



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 11:39 PM UTC

PDB ID : 3NE5 / pdb_00003ne5
Title : Crystal structure of the CusBA heavy-metal efflux complex from Escherichia coli
Authors : Su, C.-C.
Deposited on : 2010-06-08
Resolution : 2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

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

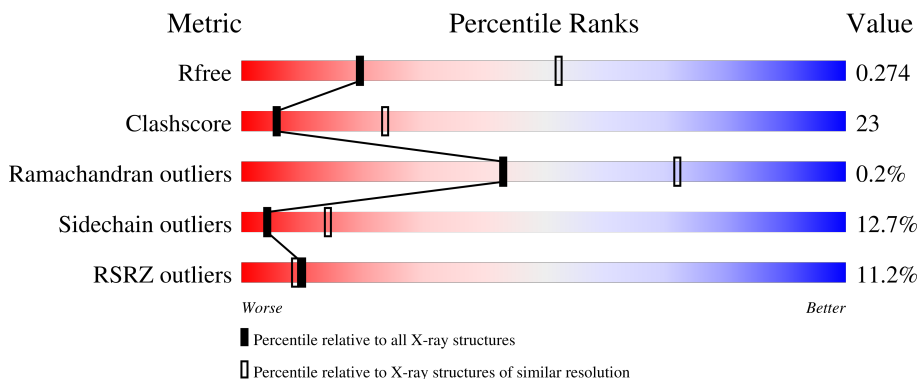
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	4% 48% 25% 5% 22%
1	C	413	2% 53% 22% • 22%
2	A	1054	15% 52% 40% 6% •

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 12873 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	1028	Total	C	N	O	S	0	0	0
			7923	5124	1330	1433	36			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	HIS	-	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	MET	-	expression tag	UNP P38054
A	1	GLY	-	expression tag	UNP P38054

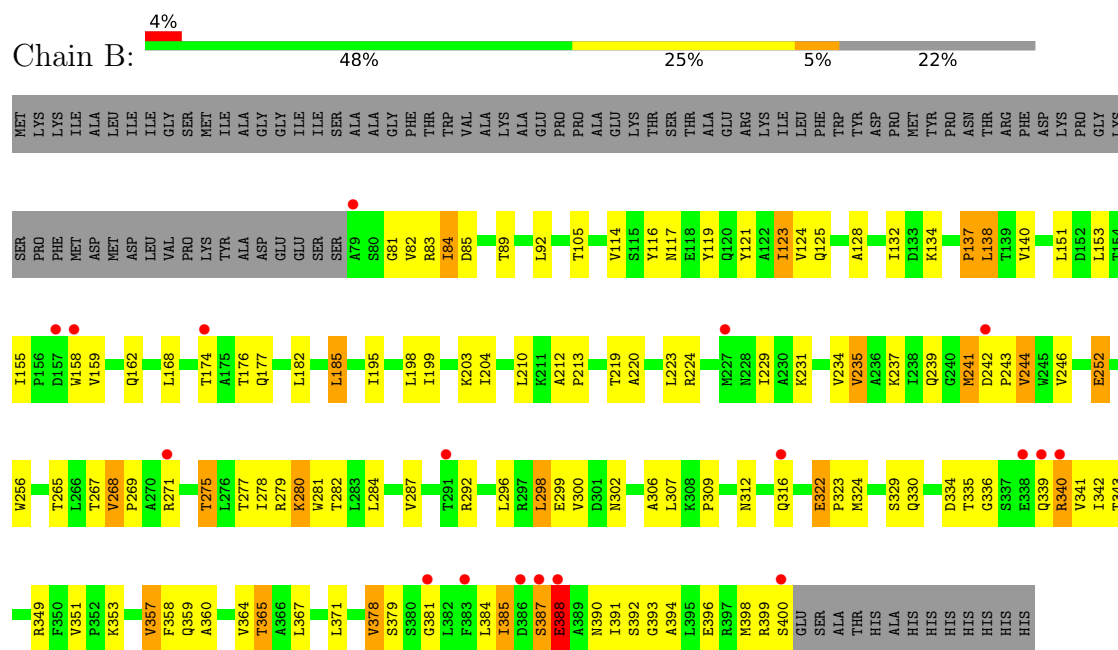
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	5	Total	O	0	0
			5	5		
3	C	10	Total	O	0	0
			10	10		
3	A	4	Total	O	0	0
			4	4		

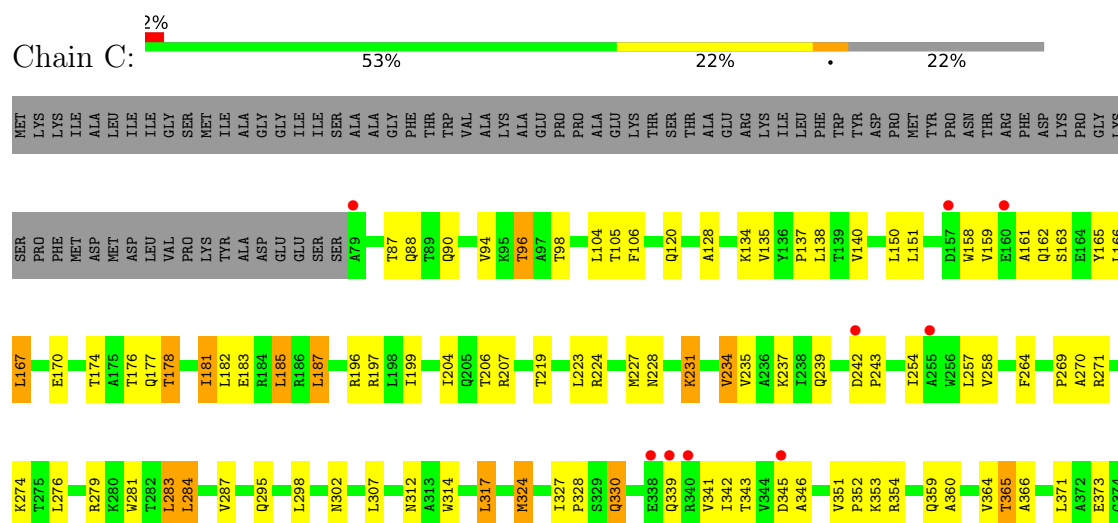
3 Residue-property plots

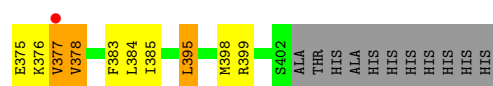
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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

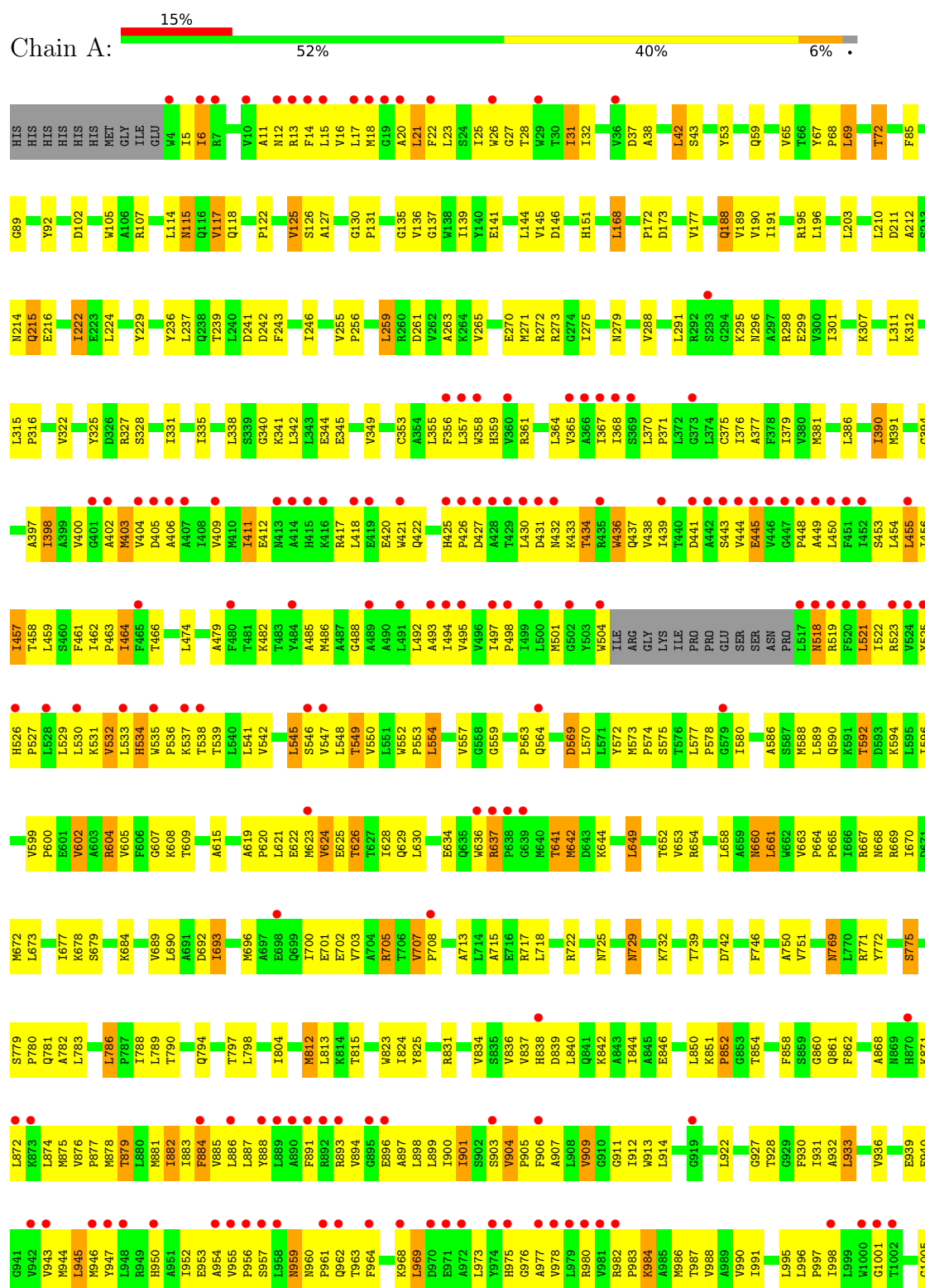


• Molecule 1: Cation efflux system protein cusB





• 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	160.27Å 160.27Å 682.84Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.49 – 2.90 39.49 – 2.90	Depositor EDS
% Data completeness (in resolution range)	78.9 (39.49-2.90) 88.5 (39.49-2.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.90 (at 2.90Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.229 , 0.267 0.237 , 0.274	Depositor DCC
R_{free} test set	3343 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	56.9	Xtriage
Anisotropy	0.357	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 51.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	12873	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.34% 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

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	0.43	2/2498 (0.1%)	0.83	6/3401 (0.2%)
1	C	0.31	0/2513	0.76	2/3421 (0.1%)
2	A	0.32	0/8089	0.77	6/11015 (0.1%)
All	All	0.34	2/13100 (0.0%)	0.78	14/17837 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	388	GLU	CA-C	-5.22	1.45	1.52
1	B	387	SER	CA-C	-5.05	1.46	1.52

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	388	GLU	N-CA-C	7.64	127.08	110.80
2	A	860	GLY	N-CA-C	-6.68	97.36	113.18
1	B	284	LEU	CA-C-N	6.51	126.09	119.19
1	B	284	LEU	C-N-CA	6.51	126.09	119.19
1	B	381	GLY	N-CA-C	-6.25	105.27	115.46
2	A	976	GLY	N-CA-C	-6.06	107.79	115.31
1	C	284	LEU	CA-C-N	5.72	125.57	119.28
1	C	284	LEU	C-N-CA	5.72	125.57	119.28
2	A	577	LEU	CA-C-N	5.67	125.52	119.28
2	A	577	LEU	C-N-CA	5.67	125.52	119.28
1	B	387	SER	CA-C-N	-5.66	110.73	121.54
1	B	387	SER	C-N-CA	-5.66	110.73	121.54
2	A	707	VAL	CA-C-N	5.10	125.14	119.32
2	A	707	VAL	C-N-CA	5.10	125.14	119.32

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	105	0
1	C	2473	0	2533	79	0
2	A	7923	0	8166	443	0
3	A	4	0	0	0	0
3	B	5	0	0	0	0
3	C	10	0	0	0	0
All	All	12873	0	13221	603	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 23.

All (603) 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)
2:A:535:TRP:O	2:A:538:THR:HG22	1.53	1.09
1:B:280:LYS:HE3	1:B:281:TRP:H	1.17	1.06
2:A:459:LEU:HB3	2:A:882:ILE:HD11	1.38	1.05
2:A:409:VAL:HB	2:A:450:LEU:HD11	1.49	0.94
2:A:964:PHE:CZ	2:A:1043:HIS:HB3	2.03	0.93
2:A:425:HIS:HB3	2:A:426:PRO:HD2	1.51	0.92
2:A:141:GLU:HG3	2:A:288:VAL:HG12	1.53	0.91
2:A:85:PHE:HD1	2:A:812:MET:HE1	1.35	0.90
2:A:118:GLN:HE22	2:A:127:ALA:H	1.18	0.88
1:B:242:ASP:HB3	1:B:243:PRO:HD3	1.56	0.87
2:A:696:MET:HG3	2:A:854:THR:HG21	1.57	0.86
2:A:534:HIS:O	2:A:535:TRP:C	2.15	0.86
2:A:534:HIS:C	2:A:534:HIS:CD2	2.53	0.85
2:A:534:HIS:O	2:A:534:HIS:CD2	2.30	0.85
1:B:82:VAL:HG11	2:A:652:THR:HG23	1.56	0.84
1:B:280:LYS:HE3	1:B:281:TRP:N	1.92	0.83
2:A:493:ALA:HA	2:A:497:ILE:HB	1.58	0.83
2:A:660:ASN:H	2:A:660:ASN:ND2	1.75	0.83
2:A:534:HIS:O	2:A:534:HIS:HD2	1.62	0.81
2:A:398:ILE:HG13	2:A:1016:MET:HE1	1.63	0.80
1:C:254:ILE:HG22	1:C:257:LEU:HB2	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:364:LEU:O	2:A:368:ILE:HG12	1.82	0.79
1:B:174:THR:HB	1:B:177:GLN:HG3	1.64	0.79
1:C:271:ARG:HB3	1:C:274:LYS:HG3	1.65	0.79
2:A:574:PRO:HB2	2:A:658:LEU:HD11	1.63	0.78
2:A:68:PRO:O	2:A:72:THR:HG22	1.84	0.78
2:A:940:PHE:HE1	2:A:984:LYS:HZ1	1.32	0.77
1:B:390:ASN:HD22	1:B:393:GLY:H	1.29	0.77
2:A:131:PRO:HD2	2:A:615:ALA:HB3	1.65	0.76
2:A:980:ARG:O	2:A:984:LYS:HB2	1.87	0.75
2:A:533:LEU:HA	2:A:536:PRO:HG3	1.68	0.75
2:A:964:PHE:HZ	2:A:1043:HIS:HB3	1.50	0.75
1:C:106:PHE:CE2	1:C:359:GLN:HG2	2.22	0.75
2:A:361:ARG:HB3	2:A:504:TRP:HB3	1.69	0.75
1:C:359:GLN:HG3	1:C:360:ALA:N	2.02	0.74
2:A:359:HIS:CE1	2:A:361:ARG:HB2	2.23	0.74
2:A:572:TYR:HB3	2:A:626:THR:HG23	1.70	0.74
2:A:588:MET:HE2	2:A:658:LEU:HD22	1.68	0.74
1:B:342:ILE:HD12	1:B:398:MET:HE1	1.70	0.74
1:C:302:ASN:HD21	1:C:307:LEU:H	1.36	0.74
1:C:242:ASP:HB3	1:C:243:PRO:HD3	1.69	0.73
2:A:38:ALA:O	2:A:390:ILE:HG22	1.88	0.73
1:C:167:LEU:C	1:C:167:LEU:HD12	2.14	0.73
2:A:345:GLU:HG2	2:A:997:PRO:HG2	1.71	0.72
2:A:964:PHE:CE2	2:A:1043:HIS:HB3	2.24	0.72
2:A:982:ARG:HB3	2:A:983:PRO:HD3	1.70	0.72
2:A:457:ILE:HD11	2:A:936:VAL:HG22	1.70	0.72
2:A:214:ASN:H	2:A:215:GLN:NE2	1.87	0.72
2:A:878:MET:O	2:A:882:ILE:HG22	1.90	0.72
2:A:402:ALA:HB3	2:A:486:MET:HE1	1.71	0.71
2:A:239:THR:HG22	2:A:241:ASP:H	1.54	0.71
2:A:43:SER:HB2	2:A:673:LEU:HD23	1.73	0.71
1:B:252:GLU:HG3	1:C:270:ALA:HB2	1.73	0.71
2:A:349:VAL:HG11	2:A:404:VAL:HG11	1.73	0.70
2:A:535:TRP:N	2:A:536:PRO:HD3	2.06	0.70
1:B:390:ASN:HD21	1:B:392:SER:HB2	1.57	0.70
1:B:219:THR:OG1	1:B:237:LYS:HD3	1.91	0.69
2:A:960:ASN:HB2	2:A:961:PRO:HD3	1.74	0.69
1:B:399:ARG:O	1:B:400:SER:HB2	1.93	0.69
2:A:535:TRP:N	2:A:536:PRO:CD	2.54	0.69
2:A:977:ALA:O	2:A:980:ARG:HG2	1.93	0.69
2:A:85:PHE:HB2	2:A:92:TYR:HB2	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:518:ASN:HA	2:A:521:LEU:HD21	1.74	0.69
2:A:962:GLN:HG3	2:A:963:THR:N	2.07	0.69
1:C:254:ILE:HD11	2:A:797:THR:HG21	1.75	0.69
1:C:359:GLN:HG3	1:C:360:ALA:H	1.57	0.68
2:A:641:THR:HG23	2:A:644:LYS:HD2	1.76	0.68
2:A:534:HIS:O	2:A:535:TRP:O	2.10	0.68
2:A:529:LEU:O	2:A:532:VAL:HG12	1.93	0.68
2:A:570:LEU:HA	2:A:665:PRO:HD3	1.75	0.68
2:A:137:GLY:O	2:A:139:ILE:HG12	1.94	0.68
2:A:359:HIS:HE1	2:A:361:ARG:HE	1.42	0.68
2:A:454:LEU:O	2:A:458:THR:HG23	1.93	0.68
2:A:1023:ALA:HB3	2:A:1024:PRO:HD3	1.75	0.67
1:C:165:TYR:HE2	1:C:178:THR:HG23	1.59	0.67
1:C:106:PHE:HE2	1:C:359:GLN:HG2	1.59	0.67
2:A:436:TRP:CD1	2:A:436:TRP:C	2.73	0.67
2:A:574:PRO:HG2	2:A:624:VAL:HG13	1.77	0.67
1:B:123:ILE:HD13	1:B:237:LYS:HG3	1.76	0.67
1:C:353:LYS:HE2	1:C:375:GLU:OE2	1.95	0.67
2:A:684:LYS:HG2	2:A:823:TRP:CD1	2.30	0.66
2:A:453:SER:OG	2:A:939:GLU:HG2	1.95	0.66
2:A:546:SER:O	2:A:549:THR:HG22	1.96	0.66
2:A:534:HIS:HD2	2:A:535:TRP:HB3	1.60	0.66
2:A:604:ARG:CG	2:A:604:ARG:HH21	2.09	0.66
2:A:955:VAL:HG12	2:A:956:PRO:HD3	1.75	0.66
1:B:341:VAL:HG21	1:B:371:LEU:HD11	1.78	0.65
2:A:522:ILE:HG23	2:A:526:HIS:CD2	2.30	0.65
2:A:991:ILE:O	2:A:995:LEU:HB2	1.95	0.65
2:A:370:LEU:HB2	2:A:371:PRO:HD3	1.77	0.65
2:A:537:LYS:HD3	2:A:1037:LEU:HD11	1.77	0.65
2:A:526:HIS:HA	2:A:529:LEU:HB3	1.79	0.65
1:B:84:ILE:HG12	1:B:85:ASP:N	2.11	0.65
1:C:165:TYR:HB2	1:C:181:ILE:HG21	1.78	0.65
2:A:361:ARG:O	2:A:365:VAL:HG23	1.96	0.65
2:A:534:HIS:C	2:A:534:HIS:HD2	2.01	0.65
1:B:125:GLN:HE21	1:C:228:ASN:H	1.44	0.65
2:A:541:LEU:O	2:A:545:LEU:HD22	1.96	0.65
2:A:660:ASN:H	2:A:660:ASN:HD22	1.42	0.65
2:A:547:VAL:O	2:A:550:VAL:HG12	1.95	0.65
2:A:630:LEU:HD13	2:A:642:MET:HE1	1.79	0.65
2:A:940:PHE:CE2	2:A:944:MET:HG3	2.32	0.65
1:C:384:LEU:HD21	2:A:588:MET:HE3	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:572:TYR:HE1	2:A:660:ASN:HB3	1.62	0.65
2:A:136:VAL:HG22	2:A:669:ARG:HB3	1.78	0.65
2:A:620:PRO:HB2	2:A:622:GLU:HG2	1.78	0.64
1:C:94:VAL:HG21	1:C:385:ILE:HD11	1.80	0.64
2:A:518:ASN:HD22	2:A:518:ASN:H	1.46	0.64
2:A:26:TRP:HD1	2:A:379:ILE:HD13	1.63	0.63
1:B:336:GLY:H	2:A:775:SER:HG	1.45	0.63
2:A:377:ALA:O	2:A:381:MET:HG3	1.98	0.63
1:C:317:LEU:C	1:C:317:LEU:HD12	2.23	0.63
2:A:607:GLY:HA2	2:A:626:THR:HB	1.79	0.63
2:A:804:ILE:HG13	2:A:804:ILE:O	1.98	0.63
2:A:904:VAL:HG22	2:A:905:PRO:HD3	1.81	0.63
1:B:385:ILE:HG13	2:A:272:ARG:HB2	1.80	0.63
2:A:425:HIS:HB3	2:A:426:PRO:CD	2.25	0.63
1:B:174:THR:H	1:B:177:GLN:HE21	1.46	0.63
1:C:163:SER:HB3	1:C:204:ILE:HD11	1.79	0.62
1:C:96:THR:OG1	1:C:376:LYS:HE3	1.98	0.62
2:A:370:LEU:HD22	2:A:400:VAL:HG23	1.81	0.62
2:A:42:LEU:HD12	2:A:42:LEU:H	1.63	0.62
2:A:891:PHE:CE1	2:A:945:LEU:HD12	2.35	0.62
2:A:212:ALA:C	2:A:215:GLN:HE22	2.08	0.62
1:B:117:ASN:HD22	1:B:119:TYR:H	1.46	0.62
2:A:422:GLN:HG2	2:A:427:ASP:OD1	2.00	0.61
2:A:534:HIS:CD2	2:A:535:TRP:HB3	2.36	0.61
1:B:117:ASN:HD22	1:B:117:ASN:C	2.08	0.61
2:A:851:LYS:HB3	2:A:852:PRO:HD2	1.81	0.61
2:A:940:PHE:HE1	2:A:984:LYS:NZ	1.97	0.61
1:B:384:LEU:HD23	1:B:394:ALA:HB3	1.83	0.61
2:A:43:SER:HB2	2:A:673:LEU:CD2	2.31	0.61
2:A:707:VAL:HG21	2:A:840:LEU:HD23	1.82	0.61
2:A:356:PHE:HD2	2:A:986:MET:HB3	1.65	0.60
2:A:991:ILE:HG21	2:A:1020:MET:SD	2.40	0.60
1:B:387:SER:HB3	2:A:271:MET:HG3	1.83	0.60
2:A:580:ILE:HG22	2:A:622:GLU:HB2	1.84	0.60
2:A:780:PRO:O	2:A:804:ILE:HD11	2.01	0.60
1:B:336:GLY:N	2:A:775:SER:OG	2.34	0.60
1:B:117:ASN:ND2	1:B:119:TYR:H	1.99	0.60
2:A:623:MET:HE3	2:A:625:GLU:HG3	1.84	0.60
2:A:394:GLY:O	2:A:398:ILE:HG22	2.02	0.60
2:A:897:ALA:O	2:A:901:ILE:HG22	2.02	0.60
2:A:995:LEU:HD21	2:A:1016:MET:HE3	1.82	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:223:LEU:HD12	1:B:235:VAL:HG12	1.84	0.59
2:A:72:THR:HG21	2:A:117:VAL:HG21	1.83	0.59
2:A:430:LEU:HB2	2:A:434:THR:HG21	1.84	0.59
1:B:342:ILE:HB	1:B:378:VAL:CG1	2.32	0.59
2:A:441:ASP:HA	2:A:444:VAL:HG23	1.83	0.59
2:A:439:ILE:HG23	2:A:501:MET:HE2	1.82	0.59
2:A:122:PRO:HB2	2:A:125:VAL:HG13	1.83	0.59
1:B:387:SER:HA	2:A:771:ARG:HH12	1.66	0.59
2:A:449:ALA:O	2:A:453:SER:HB2	2.02	0.59
2:A:529:LEU:HD13	2:A:980:ARG:HH22	1.67	0.59
2:A:461:PHE:CZ	2:A:464:ILE:HD12	2.37	0.59
2:A:296:ASN:HB3	2:A:299:GLU:HB3	1.84	0.58
1:B:84:ILE:HD11	2:A:594:LYS:HD2	1.86	0.58
2:A:667:ARG:HH11	2:A:861:GLN:HE22	1.50	0.58
1:B:89:THR:H	2:A:590:GLN:HE22	1.51	0.58
1:B:302:ASN:HD21	1:B:307:LEU:H	1.52	0.58
1:B:340:ARG:HB3	1:B:353:LYS:O	2.04	0.58
1:B:343:THR:OG1	1:B:351:VAL:HG23	2.03	0.58
2:A:275:ILE:HB	2:A:609:THR:OG1	2.03	0.58
2:A:893:ARG:HB3	2:A:896:GLU:HB3	1.84	0.58
2:A:834:VAL:HG22	2:A:838:HIS:CD2	2.38	0.57
2:A:876:VAL:HB	2:A:877:PRO:HD3	1.86	0.57
1:B:123:ILE:HB	1:C:227:MET:CG	2.35	0.57
1:B:388:GLU:OE1	1:B:388:GLU:HA	2.05	0.57
1:C:219:THR:OG1	1:C:237:LYS:HD2	2.04	0.57
2:A:940:PHE:CE2	2:A:1027:SER:HB2	2.39	0.57
2:A:746:PHE:O	2:A:750:ALA:HB3	2.05	0.57
2:A:189:VAL:HG22	2:A:265:VAL:HG22	1.87	0.57
2:A:391:MET:HG2	2:A:474:LEU:O	2.05	0.57
2:A:940:PHE:C	2:A:940:PHE:CD2	2.82	0.57
1:B:125:GLN:NE2	1:C:228:ASN:H	2.03	0.56
1:B:387:SER:O	1:B:388:GLU:HB2	2.04	0.56
1:C:242:ASP:CB	1:C:243:PRO:HD3	2.35	0.56
2:A:572:TYR:CE1	2:A:660:ASN:HB3	2.40	0.56
2:A:559:GLY:H	2:A:834:VAL:HG12	1.70	0.56
2:A:661:LEU:HD22	2:A:663:VAL:HG13	1.87	0.56
2:A:677:ILE:HG22	2:A:679:SER:H	1.70	0.56
2:A:907:ALA:HB1	2:A:933:LEU:HD11	1.86	0.56
2:A:837:VAL:HG21	2:A:862:PHE:CE2	2.40	0.56
1:C:242:ASP:O	1:C:302:ASN:HB3	2.06	0.56
2:A:984:LYS:NZ	2:A:984:LYS:HB3	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1007:GLU:O	2:A:1011:ARG:HD3	2.06	0.56
1:B:268:VAL:CG2	1:B:271:ARG:HB2	2.36	0.56
1:C:242:ASP:HB3	1:C:243:PRO:CD	2.34	0.56
2:A:553:PRO:HB2	2:A:912:ILE:CG2	2.36	0.56
1:B:244:VAL:HG12	1:B:300:VAL:HB	1.88	0.56
2:A:928:THR:HG21	2:A:1012:ILE:HD11	1.86	0.56
2:A:279:ASN:ND2	2:A:605:VAL:H	2.03	0.55
2:A:375:CYS:O	2:A:379:ILE:HG13	2.06	0.55
2:A:660:ASN:HD22	2:A:660:ASN:N	2.02	0.55
1:B:137:PRO:O	1:B:138:LEU:HD12	2.06	0.55
2:A:139:ILE:HG22	2:A:301:ILE:HD11	1.87	0.55
2:A:464:ILE:HD11	2:A:928:THR:HG23	1.89	0.55
2:A:578:PRO:HG2	2:A:717:ARG:HB2	1.89	0.55
2:A:950:HIS:HA	2:A:953:GLU:HB2	1.86	0.55
2:A:563:PRO:HG3	2:A:1011:ARG:HG2	1.89	0.55
1:B:390:ASN:ND2	1:B:392:SER:HB2	2.21	0.55
2:A:1036:LYS:O	2:A:1040:LEU:HG	2.06	0.55
1:B:387:SER:O	1:B:388:GLU:CB	2.50	0.55
1:B:121:TYR:OH	1:B:237:LYS:HE3	2.07	0.55
2:A:168:LEU:HB3	2:A:177:VAL:HG21	1.89	0.55
2:A:1026:LEU:O	2:A:1030:ILE:HG12	2.07	0.55
2:A:139:ILE:CG2	2:A:301:ILE:HD11	2.37	0.55
2:A:940:PHE:CE1	2:A:1024:PRO:HA	2.40	0.55
1:C:317:LEU:HD12	1:C:317:LEU:O	2.07	0.55
2:A:837:VAL:HG21	2:A:862:PHE:CD2	2.41	0.55
1:B:322:GLU:HG3	1:B:323:PRO:HD2	1.89	0.54
2:A:596:ILE:HG12	2:A:653:VAL:HG21	1.89	0.54
2:A:421:TRP:CE3	2:A:438:VAL:HB	2.42	0.54
2:A:592:THR:O	2:A:596:ILE:HG13	2.06	0.54
2:A:1022:THR:O	2:A:1026:LEU:HB2	2.08	0.54
2:A:246:ILE:HB	2:A:259:LEU:HB2	1.90	0.54
1:B:242:ASP:HB3	1:B:243:PRO:CD	2.35	0.54
2:A:940:PHE:CE1	2:A:984:LYS:NZ	2.74	0.54
1:B:158:TRP:O	1:B:162:GLN:HG3	2.07	0.54
2:A:65:VAL:O	2:A:68:PRO:HG2	2.08	0.54
2:A:327:ARG:O	2:A:331:ILE:HG12	2.08	0.54
2:A:359:HIS:CE1	2:A:361:ARG:HE	2.25	0.54
2:A:341:LYS:O	2:A:345:GLU:HG3	2.08	0.54
2:A:356:PHE:HD2	2:A:986:MET:CB	2.21	0.54
2:A:696:MET:CE	2:A:850:LEU:HA	2.38	0.54
2:A:969:LEU:HD12	2:A:969:LEU:C	2.33	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:536:PRO:HB3	2:A:1033:ALA:HB1	1.89	0.53
2:A:911:GLY:HA3	2:A:930:PHE:HE2	1.73	0.53
2:A:418:LEU:HD21	2:A:438:VAL:HG11	1.91	0.53
1:B:267:THR:HG22	1:B:275:THR:HB	1.89	0.53
1:B:339:GLN:HG3	1:B:357:VAL:HG13	1.91	0.53
1:C:281:TRP:CB	1:C:298:LEU:HD23	2.38	0.53
2:A:430:LEU:HB2	2:A:434:THR:CG2	2.38	0.53
2:A:431:ASP:CG	2:A:432:ASN:H	2.17	0.53
2:A:689:VAL:HB	2:A:692:ASP:HB2	1.91	0.53
2:A:944:MET:SD	2:A:980:ARG:HD2	2.49	0.53
2:A:349:VAL:CG1	2:A:404:VAL:HG11	2.39	0.53
2:A:580:ILE:CG2	2:A:622:GLU:HB2	2.39	0.53
2:A:834:VAL:HG22	2:A:838:HIS:HD2	1.73	0.53
2:A:224:LEU:HB2	2:A:229:TYR:CE1	2.44	0.53
2:A:6:ILE:HD13	2:A:6:ILE:O	2.09	0.53
2:A:18:MET:HA	2:A:21:LEU:HB3	1.89	0.53
2:A:364:LEU:HD23	2:A:367:ILE:HD12	1.91	0.53
2:A:85:PHE:CD1	2:A:812:MET:HE1	2.28	0.53
2:A:1001:GLY:HA2	2:A:1006:SER:HB2	1.91	0.53
1:C:327:ILE:HG13	1:C:328:PRO:O	2.08	0.53
2:A:482:LYS:O	2:A:486:MET:HG2	2.08	0.53
2:A:977:ALA:HB1	2:A:980:ARG:NH2	2.24	0.53
1:B:223:LEU:CD1	1:B:235:VAL:HG12	2.39	0.52
2:A:365:VAL:HG11	2:A:411:ILE:HD11	1.90	0.52
2:A:411:ILE:HA	2:A:501:MET:HE1	1.91	0.52
1:B:81:GLY:HA2	1:C:87:THR:HG21	1.91	0.52
1:C:223:LEU:C	1:C:224:ARG:HD2	2.33	0.52
2:A:307:LYS:O	2:A:311:LEU:HG	2.09	0.52
2:A:690:LEU:HD22	2:A:718:LEU:HD23	1.91	0.52
1:B:324:MET:HE1	1:B:358:PHE:CG	2.43	0.52
2:A:599:VAL:HG21	2:A:649:LEU:HD12	1.91	0.52
2:A:630:LEU:CD1	2:A:642:MET:HE1	2.39	0.52
1:B:334:ASP:OD2	1:B:339:GLN:HB3	2.10	0.52
2:A:769:ASN:C	2:A:769:ASN:ND2	2.68	0.52
2:A:459:LEU:C	2:A:461:PHE:H	2.16	0.52
2:A:195:ARG:HD3	2:A:261:ASP:O	2.09	0.52
2:A:534:HIS:C	2:A:536:PRO:HD3	2.34	0.52
2:A:536:PRO:O	2:A:539:THR:OG1	2.26	0.52
2:A:553:PRO:HB2	2:A:912:ILE:HG22	1.91	0.52
2:A:270:GLU:HG2	2:A:271:MET:N	2.25	0.52
2:A:877:PRO:O	2:A:881:MET:HG2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:345:GLU:O	2:A:349:VAL:HG23	2.10	0.52
2:A:973:LEU:O	2:A:977:ALA:HB2	2.10	0.52
1:B:223:LEU:C	1:B:224:ARG:HD2	2.35	0.52
1:C:151:LEU:C	1:C:151:LEU:HD12	2.35	0.52
2:A:696:MET:HE3	2:A:850:LEU:HA	1.92	0.52
2:A:168:LEU:CB	2:A:177:VAL:HG21	2.41	0.51
2:A:930:PHE:CE2	2:A:1015:PRO:HB3	2.45	0.51
1:B:280:LYS:HE3	1:B:280:LYS:HA	1.92	0.51
2:A:69:LEU:O	2:A:72:THR:HG23	2.09	0.51
2:A:552:TRP:HB3	2:A:553:PRO:HD3	1.91	0.51
2:A:933:LEU:HB2	2:A:1016:MET:HG2	1.92	0.51
2:A:842:LYS:O	2:A:846:GLU:HG2	2.11	0.51
2:A:239:THR:HG22	2:A:241:ASP:N	2.24	0.51
2:A:604:ARG:HH21	2:A:604:ARG:HG2	1.75	0.51
2:A:707:VAL:HG13	2:A:708:PRO:HD2	1.91	0.51
2:A:118:GLN:HE22	2:A:127:ALA:N	1.99	0.51
1:B:174:THR:H	1:B:177:GLN:NE2	2.08	0.51
2:A:216:GLU:HG3	2:A:236:TYR:CD1	2.45	0.51
2:A:729:ASN:C	2:A:729:ASN:HD22	2.19	0.51
1:C:183:GLU:O	1:C:187:LEU:HG	2.11	0.51
2:A:291:LEU:HD21	2:A:295:LYS:O	2.11	0.51
2:A:406:ALA:HB2	2:A:454:LEU:HD11	1.93	0.51
2:A:751:VAL:O	2:A:771:ARG:HD2	2.11	0.51
2:A:769:ASN:C	2:A:769:ASN:HD22	2.18	0.50
2:A:549:THR:HG23	2:A:913:TRP:HE1	1.77	0.50
2:A:668:ASN:O	2:A:672:MET:HG3	2.11	0.50
1:B:387:SER:O	1:B:388:GLU:OE1	2.30	0.50
2:A:532:VAL:HG21	2:A:1029:PHE:HB3	1.92	0.50
2:A:390:ILE:HD12	2:A:1005:GLY:HA3	1.94	0.50
1:B:390:ASN:HD21	1:B:392:SER:CB	2.23	0.50
2:A:522:ILE:HG23	2:A:526:HIS:NE2	2.27	0.50
2:A:884:PHE:O	2:A:888:TYR:HB2	2.12	0.50
2:A:906:PHE:CD1	2:A:1026:LEU:HD23	2.46	0.50
1:B:220:ALA:HB3	1:B:237:LYS:HB2	1.94	0.50
1:B:132:ILE:CD1	1:B:229:ILE:HB	2.42	0.50
1:C:106:PHE:CZ	1:C:359:GLN:HG2	2.46	0.50
2:A:944:MET:HE2	2:A:1027:SER:O	2.11	0.49
2:A:986:MET:O	2:A:990:VAL:HG13	2.12	0.49
2:A:1014:ALA:HB3	2:A:1015:PRO:HD3	1.94	0.49
2:A:553:PRO:O	2:A:557:VAL:HG22	2.12	0.49
1:B:342:ILE:O	1:B:378:VAL:HG12	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:107:ARG:NH1	2:A:130:GLY:O	2.46	0.49
2:A:420:GLU:HG3	2:A:421:TRP:N	2.27	0.49
2:A:529:LEU:HD22	2:A:980:ARG:NH2	2.27	0.49
1:B:242:ASP:O	1:B:302:ASN:HB3	2.12	0.49
2:A:574:PRO:HG2	2:A:624:VAL:CG1	2.43	0.49
2:A:884:PHE:CD1	2:A:884:PHE:C	2.90	0.49
1:C:341:VAL:HG21	1:C:371:LEU:HD11	1.93	0.49
2:A:525:TYR:HE2	2:A:1029:PHE:CZ	2.30	0.49
2:A:573:MET:HE3	2:A:573:MET:HB2	1.72	0.49
1:B:336:GLY:CA	2:A:775:SER:OG	2.61	0.49
2:A:678:LYS:HE2	2:A:825:TYR:CD2	2.48	0.49
2:A:954:ALA:HB3	2:A:956:PRO:HD2	1.94	0.49
2:A:959:ASN:N	2:A:959:ASN:OD1	2.44	0.49
1:B:385:ILE:CG1	2:A:272:ARG:H	2.25	0.49
2:A:456:ILE:HA	2:A:886:LEU:HD13	1.94	0.49
2:A:874:LEU:HG	2:A:878:MET:HE3	1.95	0.49
2:A:16:VAL:HG11	2:A:495:VAL:O	2.14	0.48
2:A:118:GLN:NE2	2:A:126:SER:HA	2.27	0.48
2:A:642:MET:HA	2:A:642:MET:CE	2.44	0.48
2:A:959:ASN:HA	2:A:962:GLN:HG2	1.95	0.48
1:C:165:TYR:HB2	1:C:181:ILE:CG2	2.43	0.48
2:A:188:GLN:HA	2:A:769:ASN:ND2	2.28	0.48
2:A:461:PHE:CE2	2:A:932:ALA:HB2	2.49	0.48
1:B:280:LYS:HA	1:B:280:LYS:CE	2.43	0.48
2:A:525:TYR:HE1	2:A:980:ARG:HE	1.60	0.48
1:C:345:ASP:OD1	1:C:346:ALA:N	2.43	0.48
2:A:102:ASP:HB3	2:A:105:TRP:HB3	1.96	0.48
2:A:466:THR:O	2:A:871:LYS:HE2	2.14	0.48
1:B:241:MET:HE2	1:B:309:PRO:HD3	1.96	0.48
1:B:360:ALA:HA	1:B:365:THR:HA	1.95	0.48
2:A:604:ARG:CG	2:A:604:ARG:NH2	2.70	0.48
1:B:116:TYR:CE2	1:B:309:PRO:HG2	2.49	0.48
1:B:123:ILE:HB	1:C:227:MET:HG2	1.95	0.48
1:B:174:THR:HG22	1:B:176:THR:H	1.78	0.48
2:A:888:TYR:CE2	2:A:894:VAL:HG22	2.49	0.48
1:C:165:TYR:CE2	1:C:178:THR:HG23	2.44	0.48
2:A:497:ILE:O	2:A:501:MET:HG2	2.13	0.48
1:C:166:LEU:O	1:C:170:GLU:HG2	2.14	0.47
2:A:26:TRP:CD1	2:A:379:ILE:HD13	2.46	0.47
2:A:172:PRO:O	2:A:173:ASP:HB2	2.14	0.47
2:A:904:VAL:N	2:A:905:PRO:CD	2.77	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:196:ARG:O	1:C:199:ILE:HG12	2.14	0.47
1:C:279:ARG:NH1	1:C:279:ARG:HB2	2.29	0.47
2:A:22:PHE:HA	2:A:25:ILE:HG22	1.95	0.47
2:A:868:ALA:O	2:A:872:LEU:HG	2.15	0.47
2:A:984:LYS:CA	2:A:984:LYS:HE2	2.44	0.47
2:A:433:LYS:O	2:A:436:TRP:HB3	2.14	0.47
1:B:269:PRO:HD2	1:B:312:ASN:O	2.13	0.47
2:A:6:ILE:HG13	2:A:443:SER:HB3	1.96	0.47
2:A:412:GLU:CD	2:A:982:ARG:HG2	2.39	0.47
2:A:461:PHE:HE1	2:A:479:ALA:HA	1.79	0.47
2:A:957:SER:O	2:A:961:PRO:HD2	2.14	0.47
2:A:1009:MET:O	2:A:1012:ILE:HG22	2.14	0.47
2:A:940:PHE:O	2:A:943:VAL:HG22	2.14	0.47
1:B:351:VAL:HG23	1:B:351:VAL:O	2.14	0.47
1:B:384:LEU:HD12	1:B:384:LEU:N	2.29	0.47
2:A:5:ILE:HB	2:A:494:ILE:HD11	1.96	0.47
2:A:115:ASN:C	2:A:115:ASN:ND2	2.73	0.47
2:A:689:VAL:O	2:A:693:ILE:HG23	2.15	0.47
2:A:779:SER:H	2:A:782:ALA:HB3	1.79	0.47
2:A:940:PHE:CZ	2:A:1024:PRO:HA	2.50	0.47
1:B:265:THR:HB	1:B:316:GLN:HB3	1.96	0.47
1:C:281:TRP:HB2	1:C:298:LEU:HD23	1.97	0.47
2:A:588:MET:CE	2:A:658:LEU:HD13	2.45	0.47
2:A:779:SER:HB2	2:A:780:PRO:HD2	1.97	0.47
2:A:1031:ILE:HB	2:A:1032:PRO:HD3	1.96	0.47
1:B:153:LEU:HD11	1:B:155:ILE:HD11	1.96	0.47
1:C:94:VAL:CG2	1:C:385:ILE:HD11	2.43	0.47
1:C:128:ALA:HA	1:C:231:LYS:HD3	1.97	0.47
1:C:342:ILE:HB	1:C:378:VAL:CG1	2.45	0.47
2:A:135:GLY:C	2:A:669:ARG:HG2	2.40	0.47
2:A:356:PHE:O	2:A:357:LEU:HD12	2.14	0.47
2:A:397:ALA:O	2:A:400:VAL:HG12	2.14	0.47
2:A:550:VAL:HG21	2:A:909:VAL:HA	1.97	0.47
2:A:975:HIS:C	2:A:977:ALA:H	2.23	0.47
1:C:281:TRP:HB3	1:C:298:LEU:HD23	1.97	0.47
2:A:596:ILE:HG21	2:A:628:ILE:HG12	1.95	0.47
2:A:933:LEU:HD22	2:A:933:LEU:O	2.15	0.47
2:A:955:VAL:N	2:A:956:PRO:CD	2.77	0.47
1:C:269:PRO:HG3	1:C:314:TRP:NE1	2.30	0.46
2:A:20:ALA:HA	2:A:23:LEU:HB3	1.97	0.46
2:A:102:ASP:O	2:A:105:TRP:HB3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:436:TRP:HD1	2:A:437:GLN:N	2.13	0.46
2:A:844:ILE:HD12	2:A:858:PHE:HZ	1.80	0.46
1:B:195:ILE:O	1:B:198:LEU:HB3	2.16	0.46
2:A:900:ILE:O	2:A:903:SER:HB3	2.15	0.46
2:A:42:LEU:HD13	2:A:670:ILE:HD13	1.97	0.46
2:A:275:ILE:HD13	2:A:586:ALA:HB2	1.96	0.46
1:C:383:PHE:CE1	2:A:580:ILE:HB	2.51	0.46
2:A:871:LYS:O	2:A:875:MET:HB2	2.15	0.46
2:A:984:LYS:HE2	2:A:984:LYS:HA	1.97	0.46
1:B:114:VAL:HG22	1:B:246:VAL:HG22	1.98	0.46
2:A:146:ASP:OD2	2:A:151:HIS:HD2	1.99	0.46
2:A:995:LEU:O	2:A:1017:ILE:HD11	2.15	0.46
2:A:988:VAL:HG21	2:A:1024:PRO:HB3	1.97	0.46
2:A:518:ASN:H	2:A:518:ASN:ND2	2.13	0.46
2:A:243:PHE:HB3	2:A:265:VAL:HG21	1.98	0.46
2:A:270:GLU:HG2	2:A:271:MET:H	1.81	0.46
2:A:390:ILE:HD12	2:A:1005:GLY:CA	2.46	0.46
2:A:572:TYR:HE1	2:A:660:ASN:CB	2.28	0.46
2:A:578:PRO:CG	2:A:717:ARG:HB2	2.45	0.46
2:A:831:ARG:NH2	2:A:839:ASP:OD1	2.43	0.46
2:A:896:GLU:OE1	2:A:945:LEU:HG	2.15	0.46
2:A:1020:MET:HA	2:A:1020:MET:CE	2.46	0.46
1:C:120:GLN:HE22	1:C:243:PRO:HD2	1.80	0.46
2:A:977:ALA:HA	2:A:980:ARG:CZ	2.46	0.46
1:B:153:LEU:H	1:B:153:LEU:HD23	1.81	0.46
1:B:220:ALA:HB3	1:B:237:LYS:CB	2.46	0.45
2:A:530:LEU:C	2:A:530:LEU:HD12	2.41	0.45
2:A:538:THR:O	2:A:542:VAL:HG23	2.16	0.45
2:A:947:TYR:OH	2:A:983:PRO:HG2	2.16	0.45
1:B:336:GLY:HA3	2:A:775:SER:OG	2.16	0.45
2:A:338:LEU:HG	2:A:390:ILE:HA	1.98	0.45
2:A:15:LEU:HD23	2:A:15:LEU:HA	1.80	0.45
2:A:312:LYS:HA	2:A:312:LYS:HD3	1.77	0.45
2:A:952:ILE:HG21	2:A:1039:TRP:NE1	2.32	0.45
1:B:385:ILE:HG13	2:A:272:ARG:H	1.81	0.45
1:C:158:TRP:O	1:C:162:GLN:HG3	2.16	0.45
2:A:135:GLY:O	2:A:669:ARG:HG2	2.17	0.45
2:A:370:LEU:CD2	2:A:403:MET:HG3	2.46	0.45
2:A:554:LEU:HD21	2:A:912:ILE:HG12	1.98	0.45
2:A:519:ARG:O	2:A:523:ARG:HG3	2.15	0.45
1:C:264:PHE:HE1	1:C:281:TRP:CE2	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:464:ILE:CD1	2:A:928:THR:HG23	2.47	0.45
2:A:563:PRO:HG2	2:A:1008:VAL:HA	1.98	0.45
2:A:693:ILE:HD11	2:A:718:LEU:HD22	1.99	0.45
2:A:729:ASN:HB3	2:A:732:LYS:HB2	1.99	0.45
2:A:1020:MET:HA	2:A:1020:MET:HE3	1.99	0.45
2:A:984:LYS:CE	2:A:988:VAL:HG23	2.47	0.45
2:A:301:ILE:HD12	2:A:328:SER:HB3	1.99	0.45
2:A:529:LEU:CD1	2:A:980:ARG:HH22	2.30	0.45
2:A:237:LEU:HD12	2:A:242:ASP:HB3	1.98	0.45
2:A:406:ALA:CB	2:A:454:LEU:HD11	2.47	0.45
2:A:418:LEU:HA	2:A:438:VAL:HG21	1.99	0.45
2:A:564:GLN:NE2	2:A:664:PRO:HG2	2.32	0.45
2:A:975:HIS:C	2:A:977:ALA:N	2.75	0.45
1:B:83:ARG:CZ	1:C:90:GLN:HB3	2.47	0.44
2:A:532:VAL:HG23	2:A:539:THR:HG21	1.99	0.44
1:B:162:GLN:HB2	1:B:204:ILE:HG23	1.98	0.44
1:C:324:MET:HB2	1:C:366:ALA:HB1	1.99	0.44
2:A:27:GLY:O	2:A:31:ILE:HG22	2.16	0.44
2:A:572:TYR:CD1	2:A:574:PRO:HD3	2.53	0.44
2:A:1029:PHE:CD2	2:A:1029:PHE:N	2.85	0.44
1:B:278:ILE:HG21	1:B:298:LEU:HD13	1.99	0.44
1:B:281:TRP:HB2	1:B:296:LEU:HD21	1.99	0.44
1:B:399:ARG:O	1:B:400:SER:CB	2.64	0.44
2:A:445:GLU:O	2:A:448:PRO:HD2	2.17	0.44
2:A:661:LEU:HD11	2:A:679:SER:HB3	1.98	0.44
1:B:151:LEU:HD12	1:B:151:LEU:C	2.42	0.44
2:A:725:ASN:O	2:A:804:ILE:HA	2.17	0.44
2:A:746:PHE:CZ	2:A:788:ILE:HG23	2.52	0.44
1:B:279:ARG:HE	1:B:279:ARG:HB2	1.59	0.44
1:B:302:ASN:ND2	1:B:307:LEU:H	2.14	0.44
2:A:421:TRP:HD1	2:A:421:TRP:O	2.00	0.44
1:C:302:ASN:ND2	1:C:307:LEU:H	2.10	0.44
2:A:222:ILE:HD11	2:A:224:LEU:HD21	1.99	0.44
2:A:619:ALA:HA	2:A:620:PRO:HD3	1.85	0.44
2:A:642:MET:HA	2:A:642:MET:HE3	1.99	0.44
1:C:317:LEU:C	1:C:317:LEU:CD1	2.91	0.44
2:A:402:ALA:O	2:A:405:ASP:HB3	2.17	0.44
2:A:214:ASN:C	2:A:215:GLN:HG3	2.43	0.44
2:A:604:ARG:HB2	2:A:629:GLN:HE21	1.82	0.44
1:B:292:ARG:HG3	1:C:312:ASN:HD21	1.83	0.44
2:A:930:PHE:CD2	2:A:1015:PRO:HB3	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:256:TRP:HE1	1:B:359:GLN:NE2	2.17	0.43
2:A:315:LEU:HA	2:A:316:PRO:HD3	1.92	0.43
2:A:702:GLU:O	2:A:705:ARG:HG3	2.18	0.43
2:A:940:PHE:CD1	2:A:984:LYS:HE3	2.53	0.43
1:B:387:SER:O	1:B:388:GLU:CD	2.61	0.43
1:C:197:ARG:HE	1:C:197:ARG:HB2	1.57	0.43
2:A:14:PHE:O	2:A:17:LEU:HB3	2.18	0.43
2:A:996:LEU:N	2:A:997:PRO:CD	2.81	0.43
1:C:352:PRO:HB2	1:C:398:MET:SD	2.59	0.43
2:A:836:VAL:O	2:A:840:LEU:HG	2.17	0.43
1:B:151:LEU:HD11	1:B:210:LEU:HD12	2.01	0.43
2:A:28:THR:O	2:A:32:ILE:HG13	2.18	0.43
2:A:533:LEU:HD22	2:A:1036:LYS:HD3	2.01	0.43
2:A:672:MET:HE3	2:A:678:LYS:HB3	2.01	0.43
2:A:961:PRO:HA	2:A:1043:HIS:HE1	1.83	0.43
1:C:395:LEU:O	1:C:399:ARG:HG3	2.19	0.43
2:A:53:TYR:O	2:A:89:GLY:HA2	2.19	0.43
2:A:214:ASN:H	2:A:215:GLN:HE21	1.64	0.43
2:A:255:VAL:HA	2:A:256:PRO:HD3	1.83	0.43
2:A:403:MET:HE1	2:A:485:ALA:HB1	1.99	0.43
1:B:123:ILE:CD1	1:B:237:LYS:HG3	2.45	0.43
1:C:106:PHE:HE2	1:C:359:GLN:CG	2.29	0.43
2:A:518:ASN:O	2:A:521:LEU:HG	2.19	0.43
2:A:701:GLU:O	2:A:705:ARG:HG2	2.18	0.43
2:A:927:GLY:O	2:A:931:ILE:HG12	2.18	0.43
2:A:42:LEU:HD12	2:A:42:LEU:N	2.32	0.43
2:A:272:ARG:O	2:A:621:LEU:HD11	2.18	0.43
2:A:400:VAL:HA	2:A:403:MET:CG	2.49	0.43
1:B:278:ILE:HG13	1:B:298:LEU:HD13	2.01	0.43
1:B:296:LEU:C	1:B:296:LEU:HD23	2.43	0.43
2:A:365:VAL:HG11	2:A:501:MET:HB3	2.01	0.43
2:A:418:LEU:CD2	2:A:438:VAL:HG11	2.49	0.43
2:A:533:LEU:C	2:A:536:PRO:HD3	2.43	0.43
1:B:128:ALA:HA	1:B:231:LYS:HD2	2.01	0.42
1:B:280:LYS:HE3	1:B:280:LYS:CA	2.49	0.42
1:C:167:LEU:C	1:C:167:LEU:CD1	2.86	0.42
2:A:599:VAL:HA	2:A:600:PRO:HD3	1.83	0.42
2:A:402:ALA:HB3	2:A:486:MET:CE	2.47	0.42
2:A:570:LEU:HD23	2:A:628:ILE:HB	2.00	0.42
2:A:599:VAL:HG21	2:A:649:LEU:CD1	2.48	0.42
2:A:739:THR:O	2:A:742:ASP:HB2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:174:THR:HG22	1:C:176:THR:H	1.84	0.42
2:A:599:VAL:O	2:A:602:VAL:HG13	2.20	0.42
2:A:1021:ILE:O	2:A:1025:LEU:HB2	2.18	0.42
1:B:329:SER:HA	1:B:365:THR:HG23	2.01	0.42
1:C:242:ASP:CB	1:C:243:PRO:CD	2.97	0.42
2:A:1041:HIS:C	2:A:1043:HIS:N	2.77	0.42
2:A:353:CYS:O	2:A:357:LEU:HB2	2.19	0.42
2:A:982:ARG:HH21	2:A:982:ARG:HG3	1.85	0.42
1:C:234:VAL:O	1:C:234:VAL:CG2	2.65	0.42
2:A:37:ASP:HA	2:A:331:ILE:HD12	2.01	0.42
2:A:790:THR:OG1	2:A:794:GLN:HB2	2.20	0.42
2:A:980:ARG:O	2:A:983:PRO:HD2	2.20	0.42
1:C:341:VAL:HB	1:C:377:VAL:CG2	2.50	0.42
1:C:360:ALA:HB2	1:C:365:THR:HB	2.02	0.42
2:A:21:LEU:O	2:A:21:LEU:HD22	2.20	0.42
2:A:191:ILE:HG21	2:A:196:LEU:HD11	2.01	0.42
2:A:340:GLY:O	2:A:344:GLU:HG3	2.19	0.42
2:A:518:ASN:OD1	2:A:982:ARG:NH2	2.52	0.42
2:A:525:TYR:CE1	2:A:980:ARG:NH2	2.87	0.42
2:A:771:ARG:HG3	2:A:772:TYR:N	2.35	0.42
1:C:342:ILE:O	1:C:378:VAL:HG12	2.19	0.42
2:A:191:ILE:HA	2:A:263:ALA:HB2	2.02	0.42
2:A:338:LEU:HD21	2:A:390:ILE:HG13	2.01	0.42
2:A:411:ILE:HA	2:A:501:MET:CE	2.49	0.42
2:A:436:TRP:CD1	2:A:437:GLN:N	2.88	0.42
2:A:455:LEU:HD13	2:A:459:LEU:HD13	2.01	0.42
2:A:940:PHE:CZ	2:A:944:MET:HG3	2.54	0.42
1:B:185:LEU:HD12	1:B:185:LEU:HA	1.80	0.42
1:C:134:LYS:HG3	1:C:135:VAL:N	2.34	0.42
2:A:67:TYR:N	2:A:68:PRO:HD2	2.34	0.42
2:A:883:ILE:O	2:A:887:LEU:HG	2.19	0.42
2:A:365:VAL:CG1	2:A:411:ILE:HD11	2.50	0.42
2:A:431:ASP:CG	2:A:432:ASN:N	2.78	0.41
2:A:715:ALA:HB2	2:A:824:ILE:HG23	2.02	0.41
1:B:302:ASN:HD21	1:B:306:ALA:N	2.18	0.41
2:A:412:GLU:OE1	2:A:983:PRO:HG3	2.20	0.41
2:A:660:ASN:ND2	2:A:660:ASN:N	2.46	0.41
2:A:705:ARG:NH1	2:A:713:ALA:O	2.53	0.41
2:A:932:ALA:O	2:A:936:VAL:HG23	2.20	0.41
1:C:88:GLN:HG2	2:A:654:ARG:O	2.20	0.41
2:A:463:PRO:HG2	2:A:879:THR:OG1	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:952:ILE:O	2:A:952:ILE:HG22	2.20	0.41
2:A:984:LYS:NZ	2:A:984:LYS:CB	2.84	0.41
1:C:223:LEU:O	1:C:224:ARG:HD2	2.21	0.41
2:A:459:LEU:C	2:A:461:PHE:N	2.76	0.41
2:A:707:VAL:HA	2:A:708:PRO:HD3	1.88	0.41
1:C:284:LEU:HD12	1:C:295:GLN:HB2	2.03	0.41
1:C:330:GLN:CD	1:C:330:GLN:H	2.28	0.41
2:A:38:ALA:HB2	2:A:331:ILE:HD13	2.03	0.41
2:A:998:ILE:CD1	2:A:1013:ALA:HB2	2.51	0.41
2:A:1035:TYR:O	2:A:1039:TRP:HB2	2.21	0.41
1:C:161:ALA:HB3	1:C:185:LEU:HD11	2.01	0.41
2:A:425:HIS:CB	2:A:426:PRO:HD2	2.34	0.41
2:A:636:TRP:CD1	2:A:636:TRP:N	2.89	0.41
2:A:962:GLN:CG	2:A:963:THR:N	2.81	0.41
2:A:390:ILE:HD11	2:A:1008:VAL:CG1	2.50	0.41
2:A:700:ILE:HA	2:A:703:VAL:HG22	2.03	0.41
1:B:124:VAL:HB	1:B:235:VAL:HG22	2.03	0.41
1:B:335:THR:HG22	1:B:391:ILE:HD12	2.02	0.41
2:A:27:GLY:HA3	2:A:375:CYS:HB3	2.02	0.41
2:A:114:LEU:HD12	2:A:114:LEU:HA	1.86	0.41
2:A:355:LEU:C	2:A:356:PHE:HD1	2.29	0.41
2:A:526:HIS:N	2:A:527:PRO:CD	2.84	0.41
2:A:569:ASP:OD2	2:A:629:GLN:HG2	2.20	0.41
2:A:786:LEU:HB3	2:A:798:LEU:HB2	2.02	0.41
2:A:984:LYS:CA	2:A:984:LYS:CE	2.99	0.41
1:B:343:THR:HG1	1:B:351:VAL:HG23	1.85	0.41
1:C:257:LEU:HD12	1:C:257:LEU:HA	1.92	0.41
2:A:11:ALA:C	2:A:13:ARG:H	2.29	0.41
2:A:403:MET:H	2:A:403:MET:HG2	1.52	0.41
2:A:975:HIS:HA	2:A:978:VAL:HG12	2.03	0.41
1:B:242:ASP:O	1:B:302:ASN:N	2.54	0.40
1:C:219:THR:HG21	1:C:239:GLN:OE1	2.21	0.40
1:C:283:LEU:HD23	1:C:283:LEU:HA	1.80	0.40
2:A:141:GLU:HB3	2:A:325:TYR:HB3	2.01	0.40
2:A:376:ILE:HG21	2:A:488:GLY:HA3	2.03	0.40
2:A:497:ILE:HB	2:A:498:PRO:HD3	2.03	0.40
2:A:589:LEU:HD22	2:A:609:THR:HG23	2.03	0.40
2:A:637:ARG:HH11	2:A:637:ARG:HB2	1.86	0.40
2:A:914:LEU:HD23	2:A:1014:ALA:O	2.20	0.40
1:B:212:ALA:HA	1:B:213:PRO:HD3	1.86	0.40
1:C:242:ASP:OD1	1:C:242:ASP:C	2.64	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:38:ALA:O	2:A:390:ILE:CG2	2.66	0.40
2:A:608:LYS:HE2	2:A:625:GLU:HB2	2.02	0.40
2:A:898:LEU:HD23	2:A:898:LEU:O	2.21	0.40
2:A:1028:LEU:O	2:A:1032:PRO:HG2	2.22	0.40
1:C:174:THR:H	1:C:177:GLN:HE21	1.68	0.40
2:A:554:LEU:HD23	2:A:912:ILE:HG21	2.03	0.40
2:A:944:MET:HE3	2:A:944:MET:HB3	1.95	0.40
1:B:242:ASP:CB	1:B:243:PRO:HD3	2.38	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%)	304 (95%)	15 (5%)	1 (0%)	36	65
1	C	322/413 (78%)	312 (97%)	9 (3%)	1 (0%)	36	65
2	A	1024/1054 (97%)	969 (95%)	54 (5%)	1 (0%)	48	77
All	All	1666/1880 (89%)	1585 (95%)	78 (5%)	3 (0%)	43	72

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	852	PRO
1	C	137	PRO
1	B	137	PRO

5.3.2 Protein sidechains [i](#)

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%)	223 (85%)	40 (15%)	3	9
1	C	265/338 (78%)	229 (86%)	36 (14%)	3	12
2	A	847/871 (97%)	749 (88%)	98 (12%)	5	18
All	All	1375/1547 (89%)	1201 (87%)	174 (13%)	4	14

All (174) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	84	ILE
1	B	92	LEU
1	B	105	THR
1	B	123	ILE
1	B	134	LYS
1	B	138	LEU
1	B	140	VAL
1	B	159	VAL
1	B	168	LEU
1	B	182	LEU
1	B	185	LEU
1	B	199	ILE
1	B	203	LYS
1	B	234	VAL
1	B	235	VAL
1	B	239	GLN
1	B	241	MET
1	B	244	VAL
1	B	252	GLU
1	B	268	VAL
1	B	275	THR
1	B	277	THR
1	B	280	LYS
1	B	282	THR
1	B	287	VAL
1	B	298	LEU
1	B	299	GLU
1	B	322	GLU
1	B	330	GLN
1	B	340	ARG

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Mol	Chain	Res	Type
1	B	349	ARG
1	B	357	VAL
1	B	364	VAL
1	B	365	THR
1	B	367	LEU
1	B	378	VAL
1	B	379	SER
1	B	385	ILE
1	B	388	GLU
1	B	396	GLU
1	C	96	THR
1	C	98	THR
1	C	104	LEU
1	C	105	THR
1	C	138	LEU
1	C	140	VAL
1	C	150	LEU
1	C	159	VAL
1	C	167	LEU
1	C	178	THR
1	C	181	ILE
1	C	182	LEU
1	C	185	LEU
1	C	187	LEU
1	C	206	THR
1	C	207	ARG
1	C	231	LYS
1	C	234	VAL
1	C	235	VAL
1	C	258	VAL
1	C	276	LEU
1	C	283	LEU
1	C	287	VAL
1	C	317	LEU
1	C	324	MET
1	C	330	GLN
1	C	339	GLN
1	C	343	THR
1	C	351	VAL
1	C	354	ARG
1	C	364	VAL
1	C	365	THR

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Mol	Chain	Res	Type
1	C	373	GLU
1	C	377	VAL
1	C	378	VAL
1	C	395	LEU
2	A	6	ILE
2	A	12	ASN
2	A	21	LEU
2	A	31	ILE
2	A	42	LEU
2	A	59	GLN
2	A	69	LEU
2	A	72	THR
2	A	115	ASN
2	A	117	VAL
2	A	125	VAL
2	A	144	LEU
2	A	145	VAL
2	A	168	LEU
2	A	188	GLN
2	A	190	VAL
2	A	203	LEU
2	A	210	LEU
2	A	211	ASP
2	A	215	GLN
2	A	222	ILE
2	A	259	LEU
2	A	273	ARG
2	A	298	ARG
2	A	322	VAL
2	A	335	ILE
2	A	342	LEU
2	A	358	TRP
2	A	386	LEU
2	A	390	ILE
2	A	398	ILE
2	A	403	MET
2	A	411	ILE
2	A	417	ARG
2	A	434	THR
2	A	436	TRP
2	A	445	GLU
2	A	455	LEU

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Mol	Chain	Res	Type
2	A	457	ILE
2	A	462	ILE
2	A	464	ILE
2	A	492	LEU
2	A	518	ASN
2	A	521	LEU
2	A	531	LYS
2	A	532	VAL
2	A	534	HIS
2	A	545	LEU
2	A	548	LEU
2	A	549	THR
2	A	554	LEU
2	A	569	ASP
2	A	575	SER
2	A	592	THR
2	A	602	VAL
2	A	604	ARG
2	A	624	VAL
2	A	626	THR
2	A	634	GLU
2	A	637	ARG
2	A	641	THR
2	A	642	MET
2	A	649	LEU
2	A	660	ASN
2	A	661	LEU
2	A	693	ILE
2	A	705	ARG
2	A	722	ARG
2	A	729	ASN
2	A	769	ASN
2	A	775	SER
2	A	781	GLN
2	A	783	LEU
2	A	786	LEU
2	A	789	LEU
2	A	812	MET
2	A	813	LEU
2	A	815	THR
2	A	879	THR
2	A	882	ILE

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Mol	Chain	Res	Type
2	A	884	PHE
2	A	885	VAL
2	A	899	LEU
2	A	901	ILE
2	A	904	VAL
2	A	909	VAL
2	A	922	LEU
2	A	933	LEU
2	A	945	LEU
2	A	946	MET
2	A	959	ASN
2	A	968	LYS
2	A	969	LEU
2	A	984	LYS
2	A	987	THR
2	A	1020	MET
2	A	1026	LEU
2	A	1039	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	113	ASN
1	B	117	ASN
1	B	125	GLN
1	B	177	GLN
1	B	302	ASN
1	B	359	GLN
1	B	390	ASN
1	C	120	GLN
1	C	125	GLN
1	C	177	GLN
1	C	263	GLN
1	C	302	ASN
1	C	312	ASN
2	A	115	ASN
2	A	118	GLN
2	A	151	HIS
2	A	194	GLN
2	A	198	GLN
2	A	215	GLN
2	A	238	GLN

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Mol	Chain	Res	Type
2	A	279	ASN
2	A	329	GLN
2	A	337	ASN
2	A	359	HIS
2	A	415	HIS
2	A	423	HIS
2	A	432	ASN
2	A	470	GLN
2	A	526	HIS
2	A	534	HIS
2	A	629	GLN
2	A	633	GLN
2	A	635	GLN
2	A	660	ASN
2	A	668	ASN
2	A	725	ASN
2	A	729	ASN
2	A	744	GLN
2	A	769	ASN
2	A	795	GLN
2	A	838	HIS
2	A	869	ASN
2	A	1043	HIS

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

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%)	0.15	18 (5%)	30	23	20, 42, 81, 134	0
1	C	324/413 (78%)	0.03	10 (3%)	51	42	20, 43, 81, 131	0
2	A	1028/1054 (97%)	0.75	159 (15%)	5	4	20, 67, 181, 263	0
All	All	1674/1880 (89%)	0.49	187 (11%)	10	9	20, 54, 155, 263	0

All (187) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	446	VAL	7.2
1	B	386	ASP	7.2
1	B	388	GLU	6.9
2	A	6	ILE	6.8
2	A	520	PHE	6.3
2	A	4	TRP	5.9
2	A	979	LEU	5.9
1	B	387	SER	5.8
2	A	955	VAL	5.8
2	A	401	GLY	5.6
2	A	444	VAL	5.6
2	A	1001	GLY	5.3
2	A	429	THR	5.2
2	A	530	LEU	5.1
1	B	157	ASP	5.1
2	A	409	VAL	4.9
2	A	896	GLU	4.9
2	A	416	LYS	4.9
2	A	439	ILE	4.8
1	C	242	ASP	4.8
2	A	517	LEU	4.7
1	B	242	ASP	4.6
2	A	406	ALA	4.6

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Mol	Chain	Res	Type	RSRZ
2	A	443	SER	4.6
2	A	639	GLY	4.5
1	C	339	GLN	4.5
2	A	26	TRP	4.5
2	A	497	ILE	4.5
2	A	891	PHE	4.5
2	A	504	TRP	4.4
2	A	873	LYS	4.4
2	A	448	PRO	4.4
2	A	895	GLY	4.4
2	A	495	VAL	4.3
1	C	157	ASP	4.3
2	A	1037	LEU	4.2
2	A	10	VAL	4.2
2	A	15	LEU	4.1
2	A	975	HIS	4.1
2	A	890	ALA	4.1
2	A	537	LYS	4.1
1	C	340	ARG	4.1
2	A	502	GLY	4.0
2	A	426	PRO	4.0
2	A	884	PHE	3.8
2	A	528	LEU	3.8
2	A	889	LEU	3.8
1	B	339	GLN	3.8
2	A	373	GLY	3.8
2	A	980	ARG	3.7
2	A	358	TRP	3.7
2	A	405	ASP	3.7
2	A	1038	MET	3.6
2	A	888	TYR	3.6
2	A	450	LEU	3.6
2	A	958	LEU	3.6
2	A	903	SER	3.6
2	A	1000	TRP	3.6
1	B	381	GLY	3.6
2	A	1039	TRP	3.6
2	A	964	PHE	3.6
2	A	946	MET	3.6
1	B	400	SER	3.5
2	A	1036	LYS	3.5
1	C	79	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
2	A	972	ALA	3.5
2	A	413	ASN	3.5
2	A	535	TRP	3.5
2	A	366	ALA	3.5
2	A	981	VAL	3.4
2	A	521	LEU	3.4
2	A	484	TYR	3.3
2	A	538	THR	3.3
2	A	419	GLU	3.3
2	A	22	PHE	3.3
2	A	404	VAL	3.3
2	A	19	GLY	3.3
2	A	491	LEU	3.2
2	A	449	ALA	3.2
1	B	383	PHE	3.2
2	A	1035	TYR	3.2
2	A	430	LEU	3.2
2	A	365	VAL	3.1
2	A	638	PRO	3.1
2	A	498	PRO	3.1
1	B	338	GLU	3.1
2	A	7	ARG	3.0
2	A	407	ALA	2.9
2	A	435	ARG	2.9
2	A	526	HIS	2.9
2	A	1002	THR	2.9
2	A	637	ARG	2.9
2	A	1042	ARG	2.9
2	A	564	GLN	2.9
2	A	428	ALA	2.9
2	A	480	PHE	2.8
2	A	906	PHE	2.8
2	A	523	ARG	2.8
2	A	943	VAL	2.8
2	A	367	ILE	2.8
2	A	870	HIS	2.8
2	A	445	GLU	2.8
2	A	360	VAL	2.8
2	A	493	ALA	2.8
2	A	970	ASP	2.8
2	A	519	ARG	2.8
2	A	978	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
2	A	947	TYR	2.8
2	A	368	ILE	2.8
2	A	533	LEU	2.8
1	B	340	ARG	2.7
1	C	338	GLU	2.7
1	B	79	ALA	2.7
2	A	20	ALA	2.6
2	A	414	ALA	2.6
2	A	451	PHE	2.6
1	B	227	MET	2.6
1	B	158	TRP	2.6
2	A	971	GLU	2.6
2	A	421	TRP	2.6
2	A	950	HIS	2.6
1	C	160	GLU	2.6
2	A	957	SER	2.6
2	A	579	GLY	2.6
2	A	415	HIS	2.5
2	A	948	LEU	2.5
2	A	961	PRO	2.5
2	A	14	PHE	2.5
2	A	425	HIS	2.5
2	A	427	ASP	2.5
2	A	293	SER	2.5
2	A	956	PRO	2.5
2	A	919	GLY	2.5
2	A	998	ILE	2.5
2	A	968	LYS	2.5
2	A	1012	ILE	2.5
2	A	954	ALA	2.5
1	C	255	ALA	2.4
2	A	418	LEU	2.4
2	A	12	ASN	2.4
2	A	441	ASP	2.4
2	A	29	TRP	2.4
2	A	17	LEU	2.4
2	A	500	LEU	2.4
2	A	447	GLY	2.4
2	A	892	ARG	2.4
2	A	893	ARG	2.4
2	A	432	ASN	2.3
2	A	465	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
2	A	698	GLU	2.3
1	B	316	GLN	2.3
2	A	962	GLN	2.3
1	B	271	ARG	2.3
2	A	489	ALA	2.3
2	A	369	SER	2.3
2	A	518	ASN	2.3
2	A	452	ILE	2.3
2	A	1030	ILE	2.3
2	A	982	ARG	2.3
2	A	13	ARG	2.2
2	A	942	VAL	2.2
1	C	345	ASP	2.2
1	C	377	VAL	2.2
2	A	636	TRP	2.2
2	A	525	TYR	2.2
2	A	974	TYR	2.2
2	A	357	LEU	2.2
2	A	1034	ALA	2.2
2	A	431	ASP	2.2
2	A	886	LEU	2.2
2	A	402	ALA	2.2
2	A	838	HIS	2.2
2	A	977	ALA	2.2
2	A	547	VAL	2.1
2	A	708	PRO	2.1
2	A	623	MET	2.1
2	A	872	LEU	2.1
2	A	494	ILE	2.1
1	B	174	THR	2.1
2	A	356	PHE	2.1
2	A	442	ALA	2.1
2	A	18	MET	2.1
2	A	524	VAL	2.1
2	A	36	VAL	2.0
2	A	455	LEU	2.0
2	A	546	SER	2.0
1	B	291	THR	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 [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.