



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 02:49 PM GMT

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 validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

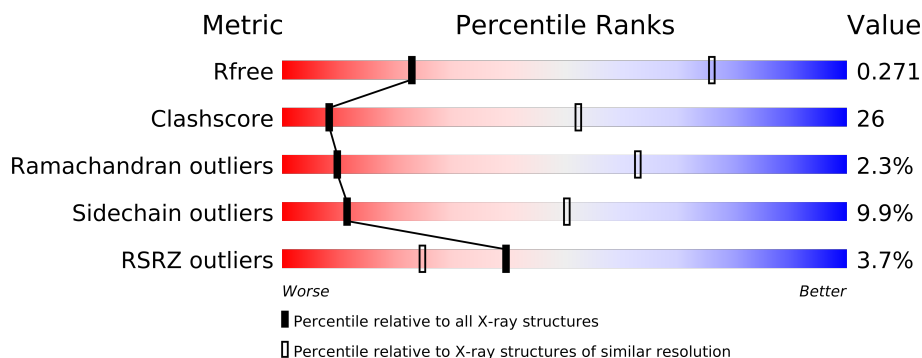
The following versions of software and data (see [references](#)) were used in the production of this report:

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 3.68 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}	66092	1013 (3.96-3.40)
Clashscore	79885	1006 (3.92-3.44)
Ramachandran outliers	78287	1218 (3.96-3.40)
Sidechain outliers	78261	1216 (3.96-3.40)
RSRZ outliers	66119	1013 (3.96-3.40)

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 ≥ 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	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 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 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.

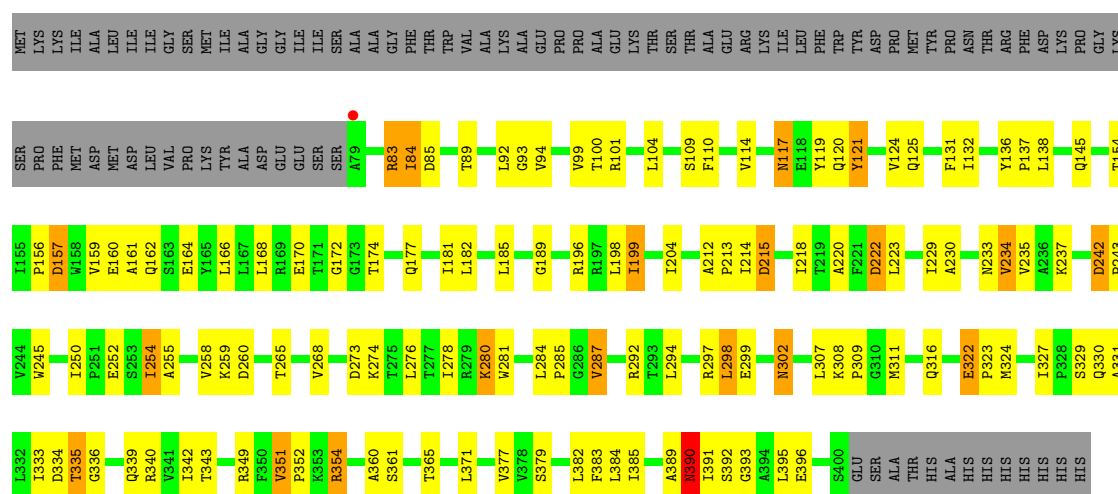
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	4	Total O 4 4	0	0
4	A	1	Total O 1 1	0	0

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 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.

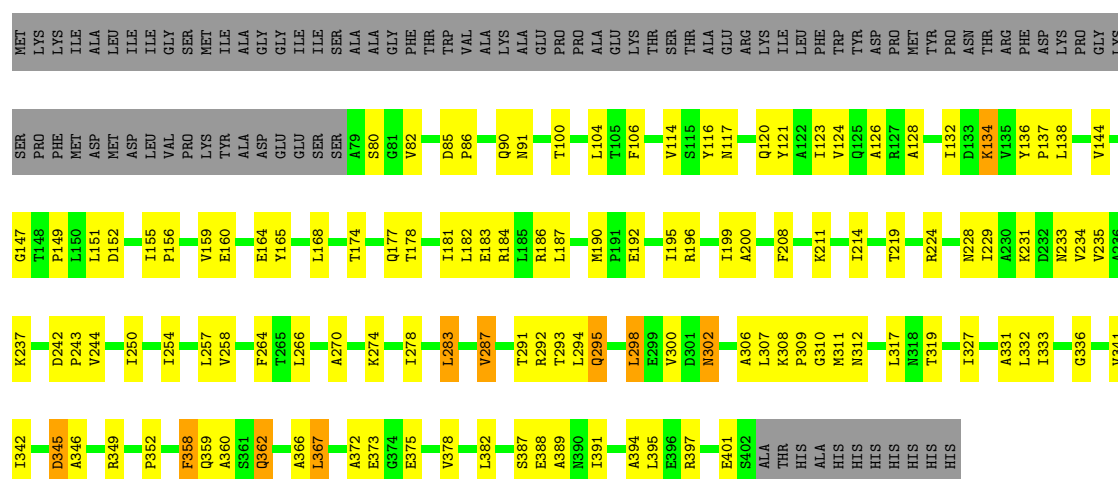
• Molecule 1: Cation efflux system protein CusB

Chain B:



• Molecule 1: Cation efflux system protein CusB

Chain C:



• Molecule 2: Cation efflux system protein CusA

Chain A:





4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	1.68 (at 3.67Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.244 , 0.272 0.239 , 0.271	Depositor DCC
R_{free} test set	1871 reflections (5.07%)	DCC
Wilson B-factor (Å ²)	83.3	Xtriage
Anisotropy	0.241	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 53.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 36934 reflections	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	12887	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities 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: 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 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	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	4	0	0	0	0
All	All	12887	0	13253	686	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 26.

All (686) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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:40:PRO:HD2	2:A:666:ILE:HG21	1.67	0.77
2:A:637:ARG:HH11	2:A:637:ARG:HB2	1.50	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
1:C:278:ILE:HD13	1:C:298:LEU:HD22	1.71	0.73
1:B:250:ILE:HG21	1:B:258:VAL:HG11	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:327:ARG:NH1	2:A:666:ILE:HG13	2.03	0.70
2:A:370:LEU:HD22	2:A:400:VAL:HG23	1.73	0.70
2:A:416:LYS:HA	2:A:416:LYS:HE3	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:458:THR:HB	2:A:483:THR:OG1	1.92	0.69
2:A:418:LEU:HD21	2:A:438:VAL:HB	1.73	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
1:B:120:GLN:NE2	1:B:243:PRO:HD2	2.07	0.68
2:A:417:ARG:HG2	2:A:441:ASP:HB3	1.75	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:456:ILE:HD12	2:A:883:ILE:HD13	1.76	0.66
1:B:204:ILE:HD12	1:B:204:ILE:H	1.61	0.66
2:A:729:ASN:HD22	2:A:729:ASN:C	1.98	0.66

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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
1:B:242:ASP:HB3	1:B:243:PRO:CD	2.27	0.65
2:A:83:ARG:HG2	2:A:675:THR:HG21	1.79	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:554:LEU:HD21	2:A:912:ILE:HD13	1.80	0.63
2:A:718:LEU:HD11	2:A:812:MET:O	1.98	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:381:MET:HG2	2:A:386:LEU:HD11	1.80	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:525:TYR:HE1	2:A:977:ALA:HB1	1.64	0.62
2:A:381:MET:HG2	2:A:386:LEU:CD1	2.29	0.62
2:A:203:LEU:HD11	2:A:750:ALA:HB2	1.80	0.62
2:A:746:PHE:O	2:A:750:ALA:HB3	1.98	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:A:680:PRO:HD2	2:A:827:ASP:HB2	1.81	0.61
2:A:786:LEU:HD22	2:A:787:PRO:HD2	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
1:B:242:ASP:CB	1:B:243:PRO:HD3	2.32	0.59
2:A:244:ASN:HB3	2:A:260:ARG:HB3	1.83	0.59
2:A:165:LYS:HE2	2:A:177:VAL:O	2.02	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:876:VAL:N	2:A:877:PRO:HD2	2.18	0.59
2:A:1006:SER:HA	2:A:1009:MET:HB2	1.85	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: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:571:LEU:HD12	2:A:663:VAL:HG23	1.84	0.59
1:C:242:ASP:HB3	1:C:243:PRO:CD	2.31	0.58
2:A:547:VAL:HG11	2:A:905:PRO:HB2	1.85	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:411:ILE:HG12	2:A:497:ILE:HD12	1.85	0.58
2:A:13:ARG:HH21	2:A:499:ILE:HD11	1.66	0.58
2:A:405:ASP:O	2:A:408:ILE:HG13	2.04	0.58
2:A:904:VAL:HG23	2:A:905:PRO:HD3	1.84	0.58
2:A:885:VAL:O	2:A:889:LEU:HB2	2.03	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:A:550:VAL:O	2:A:554:LEU:HB3	2.04	0.58
2:A:355:LEU:HD12	2:A:356:PHE:CE1	2.38	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
1:B:307:LEU:HA	1:B:311:MET:HE1	1.86	0.57
2:A:413:ASN:O	2:A:417:ARG:HB2	2.04	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:572:TYR:CE2	2:A:574:PRO:HG3	2.39	0.57
2:A:1031:ILE:HB	2:A:1032:PRO:HD3	1.85	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:956:PRO:HB3	2:A:968:LYS:HG3	1.88	0.56
1:B:84:ILE:HD11	2:A:594:LYS:HD3	1.88	0.56
2:A:189:VAL:HB	2:A:770:LEU:HD12	1.87	0.56
1:C:378:VAL:HG13	1:C:382:LEU:HD23	1.87	0.56
2:A:571:LEU:HD22	2:A:626:THR:O	2.05	0.56
2:A:387:ASN:H	2:A:387:ASN:ND2	2.04	0.56
2:A:333:ARG:HH21	2:A:1004:ALA:HB2	1.71	0.56
2:A:457:ILE:O	2:A:461:PHE:HB2	2.05	0.55
2:A:486:MET:HE2	2:A:487:ALA:N	2.21	0.55
1:B:84:ILE:HD13	1:B:85:ASP:N	2.21	0.55
2:A:533:LEU:HD22	2:A:1036:LYS:NZ	2.22	0.55
2:A:837:VAL:O	2:A:841:GLN:HG3	2.06	0.55
2:A:616:THR:O	2:A:673:LEU:HD21	2.06	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:525:TYR:CE1	2:A:977:ALA:HB1	2.41	0.55
2:A:747:VAL:O	2:A:751:VAL:HG12	2.07	0.55
1:B:131:PHE:CE2	1:B:154:THR:HB	2.42	0.55
2:A:456:ILE:HD13	2:A:886:LEU:HD12	1.89	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:C:387:SER:HB3	2:A:577:LEU:HD23	1.88	0.54
1:B:132:ILE:HD11	1:B:229:ILE:HB	1.89	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
1:B:83:ARG:HH22	1:C:90:GLN:HB3	1.73	0.54
2:A:346:PHE:C	2:A:346:PHE:HD1	2.11	0.54
2:A:1038:MET:O	2:A:1042:ARG:HD3	2.06	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:904:VAL:N	2:A:905:PRO:CD	2.72	0.53
2:A:346:PHE:CD1	2:A:346:PHE:C	2.81	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: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:687:GLY:HA3	2:A:854:THR:HG22	1.91	0.53
2:A:144:LEU:HD11	2:A:164:LEU:HD11	1.91	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
2:A:574:PRO:HD2	2:A:624:VAL:O	2.08	0.52
2:A:419:GLU:O	2:A:423:HIS:HB2	2.09	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:955:VAL:CG1	2:A:956:PRO:HD3	2.35	0.52
2:A:440:THR:O	2:A:444:VAL:HG23	2.10	0.52
1:C:164:GLU:O	1:C:168:LEU:HD13	2.10	0.52
2:A:531:LYS:HA	2:A:531:LYS:HE3	1.91	0.52
2:A:203:LEU:CD1	2:A:750:ALA:HB2	2.40	0.51
1:C:266:LEU:HG	1:C:278:ILE:HD11	1.92	0.51
2:A:562:LEU:HB2	2:A:563:PRO:HD3	1.92	0.51
2:A:926:THR:HG22	2:A:1011:ARG:O	2.09	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: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:89:THR:H	2:A:590:GLN:HE22	1.58	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
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: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:207:LYS:HG3	2:A:756:VAL:HG21	1.92	0.51
2:A:572:TYR:HB3	2:A:628:ILE:HD11	1.92	0.51
2:A:51:THR:OG1	2:A:91:SER:HB3	2.11	0.51
2:A:779:SER:HB2	2:A:780:PRO:HD2	1.93	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:475:PHE:HA	2:A:478:LEU:HD12	1.92	0.51
2:A:979:LEU:O	2:A:983:PRO:HD3	2.11	0.51
2:A:13:ARG:NH2	2:A:499:ILE:HD11	2.25	0.51
2:A:365:VAL:HG21	2:A:500:LEU:HB2	1.93	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
2:A:118:GLN:HE22	2:A:127:ALA:H	1.58	0.50
2:A:693:ILE:HA	2:A:696:MET:HG2	1.93	0.50
1:C:165:TYR:CE2	1:C:178:THR:HG23	2.45	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:384:LEU:N	1:B:384:LEU:HD12	2.25	0.50
2:A:451:PHE:O	2:A:455:LEU:HB2	2.11	0.50
2:A:868:ALA:O	2:A:872:LEU:HG	2.10	0.50
2:A:678:LYS:HA	2:A:861:GLN:HE21	1.77	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: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:833:MET:HE2	2:A:862:PHE:HB3	1.93	0.50
2:A:69:LEU:O	2:A:73:MET:HG2	2.12	0.50
2:A:38:ALA:H	2:A:331:ILE:HG12	1.75	0.50
2:A:955:VAL:N	2:A:956:PRO:CD	2.74	0.50
2:A:32:ILE:HG13	2:A:33:ASN:H	1.77	0.50
2:A:725:ASN:O	2:A:804:ILE:HA	2.11	0.50
1:C:117:ASN:HB3	1:C:120:GLN:HG3	1.94	0.50
2:A:256:PRO:HG2	2:A:258:TYR:CE1	2.47	0.50
1:C:317:LEU:HD11	1:C:319:THR:OG1	2.11	0.50
1:B:390:ASN:ND2	1:B:393:GLY:H	2.10	0.50
2:A:457:ILE:HD11	2:A:932:ALA:HA	1.94	0.50
2:A:474:LEU:HD23	2:A:475:PHE:CE1	2.46	0.50
2:A:30:THR:O	2:A:34:THR:HB	2.12	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:517:LEU:O	2:A:521:LEU:HG	2.11	0.49
2:A:163:PHE:O	2:A:167:GLU:HG2	2.10	0.49
1:B:390:ASN:HD21	1:B:392:SER:HB2	1.76	0.49
2:A:666:ILE:N	2:A:666:ILE:HD12	2.27	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
1:B:136:TYR:HB3	1:B:137:PRO:HD2	1.93	0.49
2:A:102:ASP:OD1	2:A:103:PRO:HD2	2.13	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
2:A:816:GLU:HB3	2:A:821:THR:HG21	1.94	0.49
2:A:435:ARG:CD	2:A:435:ARG:H	2.25	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:124:VAL:O	1:C:235:VAL:HG12	2.12	0.49
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
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:1014:ALA:HB3	2:A:1015:PRO:HD3	1.95	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
1:B:125:GLN:HE21	1:C:228:ASN:HD22	1.59	0.48
2:A:491:LEU:O	2:A:495:VAL:HG23	2.12	0.48
1:C:244:VAL:HG11	1:C:307:LEU:HD23	1.94	0.48
2:A:977:ALA:HA	2:A:980:ARG:HD3	1.96	0.48
2:A:677:ILE:HD13	2:A:677:ILE:N	2.28	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: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:952:ILE:CG1	2:A:1039:TRP:HE1	2.23	0.48
2:A:356:PHE:CE2	2:A:986:MET:HB3	2.48	0.48
2:A:365:VAL:CG2	2:A:496:VAL:HB	2.44	0.48
2:A:714:LEU:HD22	2:A:717:ARG:HB2	1.94	0.48
2:A:533:LEU:HD22	2:A:1036:LYS:HZ2	1.77	0.48
2:A:707:VAL:HG11	2:A:840:LEU:HD21	1.95	0.48
2:A:623:MET:CE	2:A:625:GLU:HG3	2.44	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:322:GLU:O	1:B:324:MET:HG3	2.14	0.48
1:B:101:ARG:HB2	1:B:101:ARG:NH1	2.29	0.48
1:B:342:ILE:CD1	1:B:395:LEU:HD11	2.44	0.47
1:B:330:GLN:HA	1:B:330:GLN:HE21	1.79	0.47
2:A:960:ASN:N	2:A:961:PRO:HD2	2.29	0.47
2:A:97:PHE:CE1	2:A:106:ALA:HB1	2.49	0.47
1:C:116:TYR:CE2	1:C:309:PRO:HG2	2.49	0.47
1:B:117:ASN:HD22	1:B:117:ASN:C	2.17	0.47
1:C:242:ASP:CB	1:C:243:PRO:HD3	2.36	0.47
1:B:84:ILE:HD11	2:A:594:LYS:HB2	1.96	0.47
2:A:346:PHE:CD1	2:A:367:ILE:HG12	2.50	0.47
2:A:569:ASP:HB3	2:A:629:GLN:HA	1.95	0.47
1:C:106:PHE:CE2	1:C:359:GLN:HG2	2.49	0.47
1:B:292:ARG:HG3	1:C:312:ASN:HD21	1.78	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:A:138:TRP:CZ3	2:A:288:VAL:HG11	2.49	0.47
2:A:520:PHE:O	2:A:524:VAL:HG23	2.14	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
1:B:360:ALA:CB	1:B:365:THR:HG22	2.42	0.47
2:A:526:HIS:HB3	2:A:974:TYR:OH	2.14	0.47
2:A:346:PHE:CZ	2:A:367:ILE:HG21	2.49	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:298:ARG:HA	2:A:301:ILE:HD12	1.97	0.47
1:B:117:ASN:HD21	1:B:119:TYR:HB2	1.80	0.47
2:A:988:VAL:HA	2:A:1020:MET:HE1	1.96	0.47
2:A:406:ALA:HB2	2:A:939:GLU:OE2	2.14	0.47
1:B:349:ARG:NE	1:B:349:ARG:HA	2.29	0.47
2:A:969:LEU:O	2:A:973:LEU:HD13	2.15	0.47
2:A:42:LEU:HD12	2:A:43:SER:N	2.28	0.47
1:C:266:LEU:HD11	1:C:298:LEU:HD13	1.97	0.47
2:A:952:ILE:O	2:A:957:SER:HB3	2.15	0.47
2:A:500:LEU:O	2:A:504:TRP:HB2	2.15	0.47
1:C:342:ILE:HB	1:C:378:VAL:CG1	2.45	0.47
2:A:747:VAL:HA	2:A:751:VAL:HG12	1.96	0.47
2:A:711:ALA:HB1	2:A:826:ILE:HG22	1.97	0.47
1:C:183:GLU:O	1:C:187:LEU:HG	2.15	0.47
2:A:574:PRO:HB2	2:A:658:LEU:CD1	2.41	0.47
1:C:382:LEU:HD22	1:C:382:LEU:O	2.15	0.47
1:B:196:ARG:O	1:B:199:ILE:HD13	2.14	0.47
2:A:464:ILE:N	2:A:464:ILE:HD12	2.29	0.47
2:A:357:LEU:HD23	2:A:415:HIS:CE1	2.50	0.47
1:C:199:ILE:HD12	1:C:200:ALA:N	2.29	0.47
2:A:327:ARG:HH11	2:A:666:ILE:CG1	2.13	0.46
2:A:275:ILE:O	2:A:608:LYS:HA	2.15	0.46
2:A:588:MET:O	2:A:592:THR:HG22	2.15	0.46
2:A:185:LYS:O	2:A:767:PRO:HD2	2.15	0.46
2:A:346:PHE:CE2	2:A:367:ILE:HG21	2.50	0.46
1:C:134:LYS:HB3	1:C:152:ASP:HB2	1.96	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:333:ILE:HD12	1:B:342:ILE:HD11	1.97	0.46
2:A:237:LEU:HD23	2:A:243:PHE:CE1	2.50	0.46
1:B:132:ILE:HD12	1:B:132:ILE:H	1.80	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
1:B:162:GLN:NE2	1:B:204:ILE:HG23	2.30	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
2:A:368:ILE:O	2:A:368:ILE:HG22	2.16	0.46
1:C:106:PHE:HE2	1:C:359:GLN:HG2	1.80	0.46
2:A:376:ILE:HG21	2:A:485:ALA:HA	1.98	0.46
1:B:242:ASP:O	1:B:302:ASN:HB2	2.15	0.46
2:A:461:PHE:HB3	2:A:479:ALA:CB	2.42	0.46
2:A:991:ILE:HD12	2:A:1020:MET:HE3	1.98	0.46
2:A:996:LEU:O	2:A:1000:TRP:HD1	1.98	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
2:A:602:VAL:HA	2:A:630:LEU:HA	1.97	0.46
2:A:608:LYS:O	2:A:624:VAL:HG23	2.15	0.46
2:A:954:ALA:HB3	2:A:956:PRO:HD2	1.98	0.46
2:A:518:ASN:HA	2:A:521:LEU:HD21	1.97	0.46
2:A:729:ASN:ND2	2:A:732:LYS:H	2.14	0.46
1:C:327:ILE:HD13	1:C:367:LEU:HD21	1.97	0.46
1:B:161:ALA:HB1	1:B:181:ILE:HD11	1.96	0.46
2:A:898:LEU:HD23	2:A:899:LEU:N	2.31	0.46
2:A:570:LEU:HD12	2:A:628:ILE:HD13	1.98	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:525:TYR:HE2	2:A:1028:LEU:CD1	2.29	0.45
1:C:333:ILE:CG1	1:C:382:LEU:HD11	2.46	0.45
2:A:672:MET:CE	2:A:672:MET:HA	2.46	0.45
2:A:345:GLU:HA	2:A:348:VAL:HB	1.98	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:341:LYS:CG	2:A:998:ILE:HG12	2.47	0.45
1:B:340:ARG:HG3	1:B:354:ARG:HA	1.99	0.45
2:A:829:ARG:HD3	2:A:829:ARG:HA	1.73	0.45
2:A:458:THR:HG23	2:A:459:LEU:H	1.82	0.45
1:B:242:ASP:CB	1:B:243:PRO:CD	2.91	0.45
1:B:124:VAL:HB	1:B:235:VAL:HG22	1.97	0.45
1:C:367:LEU:HD22	1:C:367:LEU:H	1.81	0.45
2:A:308:LEU:C	2:A:310:THR:H	2.20	0.45
2:A:212:ALA:C	2:A:215:GLN:HE22	2.19	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:A:925:ALA:HB1	2:A:1012:ILE:CG2	2.40	0.45
2:A:387:ASN:HD22	2:A:387:ASN:H	1.63	0.45
1:C:128:ALA:HB3	1:C:155:ILE:HG21	1.99	0.45
2:A:489:ALA:O	2:A:493:ALA:HB2	2.17	0.45
2:A:355:LEU:HD12	2:A:356:PHE:CD1	2.52	0.45
2:A:948:LEU:HD23	2:A:1035:TYR:HD2	1.82	0.45
1:C:287:VAL:HG23	1:C:293:THR:O	2.16	0.45
2:A:180:VAL:HG12	2:A:286:GLY:C	2.37	0.45
2:A:410:MET:HG2	2:A:497:ILE:HG13	1.98	0.45
2:A:356:PHE:HB3	2:A:982:ARG:NH2	2.30	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:411:ILE:HG12	2:A:497:ILE:CD1	2.46	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:227:ALA:HB3	2:A:229:TYR:HE1	1.82	0.45
2:A:420:GLU:O	2:A:424:GLN:HG3	2.16	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:649:LEU:HB3	2:A:662:TRP:CH2	2.51	0.44
2:A:468:GLU:HG3	2:A:472:GLY:CA	2.45	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:29:TRP:HD1	2:A:30:THR:HG23	1.82	0.44
2:A:640:MET:HA	2:A:644:LYS:HD2	2.00	0.44
2:A:907:ALA:C	2:A:933:LEU:HD11	2.38	0.44
2:A:359:HIS:HB3	2:A:361:ARG:NE	2.32	0.44
2:A:462:ILE:N	2:A:463:PRO:CD	2.80	0.44
2:A:1028:LEU:HD12	2:A:1028:LEU:C	2.38	0.44
1:C:174:THR:HB	1:C:177:GLN:HG3	1.99	0.44
1:C:136:TYR:CE2	1:C:149:PRO:HB2	2.53	0.44
1:B:342:ILE:O	1:B:377:VAL:HG23	2.18	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
2:A:930:PHE:CE2	2:A:1015:PRO:HB3	2.52	0.44
1:B:384:LEU:HD23	1:B:391:ILE:HA	1.99	0.44
2:A:421:TRP:CD1	2:A:421:TRP:C	2.91	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:254:ILE:HD11	2:A:797:THR:HG21	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
1:B:390:ASN:HD22	1:B:390:ASN:C	2.21	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
2:A:599:VAL:HA	2:A:600:PRO:HD3	1.88	0.44
1:B:99:VAL:HG22	1:B:327:ILE:HG22	1.99	0.44
2:A:633:GLN:HA	2:A:636:TRP:NE1	2.33	0.44
2:A:484:TYR:HD2	2:A:484:TYR:HA	1.75	0.44
2:A:279:ASN:ND2	2:A:605:VAL:H	2.15	0.44
2:A:574:PRO:CG	2:A:624:VAL:HG13	2.42	0.43
2:A:76:VAL:O	2:A:76:VAL:HG13	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: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
2:A:664:PRO:HB2	2:A:667:ARG:HB2	2.00	0.43
1:B:185:LEU:HD12	1:B:185:LEU:HA	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: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:109:ARG:HD3	2:A:112:GLU:OE1	2.18	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:4:TRP:CD1	2:A:8:ARG:HG2	2.52	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:685:VAL:HG21	2:A:696:MET:HG3	2.01	0.43
2:A:43:SER:HB3	2:A:670:ILE:HD12	2.00	0.43
2:A:436:TRP:HD1	2:A:436:TRP:O	2.02	0.43
2:A:557:VAL:HG22	2:A:558:GLY:N	2.27	0.43
1:B:174:THR:O	1:B:177:GLN:HB2	2.19	0.43
2:A:876:VAL:O	2:A:880:LEU:HG	2.19	0.43
1:C:174:THR:H	1:C:177:GLN:HE21	1.66	0.43
2:A:1033:ALA:O	2:A:1037:LEU:HD13	2.18	0.43
1:C:138:LEU:HD21	1:C:144:VAL:HG11	2.00	0.43
2:A:39:LEU:HD11	2:A:327:ARG:NH2	2.33	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:A:751:VAL:HG23	2:A:777:ARG:HB3	1.99	0.43
2:A:144:LEU:HD21	2:A:164:LEU:HD12	1.99	0.43
2:A:736:TYR:CE1	2:A:796:ILE:HG21	2.54	0.43
2:A:439:ILE:HD13	2:A:498:PRO:HG2	2.00	0.43
2:A:346:PHE:CE1	2:A:367:ILE:HG12	2.53	0.43
2:A:114:LEU:HA	2:A:117:VAL:HG12	2.01	0.43
1:C:274:LYS:HB3	1:C:274:LYS:HE2	1.77	0.43
2:A:49:ILE:HG23	2:A:129:LEU:HD12	1.99	0.43
1:C:192:GLU:O	1:C:196:ARG:HG3	2.19	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:352:VAL:CG1	2:A:986:MET:HB2	2.49	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:54:PRO:O	2:A:56:GLN:HG2	2.19	0.42
2:A:666:ILE:H	2:A:666:ILE:HD12	1.84	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:6:ILE:HG21	2:A:443:SER:HB3	1.99	0.42
2:A:402:ALA:HB3	2:A:482:LYS:HE2	2.01	0.42
2:A:693:ILE:HA	2:A:696:MET:CG	2.49	0.42
1:C:178:THR:HA	1:C:181:ILE:HG22	2.00	0.42
2:A:684:LYS:HD3	2:A:823:TRP:CZ3	2.54	0.42
1:C:373:GLU:H	1:C:373:GLU:CD	2.21	0.42
1:C:295:GLN:NE2	1:C:295:GLN:HA	2.21	0.42
2:A:547:VAL:HG11	2:A:905:PRO:CB	2.49	0.42
1:C:132:ILE:N	1:C:132:ILE:HD12	2.33	0.42
1:C:331:ALA:O	1:C:341:VAL:HG12	2.20	0.42
2:A:53:TYR:O	2:A:89:GLY:HA2	2.19	0.42
2:A:680:PRO:CG	2:A:827:ASP:HB2	2.50	0.42
2:A:491:LEU:HD12	2:A:491:LEU:C	2.40	0.42
2:A:636:TRP:CD1	2:A:636:TRP:N	2.87	0.42
2:A:914:LEU:CD2	2:A:1017:ILE:HB	2.49	0.42
2:A:156:LEU:O	2:A:159:LEU:HB3	2.19	0.42
2:A:353:CYS:O	2:A:357:LEU:HB2	2.19	0.42
1:B:137:PRO:C	1:B:138:LEU:HD12	2.39	0.42
2:A:728:ILE:HA	2:A:802:ALA:HB2	2.02	0.42
2:A:42:LEU:HD11	2:A:134:THR:HG21	2.01	0.42
2:A:398:ILE:HD11	2:A:1012:ILE:HG13	2.02	0.42
1:C:264:PHE:CE2	1:C:317:LEU:HD13	2.54	0.42
1:B:159:VAL:HG23	1:B:160:GLU:H	1.85	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:A:357:LEU:HD23	2:A:415:HIS:NE2	2.34	0.42
1:C:387:SER:O	1:C:391:ILE:HG13	2.19	0.42
1:C:359:GLN:HG3	1:C:360:ALA:N	2.35	0.42
2:A:56:GLN:HB3	2:A:60:ILE:HD12	2.00	0.42
2:A:470:GLN:OE1	2:A:474:LEU:HD13	2.20	0.42
1:B:308:LYS:O	1:B:311:MET:HG3	2.19	0.42
2:A:417:ARG:HE	2:A:417:ARG:HA	1.85	0.42
2:A:195:ARG:CB	2:A:262:VAL:HA	2.50	0.42
2:A:87:GLN:HG2	2:A:812:MET:HG3	2.02	0.42
1:C:126:ALA:HB2	1:C:229:ILE:HD11	2.02	0.42
2:A:948:LEU:HB3	2:A:1035:TYR:CD2	2.55	0.42
2:A:49:ILE:HG13	2:A:93:VAL:HB	2.01	0.42
2:A:159:LEU:HD21	2:A:319:VAL:HG11	2.01	0.42
2:A:541:LEU:O	2:A:545:LEU:HB2	2.19	0.42
2:A:265:VAL:O	2:A:265:VAL:HG13	2.20	0.42
2:A:819:ARG:HH21	2:A:819:ARG:HG3	1.85	0.42
2:A:567:GLU:CD	2:A:666:ILE:HD13	2.40	0.42
2:A:996:LEU:O	2:A:999:LEU:HB3	2.20	0.42
2:A:353:CYS:SG	2:A:363:ALA:HA	2.60	0.42
2:A:683:ILE:HG12	2:A:858:PHE:CD2	2.54	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: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
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
1:C:85:ASP:HA	1:C:86:PRO:HD3	1.94	0.41
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
2:A:906:PHE:CE2	2:A:1030:ILE:HG13	2.55	0.41
1:B:284:LEU:HB3	1:B:285:PRO:HD2	2.01	0.41
2:A:941:GLY:HA2	2:A:1031:ILE:CD1	2.50	0.41
2:A:59:GLN:NE2	2:A:813:LEU:HD21	2.36	0.41
1:C:345:ASP:CG	1:C:346:ALA:N	2.72	0.41
2:A:1008:VAL:C	2:A:1010:SER:H	2.23	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:956:PRO:HA	2:A:968:LYS:HD3	2.01	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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: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: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:292:ARG:O	2:A:293:SER:C	2.58	0.41
2:A:16:VAL:CG1	2:A:492:LEU:HD13	2.51	0.41
1:C:283:LEU:HA	1:C:283:LEU:HD23	1.72	0.41
2:A:962:GLN:HB2	2:A:962:GLN:HE21	1.58	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:41:ASP:OD2	2:A:41:ASP:N	2.54	0.41
2:A:475:PHE:HA	2:A:478:LEU:CD1	2.51	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
1:B:371:LEU:O	1:B:371:LEU:HD12	2.21	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:714:LEU:HB3	2:A:823:TRP:O	2.20	0.41
2:A:224:LEU:HG	2:A:229:TYR:CD1	2.56	0.41
1:C:159:VAL:HG13	1:C:160:GLU:N	2.36	0.41
1:B:212:ALA:HA	1:B:213:PRO:HD3	1.90	0.41
1:C:190:MET:HG2	1:C:195:ILE:HG13	2.03	0.41
2:A:459:LEU:H	2:A:459:LEU:HD22	1.86	0.41
2:A:240:LEU:O	2:A:243:PHE:HB2	2.20	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:672:MET:C	2:A:674:SER:H	2.23	0.41
2:A:664:PRO:HA	2:A:665:PRO:HD3	1.97	0.41
2:A:906:PHE:HA	2:A:909:VAL:HG12	2.03	0.41
2:A:595:LEU:O	2:A:598:SER:HB3	2.21	0.41
2:A:46:GLN:HB2	2:A:96:ILE:HD13	2.03	0.41
2:A:865:LEU:HD13	2:A:865:LEU:C	2.41	0.40
2:A:522:ILE:HD13	2:A:978:VAL:HG23	2.03	0.40
2:A:413:ASN:HD21	2:A:442:ALA:HA	1.84	0.40
2:A:405:ASP:O	2:A:409:VAL:HG23	2.20	0.40
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: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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:A:933:LEU:O	2:A:933:LEU:HD22	2.21	0.40
1:B:145:GLN:HA	1:B:215:ASP:CB	2.45	0.40
2:A:69:LEU:CD1	2:A:121:LEU:HD21	2.50	0.40
1:B:255:ALA:HB3	1:C:270:ALA:HB1	2.03	0.40
2:A:224:LEU:O	2:A:225:ALA:HB3	2.20	0.40
2:A:995:LEU:HB3	2:A:1017:ILE:HD11	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
1:B:302:ASN:OD1	1:B:307:LEU:HB2	2.21	0.40
2:A:876:VAL:HG23	2:A:877:PRO:HD3	2.03	0.40
2:A:58:PRO:HD2	2:A:723:TYR:OH	2.21	0.40
2:A:421:TRP:O	2:A:421:TRP:HD1	2.04	0.40
2:A:114:LEU:HD12	2:A:117:VAL:CG1	2.51	0.40
2:A:867:ARG:O	2:A:871:LYS:HB2	2.21	0.40
1:C:298:LEU:O	1:C:298:LEU:HD12	2.21	0.40
2:A:633:GLN:HA	2:A:636:TRP:CE2	2.57	0.40
2:A:56:GLN:HB3	2:A:60:ILE:HG23	2.02	0.40
1:B:287:VAL:CG1	1:B:294:LEU:HD23	2.52	0.40
2:A:404:VAL:HA	2:A:407:ALA:HB3	2.04	0.40
2:A:232:ARG:HG2	2:A:233:ALA:N	2.36	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%)	10	64
1	C	322/413 (78%)	294 (91%)	25 (8%)	3 (1%)	25	81
2	A	1027/1054 (97%)	891 (87%)	107 (10%)	29 (3%)	8	58
All	All	1669/1880 (89%)	1465 (88%)	165 (10%)	39 (2%)	10	63

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
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%)	16	61
1	C	265/338 (78%)	244 (92%)	21 (8%)	18	64
2	A	850/872 (98%)	756 (89%)	94 (11%)	9	43
All	All	1378/1548 (89%)	1241 (90%)	137 (10%)	11	50

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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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 ⓘ

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 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.

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, 95th 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 ²)	Q<0.9
1	B	322/413 (77%)	0.20	1 (0%) 91 82	21, 61, 104, 218	0
1	C	324/413 (78%)	0.26	0 100 100	27, 62, 105, 170	0
2	A	1031/1054 (97%)	0.50	61 (5%) 22 14	20, 103, 216, 505	0
All	All	1677/1880 (89%)	0.40	62 (3%) 39 25	20, 74, 202, 505	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	504	TRP	10.0
2	A	503	TYR	6.8
2	A	501	MET	5.7
2	A	364	LEU	4.6
2	A	498	PRO	4.4
2	A	971	GLU	4.3
2	A	497	ILE	4.1
2	A	921	HIS	4.0
2	A	975	HIS	3.9
2	A	967	GLN	3.9
2	A	951	ALA	3.8
2	A	429	THR	3.6
2	A	1036	LYS	3.6
2	A	970	ASP	3.6
2	A	531	LYS	3.5
2	A	952	ILE	3.5
2	A	956	PRO	3.5
2	A	353	CYS	3.4
2	A	716	PHE	3.3
2	A	920	PHE	3.1
2	A	968	LYS	3.1
2	A	1035	TYR	3.1
1	B	79	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
2	A	530	LEU	3.0
2	A	998	ILE	3.0
2	A	955	VAL	2.9
2	A	502	GLY	2.9
2	A	1043	HIS	2.9
2	A	1016	MET	2.8
2	A	564	GLN	2.8
2	A	717	ARG	2.7
2	A	537	LYS	2.7
2	A	415	HIS	2.6
2	A	428	ALA	2.6
2	A	436	TRP	2.5
2	A	1014	ALA	2.5
2	A	480	PHE	2.5
2	A	431	ASP	2.5
2	A	420	GLU	2.4
2	A	552	TRP	2.4
2	A	421	TRP	2.3
2	A	995	LEU	2.3
2	A	475	PHE	2.3
2	A	918	MET	2.3
2	A	439	ILE	2.3
2	A	434	THR	2.2
2	A	519	ARG	2.2
2	A	1025	LEU	2.2
2	A	435	ARG	2.1
2	A	1013	ALA	2.1
2	A	711	ALA	2.1
2	A	400	VAL	2.1
2	A	468	GLU	2.1
2	A	526	HIS	2.1
2	A	469	GLY	2.1
2	A	980	ARG	2.1
2	A	959	ASN	2.1
2	A	494	ILE	2.1
2	A	342	LEU	2.1
2	A	715	ALA	2.0
2	A	556	LYS	2.0
2	A	500	LEU	2.0

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, 95th 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(Å ²)	Q<0.9
3	CU	A	1101	1/1	0.09	-5.08	51,51,51,51	0

6.5 Other polymers

There are no such residues in this entry.