



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 09:02 PM GMT

PDB ID : 2PV0  
Title : DNA methyltransferase 3 like protein (DNMT3L)  
Authors : Cheng, X.  
Deposited on : 2007-05-09  
Resolution : 3.30 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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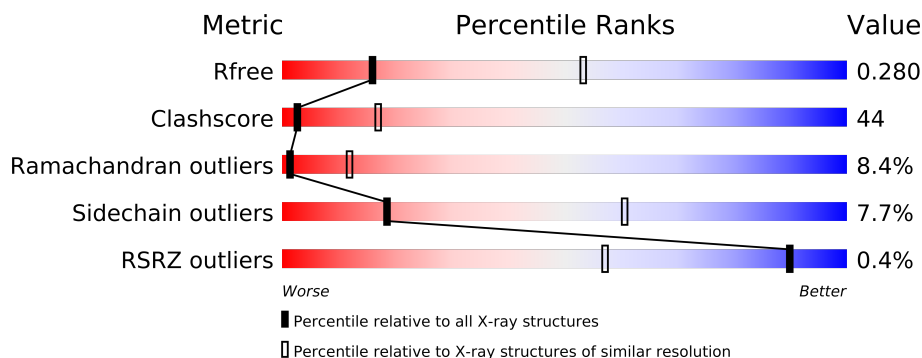
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 3.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	66092	1341 (3.40-3.20)
Clashscore	79885	1696 (3.40-3.20)
Ramachandran outliers	78287	1664 (3.40-3.20)
Sidechain outliers	78261	1662 (3.40-3.20)
RSRZ outliers	66119	1342 (3.40-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	386	
1	B	386	
1	C	386	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	ZN	C	508	-	X

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7861 atoms, of which 0 are hydrogen and 0 are deuterium.

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

- Molecule 1 is a protein called DNA (cytosine-5)-methyltransferase3-like.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	347	Total	C	N	O	S	0	0	0
			2737	1748	463	505	21			
1	A	347	Total	C	N	O	S	0	0	0
			2744	1753	467	503	21			
1	C	347	Total	C	N	O	S	0	0	0
			2371	1478	415	459	19			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	278	GLY	ARG	CONFLICT	UNP Q9UJW3
B	?	-	SER	DELETION	UNP Q9UJW3
A	278	GLY	ARG	CONFLICT	UNP Q9UJW3
A	?	-	SER	DELETION	UNP Q9UJW3
C	278	GLY	ARG	CONFLICT	UNP Q9UJW3
C	?	-	SER	DELETION	UNP Q9UJW3

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

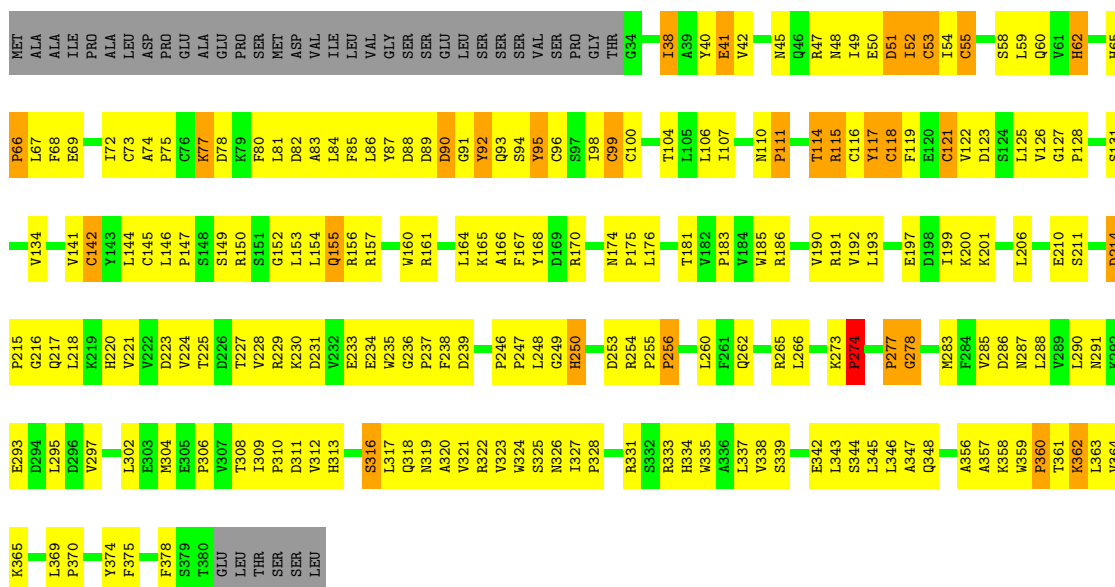
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	3	Total	Zn	0	0
			3	3		
2	A	3	Total	Zn	0	0
			3	3		
2	C	3	Total	Zn	0	0
			3	3		

### 3 Residue-property plots

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

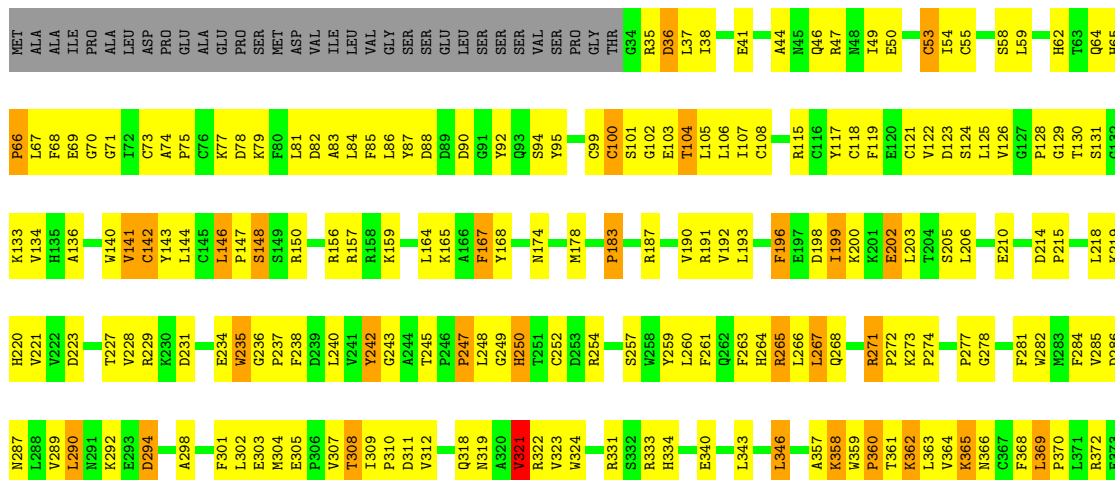
- Molecule 1: DNA (cytosine-5)-methyltransferase3-like

Chain B:



- Molecule 1: DNA (cytosine-5)-methyltransferase3-like

Chain A:



Y374  
F375  
K376  
Y377  
F378  
S379  
T380  
GLU  
LEU  
THR  
SER  
SER  
LEU

- Molecule 1: DNA (cytosine-5)-methyltransferase3-like

Chain C: 

MET  
ALA  
ALA  
ILE  
PRO  
ALA  
LEU  
ASP  
PRO  
GLU  
ALA  
GLU  
PRO  
SER  
MET  
ASP  
VAL  
ILE  
LEU  
VAL  
GLY  
SER  
SER  
GLU  
LEU  
SER  
SER  
VAL  
SER  
PRO  
GLY  
THR  
G34  
R35  
D36  
L37  
I38  
E41  
V42  
M45  
Q46  
R47  
M48  
I49  
E50  
D51  
I52  
C53  
I54  
C55  
C56  
G57  
S58  
L59  
H62  
T63

Q64  
H65  
P66  
L67  
F68  
E69  
G70  
G71  
I72  
C73  
A74  
P75  
A83  
L84  
F85  
L86  
Y87  
D88  
D89  
D90  
G91  
Y92  
Q93  
S94  
Y95  
C96  
S97  
I98  
C99  
C100  
E103  
T104  
L105  
L106  
I107  
C108  
G109  
M110  
P111  
D112  
Y117  
C118  
F119  
E120  
C121  
V122  
D123  
S124  
L125  
G126  
V127  
P128  
G129  
T130  
V134  
P215

M137  
S138  
M139  
W140  
V141  
C142  
Y143  
L144  
C145  
L153  
L154  
Q155  
R156  
R157  
R158  
K159  
W160  
R161  
S162  
Q163  
Y168  
D169  
S172  
E173  
M174  
P175  
L176  
E177  
M178  
F179  
E180  
T181  
V182  
P183  
R187  
Q188  
P189  
V190  
R191  
V192  
L193  
S194  
F196  
E197  
D198  
I199  
K200  
K201  
E202  
L203  
E210  
D214  
P215

G216  
Q217  
L218  
K219  
H220  
V224  
T225  
D226  
T227  
V228  
R229  
K230  
D231  
V232  
G236  
P237  
F238  
D239  
L240  
V241  
Y242  
G243  
L244  
T245  
P246  
P247  
L248  
G249  
H250  
T251  
C252  
P255  
P256  
L260  
F261  
Q262  
F263  
H264  
R265  
L266  
L267  
Q268  
R271  
P272  
K273  
P274  
G275  
S276  
P277  
G278  
P279  
F280  
W281  
W282  
M283

F284  
V285  
D286  
N287  
E293  
D294  
L295  
D296  
V297  
A298  
S299  
R300  
E303  
P306  
I309  
F310  
D311  
V312  
H313  
C314  
G315  
S316  
L317  
A320  
V323  
S326  
N326  
I327  
P328  
A329  
I330  
W335  
A336  
L337  
V338  
S339  
E342  
L343  
S344  
L345  
L346  
A347  
Q348  
N349  
K350  
Q351  
A356  
A357  
K358  
W359

P360  
T361  
K362  
L363  
V364  
K365  
N366  
C367  
F368  
L369  
P370  
L371  
R372  
E373  
Y374  
F375  
K376  
Y377  
F378  
S379  
T380  
GLU  
LEU  
THR  
SER  
SER  
LEU

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	267.20Å 267.20Å 149.50Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.74 – 3.30 34.37 – 3.29	Depositor EDS
% Data completeness (in resolution range)	98.8 (29.74-3.30) 98.8 (34.37-3.29)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.72 (at 3.32Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.248 , 0.272 0.263 , 0.280	Depositor DCC
$R_{free}$ test set	2344 reflections (4.99%)	DCC
Wilson B-factor (Å <sup>2</sup> )	108.2	Xtriage
Anisotropy	0.020	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 70.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.53$ , $\langle L^2 \rangle = 0.36$	Xtriage
Outliers	0 of 47265 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	7861	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	113.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.80% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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	0.42	0/2821	0.68	1/3840 (0.0%)
1	B	0.42	0/2814	0.69	0/3833
1	C	0.31	0/2431	0.57	0/3348
All	All	0.39	0/8066	0.65	1/11021 (0.0%)

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	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	369	LEU	CA-CB-CG	-5.19	103.37	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	374	TYR	Sidechain

### 5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens

added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2744	0	2625	212	0
1	B	2737	0	2605	237	0
1	C	2371	0	1927	217	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
2	C	3	0	0	0	0
All	All	7861	0	7157	659	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 44.

All (659) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:118:CYS:HB2	1:A:121:CYS:HB2	1.18	1.13
1:B:155:GLN:HA	1:B:155:GLN:HE21	1.17	1.06
1:C:47:ARG:HB3	1:C:47:ARG:HH11	1.15	1.05
1:B:65:HIS:ND1	1:B:72:ILE:HD11	1.72	1.04
1:C:118:CYS:HB2	1:C:121:CYS:HB2	1.38	1.03
1:B:144:LEU:HA	1:B:156:ARG:HD3	1.44	1.00
1:C:74:ALA:HB3	1:C:75:PRO:HD3	1.45	0.97
1:B:65:HIS:HD2	1:B:68:PHE:H	1.05	0.97
1:A:118:CYS:CB	1:A:121:CYS:HB2	1.96	0.95
1:B:106:LEU:HD13	1:B:134:VAL:HG11	1.46	0.94
1:A:159:LYS:HE2	1:A:159:LYS:H	1.31	0.94
1:A:83:ALA:HA	1:A:86:LEU:HD12	1.47	0.93
1:C:268:GLN:H	1:C:268:GLN:NE2	1.66	0.93
1:A:67:LEU:HD23	1:A:144:LEU:HD11	1.48	0.93
1:B:122:VAL:O	1:B:126:VAL:HG12	1.68	0.93
1:C:65:HIS:HD2	1:C:68:PHE:H	1.16	0.92
1:C:95:TYR:HB3	1:C:100:CYS:HA	1.54	0.90
1:C:281:PHE:HA	1:C:326:ASN:HD21	1.35	0.89
1:C:268:GLN:H	1:C:268:GLN:HE21	1.18	0.88
1:B:83:ALA:HA	1:B:86:LEU:HD23	1.55	0.88
1:A:191:ARG:NH1	1:A:237:PRO:HG2	1.88	0.87
1:C:240:LEU:HA	1:C:281:PHE:O	1.73	0.87
1:B:92:TYR:HD2	1:B:114:THR:HA	1.39	0.86
1:C:312:VAL:HG12	1:C:317:LEU:HA	1.55	0.85
1:B:115:ARG:HD2	1:B:144:LEU:HD12	1.55	0.85

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:144:LEU:HA	1:B:156:ARG:CD	2.06	0.85
1:B:285:VAL:HG22	1:B:323:VAL:HG22	1.60	0.84
1:B:155:GLN:HA	1:B:155:GLN:NE2	1.93	0.83
1:A:144:LEU:HA	1:A:156:ARG:HD3	1.60	0.83
1:C:65:HIS:ND1	1:C:72:ILE:HD11	1.94	0.82
1:B:247:PRO:HG3	1:B:359:TRP:HE3	1.43	0.81
1:B:73:CYS:SG	1:B:75:PRO:HD2	2.20	0.81
1:A:118:CYS:HB2	1:A:121:CYS:CB	2.07	0.81
1:C:153:LEU:O	1:C:153:LEU:HD23	1.80	0.81
1:A:319:ASN:HA	1:A:346:LEU:HD11	1.63	0.81
1:C:306:PRO:HG3	1:C:324:TRP:HE1	1.45	0.80
1:B:69:GLU:HB3	1:B:155:GLN:HB3	1.62	0.80
1:C:346:LEU:HD12	1:C:346:LEU:H	1.47	0.79
1:C:278:GLY:H	1:C:279:PRO:HD3	1.45	0.79
1:C:247:PRO:HA	1:C:287:ASN:ND2	1.98	0.79
1:C:54:ILE:O	1:C:54:ILE:HG13	1.83	0.78
1:A:103:GLU:O	1:A:105:LEU:HG	1.82	0.78
1:A:159:LYS:N	1:A:159:LYS:HE2	1.96	0.78
1:C:47:ARG:HB3	1:C:47:ARG:NH1	1.96	0.78
1:A:247:PRO:HA	1:A:287:ASN:HD22	1.47	0.78
1:A:118:CYS:HB3	1:A:121:CYS:H	1.49	0.78
1:C:168:TYR:HD1	1:C:178:MET:SD	2.07	0.78
1:B:65:HIS:CD2	1:B:68:PHE:H	1.96	0.78
1:B:66:PRO:O	1:B:157:ARG:HD2	1.83	0.77
1:B:48:ASN:HD22	1:B:50:GLU:HB2	1.49	0.77
1:C:53:CYS:HB3	1:C:58:SER:H	1.49	0.76
1:B:92:TYR:CD2	1:B:114:THR:HA	2.21	0.76
1:C:117:TYR:N	1:C:117:TYR:CD1	2.53	0.76
1:B:317:LEU:HD11	1:B:346:LEU:HD21	1.68	0.75
1:B:87:TYR:H	1:B:333:ARG:NH2	1.85	0.75
1:B:92:TYR:HB3	1:B:114:THR:O	1.87	0.75
1:A:74:ALA:HB3	1:A:75:PRO:HD3	1.66	0.75
1:B:319:ASN:HA	1:B:346:LEU:HD23	1.68	0.75
1:A:304:MET:HE2	1:A:331:ARG:HH21	1.51	0.74
1:B:277:PRO:HG2	1:B:278:GLY:H	1.51	0.74
1:A:67:LEU:N	1:A:67:LEU:HD12	2.01	0.73
1:C:245:THR:HB	1:C:246:PRO:HD2	1.70	0.73
1:B:175:PRO:O	1:B:176:LEU:HD23	1.87	0.73
1:C:53:CYS:SG	1:C:55:CYS:HB3	2.28	0.73
1:C:95:TYR:HB3	1:C:100:CYS:CA	2.19	0.72
1:B:287:ASN:HB2	1:B:359:TRP:CH2	2.24	0.72
1:B:106:LEU:HD13	1:B:134:VAL:CG1	2.18	0.72

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:47:ARG:HH12	1:B:59:LEU:CD2	2.03	0.72
1:A:193:LEU:HB2	1:A:238:PHE:CE1	2.25	0.72
1:C:83:ALA:HA	1:C:86:LEU:HD23	1.71	0.71
1:B:55:CYS:SG	1:B:99:CYS:HA	2.30	0.71
1:C:95:TYR:HD1	1:C:100:CYS:HB3	1.54	0.71
1:C:306:PRO:HG3	1:C:324:TRP:NE1	2.05	0.71
1:C:260:LEU:HG	1:C:298:ALA:CB	2.21	0.71
1:A:54:ILE:HB	1:A:125:LEU:HD21	1.70	0.71
1:B:287:ASN:HB2	1:B:359:TRP:CZ3	2.26	0.71
1:B:88:ASP:C	1:B:90:ASP:H	1.94	0.70
1:C:228:VAL:HG22	1:C:231:ASP:OD2	1.90	0.70
1:A:144:LEU:HA	1:A:156:ARG:CD	2.21	0.70
1:A:285:VAL:HG11	1:A:359:TRP:HZ2	1.56	0.70
1:A:118:CYS:O	1:A:122:VAL:HG23	1.92	0.70
1:C:74:ALA:CB	1:C:75:PRO:HD3	2.20	0.70
1:B:155:GLN:CA	1:B:155:GLN:HE21	1.97	0.70
1:C:108:CYS:SG	1:C:110:ASN:HB2	2.32	0.70
1:C:268:GLN:N	1:C:268:GLN:NE2	2.41	0.69
1:A:53:CYS:SG	1:A:55:CYS:HB2	2.32	0.69
1:B:328:PRO:HG2	1:B:370:PRO:HB2	1.73	0.69
1:B:107:ILE:HD13	1:B:116:CYS:CB	2.22	0.69
1:B:164:LEU:O	1:B:167:PHE:HB3	1.92	0.69
1:B:104:THR:HB	1:B:119:PHE:CD1	2.27	0.69
1:C:49:ILE:HG13	1:C:69:GLU:HG2	1.75	0.69
1:C:41:GLU:HA	1:C:45:ASN:OD1	1.92	0.69
1:B:83:ALA:CA	1:B:86:LEU:HD23	2.23	0.68
1:A:308:THR:HG23	1:A:334:HIS:CE1	2.28	0.68
1:A:202:GLU:CD	1:A:202:GLU:H	1.95	0.68
1:A:117:TYR:CE2	1:A:142:CYS:HB2	2.28	0.68
1:A:271:ARG:HG3	1:A:271:ARG:HH11	1.59	0.68
1:C:276:SER:OG	1:C:277:PRO:HD2	1.95	0.67
1:A:106:LEU:HD13	1:A:134:VAL:HG11	1.76	0.67
1:A:146:LEU:HB2	1:A:147:PRO:HD2	1.76	0.67
1:A:307:VAL:HG21	1:A:331:ARG:HA	1.74	0.67
1:B:95:TYR:N	1:B:95:TYR:HD2	1.91	0.67
1:C:268:GLN:HA	1:C:271:ARG:HG3	1.77	0.67
1:C:182:VAL:HG23	1:C:374:TYR:HD2	1.58	0.67
1:C:122:VAL:HG12	1:C:126:VAL:HG21	1.78	0.66
1:B:88:ASP:O	1:B:90:ASP:N	2.28	0.66
1:A:245:THR:HG21	1:A:290:LEU:HD21	1.77	0.66
1:C:69:GLU:OE2	1:C:155:GLN:HG2	1.95	0.66
1:C:260:LEU:HG	1:C:298:ALA:HB1	1.76	0.66

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:191:ARG:NH1	1:B:237:PRO:HG2	2.10	0.66
1:A:133:LYS:O	1:A:136:ALA:HB3	1.96	0.66
1:A:75:PRO:O	1:A:79:LYS:HG2	1.95	0.65
1:B:38:ILE:HD11	1:B:125:LEU:HD23	1.79	0.65
1:C:278:GLY:H	1:C:279:PRO:CD	2.08	0.65
1:C:65:HIS:CD2	1:C:68:PHE:H	2.07	0.65
1:B:290:LEU:HB2	1:B:295:LEU:HD13	1.79	0.65
1:A:35:ARG:O	1:A:38:ILE:HG12	1.96	0.65
1:B:286:ASP:OD2	1:B:290:LEU:HG	1.96	0.65
1:B:325:SER:OG	1:B:327:ILE:HG13	1.96	0.65
1:B:119:PHE:CD2	1:B:131:SER:HB2	2.32	0.64
1:A:193:LEU:HB2	1:A:238:PHE:CZ	2.32	0.64
1:B:309:ILE:O	1:B:309:ILE:HG13	1.97	0.64
1:B:58:SER:OG	1:B:60:GLN:HG2	1.97	0.64
1:C:346:LEU:HD12	1:C:346:LEU:N	2.12	0.64
1:B:317:LEU:HD13	1:B:318:GLN:N	2.12	0.64
1:B:107:ILE:HD13	1:B:116:CYS:HB3	1.80	0.64
1:B:306:PRO:HG3	1:B:324:TRP:CE2	2.32	0.64
1:A:47:ARG:NH1	1:A:59:LEU:HD23	2.12	0.64
1:B:248:LEU:HD21	1:B:288:LEU:O	1.97	0.64
1:B:234:GLU:O	1:B:236:GLY:N	2.30	0.64
1:B:309:ILE:HD11	1:B:363:LEU:HB3	1.80	0.64
1:A:242:TYR:CD2	1:A:243:GLY:N	2.66	0.64
1:B:262:GLN:HE22	1:B:265:ARG:NH1	1.96	0.63
1:C:311:ASP:HB2	1:C:363:LEU:HD11	1.78	0.63
1:B:317:LEU:HD22	1:B:318:GLN:H	1.62	0.63
1:A:66:PRO:HB2	1:A:67:LEU:HD12	1.79	0.63
1:B:83:ALA:HA	1:B:86:LEU:CD2	2.25	0.63
1:C:243:GLY:O	1:C:284:PHE:HA	1.99	0.63
1:C:266:LEU:H	1:C:266:LEU:HD12	1.63	0.63
1:B:175:PRO:C	1:B:176:LEU:HD23	2.19	0.63
1:C:306:PRO:CG	1:C:324:TRP:HE1	2.11	0.63
1:A:308:THR:HG23	1:A:334:HIS:HE1	1.63	0.63
1:A:104:THR:HB	1:A:119:PHE:H	1.63	0.63
1:C:95:TYR:N	1:C:95:TYR:HD2	1.96	0.63
1:A:190:VAL:HB	1:A:375:PHE:CD1	2.34	0.62
1:B:119:PHE:HD2	1:B:131:SER:HB2	1.63	0.62
1:A:183:PRO:O	1:A:187:ARG:HG3	2.00	0.62
1:B:47:ARG:HH12	1:B:59:LEU:HD23	1.64	0.62
1:B:185:TRP:CD1	1:B:186:ARG:HG3	2.34	0.62
1:C:95:TYR:N	1:C:95:TYR:CD2	2.68	0.62
1:B:214:ASP:C	1:B:216:GLY:H	2.02	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:123:ASP:HA	1:B:127:GLY:O	2.00	0.61
1:A:286:ASP:HB3	1:A:322:ARG:HB2	1.80	0.61
1:C:47:ARG:CB	1:C:47:ARG:HH11	2.03	0.61
1:B:92:TYR:HA	1:B:114:THR:HG22	1.82	0.61
1:B:260:LEU:HD13	1:B:260:LEU:C	2.21	0.61
1:C:281:PHE:HA	1:C:326:ASN:ND2	2.09	0.61
1:C:224:VAL:HG21	1:C:262:GLN:HB3	1.83	0.61
1:B:69:GLU:CB	1:B:155:GLN:HB3	2.30	0.61
1:B:99:CYS:HB3	1:B:121:CYS:SG	2.41	0.61
1:A:193:LEU:HD22	1:A:238:PHE:CE1	2.36	0.61
1:A:146:LEU:H	1:A:146:LEU:HD13	1.66	0.60
1:C:175:PRO:O	1:C:176:LEU:HD23	2.01	0.60
1:A:260:LEU:HD21	1:A:302:LEU:HD21	1.83	0.60
1:A:129:GLY:HA2	1:C:123:ASP:OD2	2.01	0.60
1:B:304:MET:CE	1:B:331:ARG:HH21	2.13	0.60
1:A:240:LEU:HA	1:A:281:PHE:O	2.02	0.60
1:A:115:ARG:CD	1:A:144:LEU:HD12	2.31	0.60
1:B:293:GLU:O	1:B:297:VAL:HG23	2.01	0.60
1:C:47:ARG:NH1	1:C:51:ASP:HB2	2.16	0.60
1:B:106:LEU:HD22	1:B:134:VAL:HG12	1.83	0.60
1:B:161:ARG:NH1	1:B:181:THR:HB	2.17	0.60
1:A:206:LEU:HD11	1:A:365:LYS:HG3	1.84	0.59
1:A:199:ILE:HG13	1:A:242:TYR:CD1	2.37	0.59
1:A:219:LYS:HE2	1:A:235:TRP:CE2	2.37	0.59
1:B:95:TYR:N	1:B:95:TYR:CD2	2.63	0.59
1:A:119:PHE:HD2	1:A:131:SER:HB2	1.67	0.59
1:C:47:ARG:HH12	1:C:51:ASP:HB2	1.67	0.59
1:A:41:GLU:O	1:A:47:ARG:HB3	2.03	0.59
1:C:72:ILE:HG22	1:C:73:CYS:N	2.18	0.59
1:B:304:MET:HE1	1:B:331:ARG:HH21	1.67	0.59
1:C:74:ALA:HB3	1:C:75:PRO:CD	2.25	0.59
1:B:214:ASP:C	1:B:216:GLY:N	2.54	0.59
1:A:106:LEU:HD22	1:A:134:VAL:HG12	1.84	0.59
1:B:65:HIS:O	1:B:157:ARG:NE	2.33	0.58
1:B:92:TYR:HD1	1:B:92:TYR:H	1.50	0.58
1:B:262:GLN:HE22	1:B:265:ARG:HH12	1.51	0.58
1:C:49:ILE:N	1:C:49:ILE:HD13	2.17	0.58
1:B:247:PRO:HG3	1:B:359:TRP:CE3	2.31	0.58
1:C:130:THR:O	1:C:134:VAL:HG23	2.04	0.58
1:C:168:TYR:CD1	1:C:178:MET:SD	2.93	0.58
1:A:50:GLU:OE1	1:A:69:GLU:HG3	2.04	0.57
1:A:248:LEU:HD22	1:A:248:LEU:N	2.19	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:199:ILE:HG22	1:A:203:LEU:HG	1.87	0.57
1:B:117:TYR:CD2	1:B:117:TYR:N	2.72	0.57
1:C:65:HIS:O	1:C:157:ARG:NH1	2.37	0.57
1:A:123:ASP:OD2	1:C:129:GLY:HA2	2.05	0.57
1:B:106:LEU:HD21	1:B:119:PHE:HE2	1.70	0.57
1:C:55:CYS:SG	1:C:99:CYS:HA	2.44	0.57
1:A:304:MET:CE	1:A:331:ARG:HH21	2.16	0.57
1:C:181:THR:HG22	1:C:182:VAL:H	1.70	0.57
1:C:181:THR:HG22	1:C:182:VAL:N	2.19	0.57
1:C:49:ILE:H	1:C:49:ILE:HD13	1.69	0.57
1:A:122:VAL:HG12	1:A:130:THR:OG1	2.05	0.56
1:B:99:CYS:O	1:B:100:CYS:HB2	2.05	0.56
1:C:49:ILE:HD11	1:C:69:GLU:OE1	2.05	0.56
1:B:322:ARG:HH11	1:B:322:ARG:HG2	1.70	0.56
1:B:193:LEU:HB2	1:B:238:PHE:CZ	2.40	0.56
1:B:167:PHE:HA	1:B:170:ARG:HH21	1.70	0.56
1:B:104:THR:HB	1:B:119:PHE:HD1	1.69	0.56
1:C:65:HIS:HB3	1:C:68:PHE:O	2.05	0.56
1:C:69:GLU:HB3	1:C:155:GLN:HB3	1.87	0.56
1:A:164:LEU:HD23	1:A:164:LEU:O	2.05	0.56
1:B:83:ALA:C	1:B:86:LEU:HD23	2.24	0.56
1:A:67:LEU:N	1:A:67:LEU:CD1	2.69	0.56
1:C:72:ILE:HG22	1:C:73:CYS:H	1.71	0.56
1:C:284:PHE:O	1:C:324:TRP:HE3	1.89	0.56
1:C:247:PRO:HA	1:C:287:ASN:HD21	1.68	0.56
1:B:328:PRO:HG2	1:B:370:PRO:CB	2.36	0.56
1:A:361:THR:HG22	1:A:362:LYS:N	2.19	0.56
1:C:48:ASN:HB3	1:C:51:ASP:OD2	2.06	0.56
1:A:260:LEU:HD21	1:A:302:LEU:CD2	2.35	0.56
1:A:117:TYR:HE2	1:A:142:CYS:HB2	1.70	0.56
1:C:71:GLY:O	1:C:72:ILE:HD13	2.06	0.56
1:A:191:ARG:HH11	1:A:237:PRO:HG2	1.66	0.56
1:B:141:VAL:O	1:B:146:LEU:HD23	2.06	0.56
1:A:147:PRO:HA	1:A:156:ARG:HH21	1.69	0.55
1:C:346:LEU:CD1	1:C:346:LEU:H	2.16	0.55
1:A:99:CYS:O	1:A:100:CYS:HB2	2.06	0.55
1:C:359:TRP:O	1:C:361:THR:N	2.38	0.55
1:B:218:LEU:C	1:B:218:LEU:HD23	2.27	0.55
1:A:196:PHE:CD1	1:A:259:TYR:HD2	2.25	0.55
1:B:95:TYR:HB3	1:B:100:CYS:HA	1.89	0.55
1:C:293:GLU:C	1:C:295:LEU:H	2.09	0.55
1:B:214:ASP:N	1:B:215:PRO:HD3	2.21	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:214:ASP:N	1:A:215:PRO:CD	2.70	0.55
1:B:88:ASP:C	1:B:90:ASP:N	2.60	0.55
1:C:88:ASP:O	1:C:91:GLY:N	2.39	0.55
1:A:311:ASP:OD1	1:A:318:GLN:HB2	2.07	0.54
1:B:152:GLY:O	1:B:153:LEU:HD23	2.07	0.54
1:A:77:LYS:HE3	1:A:78:ASP:OD2	2.07	0.54
1:B:74:ALA:HB3	1:B:75:PRO:HD3	1.89	0.54
1:B:94:SER:C	1:B:95:TYR:HD2	2.10	0.54
1:B:288:LEU:HD11	1:B:320:ALA:HB3	1.90	0.54
1:A:198:ASP:HB2	1:A:220:HIS:CD2	2.43	0.54
1:B:98:ILE:HD13	1:B:154:LEU:HD11	1.90	0.54
1:B:230:LYS:O	1:B:234:GLU:HB2	2.08	0.54
1:B:224:VAL:HB	1:B:266:LEU:HD21	1.90	0.54
1:B:193:LEU:HD22	1:B:238:PHE:CE1	2.42	0.54
1:B:122:VAL:C	1:B:126:VAL:HG12	2.26	0.54
1:B:53:CYS:O	1:B:55:CYS:N	2.40	0.54
1:C:110:ASN:OD1	1:C:145:CYS:SG	2.66	0.54
1:A:260:LEU:HD23	1:A:284:PHE:CE2	2.43	0.54
1:B:53:CYS:SG	1:B:55:CYS:HB2	2.48	0.54
1:A:196:PHE:N	1:A:196:PHE:CD2	2.74	0.54
1:C:247:PRO:O	1:C:249:GLY:N	2.40	0.54
1:A:268:GLN:NE2	1:A:271:ARG:HH12	2.06	0.54
1:A:66:PRO:O	1:A:157:ARG:HD2	2.08	0.54
1:B:346:LEU:HD12	1:B:346:LEU:N	2.23	0.54
1:A:307:VAL:CG2	1:A:331:ARG:HA	2.38	0.54
1:A:282:TRP:CZ3	1:A:302:LEU:HD12	2.43	0.54
1:C:160:TRP:O	1:C:163:GLN:N	2.41	0.54
1:A:104:THR:O	1:A:118:CYS:HA	2.09	0.53
1:C:224:VAL:HG23	1:C:262:GLN:CD	2.28	0.53
1:B:347:ALA:HB3	1:B:348:GLN:OE1	2.08	0.53
1:B:81:LEU:HD21	1:B:167:PHE:CE2	2.43	0.53
1:B:322:ARG:HG2	1:B:322:ARG:NH1	2.23	0.53
1:B:92:TYR:CB	1:B:114:THR:O	2.57	0.53
1:A:289:VAL:HG22	1:A:289:VAL:O	2.09	0.53
1:B:359:TRP:HD1	1:B:361:THR:HG23	1.73	0.53
1:B:118:CYS:O	1:B:122:VAL:HG23	2.09	0.53
1:C:94:SER:C	1:C:95:TYR:HD2	2.12	0.53
1:C:49:ILE:CG1	1:C:69:GLU:HG2	2.37	0.53
1:B:317:LEU:CD1	1:B:346:LEU:HD21	2.39	0.53
1:B:291:ASN:O	1:B:295:LEU:HB2	2.09	0.53
1:B:190:VAL:HG13	1:B:192:VAL:HG23	1.90	0.53
1:C:285:VAL:HA	1:C:323:VAL:HG23	1.90	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:122:VAL:CG1	1:B:126:VAL:HG11	2.39	0.53
1:C:160:TRP:HA	1:C:163:GLN:HB3	1.91	0.53
1:B:360:PRO:HB3	1:B:363:LEU:HD23	1.90	0.52
1:A:290:LEU:HD23	1:A:290:LEU:N	2.24	0.52
1:C:369:LEU:O	1:C:371:LEU:N	2.42	0.52
1:A:54:ILE:HB	1:A:125:LEU:CD2	2.39	0.52
1:C:99:CYS:O	1:C:100:CYS:HB2	2.09	0.52
1:B:92:TYR:N	1:B:92:TYR:CD1	2.77	0.52
1:A:99:CYS:O	1:A:100:CYS:CB	2.57	0.52
1:C:300:ARG:CZ	1:C:300:ARG:HA	2.40	0.52
1:A:53:CYS:HB2	1:A:73:CYS:H	1.74	0.52
1:C:83:ALA:CA	1:C:86:LEU:HD23	2.40	0.52
1:B:117:TYR:CE2	1:B:142:CYS:HB2	2.45	0.52
1:C:59:LEU:N	1:C:59:LEU:HD12	2.24	0.52
1:B:168:TYR:CD1	1:B:168:TYR:C	2.83	0.52
1:B:118:CYS:SG	1:B:121:CYS:HB2	2.50	0.52
1:B:87:TYR:H	1:B:333:ARG:HH22	1.55	0.52
1:A:304:MET:HG3	1:A:324:TRP:HD1	1.75	0.52
1:C:225:THR:HG23	1:C:226:ASP:N	2.24	0.52
1:B:325:SER:OG	1:B:326:ASN:N	2.40	0.51
1:A:95:TYR:N	1:A:95:TYR:CD2	2.77	0.51
1:A:357:ALA:O	1:A:358:LYS:C	2.48	0.51
1:A:47:ARG:CZ	1:A:59:LEU:HD23	2.41	0.51
1:B:67:LEU:N	1:B:67:LEU:HD23	2.23	0.51
1:C:68:PHE:CE2	1:C:144:LEU:HD21	2.45	0.51
1:A:228:VAL:O	1:A:231:ASP:HB2	2.11	0.51
1:B:122:VAL:HG12	1:B:126:VAL:HG11	1.92	0.51
1:A:287:ASN:HA	1:A:321:VAL:HG23	1.92	0.51
1:A:77:LYS:CE	1:A:78:ASP:OD2	2.59	0.51
1:A:266:LEU:H	1:A:266:LEU:HD12	1.75	0.51
1:A:242:TYR:CD2	1:A:242:TYR:C	2.83	0.51
1:C:83:ALA:HA	1:C:86:LEU:CD2	2.40	0.51
1:A:266:LEU:N	1:A:266:LEU:HD12	2.25	0.51
1:C:62:HIS:O	1:C:63:THR:HG23	2.10	0.51
1:A:199:ILE:HD11	1:A:242:TYR:CZ	2.46	0.51
1:A:298:ALA:O	1:A:302:LEU:HD23	2.11	0.51
1:C:190:VAL:HG23	1:C:375:PHE:CE2	2.46	0.51
1:A:106:LEU:HD12	1:A:122:VAL:HG21	1.93	0.51
1:C:285:VAL:CA	1:C:323:VAL:HG23	2.41	0.51
1:B:310:PRO:HB3	1:B:338:VAL:HG21	1.92	0.51
1:C:65:HIS:CG	1:C:72:ILE:HD11	2.45	0.50
1:C:192:VAL:O	1:C:218:LEU:HA	2.11	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:359:TRP:HH2	1:A:364:VAL:HG21	1.76	0.50
1:A:81:LEU:HD23	1:A:167:PHE:HE2	1.75	0.50
1:A:364:VAL:O	1:A:366:ASN:N	2.44	0.50
1:C:300:ARG:NE	1:C:300:ARG:HA	2.26	0.50
1:A:165:LYS:HE2	1:A:178:MET:O	2.11	0.50
1:B:92:TYR:HB3	1:B:114:THR:CA	2.41	0.50
1:C:281:PHE:CE2	1:C:328:PRO:HD3	2.46	0.50
1:B:346:LEU:HD12	1:B:346:LEU:H	1.76	0.50
1:B:277:PRO:HG2	1:B:278:GLY:N	2.23	0.50
1:C:241:VAL:HB	1:C:282:TRP:CB	2.41	0.50
1:C:65:HIS:CB	1:C:72:ILE:HD11	2.41	0.50
1:B:248:LEU:H	1:B:287:ASN:HD22	1.58	0.50
1:A:264:HIS:ND1	1:A:301:PHE:HD2	2.09	0.50
1:C:117:TYR:OH	1:C:142:CYS:HB2	2.12	0.50
1:A:322:ARG:O	1:A:323:VAL:HG23	2.10	0.50
1:B:335:TRP:C	1:B:337:LEU:N	2.64	0.50
1:B:66:PRO:HG3	1:B:167:PHE:CG	2.47	0.50
1:B:48:ASN:HD22	1:B:50:GLU:CB	2.23	0.50
1:A:268:GLN:HE21	1:A:271:ARG:HH12	1.59	0.50
1:A:54:ILE:HD13	1:A:70:GLY:HA3	1.92	0.49
1:C:74:ALA:CB	1:C:75:PRO:CD	2.88	0.49
1:A:271:ARG:HG3	1:A:271:ARG:NH1	2.27	0.49
1:C:42:VAL:HG11	1:C:153:LEU:HD11	1.93	0.49
1:C:241:VAL:HB	1:C:282:TRP:HA	1.93	0.49
1:A:340:GLU:O	1:A:343:LEU:N	2.45	0.49
1:A:115:ARG:NE	1:A:144:LEU:HD12	2.27	0.49
1:B:290:LEU:CB	1:B:295:LEU:HD13	2.41	0.49
1:C:225:THR:HG23	1:C:226:ASP:H	1.76	0.49
1:B:210:GLU:HB3	1:B:378:PHE:CD1	2.48	0.49
1:A:307:VAL:HG12	1:A:307:VAL:O	2.13	0.49
1:A:202:GLU:CD	1:A:202:GLU:N	2.65	0.49
1:B:80:PHE:HA	1:B:100:CYS:SG	2.52	0.49
1:A:359:TRP:CD1	1:A:360:PRO:HD2	2.47	0.49
1:C:96:CYS:HB3	1:C:100:CYS:H	1.76	0.49
1:B:93:GLN:H	1:B:114:THR:HB	1.78	0.49
1:C:182:VAL:O	1:C:187:ARG:NH2	2.46	0.49
1:B:51:ASP:N	1:B:51:ASP:OD2	2.45	0.49
1:C:85:PHE:O	1:C:87:TYR:HD1	1.96	0.49
1:B:66:PRO:HG3	1:B:167:PHE:CD1	2.48	0.49
1:C:183:PRO:O	1:C:187:ARG:HB2	2.12	0.49
1:B:274:PRO:HB3	1:A:274:PRO:HB3	1.94	0.49
1:C:306:PRO:HG3	1:C:324:TRP:CE2	2.47	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:227:THR:O	1:B:265:ARG:NH2	2.46	0.48
1:B:356:ALA:C	1:B:358:LYS:H	2.16	0.48
1:C:306:PRO:HG3	1:C:324:TRP:CZ2	2.48	0.48
1:A:219:LYS:HE2	1:A:235:TRP:CD2	2.48	0.48
1:B:346:LEU:H	1:B:346:LEU:CD1	2.27	0.48
1:A:199:ILE:HG22	1:A:199:ILE:O	2.12	0.48
1:B:228:VAL:O	1:B:229:ARG:C	2.51	0.48
1:A:199:ILE:CG2	1:A:203:LEU:HG	2.44	0.48
1:C:314:GLY:C	1:C:316:SER:H	2.16	0.48
1:C:95:TYR:CD1	1:C:100:CYS:HB3	2.41	0.48
1:C:339:SER:HB3	1:C:342:GLU:CB	2.44	0.48
1:B:364:VAL:O	1:B:365:LYS:C	2.51	0.48
1:B:42:VAL:CG2	1:B:52:ILE:HD11	2.44	0.48
1:C:117:TYR:N	1:C:117:TYR:HD1	2.10	0.48
1:C:190:VAL:HG23	1:C:375:PHE:CD2	2.49	0.48
1:C:344:SER:O	1:C:347:ALA:HB3	2.14	0.48
1:C:268:GLN:N	1:C:268:GLN:HE21	1.98	0.48
1:C:96:CYS:C	1:C:98:ILE:H	2.16	0.48
1:A:268:GLN:HE21	1:A:271:ARG:NH1	2.12	0.48
1:A:44:ALA:O	1:A:46:GLN:HG3	2.14	0.48
1:B:192:VAL:O	1:B:218:LEU:HA	2.14	0.48
1:A:94:SER:C	1:A:95:TYR:HD2	2.17	0.48
1:B:274:PRO:HB3	1:A:274:PRO:CG	2.44	0.48
1:A:210:GLU:N	1:A:378:PHE:CE1	2.82	0.48
1:C:309:ILE:HG13	1:C:309:ILE:O	2.14	0.48
1:B:197:GLU:HA	1:B:197:GLU:OE2	2.14	0.48
1:B:220:HIS:HD2	1:B:221:VAL:H	1.61	0.48
1:A:121:CYS:O	1:A:125:LEU:HD12	2.14	0.47
1:A:346:LEU:HD23	1:A:346:LEU:O	2.14	0.47
1:B:295:LEU:HD21	1:B:322:ARG:NE	2.29	0.47
1:A:369:LEU:N	1:A:370:PRO:CD	2.78	0.47
1:C:168:TYR:HD1	1:C:178:MET:CE	2.27	0.47
1:A:363:LEU:N	1:A:363:LEU:HD22	2.29	0.47
1:A:199:ILE:HG13	1:A:242:TYR:CE1	2.49	0.47
1:B:234:GLU:C	1:B:236:GLY:H	2.15	0.47
1:C:224:VAL:HB	1:C:266:LEU:HD11	1.96	0.47
1:B:161:ARG:NH1	1:B:161:ARG:HG2	2.28	0.47
1:A:199:ILE:CG2	1:A:199:ILE:O	2.61	0.47
1:C:228:VAL:HG23	1:C:230:LYS:H	1.79	0.47
1:A:261:PHE:O	1:A:264:HIS:HB3	2.14	0.47
1:C:189:PRO:O	1:C:375:PHE:HD2	1.97	0.47
1:B:122:VAL:HG12	1:B:126:VAL:CG1	2.45	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:168:TYR:HD2	1:C:172:SER:HB2	1.78	0.47
1:A:376:LYS:HD3	1:A:378:PHE:CE2	2.49	0.47
1:C:194:SER:OG	1:C:220:HIS:HA	2.14	0.47
1:A:168:TYR:CD1	1:A:168:TYR:C	2.88	0.47
1:C:191:ARG:HG2	1:C:217:GLN:CB	2.45	0.47
1:C:284:PHE:O	1:C:324:TRP:CE3	2.68	0.47
1:A:247:PRO:HG3	1:A:359:TRP:HD1	1.80	0.47
1:B:48:ASN:ND2	1:B:50:GLU:CG	2.77	0.47
1:B:295:LEU:HD12	1:B:295:LEU:HA	1.82	0.47
1:C:126:VAL:HG21	1:C:143:TYR:OH	2.14	0.47
1:A:245:THR:HG21	1:A:290:LEU:CD2	2.41	0.47
1:A:81:LEU:HD23	1:A:167:PHE:CE2	2.49	0.47
1:A:305:GLU:OE2	1:A:305:GLU:HA	2.15	0.47
1:A:263:PHE:O	1:A:267:LEU:HB2	2.15	0.47
1:C:323:VAL:HG22	1:C:324:TRP:N	2.30	0.46
1:A:193:LEU:HD22	1:A:238:PHE:HE1	1.80	0.46
1:A:59:LEU:HD12	1:A:59:LEU:N	2.30	0.46
1:C:356:ALA:O	1:C:357:ALA:HB3	2.14	0.46
1:B:339:SER:HB3	1:B:342:GLU:HG2	1.97	0.46
1:B:99:CYS:O	1:B:100:CYS:CB	2.63	0.46
1:C:117:TYR:HD1	1:C:117:TYR:H	1.62	0.46
1:C:92:TYR:N	1:C:92:TYR:CD1	2.83	0.46
1:C:140:TRP:HZ2	1:C:143:TYR:CE2	2.33	0.46
1:B:53:CYS:SG	1:B:53:CYS:O	2.72	0.46
1:A:289:VAL:HG13	1:A:290:LEU:HD23	1.98	0.46
1:A:47:ARG:NH1	1:A:59:LEU:CD2	2.79	0.46
1:B:115:ARG:HD2	1:B:144:LEU:CD1	2.37	0.46
1:C:192:VAL:HG22	1:C:240:LEU:CB	2.45	0.46
1:B:191:ARG:HB2	1:B:239:ASP:OD1	2.16	0.46
1:B:214:ASP:N	1:B:215:PRO:CD	2.78	0.46
1:C:169:ASP:HA	1:C:175:PRO:HG3	1.97	0.46
1:B:220:HIS:CD2	1:B:221:VAL:N	2.83	0.46
1:B:310:PRO:HD2	1:B:335:TRP:CE3	2.50	0.46
1:A:65:HIS:HD2	1:A:68:PHE:H	1.64	0.46
1:A:85:PHE:O	1:A:87:TYR:HD1	1.98	0.46
1:C:283:MET:HA	1:C:324:TRP:O	2.15	0.46
1:C:271:ARG:HG2	1:C:280:PHE:CZ	2.51	0.46
1:A:107:ILE:CG2	1:A:108:CYS:N	2.79	0.46
1:B:200:LYS:HG3	1:B:201:LYS:N	2.31	0.46
1:A:223:ASP:OD2	1:A:254:ARG:NH2	2.49	0.46
1:A:359:TRP:HA	1:A:360:PRO:HD3	1.68	0.45
1:B:262:GLN:NE2	1:B:265:ARG:NH1	2.64	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:88:ASP:OD2	1:A:94:SER:HA	2.15	0.45
1:A:95:TYR:N	1:A:95:TYR:HD2	2.13	0.45
1:B:67:LEU:HD22	1:B:160:TRP:CE3	2.51	0.45
1:B:42:VAL:HG23	1:B:52:ILE:HD11	1.98	0.45
1:C:364:VAL:HA	1:C:367:CYS:SG	2.56	0.45
1:A:64:GLN:HA	1:A:71:GLY:HA2	1.97	0.45
1:C:216:GLY:C	1:C:218:LEU:H	2.20	0.45
1:B:277:PRO:CG	1:B:278:GLY:H	2.19	0.45
1:C:260:LEU:HD11	1:C:298:ALA:HA	1.97	0.45
1:C:119:PHE:O	1:C:122:VAL:HG23	2.17	0.45
1:C:317:LEU:CD2	1:C:346:LEU:HD11	2.46	0.45
1:B:311:ASP:HB2	1:B:319:ASN:O	2.17	0.45
1:B:193:LEU:HB2	1:B:238:PHE:CE1	2.51	0.45
1:A:107:ILE:O	1:A:140:TRP:HE3	1.99	0.45
1:B:224:VAL:HG23	1:B:262:GLN:HE21	1.82	0.45
1:B:228:VAL:O	1:B:231:ASP:N	2.41	0.45
1:B:220:HIS:CD2	1:B:221:VAL:H	2.34	0.45
1:A:101:SER:O	1:A:103:GLU:N	2.50	0.45
1:A:147:PRO:O	1:A:148:SER:O	2.35	0.45
1:C:108:CYS:C	1:C:110:ASN:H	2.19	0.45
1:B:306:PRO:HG3	1:B:324:TRP:CZ2	2.51	0.45
1:A:219:LYS:HE3	1:A:221:VAL:CG2	2.46	0.45
1:A:364:VAL:O	1:A:365:LYS:C	2.54	0.45
1:B:181:THR:HA	1:B:374:TYR:CE2	2.52	0.45
1:A:150:ARG:HE	1:A:150:ARG:HA	1.82	0.45
1:B:96:CYS:HB3	1:B:100:CYS:H	1.81	0.45
1:C:278:GLY:N	1:C:279:PRO:HD3	2.23	0.45
1:B:310:PRO:HD2	1:B:335:TRP:HE3	1.82	0.45
1:B:229:ARG:NH1	1:A:303:GLU:OE1	2.50	0.45
1:B:150:ARG:N	1:B:155:GLN:HE22	2.15	0.45
1:C:86:LEU:HD22	1:C:86:LEU:N	2.31	0.45
1:B:369:LEU:N	1:B:370:PRO:CD	2.80	0.45
1:A:198:ASP:C	1:A:200:LYS:H	2.18	0.45
1:A:234:GLU:O	1:A:236:GLY:N	2.48	0.45
1:B:249:GLY:O	1:B:250:HIS:C	2.54	0.45
1:A:62:HIS:HB2	1:A:74:ALA:N	2.32	0.45
1:A:192:VAL:HG12	1:A:193:LEU:N	2.32	0.45
1:B:369:LEU:N	1:B:370:PRO:HD3	2.32	0.45
1:C:224:VAL:HG23	1:C:262:GLN:NE2	2.32	0.45
1:C:188:GLN:O	1:C:189:PRO:O	2.35	0.45
1:A:104:THR:HB	1:A:119:PHE:N	2.31	0.44
1:C:328:PRO:O	1:C:330:ILE:HG23	2.16	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:192:VAL:HG21	1:A:203:LEU:HD13	1.99	0.44
1:C:110:ASN:C	1:C:112:ASP:H	2.21	0.44
1:C:56:CYS:SG	1:C:58:SER:HB2	2.57	0.44
1:A:47:ARG:HH12	1:A:59:LEU:CD2	2.30	0.44
1:C:134:VAL:HA	1:C:137:MET:CE	2.47	0.44
1:B:312:VAL:HG12	1:B:313:HIS:N	2.32	0.44
1:C:179:PHE:CD2	1:C:278:GLY:HA3	2.52	0.44
1:C:110:ASN:O	1:C:112:ASP:N	2.50	0.44
1:A:202:GLU:O	1:A:205:SER:N	2.50	0.44
1:A:53:CYS:HB2	1:A:73:CYS:N	2.33	0.44
1:C:65:HIS:ND1	1:C:72:ILE:CD1	2.74	0.44
1:C:49:ILE:HB	1:C:54:ILE:HG21	1.99	0.44
1:C:160:TRP:O	1:C:161:ARG:C	2.56	0.44
1:C:369:LEU:C	1:C:371:LEU:N	2.70	0.44
1:B:335:TRP:C	1:B:337:LEU:H	2.20	0.44
1:A:64:GLN:HB2	1:A:157:ARG:HH21	1.82	0.44
1:C:317:LEU:HG	1:C:346:LEU:HD21	1.97	0.44
1:C:370:PRO:C	1:C:372:ARG:H	2.20	0.44
1:C:35:ARG:O	1:C:124:SER:HB2	2.18	0.44
1:A:257:SER:HB3	1:A:294:ASP:OD2	2.18	0.44
1:C:295:LEU:C	1:C:297:VAL:N	2.71	0.44
1:A:90:ASP:OD1	1:A:92:TYR:HD1	2.00	0.44
1:C:201:LYS:C	1:C:203:LEU:H	2.21	0.44
1:A:147:PRO:O	1:A:148:SER:C	2.56	0.44
1:A:35:ARG:O	1:A:37:LEU:N	2.51	0.44
1:B:190:VAL:HG23	1:B:375:PHE:CD1	2.53	0.44
1:C:286:ASP:CG	1:C:287:ASN:H	2.21	0.43
1:B:107:ILE:HA	1:B:116:CYS:HB3	2.00	0.43
1:C:359:TRP:HA	1:C:360:PRO:HD3	1.90	0.43
1:B:308:THR:H	1:B:334:HIS:CE1	2.36	0.43
1:C:174:ASN:O	1:C:175:PRO:O	2.35	0.43
1:B:142:CYS:SG	1:B:145:CYS:HB2	2.58	0.43
1:A:362:LYS:HG3	1:A:363:LEU:HD22	1.99	0.43
1:B:362:LYS:HE3	1:B:362:LYS:H	1.84	0.43
1:A:105:LEU:HA	1:A:117:TYR:O	2.19	0.43
1:C:121:CYS:O	1:C:122:VAL:C	2.56	0.43
1:B:229:ARG:O	1:B:233:GLU:HG3	2.17	0.43
1:B:339:SER:O	1:B:342:GLU:HB2	2.18	0.43
1:A:35:ARG:C	1:A:37:LEU:H	2.22	0.43
1:C:63:THR:HB	1:C:64:GLN:H	1.51	0.43
1:C:255:PRO:HA	1:C:256:PRO:HD3	1.84	0.43
1:A:67:LEU:HD12	1:A:67:LEU:H	1.79	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:117:TYR:OH	1:C:142:CYS:SG	2.77	0.43
1:B:223:ASP:OD2	1:B:225:THR:HG22	2.18	0.43
1:C:210:GLU:HB3	1:C:378:PHE:CD2	2.53	0.43
1:A:115:ARG:HD3	1:A:144:LEU:HD12	2.00	0.43
1:A:227:THR:HG22	1:A:228:VAL:N	2.34	0.43
1:B:273:LYS:O	1:B:274:PRO:C	2.56	0.43
1:C:65:HIS:HA	1:C:66:PRO:HD3	1.88	0.43
1:C:65:HIS:HB2	1:C:72:ILE:HD11	2.01	0.43
1:A:364:VAL:HG23	1:A:365:LYS:N	2.34	0.43
1:B:141:VAL:O	1:B:142:CYS:O	2.36	0.43
1:A:361:THR:O	1:A:363:LEU:N	2.51	0.43
1:B:206:LEU:HD21	1:B:365:LYS:HE3	2.00	0.43
1:B:45:ASN:HD22	1:B:45:ASN:N	2.16	0.43
1:A:147:PRO:HG2	1:A:148:SER:H	1.84	0.43
1:B:110:ASN:HA	1:B:111:PRO:HD3	1.84	0.43
1:B:318:GLN:HE21	1:B:318:GLN:HA	1.84	0.43
1:C:245:THR:HB	1:C:246:PRO:CD	2.45	0.43
1:A:199:ILE:HG22	1:A:203:LEU:CD1	2.49	0.43
1:C:210:GLU:O	1:C:210:GLU:HG3	2.18	0.43
1:C:104:THR:OG1	1:C:119:PHE:HB2	2.19	0.43
1:A:248:LEU:CD2	1:A:248:LEU:N	2.82	0.43
1:B:210:GLU:HB3	1:B:378:PHE:CE1	2.53	0.43
1:B:62:HIS:C	1:B:62:HIS:ND1	2.72	0.43
1:B:81:LEU:CD2	1:B:167:PHE:HE2	2.32	0.42
1:A:141:VAL:O	1:A:146:LEU:HD11	2.19	0.42
1:A:146:LEU:HB2	1:A:147:PRO:CD	2.48	0.42
1:C:168:TYR:CD2	1:C:172:SER:HB2	2.53	0.42
1:C:86:LEU:CD2	1:C:86:LEU:N	2.83	0.42
1:C:263:PHE:C	1:C:265:ARG:N	2.71	0.42
1:A:218:LEU:HD23	1:A:218:LEU:C	2.38	0.42
1:B:65:HIS:HB3	1:B:68:PHE:O	2.19	0.42
1:A:67:LEU:H	1:A:67:LEU:CD1	2.32	0.42
1:B:277:PRO:O	1:B:278:GLY:O	2.37	0.42
1:B:214:ASP:O	1:B:216:GLY:N	2.52	0.42
1:B:141:VAL:HG13	1:B:145:CYS:HB3	2.01	0.42
1:A:266:LEU:H	1:A:266:LEU:CD1	2.32	0.42
1:B:45:ASN:N	1:B:45:ASN:ND2	2.67	0.42
1:A:107:ILE:HG22	1:A:108:CYS:N	2.33	0.42
1:B:165:LYS:O	1:B:166:ALA:C	2.56	0.42
1:A:128:PRO:HG2	1:C:36:ASP:HB3	2.01	0.42
1:C:248:LEU:H	1:C:287:ASN:HD22	1.66	0.42
1:C:262:GLN:CA	1:C:262:GLN:HE21	2.31	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:295:LEU:C	1:C:297:VAL:H	2.23	0.42
1:A:369:LEU:O	1:A:372:ARG:HB3	2.19	0.42
1:B:84:LEU:HA	1:B:84:LEU:HD23	1.83	0.42
1:C:65:HIS:HB2	1:C:70:GLY:O	2.20	0.42
1:C:92:TYR:O	1:C:93:GLN:C	2.58	0.42
1:C:196:PHE:O	1:C:197:GLU:CB	2.67	0.42
1:B:72:ILE:HG22	1:B:73:CYS:O	2.19	0.42
1:B:53:CYS:C	1:B:55:CYS:H	2.22	0.42
1:C:86:LEU:H	1:C:86:LEU:CD2	2.32	0.42
1:B:85:PHE:CD2	1:B:370:PRO:HB3	2.55	0.42
1:B:302:LEU:HD23	1:B:302:LEU:HA	1.84	0.42
1:B:77:LYS:HD2	1:B:78:ASP:N	2.34	0.42
1:B:48:ASN:ND2	1:B:50:GLU:HB2	2.28	0.42
1:C:127:GLY:O	1:C:130:THR:HG23	2.19	0.42
1:B:92:TYR:HB3	1:B:114:THR:C	2.39	0.42
1:A:319:ASN:CA	1:A:346:LEU:HD11	2.40	0.42
1:B:316:SER:O	1:B:317:LEU:HB2	2.20	0.42
1:B:216:GLY:C	1:B:218:LEU:H	2.21	0.42
1:C:241:VAL:HB	1:C:282:TRP:CA	2.50	0.42
1:A:340:GLU:HA	1:A:340:GLU:OE1	2.20	0.42
1:A:273:LYS:O	1:A:274:PRO:C	2.57	0.42
1:C:248:LEU:H	1:C:287:ASN:ND2	2.18	0.42
1:A:37:LEU:O	1:A:41:GLU:HG2	2.20	0.42
1:A:311:ASP:HB2	1:A:363:LEU:HD11	2.02	0.42
1:B:149:SER:C	1:B:155:GLN:HE22	2.23	0.41
1:C:106:LEU:HD12	1:C:118:CYS:O	2.20	0.41
1:B:277:PRO:CG	1:B:278:GLY:N	2.81	0.41
1:C:202:GLU:HB3	1:C:361:THR:HG21	2.01	0.41
1:A:101:SER:HB2	1:A:118:CYS:SG	2.60	0.41
1:A:191:ARG:NH1	1:A:237:PRO:CG	2.74	0.41
1:B:190:VAL:HG23	1:B:375:PHE:CE1	2.54	0.41
1:A:234:GLU:C	1:A:236:GLY:H	2.22	0.41
1:C:349:ASN:C	1:C:351:GLN:H	2.23	0.41
1:B:343:LEU:C	1:B:345:LEU:N	2.74	0.41
1:C:49:ILE:CD1	1:C:49:ILE:H	2.33	0.41
1:C:345:LEU:C	1:C:347:ALA:H	2.23	0.41
1:B:77:LYS:HD2	1:B:77:LYS:C	2.41	0.41
1:A:106:LEU:CD1	1:A:122:VAL:HG21	2.51	0.41
1:A:144:LEU:HD23	1:A:156:ARG:HG3	2.02	0.41
1:A:53:CYS:HA	1:A:71:GLY:O	2.20	0.41
1:A:271:ARG:HA	1:A:272:PRO:HD3	1.83	0.41
1:A:84:LEU:HD12	1:A:84:LEU:HA	1.68	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:45:ASN:HB2	1:C:47:ARG:HG2	2.01	0.41
1:C:122:VAL:HG12	1:C:143:TYR:OH	2.21	0.41
1:C:232:VAL:CG2	1:C:266:LEU:HD23	2.50	0.41
1:A:368:PHE:C	1:A:370:PRO:HD2	2.41	0.41
1:B:53:CYS:C	1:B:55:CYS:N	2.74	0.41
1:C:323:VAL:HG22	1:C:324:TRP:H	1.86	0.41
1:B:306:PRO:HG3	1:B:324:TRP:NE1	2.34	0.41
1:C:202:GLU:H	1:C:202:GLU:CD	2.24	0.41
1:C:161:ARG:HG2	1:C:161:ARG:HH11	1.86	0.41
1:C:335:TRP:C	1:C:337:LEU:N	2.74	0.41
1:A:292:LYS:HB3	1:A:292:LYS:NZ	2.35	0.41
1:C:360:PRO:HB3	1:C:363:LEU:HD23	2.03	0.41
1:A:220:HIS:ND1	1:A:221:VAL:N	2.68	0.41
1:C:199:ILE:O	1:C:199:ILE:HG22	2.21	0.41
1:C:328:PRO:O	1:C:330:ILE:N	2.53	0.41
1:B:311:ASP:HB3	1:B:318:GLN:HB2	2.03	0.41
1:B:318:GLN:HA	1:B:318:GLN:NE2	2.36	0.41
1:A:38:ILE:HD11	1:A:124:SER:OG	2.21	0.41
1:C:202:GLU:HB3	1:C:361:THR:CG2	2.51	0.41
1:B:215:PRO:HB2	1:B:217:GLN:NE2	2.36	0.41
1:C:300:ARG:HH11	1:C:300:ARG:HG2	1.85	0.41
1:B:199:ILE:O	1:B:199:ILE:HG13	2.19	0.41
1:B:149:SER:OG	1:B:155:GLN:NE2	2.54	0.41
1:B:144:LEU:HA	1:B:156:ARG:HD2	1.98	0.41
1:B:246:PRO:HA	1:B:247:PRO:HD3	1.90	0.41
1:B:283:MET:HG3	1:B:325:SER:HB2	2.03	0.41
1:A:260:LEU:CD2	1:A:302:LEU:HD21	2.50	0.41
1:B:161:ARG:HH11	1:B:161:ARG:HG2	1.86	0.41
1:C:273:LYS:O	1:C:274:PRO:C	2.59	0.41
1:A:157:ARG:HH11	1:A:157:ARG:HG2	1.85	0.40
1:C:378:PHE:O	1:C:379:SER:HB3	2.21	0.40
1:B:174:ASN:N	1:B:175:PRO:HD3	2.37	0.40
1:A:146:LEU:N	1:A:146:LEU:HD13	2.33	0.40
1:A:143:TYR:O	1:A:156:ARG:HD3	2.22	0.40
1:B:265:ARG:HD2	1:A:301:PHE:CD1	2.56	0.40
1:C:293:GLU:O	1:C:295:LEU:N	2.55	0.40
1:C:88:ASP:O	1:C:89:ASP:C	2.60	0.40
1:B:98:ILE:CD1	1:B:154:LEU:HD11	2.51	0.40
1:C:191:ARG:HB2	1:C:239:ASP:OD1	2.21	0.40
1:C:364:VAL:C	1:C:366:ASN:N	2.75	0.40
1:B:49:ILE:HG13	1:B:49:ILE:H	1.63	0.40
1:B:346:LEU:N	1:B:346:LEU:CD1	2.85	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:331:ARG:C	1:A:333:ARG:H	2.25	0.40
1:A:265:ARG:HB3	1:A:266:LEU:HD12	2.03	0.40
1:B:40:TYR:O	1:B:41:GLU:C	2.59	0.40
1:A:249:GLY:O	1:A:250:HIS:C	2.60	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	345/386 (89%)	268 (78%)	53 (15%)	24 (7%)	2	17
1	B	345/386 (89%)	254 (74%)	66 (19%)	25 (7%)	2	16
1	C	345/386 (89%)	226 (66%)	81 (24%)	38 (11%)	1	6
All	All	1035/1158 (89%)	748 (72%)	200 (19%)	87 (8%)	1	12

All (87) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	89	ASP
1	B	142	CYS
1	B	147	PRO
1	B	235	TRP
1	B	277	PRO
1	B	278	GLY
1	A	148	SER
1	A	250	HIS
1	C	74	ALA
1	C	103	GLU
1	C	139	ASN
1	C	142	CYS
1	C	189	PRO
1	C	215	PRO
1	C	248	LEU

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Mol	Chain	Res	Type
1	C	277	PRO
1	C	329	ALA
1	B	53	CYS
1	B	91	GLY
1	B	211	SER
1	B	250	HIS
1	B	254	ARG
1	B	316	SER
1	A	36	ASP
1	A	58	SER
1	A	100	CYS
1	A	102	GLY
1	A	199	ILE
1	A	235	TRP
1	A	247	PRO
1	A	278	GLY
1	A	362	LYS
1	A	365	LYS
1	C	159	LYS
1	C	175	PRO
1	C	181	THR
1	C	197	GLU
1	C	255	PRO
1	B	54	ILE
1	B	90	ASP
1	B	115	ARG
1	A	53	CYS
1	A	104	THR
1	A	126	VAL
1	A	142	CYS
1	A	167	PHE
1	A	202	GLU
1	A	358	LYS
1	A	360	PRO
1	C	100	CYS
1	C	111	PRO
1	C	202	GLU
1	C	217	GLN
1	C	237	PRO
1	C	250	HIS
1	C	256	PRO
1	C	294	ASP

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Mol	Chain	Res	Type
1	B	256	PRO
1	B	274	PRO
1	B	344	SER
1	C	89	ASP
1	C	93	GLN
1	C	97	SER
1	C	161	ARG
1	C	303	GLU
1	C	360	PRO
1	B	255	PRO
1	B	357	ALA
1	B	360	PRO
1	A	265	ARG
1	A	277	PRO
1	C	98	ILE
1	C	214	ASP
1	C	274	PRO
1	C	278	GLY
1	C	287	ASN
1	B	41	GLU
1	A	321	VAL
1	B	66	PRO
1	B	214	ASP
1	A	66	PRO
1	B	111	PRO
1	C	38	ILE
1	C	54	ILE
1	C	232	VAL
1	C	328	PRO
1	C	236	GLY

### 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	301/344 (88%)	279 (93%)	22 (7%)	20	63
1	B	300/344 (87%)	278 (93%)	22 (7%)	20	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	208/344 (60%)	190 (91%)	18 (9%)	15	53
All	All	809/1032 (78%)	747 (92%)	62 (8%)	18	60

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	38	ILE
1	B	51	ASP
1	B	52	ILE
1	B	55	CYS
1	B	62	HIS
1	B	77	LYS
1	B	82	ASP
1	B	92	TYR
1	B	95	TYR
1	B	99	CYS
1	B	114	THR
1	B	117	TYR
1	B	118	CYS
1	B	121	CYS
1	B	128	PRO
1	B	155	GLN
1	B	183	PRO
1	B	253	ASP
1	B	256	PRO
1	B	274	PRO
1	B	321	VAL
1	B	362	LYS
1	A	36	ASP
1	A	49	ILE
1	A	82	ASP
1	A	141	VAL
1	A	146	LEU
1	A	174	ASN
1	A	183	PRO
1	A	196	PHE
1	A	229	ARG
1	A	242	TYR
1	A	252	CYS
1	A	267	LEU
1	A	271	ARG
1	A	290	LEU

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Mol	Chain	Res	Type
1	A	294	ASP
1	A	308	THR
1	A	309	ILE
1	A	310	PRO
1	A	312	VAL
1	A	321	VAL
1	A	346	LEU
1	A	378	PHE
1	C	47	ARG
1	C	49	ILE
1	C	63	THR
1	C	92	TYR
1	C	95	TYR
1	C	110	ASN
1	C	117	TYR
1	C	119	PHE
1	C	121	CYS
1	C	122	VAL
1	C	145	CYS
1	C	154	LEU
1	C	157	ARG
1	C	168	TYR
1	C	226	ASP
1	C	262	GLN
1	C	268	GLN
1	C	274	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	45	ASN
1	B	48	ASN
1	B	60	GLN
1	B	64	GLN
1	B	65	HIS
1	B	155	GLN
1	B	163	GLN
1	B	217	GLN
1	B	220	HIS
1	B	262	GLN
1	B	287	ASN
1	A	65	HIS

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Mol	Chain	Res	Type
1	A	155	GLN
1	A	174	ASN
1	A	264	HIS
1	A	268	GLN
1	A	287	ASN
1	A	349	ASN
1	C	48	ASN
1	C	64	GLN
1	C	65	HIS
1	C	110	ASN
1	C	135	HIS
1	C	163	GLN
1	C	262	GLN
1	C	264	HIS
1	C	268	GLN
1	C	287	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

Of 9 ligands modelled in this entry, 9 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
1	A	347/386 (89%)	-0.21	0	100 100	29, 85, 169, 195	0
1	B	347/386 (89%)	-0.19	0	100 100	33, 81, 191, 200	0
1	C	347/386 (89%)	0.11	4 (1%)	75 29	93, 166, 199, 200	0
All	All	1041/1158 (89%)	-0.10	4 (0%)	90 57	29, 112, 195, 200	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	320	ALA	4.4
1	C	250	HIS	3.6
1	C	252	CYS	2.5
1	C	376	LYS	2.4

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

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

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	ZN	C	508	1/1	0.29	2.66	104,104,104,104	1
2	ZN	B	505	1/1	0.24	1.12	13,13,13,13	1
2	ZN	A	502	1/1	0.23	0.74	48,48,48,48	1
2	ZN	B	506	1/1	0.17	0.07	67,67,67,67	0
2	ZN	A	503	1/1	0.15	-0.05	75,75,75,75	0
2	ZN	B	504	1/1	0.13	-0.19	59,59,59,59	1
2	ZN	A	501	1/1	0.11	-1.06	91,91,91,91	1
2	ZN	C	509	1/1	0.06	-1.43	127,127,127,127	0
2	ZN	C	507	1/1	0.03	-2.40	167,167,167,167	1

## 6.5 Other polymers ⓘ

There are no such residues in this entry.