



# Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 04:35 am BST

PDB ID : 4DNR  
Title : Crystal structure of the CusBA heavy-metal efflux complex from Escherichia coli, E716F mutant  
Authors : Su, C.-C.; Long, F.; Yu, E.  
Deposited on : 2012-02-08  
Resolution : 3.68 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

<https://www.wwpdb.org/validation/2017/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  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

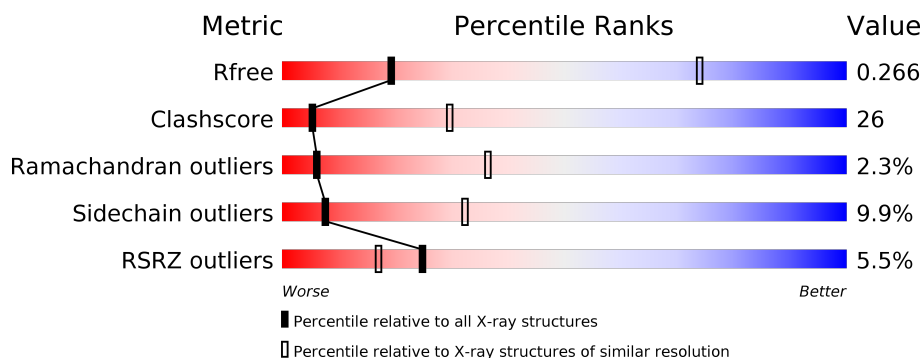
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.68 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))
$R_{free}$	130704	1013 (3.84-3.52)
Clashscore	141614	1070 (3.84-3.52)
Ramachandran outliers	138981	1036 (3.84-3.52)
Sidechain outliers	138945	1033 (3.84-3.52)
RSRZ outliers	127900	1471 (3.86-3.50)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . 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	B	413	
1	C	413	
2	A	1054	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12887 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 Cation efflux system protein CusB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	322	Total	C	N	O	S	0	0	0
			2458	1555	428	469	6			
1	C	324	Total	C	N	O	S	0	0	0
			2473	1563	430	474	6			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	408	HIS	-	EXPRESSION TAG	UNP P77239
B	409	HIS	-	EXPRESSION TAG	UNP P77239
B	410	HIS	-	EXPRESSION TAG	UNP P77239
B	411	HIS	-	EXPRESSION TAG	UNP P77239
B	412	HIS	-	EXPRESSION TAG	UNP P77239
B	413	HIS	-	EXPRESSION TAG	UNP P77239
C	408	HIS	-	EXPRESSION TAG	UNP P77239
C	409	HIS	-	EXPRESSION TAG	UNP P77239
C	410	HIS	-	EXPRESSION TAG	UNP P77239
C	411	HIS	-	EXPRESSION TAG	UNP P77239
C	412	HIS	-	EXPRESSION TAG	UNP P77239
C	413	HIS	-	EXPRESSION TAG	UNP P77239

- Molecule 2 is a protein called Cation efflux system protein CusA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	1031	Total	C	N	O	S	0	0	0
			7950	5144	1333	1436	37			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	MET	-	EXPRESSION TAG	UNP P38054
A	-5	HIS	-	EXPRESSION TAG	UNP P38054

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	HIS	-	EXPRESSION TAG	UNP P38054
A	-3	HIS	-	EXPRESSION TAG	UNP P38054
A	-2	HIS	-	EXPRESSION TAG	UNP P38054
A	-1	HIS	-	EXPRESSION TAG	UNP P38054
A	0	HIS	-	EXPRESSION TAG	UNP P38054
A	716	PHE	GLU	ENGINEERED MUTATION	UNP P38054

- Molecule 3 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Cu 1 1	0	0

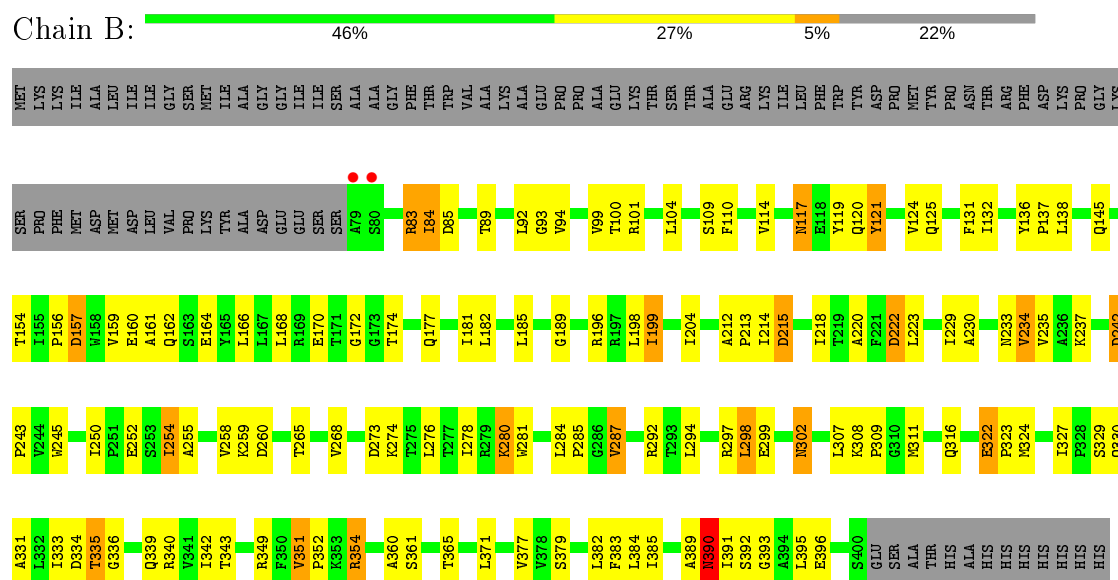
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	4	Total O 4 4	0	0
4	A	1	Total O 1 1	0	0

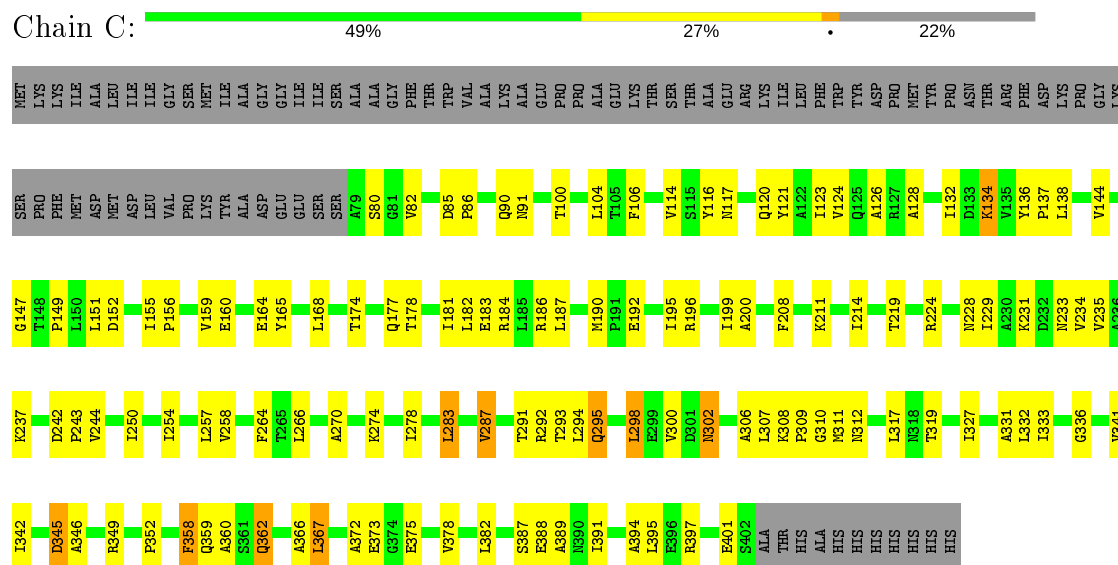
### 3 Residue-property plots

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

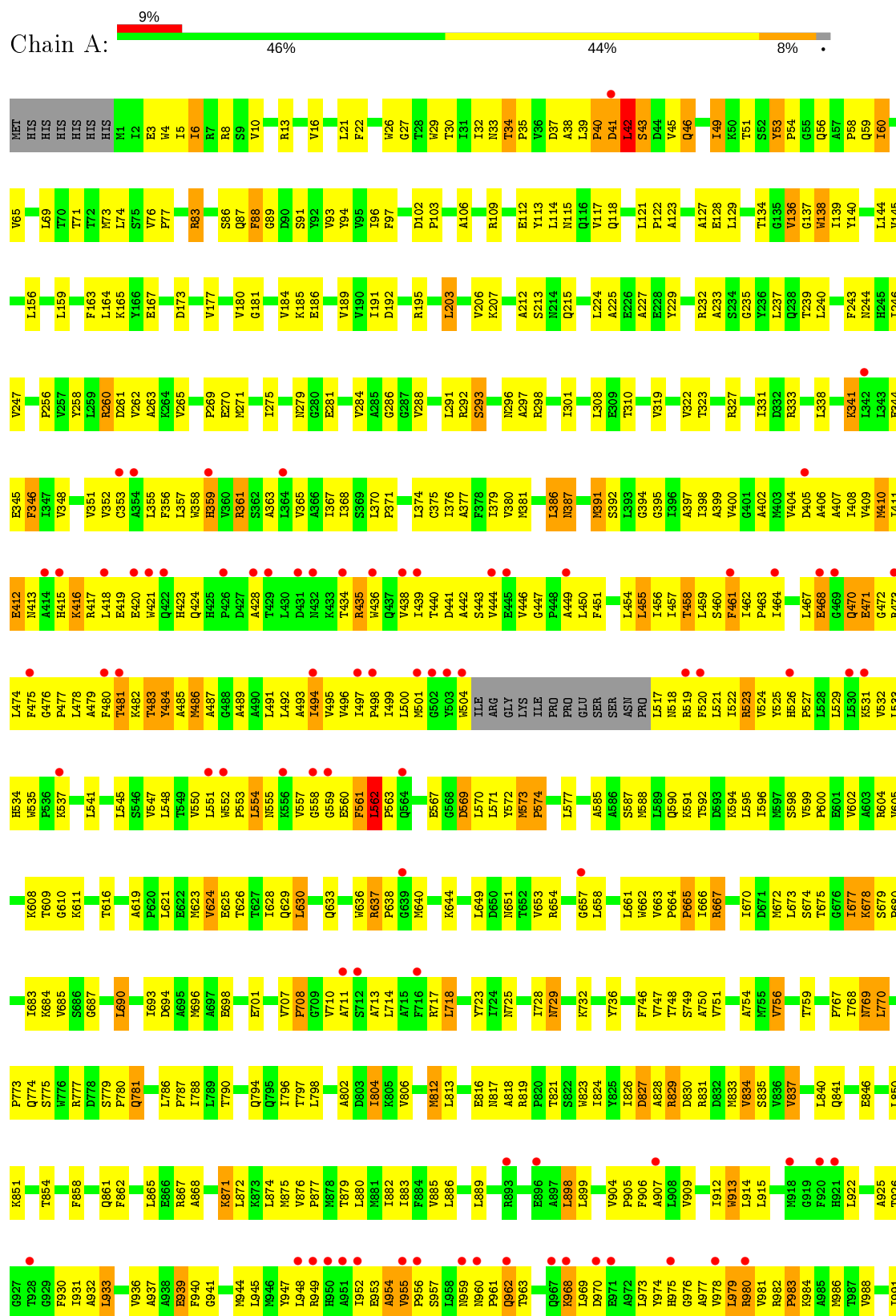
#### • Molecule 1: Cation efflux system protein CusB



#### • Molecule 1: Cation efflux system protein CusB



- Molecule 2: Cation efflux system protein CusA





## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	159.59Å 159.59Å 689.65Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	97.67 – 3.68 114.94 – 3.68	Depositor EDS
% Data completeness (in resolution range)	89.9 (97.67-3.68) 98.8 (114.94-3.68)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.68 (at 3.67Å)	Xtriage
Refinement program	PHENIX 1.6.4_486	Depositor
R, $R_{free}$	0.244 , 0.272 0.237 , 0.266	Depositor DCC
$R_{free}$ test set	1872 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	83.3	Xtriage
Anisotropy	0.241	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 93.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.86	EDS
Total number of atoms	12887	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.27% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: CU

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	B	0.21	0/2498	0.42	0/3401
1	C	0.21	0/2513	0.41	0/3421
2	A	0.22	0/8117	0.41	1/11052 (0.0%)
All	All	0.22	0/13128	0.41	1/17874 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	562	LEU	C-N-CD	5.22	139.36	128.40

There are no chirality outliers.

There are no planarity outliers.

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2458	0	2522	110	0
1	C	2473	0	2533	96	0
2	A	7950	0	8198	499	0
3	A	1	0	0	0	0
4	A	1	0	0	0	0
4	C	4	0	0	0	0
All	All	12887	0	13253	686	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 26.

All (686) 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:B:385:ILE:HG22	1:B:389:ALA:HB2	1.36	1.06
2:A:327:ARG:HH11	2:A:666:ILE:HG13	1.27	0.95
2:A:395:GLY:HA3	2:A:478:LEU:HB3	1.49	0.93
2:A:588:MET:HE2	2:A:658:LEU:HD13	1.51	0.93
2:A:51:THR:HG22	2:A:127:ALA:HA	1.49	0.90
2:A:955:VAL:HG13	2:A:956:PRO:HD3	1.55	0.88
1:B:117:ASN:HD22	1:B:119:TYR:H	1.20	0.88
1:C:295:GLN:HA	1:C:295:GLN:HE21	1.39	0.88
1:C:242:ASP:HB3	1:C:243:PRO:HD3	1.55	0.87
2:A:497:ILE:HB	2:A:498:PRO:HD3	1.56	0.86
2:A:925:ALA:HB1	2:A:1012:ILE:HG22	1.57	0.85
2:A:464:ILE:HD11	2:A:931:ILE:HG13	1.59	0.82
2:A:956:PRO:HG3	2:A:968:LYS:HE2	1.61	0.82
2:A:71:THR:HG22	2:A:818:ALA:HB1	1.61	0.81
2:A:554:LEU:HD11	2:A:912:ILE:HB	1.62	0.81
2:A:1023:ALA:HB3	2:A:1024:PRO:HD3	1.63	0.81
1:B:352:PRO:HB3	1:B:395:LEU:HD12	1.62	0.80
2:A:458:THR:HG23	2:A:459:LEU:HD22	1.63	0.80
2:A:270:GLU:HG2	2:A:271:MET:H	1.48	0.78
2:A:982:ARG:HB3	2:A:983:PRO:HD3	1.66	0.78
1:C:266:LEU:HD12	1:C:300:VAL:HG21	1.67	0.77
2:A:637:ARG:HH11	2:A:637:ARG:HB2	1.50	0.77
2:A:40:PRO:HD2	2:A:666:ILE:HG21	1.67	0.77
1:B:120:GLN:HE22	1:B:243:PRO:HD2	1.49	0.76
2:A:391:MET:HG2	2:A:474:LEU:HG	1.67	0.76
2:A:498:PRO:HA	2:A:501:MET:HG2	1.66	0.76
2:A:463:PRO:HG3	2:A:879:THR:HG21	1.68	0.76
2:A:952:ILE:HG12	2:A:1039:TRP:HE1	1.51	0.76
1:B:360:ALA:HB2	1:B:365:THR:HG22	1.67	0.76
2:A:461:PHE:HB3	2:A:479:ALA:HB1	1.68	0.75
1:B:117:ASN:ND2	1:B:119:TYR:H	1.83	0.75
1:B:242:ASP:HB3	1:B:243:PRO:HD3	1.68	0.75
2:A:6:ILE:O	2:A:10:VAL:HG23	1.87	0.75
2:A:574:PRO:HB2	2:A:658:LEU:HD11	1.68	0.74
2:A:557:VAL:HG22	2:A:558:GLY:H	1.51	0.74
2:A:574:PRO:HG2	2:A:624:VAL:HG13	1.68	0.74
2:A:468:GLU:HG3	2:A:472:GLY:HA3	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:250:ILE:HG21	1:B:258:VAL:HG11	1.71	0.73
1:C:278:ILE:HD13	1:C:298:LEU:HD22	1.71	0.73
2:A:680:PRO:HA	2:A:861:GLN:HB2	1.69	0.73
2:A:933:LEU:HB2	2:A:1016:MET:HG2	1.68	0.72
2:A:39:LEU:HD12	2:A:136:VAL:HB	1.71	0.72
2:A:690:LEU:HD22	2:A:693:ILE:HD11	1.70	0.72
2:A:370:LEU:HB2	2:A:371:PRO:HD3	1.71	0.72
1:B:223:LEU:HD12	1:B:235:VAL:HG12	1.70	0.72
2:A:327:ARG:HE	2:A:666:ILE:HD11	1.53	0.72
2:A:599:VAL:O	2:A:602:VAL:HG12	1.90	0.72
1:B:334:ASP:HA	1:B:339:GLN:HB2	1.72	0.71
2:A:1039:TRP:CE3	2:A:1039:TRP:HA	2.26	0.71
2:A:529:LEU:HA	2:A:532:VAL:HG12	1.72	0.71
2:A:370:LEU:HD22	2:A:400:VAL:HG23	1.73	0.70
2:A:327:ARG:NH1	2:A:666:ILE:HG13	2.03	0.70
2:A:416:LYS:HE3	2:A:416:LYS:HA	1.72	0.70
1:B:145:GLN:HA	1:B:215:ASP:HB3	1.73	0.70
2:A:493:ALA:O	2:A:497:ILE:HG12	1.92	0.69
2:A:559:GLY:HA2	2:A:922:LEU:HD23	1.72	0.69
2:A:418:LEU:HD21	2:A:438:VAL:HB	1.73	0.69
2:A:458:THR:HB	2:A:483:THR:OG1	1.92	0.69
1:B:230:ALA:H	1:B:233:ASN:ND2	1.91	0.69
2:A:77:PRO:HG2	2:A:109:ARG:HD2	1.75	0.69
2:A:417:ARG:HG2	2:A:441:ASP:HB3	1.75	0.68
1:B:120:GLN:NE2	1:B:243:PRO:HD2	2.07	0.68
2:A:435:ARG:HD3	2:A:435:ARG:H	1.57	0.68
1:C:308:LYS:O	1:C:311:MET:HG2	1.93	0.68
1:B:302:ASN:HD21	1:B:307:LEU:H	1.42	0.68
2:A:529:LEU:HD21	2:A:974:TYR:CD1	2.29	0.68
2:A:73:MET:O	2:A:76:VAL:HG12	1.93	0.68
2:A:817:ASN:O	2:A:818:ALA:HB3	1.94	0.67
2:A:940:PHE:CE2	2:A:1024:PRO:HG3	2.29	0.67
1:C:123:ILE:HG12	1:C:237:LYS:HG3	1.77	0.67
1:B:125:GLN:NE2	1:C:228:ASN:H	1.92	0.67
2:A:560:GLU:HG3	2:A:561:PHE:N	2.09	0.67
2:A:6:ILE:HD11	2:A:494:ILE:HG21	1.78	0.66
2:A:729:ASN:C	2:A:729:ASN:HD22	1.98	0.66
2:A:456:ILE:HD12	2:A:883:ILE:HD13	1.76	0.66
1:B:204:ILE:H	1:B:204:ILE:HD12	1.61	0.66
2:A:651:ASN:HA	2:A:654:ARG:HH21	1.61	0.66
2:A:472:GLY:O	2:A:477:PRO:HD3	1.94	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:968:LYS:HA	2:A:968:LYS:HE3	1.76	0.66
2:A:237:LEU:HD23	2:A:243:PHE:CZ	2.31	0.65
2:A:351:VAL:O	2:A:355:LEU:HB2	1.96	0.65
2:A:599:VAL:HG21	2:A:649:LEU:HD12	1.78	0.65
2:A:862:PHE:HA	2:A:865:LEU:HB3	1.77	0.65
2:A:192:ASP:HB3	2:A:195:ARG:HG2	1.79	0.65
2:A:145:VAL:HG12	2:A:284:VAL:HG11	1.79	0.65
2:A:83:ARG:HG2	2:A:675:THR:HG21	1.79	0.65
1:B:242:ASP:HB3	1:B:243:PRO:CD	2.27	0.65
2:A:395:GLY:H	2:A:478:LEU:HD22	1.62	0.65
1:B:252:GLU:HG2	1:C:270:ALA:HB2	1.78	0.65
2:A:984:LYS:HD2	2:A:1024:PRO:HB3	1.77	0.64
2:A:912:ILE:HG23	2:A:915:LEU:HD12	1.79	0.64
2:A:38:ALA:O	2:A:40:PRO:HD3	1.98	0.64
2:A:621:LEU:HD22	2:A:621:LEU:H	1.62	0.64
1:B:280:LYS:HE3	1:B:281:TRP:H	1.62	0.64
1:B:322:GLU:HG3	1:B:323:PRO:HD2	1.79	0.64
2:A:521:LEU:HD12	2:A:522:ILE:N	2.12	0.64
1:B:99:VAL:HG21	1:B:371:LEU:HD13	1.79	0.64
2:A:718:LEU:HD11	2:A:812:MET:O	1.98	0.63
2:A:554:LEU:HD21	2:A:912:ILE:HD13	1.80	0.63
2:A:381:MET:HG2	2:A:386:LEU:HD11	1.80	0.63
2:A:596:ILE:HG12	2:A:653:VAL:HG21	1.79	0.63
2:A:83:ARG:HB2	2:A:94:TYR:HB2	1.79	0.63
2:A:139:ILE:HD13	2:A:327:ARG:NH2	2.13	0.63
2:A:297:ALA:O	2:A:301:ILE:HG13	1.99	0.63
2:A:137:GLY:O	2:A:139:ILE:HG12	1.98	0.63
2:A:381:MET:HG2	2:A:386:LEU:CD1	2.29	0.62
2:A:525:TYR:HE1	2:A:977:ALA:HB1	1.64	0.62
2:A:746:PHE:O	2:A:750:ALA:HB3	1.98	0.62
2:A:203:LEU:HD11	2:A:750:ALA:HB2	1.80	0.62
2:A:86:SER:HB2	2:A:813:LEU:HB2	1.81	0.62
2:A:754:ALA:O	2:A:769:ASN:HB2	2.00	0.62
2:A:496:VAL:HA	2:A:499:ILE:HG22	1.82	0.62
1:B:174:THR:HB	1:B:177:GLN:HG3	1.80	0.62
2:A:42:LEU:HD12	2:A:43:SER:H	1.64	0.62
2:A:991:ILE:HG21	2:A:1020:MET:HG2	1.81	0.62
1:B:280:LYS:HA	1:B:280:LYS:HE3	1.80	0.62
2:A:454:LEU:HB2	2:A:486:MET:SD	2.40	0.62
2:A:406:ALA:HB1	2:A:450:LEU:HD13	1.81	0.61
2:A:786:LEU:HD22	2:A:787:PRO:HD2	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:680:PRO:HD2	2:A:827:ASP:HB2	1.81	0.61
2:A:992:ILE:O	2:A:996:LEU:HB2	2.00	0.61
1:B:265:THR:HB	1:B:316:GLN:HB3	1.83	0.61
2:A:3:GLU:O	2:A:6:ILE:HG22	2.00	0.61
2:A:243:PHE:O	2:A:246:ILE:HG12	2.00	0.61
1:C:80:SER:O	1:C:349:ARG:HD3	2.00	0.61
2:A:523:ARG:O	2:A:527:PRO:HD2	2.00	0.61
2:A:983:PRO:O	2:A:986:MET:HG3	2.01	0.60
1:B:83:ARG:NH2	1:C:90:GLN:HB3	2.15	0.60
1:B:390:ASN:HD22	1:B:393:GLY:H	1.49	0.60
2:A:637:ARG:HB2	2:A:637:ARG:NH1	2.16	0.60
2:A:139:ILE:CG2	2:A:301:ILE:HG12	2.30	0.60
1:C:165:TYR:HE2	1:C:178:THR:HG23	1.66	0.60
2:A:139:ILE:HG21	2:A:301:ILE:HG12	1.84	0.60
2:A:941:GLY:HA2	2:A:1031:ILE:HD11	1.84	0.60
2:A:550:VAL:HG13	2:A:913:TRP:HE1	1.67	0.59
2:A:165:LYS:HE2	2:A:177:VAL:O	2.02	0.59
2:A:244:ASN:HB3	2:A:260:ARG:HB3	1.83	0.59
1:B:242:ASP:CB	1:B:243:PRO:HD3	2.32	0.59
2:A:1039:TRP:HE3	2:A:1039:TRP:HA	1.66	0.59
2:A:604:ARG:HG2	2:A:604:ARG:HH21	1.67	0.59
2:A:573:MET:O	2:A:661:LEU:HB3	2.01	0.59
2:A:1006:SER:HA	2:A:1009:MET:HB2	1.85	0.59
2:A:876:VAL:N	2:A:877:PRO:HD2	2.18	0.59
2:A:474:LEU:HD23	2:A:475:PHE:CZ	2.37	0.59
2:A:191:ILE:HA	2:A:263:ALA:HB2	1.84	0.59
2:A:678:LYS:HD2	2:A:679:SER:N	2.18	0.59
1:B:109:SER:HB3	1:B:316:GLN:OE1	2.02	0.59
2:A:83:ARG:HG2	2:A:675:THR:CG2	2.32	0.59
2:A:571:LEU:HD12	2:A:663:VAL:HG23	1.84	0.59
2:A:58:PRO:HD3	2:A:88:PHE:HB2	1.85	0.59
2:A:930:PHE:CD2	2:A:1015:PRO:HB3	2.37	0.59
2:A:547:VAL:HG11	2:A:905:PRO:HB2	1.85	0.58
1:C:242:ASP:HB3	1:C:243:PRO:CD	2.31	0.58
2:A:439:ILE:HD13	2:A:498:PRO:HB2	1.85	0.58
2:A:816:GLU:O	2:A:817:ASN:HB2	2.02	0.58
2:A:13:ARG:HH21	2:A:499:ILE:HD11	1.66	0.58
2:A:411:ILE:HG12	2:A:497:ILE:HD12	1.85	0.58
2:A:405:ASP:O	2:A:408:ILE:HG13	2.04	0.58
2:A:885:VAL:O	2:A:889:LEU:HB2	2.03	0.58
2:A:904:VAL:HG23	2:A:905:PRO:HD3	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:355:LEU:HD12	2:A:356:PHE:CE1	2.38	0.58
2:A:550:VAL:O	2:A:554:LEU:HB3	2.04	0.58
1:B:222:ASP:OD1	1:B:234:VAL:HG23	2.03	0.58
2:A:415:HIS:O	2:A:419:GLU:HG2	2.03	0.58
2:A:907:ALA:HA	2:A:1023:ALA:HB2	1.85	0.57
2:A:481:THR:HG23	2:A:482:LYS:H	1.69	0.57
2:A:521:LEU:HD12	2:A:522:ILE:HG13	1.84	0.57
2:A:413:ASN:O	2:A:417:ARG:HB2	2.04	0.57
1:B:307:LEU:HA	1:B:311:MET:HE1	1.86	0.57
1:B:278:ILE:HG13	1:B:298:LEU:HD13	1.85	0.57
2:A:454:LEU:O	2:A:457:ILE:HG22	2.04	0.57
2:A:1031:ILE:HB	2:A:1032:PRO:HD3	1.85	0.57
2:A:572:TYR:CE2	2:A:574:PRO:HG3	2.39	0.57
2:A:714:LEU:HD23	2:A:717:ARG:HD2	1.86	0.57
1:B:335:THR:HG22	1:B:391:ILE:HD12	1.86	0.57
1:B:220:ALA:HB3	1:B:237:LYS:HB3	1.87	0.57
2:A:944:MET:SD	2:A:980:ARG:HD2	2.44	0.56
1:C:132:ILE:HD11	1:C:229:ILE:HB	1.87	0.56
1:B:162:GLN:HG2	1:B:198:LEU:HD22	1.87	0.56
1:B:92:LEU:HD13	2:A:281:GLU:O	2.05	0.56
2:A:191:ILE:HD13	2:A:263:ALA:HB2	1.87	0.56
2:A:590:GLN:O	2:A:594:LYS:HG3	2.06	0.56
1:C:333:ILE:HG12	1:C:382:LEU:HD11	1.87	0.56
2:A:189:VAL:HB	2:A:770:LEU:HD12	1.87	0.56
1:B:84:ILE:HD11	2:A:594:LYS:HD3	1.88	0.56
2:A:956:PRO:HB3	2:A:968:LYS:HG3	1.88	0.56
1:C:378:VAL:HG13	1:C:382:LEU:HD23	1.87	0.56
2:A:333:ARG:HH21	2:A:1004:ALA:HB2	1.71	0.56
2:A:387:ASN:H	2:A:387:ASN:ND2	2.04	0.56
2:A:571:LEU:HD22	2:A:626:THR:O	2.05	0.56
2:A:457:ILE:O	2:A:461:PHE:HB2	2.05	0.55
2:A:533:LEU:HD22	2:A:1036:LYS:NZ	2.22	0.55
2:A:486:MET:HE2	2:A:487:ALA:N	2.21	0.55
2:A:616:THR:O	2:A:673:LEU:HD21	2.06	0.55
2:A:837:VAL:O	2:A:841:GLN:HG3	2.06	0.55
1:B:84:ILE:HD13	1:B:85:ASP:N	2.21	0.55
2:A:759:THR:HG23	2:A:768:ILE:HD11	1.86	0.55
1:B:138:LEU:HD23	1:B:218:ILE:HD11	1.88	0.55
2:A:747:VAL:O	2:A:751:VAL:HG12	2.07	0.55
2:A:525:TYR:CE1	2:A:977:ALA:HB1	2.41	0.55
1:B:131:PHE:CE2	1:B:154:THR:HB	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:456:ILE:HD13	2:A:886:LEU:HD12	1.89	0.55
1:B:336:GLY:HA3	2:A:775:SER:OG	2.06	0.55
2:A:574:PRO:HG2	2:A:624:VAL:CG1	2.36	0.55
2:A:949:ARG:HG2	2:A:1035:TYR:OH	2.06	0.55
2:A:186:GLU:HG3	2:A:767:PRO:HG2	1.88	0.55
1:B:245:TRP:CE3	1:B:297:ARG:HD3	2.42	0.55
2:A:395:GLY:HA2	2:A:398:ILE:HB	1.87	0.55
2:A:696:MET:HE2	2:A:851:LYS:HD3	1.88	0.55
2:A:707:VAL:HG23	2:A:708:PRO:HD2	1.89	0.55
2:A:32:ILE:HG13	2:A:33:ASN:N	2.22	0.54
2:A:27:GLY:HA3	2:A:375:CYS:HB3	1.89	0.54
1:B:132:ILE:HD11	1:B:229:ILE:HB	1.89	0.54
1:C:387:SER:HB3	2:A:577:LEU:HD23	1.88	0.54
1:C:302:ASN:HD21	1:C:306:ALA:H	1.55	0.54
2:A:472:GLY:O	2:A:476:GLY:HA3	2.08	0.54
2:A:1038:MET:O	2:A:1042:ARG:HD3	2.06	0.54
2:A:346:PHE:C	2:A:346:PHE:HD1	2.11	0.54
1:B:83:ARG:HH22	1:C:90:GLN:HB3	1.73	0.54
1:B:360:ALA:HA	1:B:365:THR:HA	1.90	0.54
1:B:382:LEU:HD23	2:A:269:PRO:HD3	1.90	0.54
2:A:879:THR:O	2:A:882:ILE:HG22	2.07	0.54
1:C:219:THR:OG1	1:C:237:LYS:HD2	2.07	0.54
2:A:944:MET:HB3	2:A:1031:ILE:HD13	1.90	0.53
1:B:110:PHE:CE1	1:B:250:ILE:HG23	2.43	0.53
2:A:395:GLY:N	2:A:478:LEU:HD13	2.23	0.53
2:A:945:LEU:O	2:A:949:ARG:HG3	2.08	0.53
2:A:394:GLY:HA2	2:A:1009:MET:SD	2.47	0.53
2:A:346:PHE:CD1	2:A:346:PHE:C	2.81	0.53
2:A:904:VAL:N	2:A:905:PRO:CD	2.72	0.53
2:A:932:ALA:O	2:A:936:VAL:HG23	2.09	0.53
2:A:356:PHE:HB3	2:A:982:ARG:HH22	1.74	0.53
1:B:84:ILE:HG22	1:C:91:ASN:OD1	2.08	0.53
2:A:464:ILE:H	2:A:464:ILE:HD12	1.74	0.53
2:A:841:GLN:HG2	2:A:858:PHE:CE1	2.43	0.53
2:A:907:ALA:HB2	2:A:937:ALA:HB2	1.90	0.53
2:A:144:LEU:HD11	2:A:164:LEU:HD11	1.91	0.53
2:A:687:GLY:HA3	2:A:854:THR:HG22	1.91	0.53
2:A:525:TYR:CD1	2:A:981:VAL:HG21	2.43	0.53
1:B:331:ALA:HB2	1:B:379:SER:HA	1.90	0.53
2:A:409:VAL:HB	2:A:450:LEU:HD11	1.91	0.53
2:A:341:LYS:HG2	2:A:998:ILE:HG12	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:419:GLU:O	2:A:423:HIS:HB2	2.09	0.52
2:A:574:PRO:HD2	2:A:624:VAL:O	2.08	0.52
2:A:976:GLY:O	2:A:980:ARG:HD3	2.10	0.52
2:A:173:ASP:O	2:A:291:LEU:HD12	2.10	0.52
2:A:471:GLU:HA	2:A:474:LEU:HB2	1.91	0.52
1:B:83:ARG:HA	1:B:83:ARG:HE	1.74	0.52
2:A:440:THR:O	2:A:444:VAL:HG23	2.10	0.52
2:A:531:LYS:HA	2:A:531:LYS:HE3	1.91	0.52
2:A:955:VAL:CG1	2:A:956:PRO:HD3	2.35	0.52
1:C:164:GLU:O	1:C:168:LEU:HD13	2.10	0.52
2:A:203:LEU:CD1	2:A:750:ALA:HB2	2.40	0.51
2:A:562:LEU:HB2	2:A:563:PRO:HD3	1.92	0.51
1:C:266:LEU:HG	1:C:278:ILE:HD11	1.92	0.51
2:A:926:THR:HG22	2:A:1011:ARG:O	2.09	0.51
2:A:192:ASP:HB3	2:A:195:ARG:CG	2.40	0.51
2:A:959:ASN:O	2:A:963:THR:HG22	2.10	0.51
1:B:389:ALA:O	1:B:390:ASN:C	2.48	0.51
1:C:266:LEU:HD11	1:C:298:LEU:CD1	2.40	0.51
2:A:701:GLU:OE1	2:A:713:ALA:HB2	2.11	0.51
1:B:273:ASP:OD2	1:B:274:LYS:HD2	2.11	0.51
1:B:89:THR:H	2:A:590:GLN:HE22	1.58	0.51
2:A:42:LEU:HD11	2:A:134:THR:CB	2.41	0.51
2:A:213:SER:OG	2:A:246:ILE:HD12	2.10	0.51
2:A:207:LYS:HG3	2:A:756:VAL:HG21	1.92	0.51
2:A:980:ARG:O	2:A:983:PRO:HD2	2.11	0.51
1:C:128:ALA:HA	1:C:231:LYS:HD3	1.93	0.51
2:A:572:TYR:HB3	2:A:628:ILE:HD11	1.92	0.51
2:A:779:SER:HB2	2:A:780:PRO:HD2	1.93	0.51
2:A:51:THR:OG1	2:A:91:SER:HB3	2.11	0.51
2:A:341:LYS:O	2:A:344:GLU:HB2	2.11	0.51
1:B:94:VAL:HG13	1:B:383:PHE:HZ	1.76	0.51
2:A:13:ARG:NH2	2:A:499:ILE:HD11	2.25	0.51
2:A:475:PHE:HA	2:A:478:LEU:HD12	1.92	0.51
2:A:365:VAL:HG21	2:A:500:LEU:HB2	1.93	0.51
2:A:979:LEU:O	2:A:983:PRO:HD3	2.11	0.51
1:B:343:THR:OG1	1:B:351:VAL:HG23	2.11	0.51
2:A:74:LEU:HD11	2:A:818:ALA:HB3	1.93	0.50
2:A:922:LEU:N	2:A:922:LEU:HD22	2.26	0.50
2:A:786:LEU:HB3	2:A:798:LEU:HB2	1.92	0.50
2:A:828:ALA:HB1	2:A:831:ARG:HG3	1.93	0.50
1:B:114:VAL:HG12	1:B:309:PRO:HA	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:118:GLN:HE22	2:A:127:ALA:H	1.58	0.50
2:A:451:PHE:O	2:A:455:LEU:HB2	2.11	0.50
2:A:693:ILE:HA	2:A:696:MET:HG2	1.93	0.50
2:A:868:ALA:O	2:A:872:LEU:HG	2.10	0.50
1:B:384:LEU:N	1:B:384:LEU:HD12	2.25	0.50
1:C:165:TYR:CE2	1:C:178:THR:HG23	2.45	0.50
2:A:22:PHE:O	2:A:26:TRP:HB2	2.11	0.50
2:A:380:VAL:HG11	2:A:480:PHE:CE2	2.45	0.50
2:A:678:LYS:HA	2:A:861:GLN:HE21	1.77	0.50
2:A:134:THR:OG1	2:A:136:VAL:HG22	2.12	0.50
2:A:459:LEU:HD23	2:A:886:LEU:HD11	1.94	0.50
2:A:69:LEU:O	2:A:73:MET:HG2	2.12	0.50
2:A:833:MET:HE2	2:A:862:PHE:HB3	1.93	0.50
2:A:256:PRO:HG2	2:A:258:TYR:CE1	2.47	0.50
2:A:32:ILE:HG13	2:A:33:ASN:H	1.77	0.50
2:A:38:ALA:H	2:A:331:ILE:HG12	1.75	0.50
2:A:725:ASN:O	2:A:804:ILE:HA	2.11	0.50
2:A:955:VAL:N	2:A:956:PRO:CD	2.74	0.50
1:C:117:ASN:HB3	1:C:120:GLN:HG3	1.94	0.50
1:C:317:LEU:HD11	1:C:319:THR:OG1	2.11	0.50
2:A:457:ILE:HD11	2:A:932:ALA:HA	1.94	0.50
1:B:390:ASN:ND2	1:B:393:GLY:H	2.10	0.50
2:A:30:THR:O	2:A:34:THR:HB	2.12	0.50
2:A:474:LEU:HD23	2:A:475:PHE:CE1	2.46	0.50
1:C:358:PHE:CD2	1:C:358:PHE:C	2.83	0.50
1:B:121:TYR:CG	1:C:224:ARG:HD2	2.47	0.50
2:A:163:PHE:O	2:A:167:GLU:HG2	2.10	0.49
2:A:517:LEU:O	2:A:521:LEU:HG	2.11	0.49
2:A:666:ILE:N	2:A:666:ILE:HD12	2.27	0.49
1:B:390:ASN:HD21	1:B:392:SER:HB2	1.76	0.49
1:C:362:GLN:HA	1:C:362:GLN:HE21	1.78	0.49
1:B:110:PHE:CG	1:B:250:ILE:HG12	2.47	0.49
2:A:596:ILE:O	2:A:602:VAL:HG11	2.13	0.49
2:A:749:SER:HA	2:A:754:ALA:HB3	1.94	0.49
2:A:680:PRO:O	2:A:862:PHE:HD1	1.95	0.49
1:B:164:GLU:O	1:B:168:LEU:HD13	2.13	0.49
2:A:102:ASP:OD1	2:A:103:PRO:HD2	2.13	0.49
1:B:136:TYR:HB3	1:B:137:PRO:HD2	1.93	0.49
2:A:397:ALA:HB1	2:A:998:ILE:HD13	1.94	0.49
2:A:790:THR:OG1	2:A:794:GLN:HB2	2.12	0.49
2:A:41:ASP:HB2	2:A:473:ARG:HD2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:435:ARG:CD	2:A:435:ARG:H	2.25	0.49
2:A:816:GLU:HB3	2:A:821:THR:HG21	1.94	0.49
1:B:156:PRO:O	1:B:157:ASP:HB2	2.12	0.49
2:A:680:PRO:CD	2:A:827:ASP:HB2	2.43	0.49
1:C:124:VAL:O	1:C:235:VAL:HG12	2.12	0.49
2:A:1014:ALA:HB3	2:A:1015:PRO:HD3	1.95	0.48
2:A:521:LEU:HD12	2:A:522:ILE:H	1.76	0.48
2:A:585:ALA:CB	2:A:621:LEU:HB3	2.42	0.48
2:A:817:ASN:O	2:A:818:ALA:CB	2.59	0.48
1:B:250:ILE:HD13	1:B:258:VAL:HG11	1.94	0.48
1:C:257:LEU:O	1:C:317:LEU:HD21	2.13	0.48
2:A:109:ARG:O	2:A:112:GLU:HG2	2.14	0.48
2:A:491:LEU:O	2:A:495:VAL:HG23	2.12	0.48
1:B:125:GLN:HE21	1:C:228:ASN:HD22	1.59	0.48
1:C:244:VAL:HG11	1:C:307:LEU:HD23	1.94	0.48
2:A:677:ILE:HD13	2:A:677:ILE:N	2.28	0.48
2:A:977:ALA:HA	2:A:980:ARG:HD3	1.96	0.48
1:C:174:THR:H	1:C:177:GLN:NE2	2.11	0.48
2:A:572:TYR:CZ	2:A:574:PRO:HG3	2.49	0.48
2:A:862:PHE:HA	2:A:865:LEU:CB	2.41	0.48
2:A:952:ILE:CG1	2:A:1039:TRP:HE1	2.23	0.48
2:A:275:ILE:HD12	2:A:275:ILE:N	2.29	0.48
2:A:592:THR:O	2:A:596:ILE:HG13	2.13	0.48
2:A:365:VAL:CG2	2:A:496:VAL:HB	2.44	0.48
2:A:533:LEU:HD22	2:A:1036:LYS:HZ2	1.77	0.48
2:A:623:MET:CE	2:A:625:GLU:HG3	2.44	0.48
2:A:707:VAL:HG11	2:A:840:LEU:HD21	1.95	0.48
2:A:714:LEU:HD22	2:A:717:ARG:HB2	1.94	0.48
2:A:356:PHE:CE2	2:A:986:MET:HB3	2.48	0.48
1:C:327:ILE:CD1	1:C:367:LEU:HD21	2.43	0.48
2:A:461:PHE:CZ	2:A:932:ALA:HB2	2.48	0.48
2:A:729:ASN:HB3	2:A:732:LYS:HB2	1.95	0.48
1:B:101:ARG:HB2	1:B:101:ARG:NH1	2.29	0.48
1:B:322:GLU:O	1:B:324:MET:HG3	2.14	0.48
2:A:97:PHE:CE1	2:A:106:ALA:HB1	2.49	0.47
2:A:960:ASN:N	2:A:961:PRO:HD2	2.29	0.47
1:B:330:GLN:HA	1:B:330:GLN:HE21	1.79	0.47
1:B:342:ILE:CD1	1:B:395:LEU:HD11	2.44	0.47
1:C:116:TYR:CE2	1:C:309:PRO:HG2	2.49	0.47
2:A:138:TRP:CZ3	2:A:288:VAL:HG11	2.49	0.47
2:A:346:PHE:CD1	2:A:367:ILE:HG12	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:520:PHE:O	2:A:524:VAL:HG23	2.14	0.47
2:A:569:ASP:HB3	2:A:629:GLN:HA	1.95	0.47
1:B:84:ILE:HD11	2:A:594:LYS:HB2	1.96	0.47
1:B:117:ASN:HD22	1:B:117:ASN:C	2.17	0.47
1:B:292:ARG:HG3	1:C:312:ASN:HD21	1.78	0.47
1:C:106:PHE:CE2	1:C:359:GLN:HG2	2.49	0.47
1:C:242:ASP:CB	1:C:243:PRO:HD3	2.36	0.47
2:A:551:LEU:HA	2:A:554:LEU:HD22	1.95	0.47
2:A:526:HIS:CE1	2:A:978:VAL:HB	2.49	0.47
2:A:346:PHE:CZ	2:A:367:ILE:HG21	2.49	0.47
2:A:526:HIS:HB3	2:A:974:TYR:OH	2.14	0.47
1:B:360:ALA:CB	1:B:365:THR:HG22	2.42	0.47
2:A:399:ALA:HA	2:A:482:LYS:HE3	1.97	0.47
1:B:104:LEU:HD22	1:B:361:SER:HB3	1.96	0.47
2:A:413:ASN:ND2	2:A:442:ALA:HA	2.29	0.47
1:C:358:PHE:HB3	1:C:366:ALA:O	2.15	0.47
2:A:988:VAL:HA	2:A:1020:MET:HE1	1.96	0.47
2:A:298:ARG:HA	2:A:301:ILE:HD12	1.97	0.47
2:A:406:ALA:HB2	2:A:939:GLU:OE2	2.14	0.47
2:A:969:LEU:O	2:A:973:LEU:HD13	2.15	0.47
1:B:117:ASN:HD21	1:B:119:TYR:HB2	1.80	0.47
1:B:349:ARG:HA	1:B:349:ARG:NE	2.29	0.47
2:A:42:LEU:HD12	2:A:43:SER:N	2.28	0.47
2:A:500:LEU:O	2:A:504:TRP:HB2	2.15	0.47
2:A:711:ALA:HB1	2:A:826:ILE:HG22	1.97	0.47
2:A:747:VAL:HA	2:A:751:VAL:HG12	1.96	0.47
2:A:952:ILE:O	2:A:957:SER:HB3	2.15	0.47
1:C:183:GLU:O	1:C:187:LEU:HG	2.15	0.47
1:C:266:LEU:HD11	1:C:298:LEU:HD13	1.97	0.47
1:C:342:ILE:HB	1:C:378:VAL:CG1	2.45	0.47
2:A:574:PRO:HB2	2:A:658:LEU:CD1	2.41	0.47
1:B:196:ARG:O	1:B:199:ILE:HD13	2.14	0.47
1:C:382:LEU:HD22	1:C:382:LEU:O	2.15	0.47
2:A:357:LEU:HD23	2:A:415:HIS:CE1	2.50	0.47
2:A:464:ILE:N	2:A:464:ILE:HD12	2.29	0.47
1:C:199:ILE:HD12	1:C:200:ALA:N	2.29	0.47
2:A:185:LYS:O	2:A:767:PRO:HD2	2.15	0.46
2:A:327:ARG:HH11	2:A:666:ILE:CG1	2.13	0.46
2:A:346:PHE:CE2	2:A:367:ILE:HG21	2.50	0.46
2:A:588:MET:O	2:A:592:THR:HG22	2.15	0.46
2:A:275:ILE:O	2:A:608:LYS:HA	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:134:LYS:HB3	1:C:152:ASP:HB2	1.96	0.46
2:A:237:LEU:HD23	2:A:243:PHE:CE1	2.50	0.46
2:A:37:ASP:HB2	2:A:39:LEU:HD23	1.96	0.46
2:A:410:MET:HB2	2:A:494:ILE:HG12	1.96	0.46
1:B:132:ILE:HD12	1:B:132:ILE:H	1.80	0.46
1:B:333:ILE:HD12	1:B:342:ILE:HD11	1.97	0.46
1:C:389:ALA:HB1	1:C:394:ALA:HB3	1.97	0.46
2:A:112:GLU:HG3	2:A:113:TYR:CD1	2.49	0.46
2:A:623:MET:HE1	2:A:625:GLU:HG3	1.98	0.46
1:C:397:ARG:O	1:C:401:GLU:HG3	2.14	0.46
2:A:368:ILE:O	2:A:368:ILE:HG22	2.16	0.46
2:A:850:LEU:HD22	2:A:854:THR:OG1	2.15	0.46
1:B:100:THR:HG22	1:B:101:ARG:N	2.30	0.46
1:B:162:GLN:NE2	1:B:204:ILE:HG23	2.30	0.46
2:A:376:ILE:HG21	2:A:485:ALA:HA	1.98	0.46
1:C:106:PHE:HE2	1:C:359:GLN:HG2	1.80	0.46
2:A:996:LEU:O	2:A:1000:TRP:HD1	1.98	0.46
2:A:991:ILE:HD12	2:A:1020:MET:HE3	1.98	0.46
2:A:461:PHE:HB3	2:A:479:ALA:CB	2.42	0.46
2:A:876:VAL:N	2:A:877:PRO:CD	2.78	0.46
1:B:245:TRP:CD1	1:B:299:GLU:HG2	2.49	0.46
1:B:242:ASP:O	1:B:302:ASN:HB2	2.15	0.46
2:A:518:ASN:HA	2:A:521:LEU:HD21	1.97	0.46
2:A:608:LYS:O	2:A:624:VAL:HG23	2.15	0.46
2:A:602:VAL:HA	2:A:630:LEU:HA	1.97	0.46
2:A:729:ASN:ND2	2:A:732:LYS:H	2.14	0.46
2:A:898:LEU:HD23	2:A:899:LEU:N	2.31	0.46
2:A:954:ALA:HB3	2:A:956:PRO:HD2	1.98	0.46
1:B:161:ALA:HB1	1:B:181:ILE:HD11	1.96	0.46
1:C:327:ILE:HD13	1:C:367:LEU:HD21	1.97	0.46
2:A:461:PHE:CD1	2:A:479:ALA:HA	2.51	0.46
2:A:548:LEU:HB3	2:A:552:TRP:CZ2	2.51	0.46
2:A:570:LEU:HD12	2:A:628:ILE:HD13	1.98	0.46
2:A:525:TYR:HE2	2:A:1028:LEU:CD1	2.29	0.45
2:A:345:GLU:HA	2:A:348:VAL:HB	1.98	0.45
2:A:672:MET:CE	2:A:672:MET:HA	2.46	0.45
1:C:333:ILE:CG1	1:C:382:LEU:HD11	2.46	0.45
1:C:287:VAL:HG23	1:C:293:THR:C	2.37	0.45
1:C:372:ALA:O	1:C:375:GLU:HB2	2.15	0.45
2:A:829:ARG:HA	2:A:829:ARG:HD3	1.73	0.45
2:A:341:LYS:CG	2:A:998:ILE:HG12	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:340:ARG:HG3	1:B:354:ARG:HA	1.99	0.45
2:A:212:ALA:C	2:A:215:GLN:HE22	2.19	0.45
2:A:308:LEU:C	2:A:310:THR:H	2.20	0.45
2:A:458:THR:HG23	2:A:459:LEU:H	1.82	0.45
1:B:124:VAL:HB	1:B:235:VAL:HG22	1.97	0.45
1:B:242:ASP:CB	1:B:243:PRO:CD	2.91	0.45
1:C:367:LEU:HD22	1:C:367:LEU:H	1.81	0.45
2:A:387:ASN:HD22	2:A:387:ASN:H	1.63	0.45
2:A:925:ALA:HB1	2:A:1012:ILE:CG2	2.40	0.45
1:C:128:ALA:HB3	1:C:155:ILE:HG21	1.99	0.45
2:A:948:LEU:HD23	2:A:1035:TYR:HD2	1.82	0.45
2:A:180:VAL:HG12	2:A:286:GLY:C	2.37	0.45
2:A:355:LEU:HD12	2:A:356:PHE:CD1	2.52	0.45
2:A:489:ALA:O	2:A:493:ALA:HB2	2.17	0.45
1:C:287:VAL:HG23	1:C:293:THR:O	2.16	0.45
2:A:356:PHE:HB3	2:A:982:ARG:NH2	2.30	0.45
2:A:410:MET:HG2	2:A:497:ILE:HG13	1.98	0.45
2:A:685:VAL:HG21	2:A:696:MET:HB2	1.98	0.45
2:A:683:ILE:HB	2:A:824:ILE:HB	1.98	0.45
1:C:250:ILE:O	1:C:294:LEU:N	2.45	0.45
2:A:227:ALA:HB3	2:A:229:TYR:HE1	1.82	0.45
2:A:270:GLU:HG2	2:A:271:MET:N	2.25	0.45
2:A:412:GLU:HB3	2:A:983:PRO:HG3	1.97	0.45
2:A:420:GLU:O	2:A:424:GLN:HG3	2.16	0.45
2:A:411:ILE:HG12	2:A:497:ILE:CD1	2.46	0.45
2:A:462:ILE:N	2:A:463:PRO:HD2	2.32	0.45
2:A:779:SER:OG	2:A:781:GLN:HG2	2.17	0.45
1:C:291:THR:O	1:C:293:THR:HG23	2.17	0.45
1:B:166:LEU:O	1:B:170:GLU:HG3	2.17	0.44
1:C:156:PRO:O	1:C:159:VAL:HG12	2.17	0.44
2:A:949:ARG:O	2:A:953:GLU:HB2	2.17	0.44
2:A:29:TRP:HD1	2:A:30:THR:HG23	1.82	0.44
2:A:468:GLU:HG3	2:A:472:GLY:CA	2.45	0.44
2:A:640:MET:HA	2:A:644:LYS:HD2	2.00	0.44
2:A:649:LEU:HB3	2:A:662:TRP:CH2	2.51	0.44
1:B:250:ILE:HG23	1:B:254:ILE:HD11	1.99	0.44
1:C:345:ASP:HB3	1:C:349:ARG:O	2.18	0.44
2:A:359:HIS:HB3	2:A:361:ARG:NE	2.32	0.44
2:A:907:ALA:C	2:A:933:LEU:HD11	2.38	0.44
2:A:1028:LEU:HD12	2:A:1028:LEU:C	2.38	0.44
2:A:462:ILE:N	2:A:463:PRO:CD	2.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:136:TYR:CE2	1:C:149:PRO:HB2	2.53	0.44
1:C:174:THR:HB	1:C:177:GLN:HG3	1.99	0.44
2:A:930:PHE:CE2	2:A:1015:PRO:HB3	2.52	0.44
2:A:421:TRP:C	2:A:421:TRP:CD1	2.91	0.44
2:A:460:SER:O	2:A:463:PRO:HD2	2.18	0.44
2:A:457:ILE:HG21	2:A:482:LYS:HD2	2.00	0.44
1:C:254:ILE:HD11	2:A:797:THR:HG21	1.99	0.44
1:B:342:ILE:O	1:B:377:VAL:HG23	2.18	0.44
1:B:384:LEU:HD23	1:B:391:ILE:HA	1.99	0.44
2:A:355:LEU:HD12	2:A:356:PHE:HE1	1.81	0.44
2:A:356:PHE:CD1	2:A:356:PHE:N	2.85	0.44
1:C:126:ALA:HB2	1:C:229:ILE:CD1	2.47	0.44
2:A:554:LEU:HD23	2:A:555:ASN:OD1	2.18	0.44
2:A:746:PHE:CZ	2:A:788:ILE:HG23	2.53	0.44
1:B:390:ASN:HD22	1:B:390:ASN:C	2.21	0.44
2:A:484:TYR:HD2	2:A:484:TYR:HA	1.75	0.44
2:A:599:VAL:HA	2:A:600:PRO:HD3	1.88	0.44
2:A:279:ASN:ND2	2:A:605:VAL:H	2.15	0.44
2:A:633:GLN:HA	2:A:636:TRP:NE1	2.33	0.44
1:B:99:VAL:HG22	1:B:327:ILE:HG22	1.99	0.44
2:A:574:PRO:CG	2:A:624:VAL:HG13	2.42	0.43
2:A:76:VAL:HG13	2:A:76:VAL:O	2.18	0.43
2:A:996:LEU:N	2:A:997:PRO:CD	2.80	0.43
1:B:132:ILE:N	1:B:132:ILE:HD12	2.33	0.43
1:C:254:ILE:O	1:C:254:ILE:HG22	2.18	0.43
2:A:664:PRO:HB2	2:A:667:ARG:HB2	2.00	0.43
2:A:882:ILE:O	2:A:886:LEU:HG	2.17	0.43
1:B:137:PRO:O	1:B:138:LEU:HD12	2.17	0.43
1:B:185:LEU:HA	1:B:185:LEU:HD12	1.82	0.43
2:A:537:LYS:HA	2:A:1037:LEU:HD11	2.01	0.43
1:C:388:GLU:HB2	2:A:657:GLY:N	2.33	0.43
2:A:109:ARG:HD3	2:A:112:GLU:OE1	2.18	0.43
2:A:41:ASP:OD1	2:A:470:GLN:HG2	2.19	0.43
2:A:395:GLY:N	2:A:478:LEU:HD22	2.32	0.43
2:A:572:TYR:CB	2:A:628:ILE:HD11	2.48	0.43
2:A:587:SER:O	2:A:591:LYS:HG2	2.18	0.43
2:A:610:GLY:O	2:A:619:ALA:HB3	2.19	0.43
2:A:4:TRP:CD1	2:A:8:ARG:HG2	2.52	0.43
2:A:998:ILE:HG22	2:A:1009:MET:O	2.19	0.43
1:C:302:ASN:HD21	1:C:306:ALA:N	2.17	0.43
2:A:685:VAL:HG21	2:A:696:MET:HG3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1033:ALA:O	2:A:1037:LEU:HD13	2.18	0.43
2:A:436:TRP:O	2:A:436:TRP:HD1	2.02	0.43
2:A:557:VAL:HG22	2:A:558:GLY:N	2.27	0.43
2:A:43:SER:HB3	2:A:670:ILE:HD12	2.00	0.43
2:A:876:VAL:O	2:A:880:LEU:HG	2.19	0.43
1:B:174:THR:O	1:B:177:GLN:HB2	2.19	0.43
1:C:138:LEU:HD21	1:C:144:VAL:HG11	2.00	0.43
1:C:174:THR:H	1:C:177:GLN:HE21	1.66	0.43
2:A:144:LEU:HD21	2:A:164:LEU:HD12	1.99	0.43
2:A:39:LEU:HD11	2:A:327:ARG:NH2	2.33	0.43
2:A:736:TYR:CE1	2:A:796:ILE:HG21	2.54	0.43
2:A:751:VAL:HG23	2:A:777:ARG:HB3	1.99	0.43
2:A:114:LEU:HA	2:A:117:VAL:HG12	2.01	0.43
2:A:49:ILE:HG23	2:A:129:LEU:HD12	1.99	0.43
2:A:346:PHE:CE1	2:A:367:ILE:HG12	2.53	0.43
2:A:439:ILE:HD13	2:A:498:PRO:HG2	2.00	0.43
1:C:192:GLU:O	1:C:196:ARG:HG3	2.19	0.43
1:C:274:LYS:HE2	1:C:274:LYS:HB3	1.77	0.43
1:B:159:VAL:HG23	1:B:160:GLU:N	2.34	0.43
1:C:114:VAL:O	1:C:310:GLY:N	2.52	0.43
2:A:42:LEU:HA	2:A:42:LEU:HD13	1.80	0.42
2:A:54:PRO:O	2:A:56:GLN:HG2	2.19	0.42
2:A:685:VAL:HG21	2:A:696:MET:CB	2.49	0.42
2:A:718:LEU:HD22	2:A:718:LEU:HA	1.80	0.42
2:A:352:VAL:CG1	2:A:986:MET:HB2	2.49	0.42
2:A:392:SER:HA	2:A:478:LEU:HD21	2.02	0.42
2:A:41:ASP:OD1	2:A:474:LEU:HD13	2.18	0.42
2:A:402:ALA:HB3	2:A:482:LYS:HE2	2.01	0.42
2:A:666:ILE:H	2:A:666:ILE:HD12	1.84	0.42
2:A:684:LYS:HD3	2:A:823:TRP:CZ3	2.54	0.42
2:A:693:ILE:HA	2:A:696:MET:CG	2.49	0.42
2:A:6:ILE:HG21	2:A:443:SER:HB3	1.99	0.42
1:C:178:THR:HA	1:C:181:ILE:HG22	2.00	0.42
1:C:373:GLU:H	1:C:373:GLU:CD	2.21	0.42
2:A:547:VAL:HG11	2:A:905:PRO:CB	2.49	0.42
2:A:53:TYR:O	2:A:89:GLY:HA2	2.19	0.42
1:C:132:ILE:N	1:C:132:ILE:HD12	2.33	0.42
1:C:295:GLN:HA	1:C:295:GLN:NE2	2.21	0.42
1:C:331:ALA:O	1:C:341:VAL:HG12	2.20	0.42
2:A:156:LEU:O	2:A:159:LEU:HB3	2.19	0.42
2:A:491:LEU:HD12	2:A:491:LEU:C	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:636:TRP:CD1	2:A:636:TRP:N	2.87	0.42
2:A:680:PRO:CG	2:A:827:ASP:HB2	2.50	0.42
2:A:914:LEU:CD2	2:A:1017:ILE:HB	2.49	0.42
2:A:353:CYS:O	2:A:357:LEU:HB2	2.19	0.42
2:A:728:ILE:HA	2:A:802:ALA:HB2	2.02	0.42
1:B:137:PRO:C	1:B:138:LEU:HD12	2.39	0.42
2:A:398:ILE:HD11	2:A:1012:ILE:HG13	2.02	0.42
2:A:42:LEU:HD11	2:A:134:THR:HG21	2.01	0.42
1:B:159:VAL:HG23	1:B:160:GLU:H	1.85	0.42
1:C:264:PHE:CE2	1:C:317:LEU:HD13	2.54	0.42
2:A:357:LEU:HD23	2:A:415:HIS:NE2	2.34	0.42
2:A:56:GLN:HB3	2:A:60:ILE:HD12	2.00	0.42
1:C:359:GLN:HG3	1:C:360:ALA:N	2.35	0.42
1:C:387:SER:O	1:C:391:ILE:HG13	2.19	0.42
2:A:948:LEU:HB3	2:A:1035:TYR:CD2	2.55	0.42
2:A:159:LEU:HD21	2:A:319:VAL:HG11	2.01	0.42
2:A:195:ARG:CB	2:A:262:VAL:HA	2.50	0.42
2:A:265:VAL:O	2:A:265:VAL:HG13	2.20	0.42
2:A:417:ARG:HE	2:A:417:ARG:HA	1.85	0.42
2:A:470:GLN:OE1	2:A:474:LEU:HD13	2.20	0.42
2:A:49:ILE:HG13	2:A:93:VAL:HB	2.01	0.42
2:A:541:LEU:O	2:A:545:LEU:HB2	2.19	0.42
2:A:819:ARG:HH21	2:A:819:ARG:HG3	1.85	0.42
2:A:87:GLN:HG2	2:A:812:MET:HG3	2.02	0.42
1:B:308:LYS:O	1:B:311:MET:HG3	2.19	0.42
1:C:126:ALA:HB2	1:C:229:ILE:HD11	2.02	0.42
2:A:353:CYS:SG	2:A:363:ALA:HA	2.60	0.42
2:A:567:GLU:CD	2:A:666:ILE:HD13	2.40	0.42
2:A:683:ILE:HG12	2:A:858:PHE:CD2	2.54	0.42
2:A:996:LEU:O	2:A:999:LEU:HB3	2.20	0.42
1:C:147:GLY:O	1:C:211:LYS:HD3	2.20	0.42
2:A:436:TRP:O	2:A:436:TRP:CD1	2.73	0.42
2:A:816:GLU:H	2:A:821:THR:HG22	1.85	0.42
2:A:834:VAL:HG13	2:A:834:VAL:O	2.20	0.42
2:A:35:PRO:HA	2:A:296:ASN:ND2	2.35	0.41
2:A:374:LEU:O	2:A:377:ALA:HB3	2.19	0.41
2:A:442:ALA:O	2:A:446:VAL:HB	2.19	0.41
2:A:651:ASN:HA	2:A:654:ARG:NH2	2.31	0.41
2:A:875:MET:C	2:A:877:PRO:HD2	2.39	0.41
1:C:85:ASP:HA	1:C:86:PRO:HD3	1.94	0.41
2:A:906:PHE:CE2	2:A:1030:ILE:HG13	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:434:THR:O	2:A:438:VAL:HG12	2.19	0.41
2:A:748:THR:O	2:A:754:ALA:HB2	2.20	0.41
1:B:284:LEU:HB3	1:B:285:PRO:HD2	2.01	0.41
2:A:1008:VAL:C	2:A:1010:SER:H	2.23	0.41
2:A:59:GLN:NE2	2:A:813:LEU:HD21	2.36	0.41
2:A:941:GLY:HA2	2:A:1031:ILE:CD1	2.50	0.41
1:C:345:ASP:CG	1:C:346:ALA:N	2.72	0.41
2:A:74:LEU:HD11	2:A:817:ASN:O	2.20	0.41
1:C:352:PRO:HG3	1:C:395:LEU:HD12	2.01	0.41
2:A:447:GLY:O	2:A:451:PHE:HB3	2.19	0.41
2:A:16:VAL:CG1	2:A:492:LEU:HD13	2.51	0.41
2:A:191:ILE:HD13	2:A:263:ALA:CB	2.50	0.41
2:A:191:ILE:HD11	2:A:206:VAL:HG11	2.01	0.41
2:A:292:ARG:O	2:A:293:SER:C	2.58	0.41
2:A:458:THR:HB	2:A:483:THR:CG2	2.50	0.41
2:A:680:PRO:HB2	2:A:833:MET:HE1	2.02	0.41
2:A:69:LEU:HD11	2:A:121:LEU:HD21	2.03	0.41
2:A:191:ILE:O	2:A:773:PRO:HD3	2.20	0.41
2:A:88:PHE:O	2:A:88:PHE:CD1	2.73	0.41
2:A:956:PRO:HA	2:A:968:LYS:HD3	2.01	0.41
2:A:962:GLN:HB2	2:A:962:GLN:HE21	1.58	0.41
1:C:283:LEU:HD23	1:C:283:LEU:HA	1.72	0.41
2:A:10:VAL:HG12	2:A:436:TRP:HE1	1.85	0.41
1:C:138:LEU:HA	1:C:138:LEU:HD12	1.93	0.41
2:A:260:ARG:HD2	2:A:261:ASP:OD1	2.20	0.41
2:A:357:LEU:HD23	2:A:415:HIS:CD2	2.56	0.41
2:A:41:ASP:OD2	2:A:41:ASP:N	2.54	0.41
2:A:714:LEU:HB3	2:A:823:TRP:O	2.20	0.41
2:A:356:PHE:CB	2:A:982:ARG:HH22	2.33	0.41
1:B:329:SER:OG	1:B:365:THR:HG23	2.21	0.41
2:A:224:LEU:HG	2:A:229:TYR:CD1	2.56	0.41
2:A:475:PHE:HA	2:A:478:LEU:CD1	2.51	0.41
1:B:212:ALA:HA	1:B:213:PRO:HD3	1.90	0.41
1:B:371:LEU:HD12	1:B:371:LEU:O	2.21	0.41
1:C:159:VAL:HG13	1:C:160:GLU:N	2.36	0.41
1:C:190:MET:HG2	1:C:195:ILE:HG13	2.03	0.41
2:A:240:LEU:O	2:A:243:PHE:HB2	2.20	0.41
2:A:459:LEU:H	2:A:459:LEU:HD22	1.86	0.41
2:A:46:GLN:HB2	2:A:96:ILE:HD13	2.03	0.41
2:A:595:LEU:O	2:A:598:SER:HB3	2.21	0.41
2:A:664:PRO:HA	2:A:665:PRO:HD3	1.97	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:672:MET:C	2:A:674:SER:H	2.23	0.41
2:A:906:PHE:HA	2:A:909:VAL:HG12	2.03	0.41
1:C:155:ILE:HB	1:C:208:PHE:HE1	1.85	0.41
1:C:397:ARG:HB2	1:C:397:ARG:CZ	2.51	0.41
2:A:26:TRP:HD1	2:A:379:ILE:HG12	1.85	0.40
2:A:34:THR:HA	2:A:35:PRO:HD3	1.93	0.40
2:A:405:ASP:O	2:A:409:VAL:HG23	2.20	0.40
2:A:413:ASN:HD21	2:A:442:ALA:HA	1.84	0.40
2:A:552:TRP:HB2	2:A:553:PRO:HD3	2.03	0.40
2:A:829:ARG:O	2:A:830:ASP:HB2	2.21	0.40
2:A:865:LEU:C	2:A:865:LEU:HD13	2.41	0.40
2:A:522:ILE:HD13	2:A:978:VAL:HG23	2.03	0.40
2:A:69:LEU:CD1	2:A:121:LEU:HD21	2.50	0.40
2:A:224:LEU:O	2:A:225:ALA:HB3	2.20	0.40
2:A:933:LEU:HD22	2:A:933:LEU:O	2.21	0.40
2:A:995:LEU:HB3	2:A:1017:ILE:HD11	2.03	0.40
1:B:145:GLN:HA	1:B:215:ASP:CB	2.45	0.40
1:B:255:ALA:HB3	1:C:270:ALA:HB1	2.03	0.40
1:B:259:LYS:HE2	1:B:260:ASP:OD2	2.22	0.40
2:A:571:LEU:HD13	2:A:571:LEU:C	2.42	0.40
1:C:183:GLU:HG3	1:C:186:ARG:HE	1.86	0.40
1:C:336:GLY:HA3	2:A:806:VAL:O	2.22	0.40
2:A:114:LEU:HD12	2:A:117:VAL:CG1	2.51	0.40
2:A:421:TRP:O	2:A:421:TRP:HD1	2.04	0.40
2:A:58:PRO:HD2	2:A:723:TYR:OH	2.21	0.40
2:A:867:ARG:O	2:A:871:LYS:HB2	2.21	0.40
2:A:876:VAL:HG23	2:A:877:PRO:HD3	2.03	0.40
1:B:302:ASN:OD1	1:B:307:LEU:HB2	2.21	0.40
2:A:232:ARG:HG2	2:A:233:ALA:N	2.36	0.40
2:A:404:VAL:HA	2:A:407:ALA:HB3	2.04	0.40
2:A:56:GLN:HB3	2:A:60:ILE:HG23	2.02	0.40
2:A:633:GLN:HA	2:A:636:TRP:CE2	2.57	0.40
1:B:287:VAL:CG1	1:B:294:LEU:HD23	2.52	0.40
1:C:298:LEU:O	1:C:298:LEU:HD12	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	320/413 (78%)	280 (88%)	33 (10%)	7 (2%)	6	37
1	C	322/413 (78%)	294 (91%)	25 (8%)	3 (1%)	17	54
2	A	1027/1054 (97%)	891 (87%)	107 (10%)	29 (3%)	5	33
All	All	1669/1880 (89%)	1465 (88%)	165 (10%)	39 (2%)	6	36

All (39) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	157	ASP
1	B	390	ASN
2	A	123	ALA
2	A	138	TRP
2	A	293	SER
2	A	562	LEU
2	A	574	PRO
2	A	835	SER
2	A	846	GLU
1	C	233	ASN
2	A	122	PRO
2	A	428	ALA
2	A	954	ALA
1	B	172	GLY
2	A	42	LEU
2	A	43	SER
2	A	359	HIS
2	A	483	THR
2	A	561	PHE
2	A	638	PRO
2	A	708	PRO
2	A	983	PRO
1	C	137	PRO
2	A	41	ASP

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Mol	Chain	Res	Type
2	A	88	PHE
2	A	449	ALA
2	A	812	MET
2	A	40	PRO
1	B	93	GLY
2	A	235	GLY
2	A	756	VAL
2	A	834	VAL
2	A	181	GLY
1	B	189	GLY
1	B	242	ASP
1	B	254	ILE
2	A	136	VAL
2	A	665	PRO
1	C	82	VAL

### 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	B	263/338 (78%)	241 (92%)	22 (8%)	11	40
1	C	265/338 (78%)	244 (92%)	21 (8%)	12	42
2	A	850/872 (98%)	756 (89%)	94 (11%)	6	28
All	All	1378/1548 (89%)	1241 (90%)	137 (10%)	8	32

All (137) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	83	ARG
1	B	84	ILE
1	B	117	ASN
1	B	121	TYR
1	B	182	LEU
1	B	199	ILE
1	B	214	ILE

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Mol	Chain	Res	Type
1	B	215	ASP
1	B	222	ASP
1	B	234	VAL
1	B	268	VAL
1	B	276	LEU
1	B	280	LYS
1	B	287	VAL
1	B	298	LEU
1	B	302	ASN
1	B	322	GLU
1	B	335	THR
1	B	351	VAL
1	B	354	ARG
1	B	390	ASN
1	B	396	GLU
1	C	100	THR
1	C	104	LEU
1	C	121	TYR
1	C	134	LYS
1	C	151	LEU
1	C	182	LEU
1	C	184	ARG
1	C	214	ILE
1	C	234	VAL
1	C	258	VAL
1	C	283	LEU
1	C	287	VAL
1	C	292	ARG
1	C	295	GLN
1	C	298	LEU
1	C	302	ASN
1	C	332	LEU
1	C	345	ASP
1	C	358	PHE
1	C	362	GLN
1	C	367	LEU
2	A	5	ILE
2	A	6	ILE
2	A	21	LEU
2	A	34	THR
2	A	42	LEU
2	A	45	VAL

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Mol	Chain	Res	Type
2	A	46	GLN
2	A	49	ILE
2	A	53	TYR
2	A	60	ILE
2	A	65	VAL
2	A	83	ARG
2	A	115	ASN
2	A	128	GLU
2	A	140	TYR
2	A	184	VAL
2	A	203	LEU
2	A	239	THR
2	A	247	VAL
2	A	260	ARG
2	A	322	VAL
2	A	323	THR
2	A	338	LEU
2	A	341	LYS
2	A	346	PHE
2	A	358	TRP
2	A	361	ARG
2	A	386	LEU
2	A	387	ASN
2	A	391	MET
2	A	410	MET
2	A	412	GLU
2	A	416	LYS
2	A	435	ARG
2	A	455	LEU
2	A	458	THR
2	A	461	PHE
2	A	467	LEU
2	A	468	GLU
2	A	470	GLN
2	A	471	GLU
2	A	481	THR
2	A	484	TYR
2	A	486	MET
2	A	494	ILE
2	A	519	ARG
2	A	523	ARG
2	A	534	HIS

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Mol	Chain	Res	Type
2	A	535	TRP
2	A	554	LEU
2	A	562	LEU
2	A	569	ASP
2	A	573	MET
2	A	609	THR
2	A	611	LYS
2	A	624	VAL
2	A	630	LEU
2	A	637	ARG
2	A	667	ARG
2	A	677	ILE
2	A	678	LYS
2	A	690	LEU
2	A	694	ASP
2	A	698	GLU
2	A	710	VAL
2	A	718	LEU
2	A	729	ASN
2	A	769	ASN
2	A	770	LEU
2	A	774	GLN
2	A	781	GLN
2	A	804	ILE
2	A	827	ASP
2	A	829	ARG
2	A	837	VAL
2	A	871	LYS
2	A	874	LEU
2	A	898	LEU
2	A	913	TRP
2	A	933	LEU
2	A	939	GLU
2	A	947	TYR
2	A	955	VAL
2	A	962	GLN
2	A	968	LYS
2	A	970	ASP
2	A	975	HIS
2	A	979	LEU
2	A	980	ARG
2	A	998	ILE

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Mol	Chain	Res	Type
2	A	1035	TYR
2	A	1038	MET
2	A	1039	TRP
2	A	1041	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	117	ASN
1	B	120	GLN
1	B	125	GLN
1	B	177	GLN
1	B	233	ASN
1	B	239	GLN
1	B	263	GLN
1	B	330	GLN
1	B	390	ASN
1	C	125	GLN
1	C	177	GLN
1	C	205	GLN
1	C	233	ASN
1	C	239	GLN
1	C	263	GLN
1	C	295	GLN
1	C	302	ASN
1	C	316	GLN
1	C	362	GLN
2	A	115	ASN
2	A	116	GLN
2	A	215	GLN
2	A	244	ASN
2	A	279	ASN
2	A	329	GLN
2	A	413	ASN
2	A	422	GLN
2	A	470	GLN
2	A	518	ASN
2	A	526	HIS
2	A	633	GLN
2	A	635	GLN
2	A	725	ASN
2	A	729	ASN

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Mol	Chain	Res	Type
2	A	744	GLN
2	A	769	ASN
2	A	795	GLN
2	A	861	GLN
2	A	950	HIS
2	A	962	GLN

### 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](#)

Of 1 ligands modelled in this entry, 1 is 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.

No monomer is involved in short contacts.

### 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	B	322/413 (77%)	0.01	2 (0%) 89 83	21, 61, 104, 218	0
1	C	324/413 (78%)	0.05	0 100 100	27, 62, 105, 170	0
2	A	1031/1054 (97%)	0.40	91 (8%) 10 7	20, 103, 216, 505	0
All	All	1677/1880 (89%)	0.26	93 (5%) 25 17	20, 74, 202, 505	0

All (93) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	504	TRP	12.4
2	A	501	MET	6.9
2	A	503	TYR	6.7
2	A	498	PRO	5.9
2	A	970	ASP	5.4
2	A	975	HIS	5.2
2	A	497	ILE	5.1
2	A	921	HIS	5.0
2	A	429	THR	4.9
2	A	971	GLU	4.9
2	A	951	ALA	4.7
2	A	552	TRP	4.7
2	A	364	LEU	4.6
2	A	415	HIS	4.3
2	A	952	ILE	4.1
2	A	920	PHE	4.0
2	A	956	PRO	4.0
2	A	421	TRP	3.9
2	A	431	ASP	3.8
2	A	502	GLY	3.7
2	A	1043	HIS	3.7
2	A	353	CYS	3.6
2	A	420	GLU	3.6

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Mol	Chain	Res	Type	RSRZ
2	A	480	PHE	3.5
2	A	1014	ALA	3.5
2	A	998	ILE	3.4
2	A	967	GLN	3.4
2	A	530	LEU	3.4
2	A	531	LYS	3.4
1	B	79	ALA	3.1
2	A	955	VAL	3.1
2	A	475	PHE	3.1
2	A	1036	LYS	3.0
2	A	469	GLY	3.0
2	A	564	GLN	2.9
2	A	712	SER	2.9
2	A	716	PHE	2.9
2	A	428	ALA	2.9
2	A	526	HIS	2.9
2	A	959	ASN	2.9
2	A	1035	TYR	2.9
2	A	434	THR	2.9
2	A	980	ARG	2.9
2	A	405	ASP	2.8
2	A	436	TRP	2.8
2	A	949	ARG	2.8
2	A	1016	MET	2.7
2	A	414	ALA	2.7
2	A	551	LEU	2.7
2	A	494	ILE	2.6
2	A	537	LYS	2.6
2	A	1025	LEU	2.6
2	A	907	ALA	2.5
2	A	449	ALA	2.5
2	A	639	GLY	2.5
2	A	439	ILE	2.5
2	A	461	PHE	2.5
2	A	359	HIS	2.4
2	A	978	VAL	2.4
2	A	426	PRO	2.4
2	A	968	LYS	2.4
2	A	1015	PRO	2.4
2	A	711	ALA	2.4
2	A	445	GLU	2.4
2	A	418	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
2	A	948	LEU	2.4
2	A	464	ILE	2.4
2	A	354	ALA	2.3
1	B	80	SER	2.3
2	A	1013	ALA	2.3
2	A	481	THR	2.3
2	A	468	GLU	2.3
2	A	520	PHE	2.3
2	A	962	GLN	2.3
2	A	422	GLN	2.2
2	A	960	ASN	2.2
2	A	896	GLU	2.2
2	A	559	GLY	2.2
2	A	473	ARG	2.2
2	A	893	ARG	2.2
2	A	519	ARG	2.2
2	A	950	HIS	2.1
2	A	657	GLY	2.1
2	A	556	LYS	2.1
2	A	558	GLY	2.1
2	A	41	ASP	2.1
2	A	438	VAL	2.1
2	A	995	LEU	2.1
2	A	918	MET	2.0
2	A	342	LEU	2.0
2	A	432	ASN	2.0
2	A	928	THR	2.0
2	A	444	VAL	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no 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. 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	B-factors( $\text{\AA}^2$ )	Q<0.9
3	CU	A	1101	1/1	0.99	0.08	51,51,51,51	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.