



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:22 PM UTC

PDB ID : 4DNR / pdb_00004dnr
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

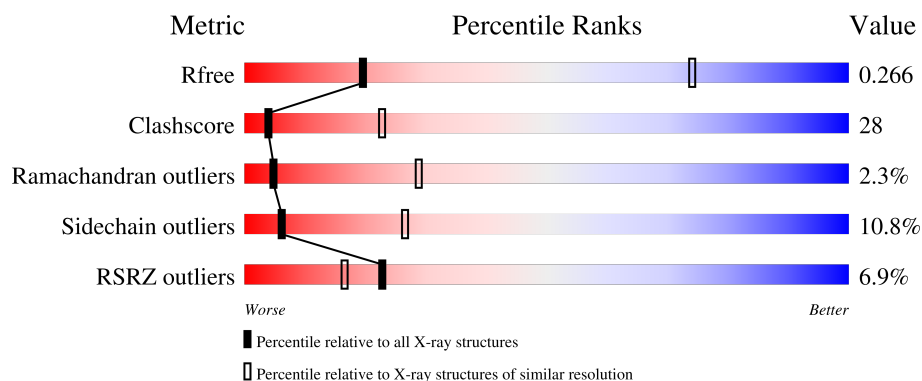
1 Overall quality at a glance

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}	180053	1263 (3.80-3.56)
Clashscore	190562	1305 (3.80-3.56)
Ramachandran outliers	187476	1259 (3.80-3.56)
Sidechain outliers	187428	1256 (3.80-3.56)
RSRZ outliers	180081	1262 (3.80-3.56)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 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 (CCD ID: CU) (formula: Cu).

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

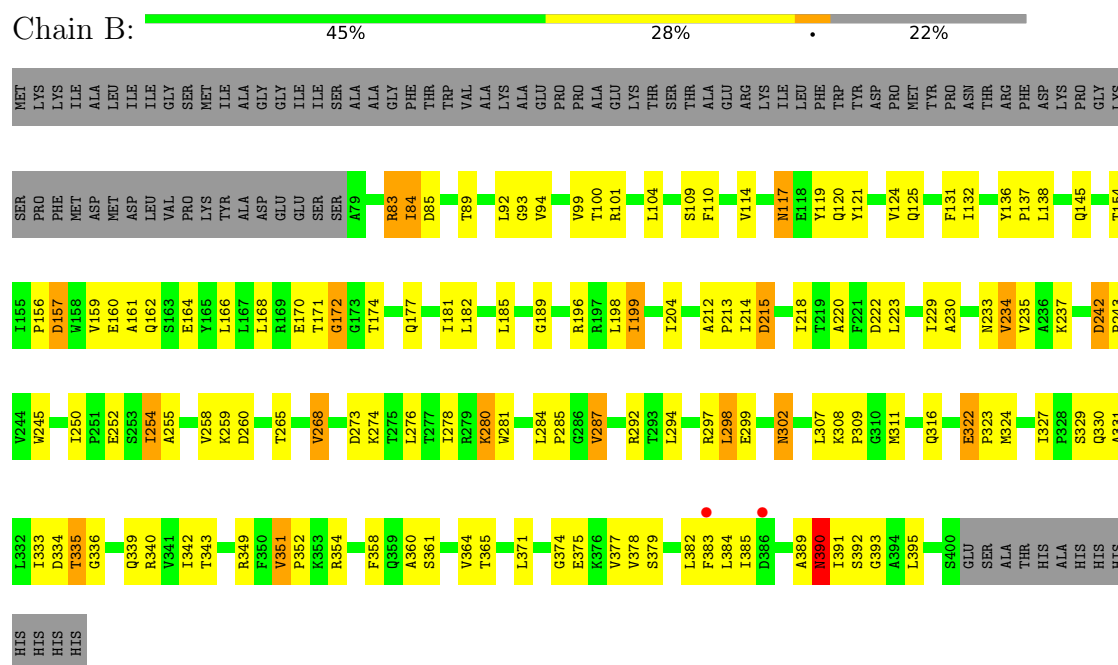
- Molecule 4 is water.

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

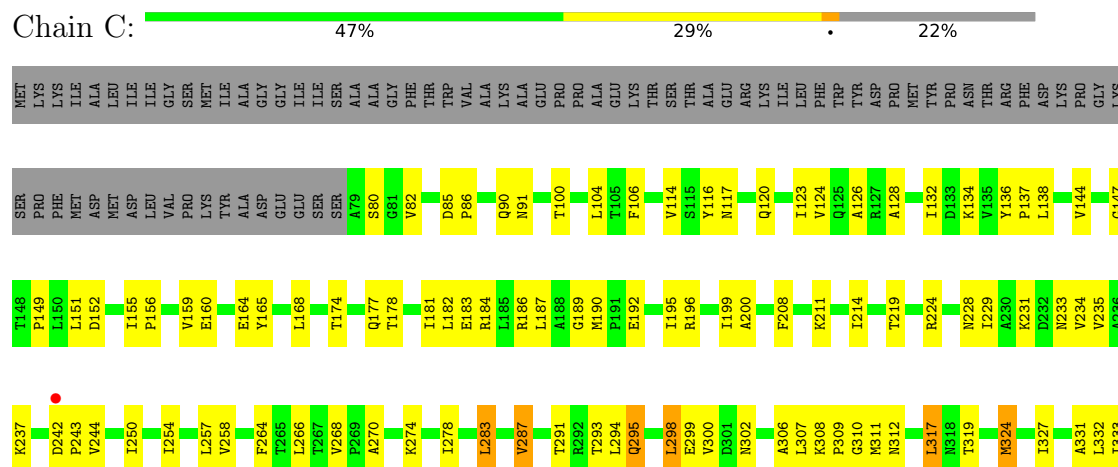
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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

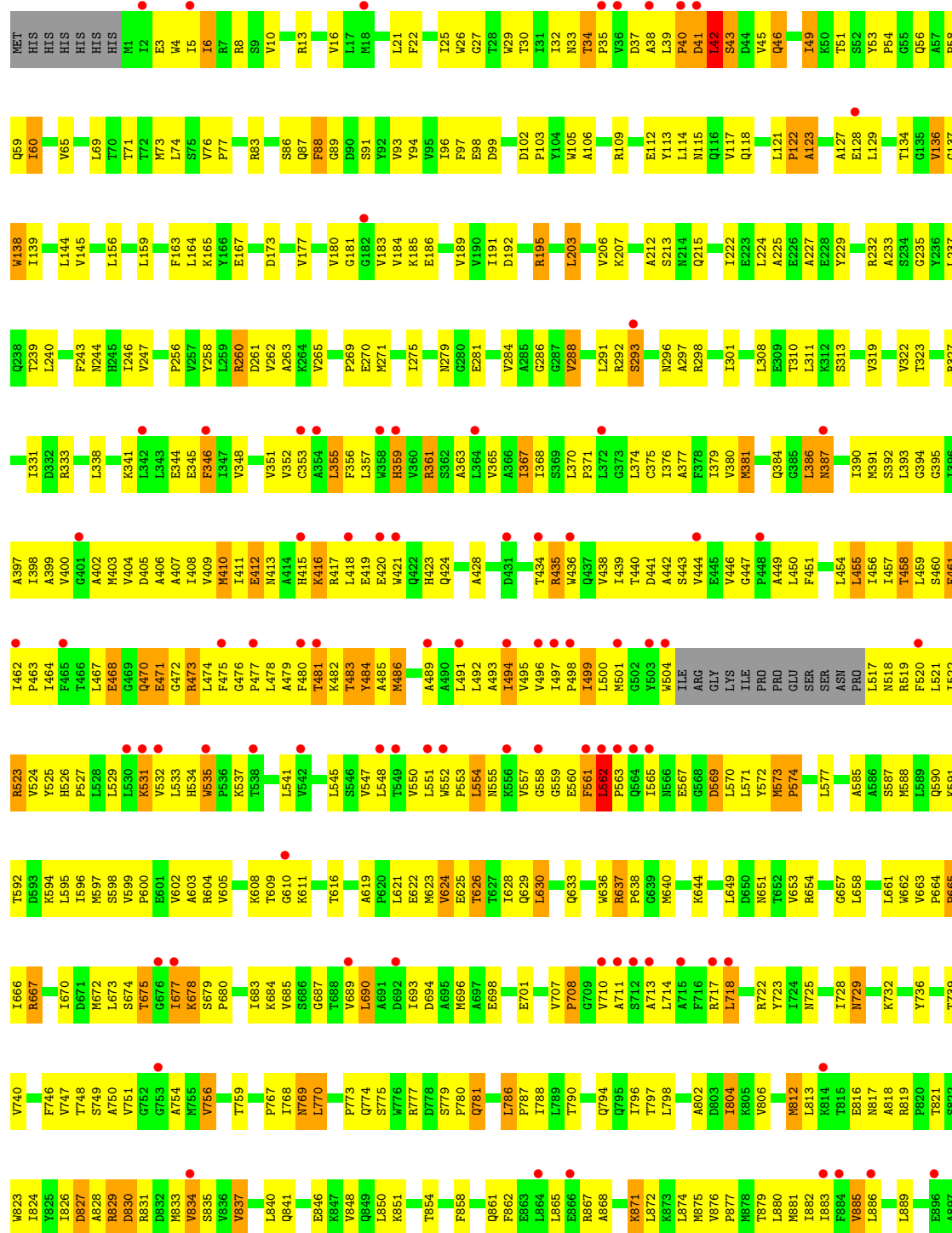


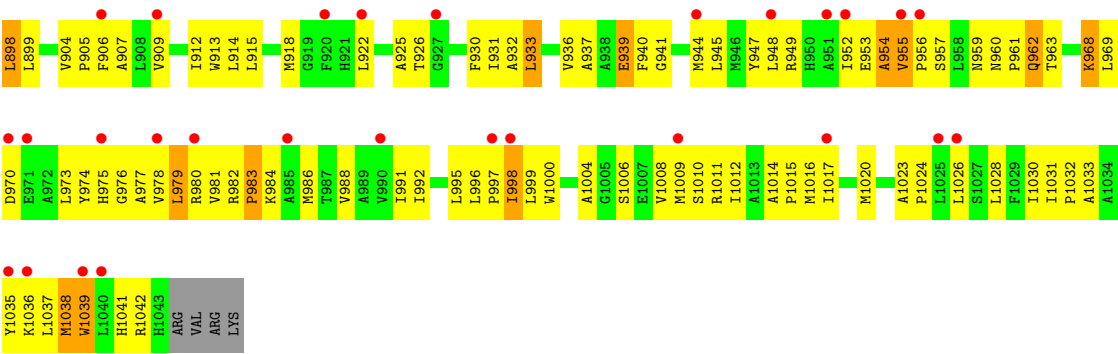
• Molecule 1: Cation efflux system protein CusB





• 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, α , β , γ	159.59Å 159.59Å 689.65Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	97.67 – 3.68 97.67 – 3.68	Depositor EDS
% Data completeness (in resolution range)	89.9 (97.67-3.68) 98.8 (97.67-3.68)	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 1.6.4_486	Depositor
R, R_{free}	0.244 , 0.272 0.238 , 0.266	Depositor DCC
R_{free} test set	1872 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	83.3	Xtriage
Anisotropy	0.241	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 111.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	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.

²Theoretical 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 ⓘ

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	0.27	0/2498	0.74	2/3401 (0.1%)
1	C	0.27	0/2513	0.74	0/3421
2	A	0.29	0/8117	0.76	6/11052 (0.1%)
All	All	0.28	0/13128	0.75	8/17874 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	562	LEU	CA-C-N	-7.41	110.57	119.84
2	A	562	LEU	C-N-CA	-7.41	110.57	119.84
2	A	535	TRP	CA-C-N	5.52	124.71	118.97
2	A	535	TRP	C-N-CA	5.52	124.71	118.97
2	A	473	ARG	N-CA-C	-5.42	106.62	113.18
1	B	268	VAL	CA-C-N	5.31	124.95	119.05
1	B	268	VAL	C-N-CA	5.31	124.95	119.05
2	A	830	ASP	CB-CA-C	-5.04	110.78	116.63

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2458	0	2522	118	0
1	C	2473	0	2533	103	0
2	A	7950	0	8198	534	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	735	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 28.

All (735) 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: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:HE21	1:C:295:GLN:HA	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:991:ILE:HD12	2:A:1020:MET:HE3	1.57	0.84
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
1:C:308:LYS:HB2	1:C:311:MET:HE3	1.63	0.80
2:A:458:THR:HG23	2:A:459:LEU:HD22	1.63	0.80
2:A:391:MET:HE3	2:A:1008:VAL:HG21	1.63	0.79
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:HB2	2:A:637:ARG:HH11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:672:MET:HA	2:A:672:MET:HE2	1.68	0.74
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
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:410:MET:HE3	2:A:493:ALA:HB1	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
2:A:729:ASN:C	2:A:729:ASN:HD22	1.98	0.71
1:B:334:ASP:HA	1:B:339:GLN:HB2	1.72	0.71
2:A:1039:TRP:HA	2:A:1039:TRP:CE3	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
1:B:145:GLN:HA	1:B:215:ASP:HB3	1.73	0.70
2:A:416:LYS:HE3	2:A:416:LYS:HA	1.72	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
1:C:384:LEU:HD21	2:A:588:MET:HE3	1.73	0.69
1:B:230:ALA:H	1:B:233:ASN:ND2	1.91	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
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
1:C:308:LYS:O	1:C:311:MET:HG2	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:435:ARG:H	2:A:435:ARG:HD3	1.57	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
1:C:123:ILE:HG12	1:C:237:LYS:HG3	1.77	0.67
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:B:125:GLN:NE2	1:C:228:ASN:H	1.92	0.67
2:A:696:MET:HE1	2:A:851:LYS:HB2	1.75	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
1:B:204:ILE:HD12	1:B:204:ILE:H	1.61	0.66
2:A:456:ILE:HD12	2:A:883:ILE:HD13	1.76	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
2:A:968:LYS:HE3	2:A:968:LYS:HA	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
1:B:252:GLU:HG2	1:C:270:ALA:HB2	1.78	0.65
2:A:395:GLY:H	2:A:478:LEU:HD22	1.62	0.65
2:A:410:MET:HE2	2:A:497:ILE:HD11	1.79	0.64
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
1:B:280:LYS:HE3	1:B:281:TRP:H	1.62	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:322:GLU:HG3	1:B:323:PRO:HD2	1.79	0.64
2:A:403:MET:HE2	2:A:403:MET:HA	1.80	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: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:596:ILE:HG12	2:A:653:VAL:HG21	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:203:LEU:HD11	2:A:750:ALA:HB2	1.80	0.62
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: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
1:B:174:THR:HB	1:B:177:GLN:HG3	1.80	0.62
2:A:496:VAL:HA	2:A:499:ILE:HG22	1.82	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:HE3	1:B:280:LYS:HA	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:455:LEU:HD22	2:A:486:MET:HE1	1.82	0.61
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: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
2:A:604:ARG:HG2	2:A:604:ARG:HH21	1.67	0.59
2:A:1039:TRP:HA	2:A:1039:TRP:HE3	1.66	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:109:SER:HB3	1:B:316:GLN:OE1	2.02	0.59
2:A:678:LYS:HD2	2:A:679:SER:N	2.18	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:346:PHE:HD1	2:A:346:PHE:C	2.11	0.59
2:A:571:LEU:HD12	2:A:663:VAL:HG23	1.84	0.59
2:A:930:PHE:CD2	2:A:1015:PRO:HB3	2.37	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: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
1:B:222:ASP:OD1	1:B:234:VAL:HG23	2.03	0.58
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
2:A:588:MET:HE2	2:A:658:LEU:HD13	1.86	0.58
2:A:415:HIS:O	2:A:419:GLU:HG2	2.03	0.58
1:B:324:MET:HE1	1:B:358:PHE:CG	2.39	0.57
2:A:907:ALA:HA	2:A:1023:ALA:HB2	1.85	0.57
2:A:346:PHE:C	2:A:346:PHE:CD1	2.81	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: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:714:LEU:HD23	2:A:717:ARG:HD2	1.86	0.57
2:A:1031:ILE:HB	2:A:1032:PRO:HD3	1.85	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
1:C:132:ILE:HD11	1:C:229:ILE:HB	1.87	0.56
2:A:944:MET:SD	2:A:980:ARG:HD2	2.44	0.56
1:B:92:LEU:HD13	2:A:281:GLU:O	2.05	0.56
1:B:162:GLN:HG2	1:B:198:LEU:HD22	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:A:956:PRO:HB3	2:A:968:LYS:HG3	1.88	0.56
1:B:389:ALA:O	1:B:390:ASN:C	2.48	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:ND2	2:A:387:ASN:H	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
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: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:138:LEU:HD23	1:B:218:ILE:HD11	1.88	0.55
2:A:759:THR:HG23	2:A:768:ILE:HD11	1.86	0.55
1:B:131:PHE:CE2	1:B:154:THR:HB	2.42	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:336:GLY:HA3	2:A:775:SER:OG	2.06	0.55
2:A:456:ILE:HD13	2:A:886:LEU:HD12	1.89	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
1:B:245:TRP:CE3	1:B:297:ARG:HD3	2.42	0.55
2:A:186:GLU:HG3	2:A:767:PRO:HG2	1.88	0.55
2:A:395:GLY:HA2	2:A:398:ILE:HB	1.87	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:944:MET:HE2	2:A:948:LEU:HD13	1.89	0.54
1:C:358:PHE:C	1:C:358:PHE:CD2	2.83	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
1:B:83:ARG:HH22	1:C:90:GLN:HB3	1.73	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:110:PHE:CE1	1:B:250:ILE:HG23	2.43	0.53
2:A:944:MET:HB3	2:A:1031:ILE:HD13	1.90	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:932:ALA:O	2:A:936:VAL:HG23	2.09	0.53
2:A:588:MET:HE2	2:A:658:LEU:HD22	1.90	0.53
1:B:84:ILE:HG22	1:C:91:ASN:OD1	2.08	0.53
2:A:356:PHE:HB3	2:A:982:ARG:HH22	1.74	0.53
2:A:464:ILE:HD12	2:A:464:ILE:H	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
1:B:331:ALA:HB2	1:B:379:SER:HA	1.90	0.53
2:A:144:LEU:HD11	2:A:164:LEU:HD11	1.91	0.53
2:A:525:TYR:CD1	2:A:981:VAL:HG21	2.43	0.53
2:A:687:GLY:HA3	2:A:854:THR:HG22	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: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
1:B:117:ASN:HD22	1:B:117:ASN:C	2.17	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:HE	1:B:83:ARG:HA	1.74	0.52
1:C:164:GLU:O	1:C:168:LEU:HD13	2.10	0.52
2:A:440:THR:O	2:A:444:VAL:HG23	2.10	0.52
2:A:531:LYS:HE3	2:A:531:LYS:HA	1.91	0.52
2:A:955:VAL:CG1	2:A:956:PRO:HD3	2.35	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: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
1:B:273:ASP:OD2	1:B:274:LYS:HD2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:701:GLU:OE1	2:A:713:ALA:HB2	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
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:980:ARG:O	2:A:983:PRO:HD2	2.11	0.51
2:A:51:THR:OG1	2:A:91:SER:HB3	2.11	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
1:B:94:VAL:HG13	1:B:383:PHE:HZ	1.76	0.51
2:A:341:LYS:O	2:A:344:GLU:HB2	2.11	0.51
1:B:343:THR:OG1	1:B:351:VAL:HG23	2.11	0.51
1:C:190:MET:HE2	1:C:195:ILE:HA	1.93	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
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: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
1:B:114:VAL:HG12	1:B:309:PRO:HA	1.92	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:384:LEU:HD12	1:B:384:LEU:N	2.25	0.50
1:C:165:TYR:CE2	1:C:178:THR:HG23	2.45	0.50
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
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:69:LEU:O	2:A:73:MET:HG2	2.12	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
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: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:256:PRO:HG2	2:A:258:TYR:CE1	2.47	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:30:THR:O	2:A:34:THR:HB	2.12	0.50
2:A:212:ALA:C	2:A:215:GLN:HE22	2.19	0.50
2:A:308:LEU:C	2:A:310:THR:H	2.20	0.50
2:A:474:LEU:HD23	2:A:475:PHE:CE1	2.46	0.50
1:B:121:TYR:CG	1:C:224:ARG:HD2	2.47	0.50
2:A:180:VAL:HG12	2:A:286:GLY:C	2.37	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
1:B:390:ASN:HD21	1:B:392:SER:HB2	1.76	0.49
1:C:362:GLN:HE21	1:C:362:GLN:HA	1.78	0.49
2:A:666:ILE:N	2:A:666:ILE:HD12	2.27	0.49
1:B:110:PHE:CG	1:B:250:ILE:HG12	2.47	0.49
2:A:533:LEU:HD22	2:A:1036:LYS:HZ2	1.76	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
1:B:164:GLU:O	1:B:168:LEU:HD13	2.13	0.49
2:A:680:PRO:O	2:A:862:PHE:HD1	1.95	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:907:ALA:C	2:A:933:LEU:HD11	2.38	0.49
1:B:156:PRO:O	1:B:157:ASP:HB2	2.12	0.49
2:A:41:ASP:HB2	2:A:473:ARG:HD2	1.94	0.49
2:A:435:ARG:H	2:A:435:ARG:CD	2.25	0.49
2:A:816:GLU:HB3	2:A:821:THR:HG21	1.94	0.49
1:C:124:VAL:O	1:C:235:VAL:HG12	2.12	0.49
1:C:287:VAL:HG23	1:C:293:THR:C	2.37	0.49
2:A:680:PRO:CD	2:A:827:ASP:HB2	2.43	0.49
2:A:1028:LEU:C	2:A:1028:LEU:HD12	2.38	0.49
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: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
2:A:1014:ALA:HB3	2:A:1015:PRO:HD3	1.95	0.48
1:B:125:GLN:HE21	1:C:228:ASN:HD22	1.59	0.48
1:B:390:ASN:HD22	1:B:390:ASN:C	2.21	0.48
1:C:244:VAL:HG11	1:C:307:LEU:HD23	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:109:ARG:O	2:A:112:GLU:HG2	2.14	0.48
2:A:391:MET:HE1	2:A:565:ILE:HD11	1.95	0.48
2:A:491:LEU:O	2:A:495:VAL:HG23	2.12	0.48
2:A:995:LEU:HD21	2:A:1016:MET:HE3	1.95	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:275:ILE:N	2:A:275:ILE:HD12	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
1:C:327:ILE:CD1	1:C:367:LEU:HD21	2.43	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: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: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
1:B:307:LEU:HA	1:B:311:MET:HE1	1.94	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:97:PHE:CE1	2:A:106:ALA:HB1	2.49	0.47
2:A:421:TRP:CD1	2:A:421:TRP:C	2.91	0.47
2:A:623:MET:HE1	2:A:625:GLU:HG3	1.96	0.47
2:A:875:MET:C	2:A:877:PRO:HD2	2.39	0.47
2:A:960:ASN:N	2:A:961:PRO:HD2	2.29	0.47
1:B:84:ILE:HD11	2:A:594:LYS:HB2	1.96	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: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
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
2:A:526:HIS:CE1	2:A:978:VAL:HB	2.49	0.47
2:A:551:LEU:HA	2:A:554:LEU:HD22	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:567:GLU:CD	2:A:666:ILE:HD13	2.40	0.47
1:B:360:ALA:CB	1:B:365:THR:HG22	2.42	0.47
1:C:373:GLU:CD	1:C:373:GLU:H	2.21	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:104:LEU:HD22	1:B:361:SER:HB3	1.96	0.47
2:A:399:ALA:HA	2:A:482:LYS:HE3	1.97	0.47
1:C:358:PHE:HB3	1:C:366:ALA:O	2.15	0.47
2:A:413:ASN:ND2	2:A:442:ALA:HA	2.29	0.47
1:B:117:ASN:HD21	1:B:119:TYR:HB2	1.80	0.47
1:B:137:PRO:C	1:B:138:LEU:HD12	2.39	0.47
1:B:349:ARG:NE	1:B:349:ARG:HA	2.29	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:491:LEU:HD12	2:A:491:LEU:C	2.40	0.47
2:A:672:MET:C	2:A:674:SER:H	2.23	0.47
2:A:969:LEU:O	2:A:973:LEU:HD13	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: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: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:574:PRO:HB2	2:A:658:LEU:CD1	2.41	0.47
1:C:199:ILE:HD12	1:C:200:ALA:N	2.29	0.47
2:A:357:LEU:HD23	2:A:415:HIS:CE1	2.50	0.47
2:A:464:ILE:HD12	2:A:464:ILE:N	2.29	0.47
1:C:134:LYS:HB3	1:C:152:ASP:HB2	1.96	0.46
2:A:185:LYS:O	2:A:767:PRO:HD2	2.15	0.46
2:A:275:ILE:O	2:A:608:LYS:HA	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
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:37:ASP:HB2	2:A:39:LEU:HD23	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:237:LEU:HD23	2:A:243:PHE:CE1	2.50	0.46
2:A:410:MET:HB2	2:A:494:ILE:HG12	1.96	0.46
1:C:397:ARG:O	1:C:401:GLU:HG3	2.14	0.46
2:A:112:GLU:HG3	2:A:113:TYR:CD1	2.49	0.46
1:C:345:ASP:CG	1:C:346:ALA:N	2.72	0.46
2:A:1008:VAL:C	2:A:1010:SER:H	2.23	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:368:ILE:O	2:A:368:ILE:HG22	2.16	0.46
2:A:588:MET:CE	2:A:658:LEU:HD13	2.45	0.46
2:A:850:LEU:HD22	2:A:854:THR:OG1	2.15	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
1:B:245:TRP:CD1	1:B:299:GLU:HG2	2.49	0.46
2:A:292:ARG:O	2:A:293:SER:C	2.58	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
2:A:996:LEU:O	2:A:1000:TRP:HD1	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:518:ASN:HA	2:A:521:LEU:HD21	1.97	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: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
2:A:988:VAL:HA	2:A:1020:MET:HE1	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:570:LEU:HD12	2:A:628:ILE:HD13	1.98	0.46
1:C:324:MET:HE2	1:C:324:MET:HA	1.98	0.45
1:C:333:ILE:CG1	1:C:382:LEU:HD11	2.46	0.45
2:A:345:GLU:HA	2:A:348:VAL:HB	1.98	0.45
2:A:525:TYR:HE2	2:A:1028:LEU:CD1	2.29	0.45
1:C:372:ALA:O	1:C:375:GLU:HB2	2.15	0.45
1:B:340:ARG:HG3	1:B:354:ARG:HA	1.99	0.45
2:A:341:LYS:CG	2:A:998:ILE:HG12	2.47	0.45
2:A:829:ARG:HA	2:A:829:ARG:HD3	1.73	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:367:LEU:H	1:C:367:LEU:HD22	1.81	0.45
2:A:458:THR:HG23	2:A:459:LEU:H	1.82	0.45
1:C:128:ALA:HB3	1:C:155:ILE:HG21	1.99	0.45
2:A:387:ASN:H	2:A:387:ASN:HD22	1.63	0.45
2:A:865:LEU:C	2:A:865:LEU:HD13	2.41	0.45
2:A:925:ALA:HB1	2:A:1012:ILE:CG2	2.40	0.45
1:C:287:VAL:HG23	1:C:293:THR:O	2.16	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
2:A:696:MET:HE1	2:A:851:LYS:CB	2.45	0.45
2:A:833:MET:HE2	2:A:862:PHE:HB3	1.99	0.45
2:A:948:LEU:HD23	2:A:1035:TYR:HD2	1.82	0.45
1:C:250:ILE:O	1:C:294:LEU:N	2.45	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:597:MET:HE1	2:A:603:ALA:O	2.16	0.45
2:A:683:ILE:HB	2:A:824:ILE:HB	1.98	0.45
2:A:685:VAL:HG21	2:A:696:MET:HB2	1.98	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:411:ILE:HG12	2:A:497:ILE:CD1	2.46	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
1:C:291:THR:O	1:C:293:THR:HG23	2.17	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: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
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: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
2:A:311:LEU:C	2:A:313:SER:H	2.25	0.44
2:A:359:HIS:HB3	2:A:361:ARG:NE	2.32	0.44
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:462:ILE:N	2:A:463:PRO:CD	2.80	0.44
1:B:342:ILE:O	1:B:377:VAL:HG23	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:384:LEU:HD23	1:B:391:ILE:HA	1.99	0.44
1:C:254:ILE:HD11	2:A:797:THR:HG21	1.99	0.44
2:A:457:ILE:HG21	2:A:482:LYS:HD2	2.00	0.44
2:A:460:SER:O	2:A:463:PRO:HD2	2.18	0.44
2:A:485:ALA:O	2:A:486:MET:C	2.61	0.44
2:A:571:LEU:C	2:A:571:LEU:HD13	2.42	0.44
2:A:930:PHE:CE2	2:A:1015:PRO:HB3	2.52	0.44
1:C:126:ALA:HB2	1:C:229:ILE:CD1	2.47	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
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:99:VAL:HG22	1:B:327:ILE:HG22	1.99	0.44
2:A:279:ASN:ND2	2:A:605:VAL:H	2.15	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:633:GLN:HA	2:A:636:TRP:NE1	2.33	0.44
2:A:714:LEU:C	2:A:714:LEU:HD13	2.43	0.44
1:B:132:ILE:HD12	1:B:132:ILE:N	2.33	0.43
2:A:76:VAL:HG13	2:A:76:VAL:O	2.18	0.43
2:A:574:PRO:CG	2:A:624:VAL:HG13	2.42	0.43
2:A:996:LEU:N	2:A:997:PRO:CD	2.80	0.43
1:B:171:THR:O	1:B:172:GLY:C	2.60	0.43
1:C:254:ILE:HG22	1:C:254:ILE:O	2.18	0.43
1:B:137:PRO:O	1:B:138:LEU:HD12	2.17	0.43
1:B:185:LEU:HD12	1:B:185:LEU:HA	1.82	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
2:A:954:ALA:C	2:A:956:PRO:HD2	2.42	0.43
1:B:371:LEU:HD12	1:B:371:LEU:C	2.43	0.43
1:C:388:GLU:HB2	2:A:657:GLY:N	2.33	0.43
2:A:537:LYS:HA	2:A:1037:LEU:HD11	2.01	0.43
2:A:672:MET:C	2:A:674:SER:N	2.74	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:41:ASP:OD1	2:A:470:GLN:HG2	2.19	0.43
2:A:109:ARG:HD3	2:A:112:GLU:OE1	2.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:640:MET:HE3	2:A:644:LYS:HB3	1.99	0.43
2:A:998:ILE:HG22	2:A:1009:MET:O	2.19	0.43
2:A:391:MET:C	2:A:393:LEU:H	2.26	0.43
2:A:685:VAL:HG21	2:A:696:MET:HG3	2.01	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: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
2:A:876:VAL:O	2:A:880:LEU:HG	2.19	0.43
2:A:1033:ALA:O	2:A:1037:LEU:HD13	2.18	0.43
2:A:39:LEU:HD11	2:A:327:ARG:NH2	2.33	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:751:VAL:HG23	2:A:777:ARG:HB3	1.99	0.43
1:C:192:GLU:O	1:C:196:ARG:HG3	2.19	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
2:A:114:LEU:HA	2:A:117:VAL:HG12	2.01	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
2:A:460:SER:C	2:A:463:PRO:HD2	2.43	0.43
2:A:933:LEU:HD13	2:A:933:LEU:C	2.44	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:357:LEU:HD13	2:A:986:MET:HE1	2.01	0.43
2:A:969:LEU:HD12	2:A:969:LEU:C	2.43	0.43
2:A:42:LEU:HD13	2:A:42:LEU:HA	1.80	0.42
2:A:54:PRO:O	2:A:56:GLN:HG2	2.19	0.42
2:A:352:VAL:CG1	2:A:986:MET:HB2	2.49	0.42
2:A:408:ILE:HD12	2:A:408:ILE:C	2.43	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
1:B:374:GLY:O	1:B:375:GLU:C	2.62	0.42
1:C:178:THR:HA	1:C:181:ILE:HG22	2.00	0.42
2:A:6:ILE:HG21	2:A:443:SER:HB3	1.99	0.42
2:A:41:ASP:OD1	2:A:474:LEU:HD13	2.18	0.42
2:A:392:SER:HA	2:A:478:LEU:HD21	2.02	0.42
2:A:402:ALA:HB3	2:A:482:LYS:HE2	2.01	0.42
2:A:666:ILE:HD12	2:A:666:ILE:H	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:53:TYR:O	2:A:89:GLY:HA2	2.19	0.42
2:A:547:VAL:HG11	2:A:905:PRO:CB	2.49	0.42
1:C:382:LEU:HD13	1:C:382:LEU:C	2.44	0.42
2:A:156:LEU:O	2:A:159:LEU:HB3	2.19	0.42
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: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: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:189:GLY:O	1:C:190:MET:C	2.62	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:56:GLN:HB3	2:A:60:ILE:HD12	2.00	0.42
2:A:122:PRO:O	2:A:123:ALA:C	2.63	0.42
2:A:357:LEU:HD23	2:A:415:HIS:NE2	2.34	0.42
2:A:918:MET:HE3	2:A:999:LEU:HD21	2.01	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:49:ILE:HG13	2:A:93:VAL:HB	2.01	0.42
2:A:87:GLN:HG2	2:A:812:MET:HG3	2.02	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: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:948:LEU:HB3	2:A:1035:TYR:CD2	2.55	0.42
1:C:147:GLY:O	1:C:211:LYS:HD3	2.20	0.42
1:C:199:ILE:HD12	1:C:199:ILE:C	2.45	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:996:LEU:O	2:A:999:LEU:HB3	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
1:C:85:ASP:HA	1:C:86:PRO:HD3	1.94	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
2:A:442:ALA:O	2:A:446:VAL:HB	2.19	0.41
2:A:455:LEU:CD2	2:A:486:MET:HE1	2.49	0.41
2:A:651:ASN:HA	2:A:654:ARG:NH2	2.31	0.41
1:B:284:LEU:HB3	1:B:285:PRO:HD2	2.01	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
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:352:PRO:HG3	1:C:395:LEU:HD12	2.01	0.41
2:A:74:LEU:HD11	2:A:817:ASN:O	2.20	0.41
1:B:383:PHE:C	1:B:384:LEU:HD12	2.46	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:69:LEU:HD11	2:A:121:LEU:HD21	2.03	0.41
2:A:88:PHE:O	2:A:88:PHE:CD1	2.73	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:458:THR:HB	2:A:483:THR:CG2	2.50	0.41
2:A:956:PRO:HA	2:A:968:LYS:HD3	2.01	0.41
1:C:283:LEU:HD23	1:C:283:LEU:HA	1.72	0.41
2:A:962:GLN:HE21	2:A:962:GLN:HB2	1.58	0.41
1:B:307:LEU:HA	1:B:311:MET:CE	2.51	0.41
1:C:138:LEU:HD12	1:C:138:LEU:HA	1.93	0.41
2:A:10:VAL:HG12	2:A:436:TRP:HE1	1.85	0.41
1:B:212:ALA:HA	1:B:213:PRO:HD3	1.90	0.41
1:B:329:SER:OG	1:B:365:THR:HG23	2.21	0.41
1:B:329:SER:C	1:B:331:ALA:H	2.29	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:41:ASP:OD2	2:A:41:ASP:N	2.54	0.41
2:A:60:ILE:C	2:A:60:ILE:HD13	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:98:GLU:O	2:A:99:ASP:C	2.61	0.41
2:A:224:LEU:HG	2:A:229:TYR:CD1	2.56	0.41
2:A:260:ARG:HD2	2:A:261:ASP:OD1	2.20	0.41
2:A:356:PHE:CB	2:A:982:ARG:HH22	2.33	0.41
2:A:357:LEU:HD23	2:A:415:HIS:CD2	2.56	0.41
2:A:475:PHE:HA	2:A:478:LEU:CD1	2.51	0.41
2:A:714:LEU:HB3	2:A:823:TRP:O	2.20	0.41
2:A:877:PRO:O	2:A:881:MET:HE2	2.21	0.41
1:C:155:ILE:HB	1:C:208:PHE:HE1	1.85	0.41
1:C:397:ARG:CZ	1:C:397:ARG:HB2	2.51	0.41
2:A:46:GLN:HB2	2:A:96:ILE:HD13	2.03	0.41
2:A:240:LEU:O	2:A:243:PHE:HB2	2.20	0.41
2:A:459:LEU:HD22	2:A:459:LEU:H	1.86	0.41
2:A:483:THR:O	2:A:486:MET:HE2	2.20	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
2:A:906:PHE:HA	2:A:909:VAL:HG12	2.03	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:311:LEU:C	2:A:313:SER:N	2.79	0.40
2:A:405:ASP:O	2:A:409:VAL:HG23	2.20	0.40
2:A:412:GLU:CD	2:A:982:ARG:HG3	2.45	0.40
2:A:413:ASN:HD21	2:A:442:ALA:HA	1.84	0.40
2:A:522:ILE:HD13	2:A:978:VAL:HG23	2.03	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
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: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: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:739:THR:O	2:A:740:VAL:C	2.65	0.40
2:A:1038:MET:HE2	2:A:1038:MET:HB3	1.99	0.40
1:B:302:ASN:OD1	1:B:307:LEU:HB2	2.21	0.40
1:B:390:ASN:C	1:B:390:ASN:ND2	2.80	0.40
2:A:58:PRO:HD2	2:A:723:TYR:OH	2.21	0.40
2:A:114:LEU:HD12	2:A:117:VAL:CG1	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:421:TRP:HD1	2:A:421:TRP:O	2.04	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:287:VAL:CG1	1:B:294:LEU:HD23	2.52	0.40
1:C:298:LEU:HD12	1:C:298:LEU:O	2.21	0.40
2:A:56:GLN:HB3	2:A:60:ILE:HG23	2.02	0.40
2:A:105:TRP:CD1	2:A:105:TRP:C	2.98	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:633:GLN:HA	2:A:636:TRP:CE2	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	320/413 (78%)	280 (88%)	33 (10%)	7 (2%)	5	29
1	C	322/413 (78%)	294 (91%)	25 (8%)	3 (1%)	14	45
2	A	1027/1054 (97%)	891 (87%)	107 (10%)	29 (3%)	4	26
All	All	1669/1880 (89%)	1465 (88%)	165 (10%)	39 (2%)	5	29

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

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Mol	Chain	Res	Type
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%)	243 (92%)	20 (8%)	12	38
1	C	265/338 (78%)	242 (91%)	23 (9%)	9	33
2	A	850/872 (98%)	744 (88%)	106 (12%)	4	21
All	All	1378/1548 (89%)	1229 (89%)	149 (11%)	6	26

All (149) 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	182	LEU
1	B	199	ILE
1	B	214	ILE
1	B	215	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	364	VAL
1	B	378	VAL
1	B	390	ASN
1	C	100	THR
1	C	104	LEU
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	268	VAL
1	C	283	LEU
1	C	287	VAL
1	C	295	GLN
1	C	298	LEU
1	C	299	GLU

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Mol	Chain	Res	Type
1	C	317	LEU
1	C	324	MET
1	C	332	LEU
1	C	345	ASP
1	C	362	GLN
1	C	364	VAL
1	C	367	LEU
1	C	373	GLU
1	C	396	GLU
2	A	5	ILE
2	A	6	ILE
2	A	21	LEU
2	A	25	ILE
2	A	34	THR
2	A	42	LEU
2	A	45	VAL
2	A	46	GLN
2	A	49	ILE
2	A	60	ILE
2	A	65	VAL
2	A	115	ASN
2	A	128	GLU
2	A	183	VAL
2	A	184	VAL
2	A	195	ARG
2	A	203	LEU
2	A	222	ILE
2	A	239	THR
2	A	247	VAL
2	A	260	ARG
2	A	288	VAL
2	A	322	VAL
2	A	323	THR
2	A	338	LEU
2	A	346	PHE
2	A	355	LEU
2	A	361	ARG
2	A	367	ILE
2	A	381	MET
2	A	384	GLN
2	A	386	LEU
2	A	387	ASN

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Mol	Chain	Res	Type
2	A	390	ILE
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	499	ILE
2	A	519	ARG
2	A	523	ARG
2	A	531	LYS
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	622	GLU
2	A	624	VAL
2	A	626	THR
2	A	630	LEU
2	A	637	ARG
2	A	667	ARG
2	A	675	THR
2	A	677	ILE
2	A	678	LYS
2	A	689	VAL
2	A	690	LEU
2	A	694	ASP
2	A	698	GLU
2	A	710	VAL

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Mol	Chain	Res	Type
2	A	718	LEU
2	A	722	ARG
2	A	729	ASN
2	A	769	ASN
2	A	770	LEU
2	A	774	GLN
2	A	781	GLN
2	A	786	LEU
2	A	804	ILE
2	A	827	ASP
2	A	829	ARG
2	A	837	VAL
2	A	848	VAL
2	A	871	LYS
2	A	874	LEU
2	A	885	VAL
2	A	898	LEU
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	998	ILE
2	A	1026	LEU
2	A	1038	MET
2	A	1039	TRP
2	A	1041	HIS

Sometimes 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

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Mol	Chain	Res	Type
1	B	390	ASN
1	C	90	GLN
1	C	125	GLN
1	C	145	GLN
1	C	177	GLN
1	C	205	GLN
1	C	263	GLN
1	C	295	GLN
1	C	302	ASN
1	C	316	GLN
1	C	362	GLN
2	A	63	ASN
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	629	GLN
2	A	633	GLN
2	A	635	GLN
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 molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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, 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%)	-0.02	2 (0%) 85 65	21, 61, 104, 218	0
1	C	324/413 (78%)	-0.04	1 (0%) 90 76	27, 62, 105, 170	0
2	A	1031/1054 (97%)	0.66	112 (10%) 10 11	20, 103, 216, 505	0
All	All	1677/1880 (89%)	0.40	115 (6%) 23 16	20, 74, 202, 505	0

All (115) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	715	ALA	4.9
2	A	717	ARG	4.9
2	A	1036	LYS	4.6
2	A	980	ARG	4.3
2	A	563	PRO	4.3
2	A	1025	LEU	4.2
2	A	970	ASP	4.1
2	A	444	VAL	4.0
2	A	489	ALA	3.9
2	A	866	GLU	3.9
2	A	504	TRP	3.9
2	A	864	LEU	3.9
2	A	538	THR	3.8
2	A	501	MET	3.8
2	A	552	TRP	3.7
2	A	481	THR	3.7
2	A	834	VAL	3.7
2	A	36	VAL	3.7
2	A	951	ALA	3.7
2	A	475	PHE	3.6
2	A	40	PRO	3.5
2	A	498	PRO	3.5
2	A	480	PHE	3.5

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Mol	Chain	Res	Type	RSRZ
2	A	182	GLY	3.5
1	B	386	ASP	3.5
2	A	415	HIS	3.4
2	A	364	LEU	3.4
2	A	448	PRO	3.4
2	A	1009	MET	3.4
2	A	556	LYS	3.3
2	A	401	GLY	3.3
2	A	549	THR	3.3
2	A	927	GLY	3.2
2	A	551	LEU	3.2
2	A	2	ILE	3.2
2	A	1035	TYR	3.1
2	A	884	PHE	3.1
2	A	971	GLU	3.1
2	A	1040	LEU	3.0
2	A	886	LEU	3.0
2	A	420	GLU	2.9
2	A	909	VAL	2.9
2	A	558	GLY	2.9
2	A	712	SER	2.9
2	A	418	LEU	2.9
2	A	353	CYS	2.9
2	A	561	PHE	2.8
2	A	944	MET	2.8
2	A	491	LEU	2.8
2	A	753	GLY	2.8
2	A	920	PHE	2.8
2	A	497	ILE	2.7
2	A	41	ASP	2.7
2	A	531	LYS	2.7
2	A	530	LEU	2.7
2	A	948	LEU	2.7
2	A	956	PRO	2.7
2	A	562	LEU	2.7
2	A	710	VAL	2.6
2	A	998	ILE	2.6
2	A	38	ALA	2.6
2	A	896	GLU	2.6
2	A	462	ILE	2.6
2	A	1017	ILE	2.6
2	A	713	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
2	A	1026	LEU	2.6
2	A	883	ILE	2.6
2	A	434	THR	2.5
2	A	692	ASP	2.5
2	A	718	LEU	2.5
2	A	494	ILE	2.5
2	A	975	HIS	2.5
2	A	548	LEU	2.5
2	A	1039	TRP	2.4
2	A	990	VAL	2.4
2	A	814	LYS	2.4
2	A	676	GLY	2.4
2	A	542	VAL	2.4
2	A	985	ALA	2.4
2	A	387	ASN	2.3
2	A	436	TRP	2.3
2	A	5	ILE	2.3
2	A	520	PHE	2.3
2	A	346	PHE	2.3
2	A	677	ILE	2.3
1	C	242	ASP	2.3
2	A	610	GLY	2.3
2	A	18	MET	2.3
2	A	922	LEU	2.3
1	B	383	PHE	2.3
2	A	952	ILE	2.2
2	A	906	PHE	2.2
2	A	465	PHE	2.2
2	A	503	TYR	2.2
2	A	532	VAL	2.2
2	A	535	TRP	2.2
2	A	35	PRO	2.2
2	A	477	PRO	2.2
2	A	359	HIS	2.1
2	A	431	ASP	2.1
2	A	358	TRP	2.1
2	A	689	VAL	2.1
2	A	978	VAL	2.1
2	A	372	LEU	2.1
2	A	564	GLN	2.1
2	A	128	GLU	2.1
2	A	293	SER	2.1

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Mol	Chain	Res	Type	RSRZ
2	A	354	ALA	2.1
2	A	711	ALA	2.1
2	A	496	VAL	2.1
2	A	421	TRP	2.0
2	A	997	PRO	2.0
2	A	955	VAL	2.0
2	A	565	ILE	2.0
2	A	342	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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, 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	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	CU	A	1101	1/1	0.99	0.04	51,51,51,51	0

6.5 Other polymers [i](#)

There are no such residues in this entry.