU:HD23	1:D:387:ALA:N	2.35	0.41
1:A:243:LEU:O	1:A:247:ILE:HG13	2.20	0.41
1:C:256:SER:OG	1:C:403:GLY:HA3	2.20	0.41
1:C:167:LEU:HD23	1:C:221:ILE:CG1	2.49	0.41
1:C:131:GLN:OE1	1:C:376:THR:CG2	2.63	0.41
1:D:254:THR:HA	2:D:501:HEM:HBB1	2.02	0.41
1:D:389:GLU:HG3	1:D:390:ARG:N	2.35	0.41
1:D:44:VAL:CG1	1:D:315:VAL:HG12	2.46	0.41
1:D:164:CYS:SG	1:D:178:ARG:NE	2.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:92:ALA:O	1:D:95:ARG:CG	2.65	0.41
1:D:95:ARG:C	1:D:95:ARG:NE	2.74	0.41
1:D:216:PRO:HB2	1:D:222:SER:OG	2.20	0.41
1:C:301:LEU:C	1:C:302:ARG:HG3	2.40	0.41
1:D:189:SER:C	1:D:190:THR:CG2	2.88	0.41
1:C:51:THR:O	1:C:52:ARG:CB	2.68	0.41
1:A:198:LEU:HA	1:A:198:LEU:HD23	1.82	0.41
1:B:174:LEU:O	1:B:175:GLU:CB	2.69	0.41
1:C:77:ILE:CA	1:C:82:PHE:CD2	2.73	0.41
1:B:159:SER:HB3	1:B:255:THR:HG22	1.99	0.41
1:D:394:VAL:HG11	1:D:405:GLU:HB3	2.01	0.41
1:D:175:GLU:O	1:D:179:ASP:CB	2.68	0.41
1:C:42:ASP:OD1	1:C:45:ALA:CA	2.68	0.41
1:C:345:ARG:HH11	1:C:345:ARG:CG	2.34	0.41
1:D:393:VAL:HG11	1:D:407:LEU:CD2	2.49	0.41
1:B:198:LEU:HA	1:B:198:LEU:HD23	1.76	0.41
1:B:202:PHE:CD1	1:B:240:LEU:HD12	2.53	0.41
1:B:70:ASP:OD1	1:B:71:PRO:HD2	2.21	0.41
1:C:115:LEU:HD23	1:C:361:VAL:HG13	2.01	0.41
1:B:190:THR:HG22	1:B:193:GLN:H	1.85	0.41
1:D:256:SER:OG	1:D:403:GLY:HA3	2.20	0.41
1:C:92:ALA:HA	1:C:95:ARG:CG	2.50	0.41
1:C:95:ARG:NH1	1:C:97:ARG:HD3	2.35	0.41
1:B:174:LEU:HD13	1:B:204:LEU:HD21	2.02	0.41
1:C:411:TRP:C	1:C:412:HIS:ND1	2.74	0.41
1:D:174:LEU:C	1:D:176:PHE:N	2.74	0.41
1:B:34:GLU:N	1:B:34:GLU:CD	2.72	0.41
1:D:56:TRP:NE1	1:D:316:PRO:HD2	2.36	0.41
1:B:190:THR:HG21	1:B:193:GLN:CB	2.51	0.41
1:C:137:ILE:HD13	1:C:157:ALA:HB3	2.01	0.41
1:D:335:PHE:O	1:D:338:PRO:HD3	2.21	0.41
1:B:257:MET:HE1	1:B:290:LEU:HA	2.03	0.41
1:A:217:ARG:O	1:A:222:SER:CB	2.69	0.41
1:A:234:VAL:HG12	1:A:238:GLN:NE2	2.35	0.41
1:A:86:GLY:CA	1:A:89:GLU:OE2	2.68	0.41
1:B:177:PHE:HD2	1:B:177:PHE:O	2.04	0.41
1:A:114:LEU:HD12	1:A:114:LEU:C	2.41	0.41
1:A:73:VAL:CG2	1:A:308:ILE:HD13	2.41	0.41
1:B:21:PHE:HB2	1:B:47:VAL:CG2	2.51	0.41
1:A:175:GLU:O	1:A:179:ASP:N	2.41	0.41
1:D:44:VAL:HG11	1:D:315:VAL:CG1	2.44	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:270:GLU:O	1:D:273:ALA:HB3	2.21	0.41
1:C:95:ARG:HG3	1:C:95:ARG:H	1.52	0.41
1:D:133:ARG:O	1:D:137:ILE:HG13	2.20	0.41
1:D:390:ARG:O	1:D:391:ASP:CB	2.69	0.41
1:D:138:LEU:HA	1:D:138:LEU:HD23	1.91	0.41
1:A:216:PRO:HG3	1:A:226:THR:HG21	2.03	0.41
1:A:268:ARG:O	1:A:272:PRO:HD2	2.20	0.41
1:D:46:ARG:CZ	1:D:54:GLU:HB3	2.51	0.41
1:C:243:LEU:O	1:C:247:ILE:HG13	2.21	0.41
1:C:45:ALA:HB3	1:C:57:VAL:HG12	1.98	0.41
1:B:234:VAL:HG13	1:B:238:GLN:HB3	2.03	0.41
1:A:220:LEU:HD22	1:A:224:LEU:HG	2.02	0.41
1:A:374:LEU:HD23	1:A:374:LEU:HA	1.85	0.41
1:A:128:PRO:HG2	1:A:129:ALA:N	2.36	0.41
1:A:171:ARG:O	1:A:174:LEU:O	2.39	0.41
1:C:404:LEU:HD13	1:C:407:LEU:HG	2.02	0.41
1:D:346:THR:OG1	1:D:347:ASP:OD2	2.39	0.41
1:D:187:ARG:CG	1:D:188:ASN:H	2.33	0.41
1:D:164:CYS:SG	1:D:178:ARG:CD	3.09	0.40
1:D:299:ILE:N	1:D:300:PRO:HD2	2.36	0.40
1:A:384:LEU:HD13	1:A:385:ARG:N	2.36	0.40
1:C:408:MET:SD	1:C:408:MET:N	2.91	0.40
1:A:163:ILE:O	1:A:163:ILE:HG22	2.21	0.40
1:D:110:TYR:O	1:D:113:MET:CB	2.65	0.40
1:D:288:GLU:OE1	1:D:291:ARG:NH1	2.54	0.40
1:D:149:ASP:OD2	1:D:407:LEU:O	2.38	0.40
1:A:290:LEU:HD13	1:A:353:PHE:HE2	1.85	0.40
1:D:384:LEU:C	1:D:384:LEU:HD13	2.42	0.40
1:D:413:HIS:O	1:D:414:HIS:CB	2.69	0.40
1:C:138:LEU:HD21	1:C:141:MET:HE2	1.99	0.40
1:B:260:LEU:HD22	1:B:293:LEU:HD22	2.02	0.40
1:D:28:PRO:HG2	1:D:29:PHE:CD1	2.56	0.40
1:A:190:THR:HG22	1:A:193:GLN:HB3	1.68	0.40
1:C:56:TRP:HE1	1:C:316:PRO:HD2	1.86	0.40
1:C:142:LEU:HA	1:C:142:LEU:HD23	1.94	0.40
1:D:189:SER:O	1:D:190:THR:CG2	2.69	0.40
1:A:20:ASP:HA	1:A:48:THR:O	2.21	0.40
1:A:405:GLU:HG2	1:A:405:GLU:O	2.20	0.40
1:A:103:ASP:O	1:A:104:ALA:CB	2.69	0.40
1:A:389:GLU:HB3	1:A:392:GLN:CG	2.52	0.40
1:B:177:PHE:HD2	1:B:177:PHE:C	2.25	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:LEU:CD2	1:A:201:LEU:C	2.90	0.40
1:B:119:THR:HG21	1:D:333:GLU:OE1	2.22	0.40
1:C:186:SER:O	1:C:187:ARG:CB	2.69	0.40

All (31) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:193:GLN:CD	1:C:95:ARG:CZ[3_444]	0.53	1.67
1:A:193:GLN:OE1	1:D:95:ARG:NH2[2_565]	0.57	1.63
1:A:193:GLN:NE2	1:D:95:ARG:NH1[2_565]	0.69	1.51
1:A:193:GLN:CD	1:D:95:ARG:CZ[2_565]	0.90	1.30
1:B:193:GLN:CD	1:C:95:ARG:NH2[3_444]	1.04	1.16
1:B:193:GLN:NE2	1:C:95:ARG:NH1[3_444]	1.12	1.08
1:A:193:GLN:CD	1:D:95:ARG:NH1[2_565]	1.14	1.06
1:A:193:GLN:OE1	1:D:95:ARG:CZ[2_565]	1.14	1.06
1:B:193:GLN:NE2	1:C:95:ARG:CZ[3_444]	1.14	1.06
1:B:193:GLN:OE1	1:C:95:ARG:NH2[3_444]	1.16	1.04
1:B:193:GLN:OE1	1:C:96:PHE:O[3_444]	1.38	0.82
1:A:193:GLN:CD	1:D:95:ARG:NH2[2_565]	1.44	0.76
1:A:193:GLN:NE2	1:D:95:ARG:CZ[2_565]	1.62	0.58
1:B:193:GLN:CG	1:C:95:ARG:NH2[3_444]	1.64	0.56
1:B:193:GLN:OE1	1:C:95:ARG:CZ[3_444]	1.65	0.55
1:B:193:GLN:NE2	1:C:95:ARG:NE[3_444]	1.66	0.54
1:B:193:GLN:CD	1:C:95:ARG:NH1[3_444]	1.70	0.50
1:C:172:HIS:NE2	1:D:171:ARG:NH1[6_555]	1.72	0.48
1:B:193:GLN:CD	1:C:95:ARG:NE[3_444]	1.74	0.46
1:C:172:HIS:NE2	1:D:171:ARG:CZ[6_555]	1.84	0.36
1:B:193:GLN:CG	1:C:95:ARG:CZ[3_444]	1.89	0.31
1:C:172:HIS:CE1	1:D:171:ARG:NH2[6_555]	1.91	0.29
1:B:193:GLN:CB	1:C:95:ARG:NH1[3_444]	1.99	0.21
1:A:193:GLN:OE1	1:D:95:ARG:NE[2_565]	2.01	0.19
1:A:193:GLN:CG	1:D:95:ARG:NH1[2_565]	2.03	0.17
1:B:193:GLN:OE1	1:C:95:ARG:NE[3_444]	2.06	0.14
1:B:193:GLN:NE2	1:C:95:ARG:CD[3_444]	2.08	0.12
1:A:193:GLN:OE1	1:D:96:PHE:O[2_565]	2.10	0.10
1:C:172:HIS:CD2	1:D:171:ARG:NH1[6_555]	2.13	0.07
1:A:193:GLN:CD	1:D:95:ARG:NE[2_565]	2.16	0.04
1:B:193:GLN:CG	1:C:95:ARG:NH1[3_444]	2.19	0.01

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	395/417 (95%)	374 (95%)	18 (5%)	3 (1%)	24	60
1	B	395/417 (95%)	378 (96%)	13 (3%)	4 (1%)	19	54
1	C	396/417 (95%)	375 (95%)	13 (3%)	8 (2%)	9	33
1	D	397/417 (95%)	371 (94%)	20 (5%)	6 (2%)	13	42
All	All	1583/1668 (95%)	1498 (95%)	64 (4%)	21 (1%)	15	46

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	104	ALA
1	B	104	ALA
1	C	104	ALA
1	C	391	ASP
1	C	412	HIS
1	D	104	ALA
1	D	391	ASP
1	D	413	HIS
1	D	414	HIS
1	A	187	ARG
1	B	187	ARG
1	C	175	GLU
1	C	395	VAL
1	D	187	ARG
1	D	191	ALA
1	B	96	PHE
1	C	187	ARG
1	A	297	ASP
1	B	297	ASP
1	C	190	THR
1	C	300	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	330/347 (95%)	249 (76%)	81 (24%)	1	2
1	B	330/347 (95%)	249 (76%)	81 (24%)	1	2
1	C	331/347 (95%)	244 (74%)	87 (26%)	0	2
1	D	332/347 (96%)	247 (74%)	85 (26%)	0	2
All	All	1323/1388 (95%)	989 (75%)	334 (25%)	1	2

All (334) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	ARG
1	A	20	ASP
1	A	25	ARG
1	A	34	GLU
1	A	48	THR
1	A	52	ARG
1	A	57	VAL
1	A	59	THR
1	A	67	LEU
1	A	77	ILE
1	A	78	ARG
1	A	91	GLU
1	A	95	ARG
1	A	97	ARG
1	A	112	ARG
1	A	122	ARG
1	A	124	ARG
1	A	127	ARG
1	A	141	MET
1	A	148	VAL
1	A	152	SER
1	A	160	THR
1	A	167	LEU
1	A	175	GLU

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Mol	Chain	Res	Type
1	A	177	PHE
1	A	178	ARG
1	A	179	ASP
1	A	180	VAL
1	A	182	ARG
1	A	186	SER
1	A	187	ARG
1	A	195	SER
1	A	201	LEU
1	A	211	GLU
1	A	217	ARG
1	A	219	ASP
1	A	220	LEU
1	A	222	SER
1	A	223	LYS
1	A	227	ASP
1	A	231	PRO
1	A	234	VAL
1	A	240	LEU
1	A	251	ARG
1	A	252	GLU
1	A	253	THR
1	A	254	THR
1	A	260	LEU
1	A	261	SER
1	A	263	LEU
1	A	267	ASP
1	A	269	PRO
1	A	278	ASP
1	A	291	ARG
1	A	292	VAL
1	A	298	SER
1	A	300	PRO
1	A	302	ARG
1	A	306	GLU
1	A	307	ASP
1	A	309	GLU
1	A	314	THR
1	A	319	ASP
1	A	321	VAL
1	A	324	LEU
1	A	345	ARG

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Mol	Chain	Res	Type
1	A	346	THR
1	A	348	ASN
1	A	357	VAL
1	A	365	LEU
1	A	369	GLU
1	A	376	THR
1	A	384	LEU
1	A	385	ARG
1	A	386	LEU
1	A	389	GLU
1	A	391	ASP
1	A	397	HIS
1	A	399	SER
1	A	407	LEU
1	A	412	HIS
1	B	19	ARG
1	B	20	ASP
1	B	25	ARG
1	B	34	GLU
1	B	46	ARG
1	B	52	ARG
1	B	57	VAL
1	B	59	THR
1	B	67	LEU
1	B	69	SER
1	B	77	ILE
1	B	78	ARG
1	B	90	GLN
1	B	91	GLU
1	B	95	ARG
1	B	96	PHE
1	B	97	ARG
1	B	106	GLU
1	B	112	ARG
1	B	127	ARG
1	B	141	MET
1	B	150	LEU
1	B	152	SER
1	B	160	THR
1	B	167	LEU
1	B	175	GLU
1	B	176	PHE

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Mol	Chain	Res	Type
1	B	177	PHE
1	B	178	ARG
1	B	179	ASP
1	B	180	VAL
1	B	184	SER
1	B	186	SER
1	B	187	ARG
1	B	193	GLN
1	B	195	SER
1	B	204	LEU
1	B	211	GLU
1	B	216	PRO
1	B	219	ASP
1	B	220	LEU
1	B	222	SER
1	B	226	THR
1	B	227	ASP
1	B	252	GLU
1	B	253	THR
1	B	254	THR
1	B	255	THR
1	B	260	LEU
1	B	261	SER
1	B	263	LEU
1	B	267	ASP
1	B	278	ASP
1	B	291	ARG
1	B	292	VAL
1	B	298	SER
1	B	302	ARG
1	B	306	GLU
1	B	307	ASP
1	B	313	ARG
1	B	314	THR
1	B	319	ASP
1	B	321	VAL
1	B	324	LEU
1	B	340	ARG
1	B	345	ARG
1	B	348	ASN
1	B	351	VAL
1	B	357	VAL

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Mol	Chain	Res	Type
1	B	365	LEU
1	B	370	LEU
1	B	376	THR
1	B	382	PRO
1	B	384	LEU
1	B	385	ARG
1	B	386	LEU
1	B	391	ASP
1	B	397	HIS
1	B	398	ASP
1	B	399	SER
1	B	407	LEU
1	C	19	ARG
1	C	25	ARG
1	C	34	GLU
1	C	39	ARG
1	C	40	THR
1	C	46	ARG
1	C	49	LEU
1	C	52	ARG
1	C	58	VAL
1	C	59	THR
1	C	65	ARG
1	C	67	LEU
1	C	69	SER
1	C	80	PRO
1	C	82	PHE
1	C	83	PRO
1	C	87	GLU
1	C	90	GLN
1	C	95	ARG
1	C	97	ARG
1	C	98	PRO
1	C	99	PHE
1	C	103	ASP
1	C	111	ARG
1	C	112	ARG
1	C	114	LEU
1	C	122	ARG
1	C	124	ARG
1	C	127	ARG
1	C	141	MET

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Mol	Chain	Res	Type
1	C	160	THR
1	C	167	LEU
1	C	172	HIS
1	C	178	ARG
1	C	179	ASP
1	C	180	VAL
1	C	187	ARG
1	C	188	ASN
1	C	195	SER
1	C	196	GLU
1	C	204	LEU
1	C	211	GLU
1	C	213	ARG
1	C	214	GLU
1	C	215	GLU
1	C	219	ASP
1	C	220	LEU
1	C	226	THR
1	C	231	PRO
1	C	234	VAL
1	C	240	LEU
1	C	246	THR
1	C	251	ARG
1	C	252	GLU
1	C	253	THR
1	C	255	THR
1	C	256	SER
1	C	260	LEU
1	C	261	SER
1	C	263	LEU
1	C	277	LYS
1	C	278	ASP
1	C	281	LEU
1	C	291	ARG
1	C	307	ASP
1	C	313	ARG
1	C	314	THR
1	C	321	VAL
1	C	322	ILE
1	C	324	LEU
1	C	340	ARG
1	C	345	ARG

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Mol	Chain	Res	Type
1	C	348	ASN
1	C	357	VAL
1	C	368	LEU
1	C	376	THR
1	C	383	THR
1	C	384	LEU
1	C	385	ARG
1	C	386	LEU
1	C	390	ARG
1	C	396	LYS
1	C	398	ASP
1	C	407	LEU
1	C	408	MET
1	C	412	HIS
1	C	414	HIS
1	D	19	ARG
1	D	25	ARG
1	D	28	PRO
1	D	34	GLU
1	D	40	THR
1	D	42	ASP
1	D	46	ARG
1	D	49	LEU
1	D	52	ARG
1	D	58	VAL
1	D	59	THR
1	D	65	ARG
1	D	67	LEU
1	D	74	SER
1	D	78	ARG
1	D	79	ARG
1	D	82	PHE
1	D	95	ARG
1	D	97	ARG
1	D	99	PHE
1	D	103	ASP
1	D	106	GLU
1	D	111	ARG
1	D	114	LEU
1	D	121	ARG
1	D	122	ARG
1	D	127	ARG

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Mol	Chain	Res	Type
1	D	141	MET
1	D	148	VAL
1	D	160	THR
1	D	161	SER
1	D	167	LEU
1	D	175	GLU
1	D	176	PHE
1	D	178	ARG
1	D	180	VAL
1	D	187	ARG
1	D	192	GLU
1	D	195	SER
1	D	201	LEU
1	D	204	LEU
1	D	213	ARG
1	D	214	GLU
1	D	215	GLU
1	D	217	ARG
1	D	220	LEU
1	D	223	LYS
1	D	226	THR
1	D	240	LEU
1	D	242	THR
1	D	246	THR
1	D	252	GLU
1	D	253	THR
1	D	255	THR
1	D	256	SER
1	D	260	LEU
1	D	261	SER
1	D	263	LEU
1	D	270	GLU
1	D	277	LYS
1	D	291	ARG
1	D	295	VAL
1	D	300	PRO
1	D	303	VAL
1	D	307	ASP
1	D	310	LEU
1	D	311	SER
1	D	313	ARG
1	D	314	THR

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Mol	Chain	Res	Type
1	D	316	PRO
1	D	321	VAL
1	D	322	ILE
1	D	324	LEU
1	D	347	ASP
1	D	348	ASN
1	D	357	VAL
1	D	376	THR
1	D	383	THR
1	D	384	LEU
1	D	385	ARG
1	D	386	LEU
1	D	389	GLU
1	D	390	ARG
1	D	407	LEU
1	D	408	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	228	HIS
1	A	238	GLN
1	A	248	ASN
1	A	344	HIS
1	A	358	HIS
1	B	24	GLN
1	B	90	GLN
1	B	228	HIS
1	B	238	GLN
1	B	358	HIS
1	B	359	GLN
1	B	363	GLN
1	C	238	GLN
1	C	330	HIS
1	C	344	HIS
1	C	348	ASN
1	C	359	GLN
1	C	392	GLN
1	D	228	HIS
1	D	238	GLN
1	D	348	ASN
1	D	358	HIS

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Mol	Chain	Res	Type
1	D	359	GLN
1	D	412	HIS
1	D	415	HIS

### 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 carbohydrates 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).

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	2.61	8 (26%)	24,82,82	2.96	11 (45%)
2	HEM	B	501	1	30,50,50	2.62	8 (26%)	24,82,82	2.91	10 (41%)
2	HEM	C	501	1	30,50,50	2.49	9 (30%)	24,82,82	3.05	11 (45%)
2	HEM	D	501	1	30,50,50	2.46	7 (23%)	24,82,82	3.07	10 (41%)

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
2	HEM	C	501	1	-	0/10/54/54	0/0/8/8
2	HEM	D	501	1	-	0/10/54/54	0/0/8/8

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	HEM	C3B-C4B	-8.42	1.44	1.51
2	A	501	HEM	C3B-C4B	-8.23	1.44	1.51
2	C	501	HEM	C3B-C4B	-7.31	1.45	1.51
2	D	501	HEM	C3B-C4B	-7.22	1.45	1.51
2	B	501	HEM	C2D-C3D	-6.67	1.34	1.54
2	A	501	HEM	C2D-C3D	-6.64	1.34	1.54
2	C	501	HEM	C2D-C3D	-6.27	1.35	1.54
2	D	501	HEM	C2D-C3D	-5.94	1.36	1.54
2	D	501	HEM	C3D-C4D	-4.39	1.45	1.51
2	A	501	HEM	C3D-C4D	-4.13	1.46	1.51
2	C	501	HEM	C3D-C4D	-3.84	1.46	1.51
2	B	501	HEM	C3D-C4D	-3.64	1.46	1.51
2	D	501	HEM	C2C-C1C	-2.73	1.47	1.52
2	C	501	HEM	C2C-C1C	-2.56	1.47	1.52
2	B	501	HEM	C2C-C1C	-2.38	1.48	1.52
2	A	501	HEM	C2C-C1C	-2.35	1.48	1.52
2	C	501	HEM	CAA-C2A	2.01	1.55	1.52
2	B	501	HEM	C3C-CAC	2.05	1.55	1.51
2	C	501	HEM	C1C-NC	2.17	1.38	1.36
2	A	501	HEM	C1C-NC	2.37	1.38	1.36
2	D	501	HEM	C4C-NC	2.44	1.39	1.36
2	A	501	HEM	C4C-NC	2.47	1.39	1.36
2	B	501	HEM	C4C-NC	2.62	1.39	1.36
2	C	501	HEM	C4C-NC	2.82	1.39	1.36
2	D	501	HEM	CBB-CAB	4.08	1.52	1.29
2	C	501	HEM	CBB-CAB	4.14	1.53	1.29
2	A	501	HEM	CBB-CAB	4.23	1.53	1.29
2	D	501	HEM	CBC-CAC	4.28	1.54	1.29
2	A	501	HEM	CBC-CAC	4.28	1.54	1.29
2	B	501	HEM	CBC-CAC	4.29	1.54	1.29
2	C	501	HEM	CBC-CAC	4.33	1.54	1.29
2	B	501	HEM	CBB-CAB	4.38	1.54	1.29

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	HEM	C3B-CAB-CBB	-7.23	113.36	124.46
2	C	501	HEM	C3B-CAB-CBB	-7.22	113.38	124.46
2	D	501	HEM	C3B-CAB-CBB	-7.17	113.47	124.46
2	D	501	HEM	C3C-CAC-CBC	-7.02	113.69	124.46
2	B	501	HEM	C3B-CAB-CBB	-6.97	113.76	124.46
2	C	501	HEM	C3C-CAC-CBC	-6.93	113.83	124.46
2	A	501	HEM	C3C-CAC-CBC	-6.34	114.73	124.46
2	B	501	HEM	C3C-CAC-CBC	-6.08	115.14	124.46
2	D	501	HEM	CMA-C3A-C4A	-2.74	123.83	128.36
2	C	501	HEM	CMA-C3A-C4A	-2.70	123.90	128.36
2	B	501	HEM	CMA-C3A-C4A	-2.26	124.62	128.36
2	C	501	HEM	CAA-C2A-C1A	-2.23	124.58	127.01
2	A	501	HEM	CMA-C3A-C4A	-2.20	124.73	128.36
2	A	501	HEM	CAA-C2A-C1A	-2.01	124.83	127.01
2	A	501	HEM	C3B-C4B-CHC	2.11	126.14	123.16
2	B	501	HEM	C3B-C4B-CHC	2.14	126.17	123.16
2	C	501	HEM	C3B-C4B-CHC	2.16	126.20	123.16
2	D	501	HEM	C3B-C4B-CHC	2.23	126.30	123.16
2	B	501	HEM	CMD-C2D-C3D	2.88	127.10	114.35
2	A	501	HEM	CMD-C2D-C3D	2.90	127.16	114.35
2	C	501	HEM	CMD-C2D-C3D	2.90	127.20	114.35
2	D	501	HEM	CMD-C2D-C3D	2.99	127.56	114.35
2	D	501	HEM	C2D-C3D-C4D	3.04	106.66	101.50
2	C	501	HEM	C2D-C3D-C4D	3.25	107.00	101.50
2	A	501	HEM	C2D-C3D-C4D	3.33	107.15	101.50
2	B	501	HEM	C2D-C3D-C4D	3.36	107.19	101.50
2	C	501	HEM	CAD-C3D-C4D	3.87	126.12	112.47
2	D	501	HEM	CAD-C3D-C4D	3.89	126.19	112.47
2	A	501	HEM	CAD-C3D-C4D	3.91	126.27	112.47
2	B	501	HEM	CAD-C3D-C4D	3.93	126.32	112.47
2	A	501	HEM	CMB-C2B-C3B	4.33	127.35	116.53
2	B	501	HEM	CMB-C2B-C3B	4.35	127.40	116.53
2	C	501	HEM	CMB-C2B-C3B	4.59	127.98	116.53
2	B	501	HEM	CAD-C3D-C2D	4.61	126.48	113.22
2	A	501	HEM	CAD-C3D-C2D	4.65	126.58	113.22
2	D	501	HEM	CMB-C2B-C3B	4.73	128.34	116.53
2	C	501	HEM	CAD-C3D-C2D	4.75	126.88	113.22
2	D	501	HEM	CAD-C3D-C2D	4.85	127.16	113.22
2	B	501	HEM	CMC-C2C-C3C	4.96	128.92	116.53
2	C	501	HEM	CMC-C2C-C3C	4.99	128.99	116.53
2	A	501	HEM	CMC-C2C-C3C	5.01	129.04	116.53
2	D	501	HEM	CMC-C2C-C3C	5.04	129.10	116.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	HEM	5	0
2	B	501	HEM	4	0
2	C	501	HEM	4	0
2	D	501	HEM	6	0

## 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

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	397/417 (95%)	0.28	7 (1%) 71 68	37, 64, 93, 102	2 (0%)
1	B	397/417 (95%)	0.29	6 (1%) 76 74	38, 63, 92, 103	2 (0%)
1	C	398/417 (95%)	0.42	20 (5%) 32 26	43, 74, 100, 127	2 (0%)
1	D	399/417 (95%)	0.40	16 (4%) 42 35	46, 74, 99, 130	2 (0%)
All	All	1591/1668 (95%)	0.35	49 (3%) 52 45	37, 68, 96, 130	8 (0%)

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	21	PHE	5.6
1	C	93	GLY	5.3
1	D	172	HIS	4.8
1	D	95	ARG	4.5
1	C	86	GLY	4.5
1	C	95	ARG	4.5
1	C	90	GLN	4.4
1	C	89	GLU	4.4
1	B	21	PHE	4.3
1	D	93	GLY	4.3
1	C	83	PRO	3.8
1	C	96	PHE	3.8
1	D	90	GLN	3.5
1	D	21	PHE	3.4
1	D	77	ILE	3.4
1	D	92	ALA	3.3
1	A	21	PHE	3.2
1	D	94	ALA	3.1
1	C	77	ILE	3.1
1	D	397	HIS	3.0
1	B	193	GLN	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	89	GLU	2.9
1	C	94	ALA	2.9
1	C	91	GLU	2.8
1	C	85	LEU	2.8
1	D	369	GLU	2.8
1	B	182	ARG	2.7
1	C	397	HIS	2.7
1	D	83	PRO	2.6
1	B	172	HIS	2.6
1	C	97	ARG	2.6
1	C	193	GLN	2.5
1	D	85	LEU	2.5
1	D	86	GLY	2.5
1	B	312	GLY	2.4
1	C	172	HIS	2.3
1	A	182	ARG	2.3
1	A	94	ALA	2.3
1	D	193	GLN	2.2
1	A	196	GLU	2.1
1	A	312	GLY	2.1
1	D	404	LEU	2.1
1	C	76	ASP	2.1
1	C	182	ARG	2.1
1	C	184	SER	2.1
1	A	77	ILE	2.0
1	A	193	GLN	2.0
1	C	300	PRO	2.0
1	B	240	LEU	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(Å <sup>2</sup> )	Q<0.9
2	HEM	B	501	43/43	0.97	0.26	1.15	30,38,51,55	0
2	HEM	A	501	43/43	0.97	0.26	1.09	31,40,50,55	0
2	HEM	D	501	43/43	0.97	0.27	0.58	48,50,56,57	0
2	HEM	C	501	43/43	0.97	0.26	0.35	47,50,56,59	0

## 6.5 Other polymers

There are no such residues in this entry.