Full wwPDB X-ray Structure Validation Report (i)

Feb 17, 2024 – 04:33 PM EST

PDB ID	:	3T56
Title	:	Crystal structure of the pre-extrusion state of the CusBA adaptor-transporter complex
Authors	:	Su, C.-C.; Long, F.; Yu, E.W.
Deposited on	:	2011-07-26
Resolution	:	3.42 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 (i) 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 (1)) were used in the production of this report:

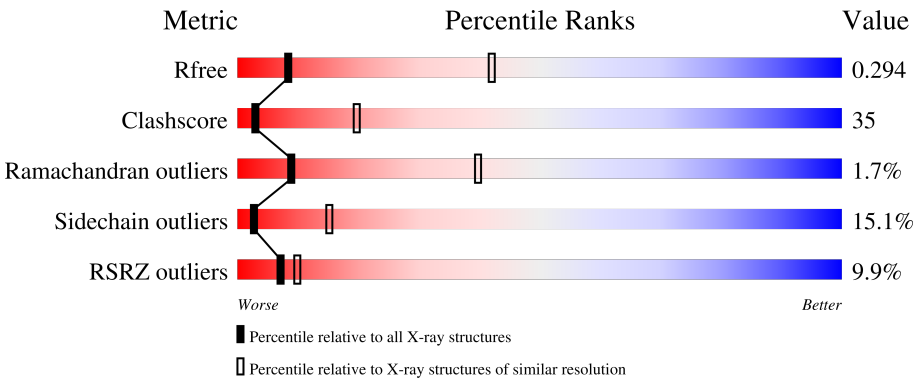
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.42 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1486 (3.50-3.34)
Clashscore	141614	1572 (3.50-3.34)
Ramachandran outliers	138981	1534 (3.50-3.34)
Sidechain outliers	138945	1535 (3.50-3.34)
RSRZ outliers	127900	1395 (3.50-3.34)

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 <=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	A	1054	15% 38% 49% 10% •
2	B	336	% 53% 35% 8% •
2	C	336	% 60% 32% 5% •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CU	A	1048	-	-	-	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 13860 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 CusA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1027	8913	5754	1502	1615	42	0	225	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	GLY	-	expression tag	UNP P38054
A	-5	HIS	-	expression tag	UNP P38054
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

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

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

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

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Chain	Residue	Modelled	Actual	Comment	Reference
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 3 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

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

- Molecule 4 is water.

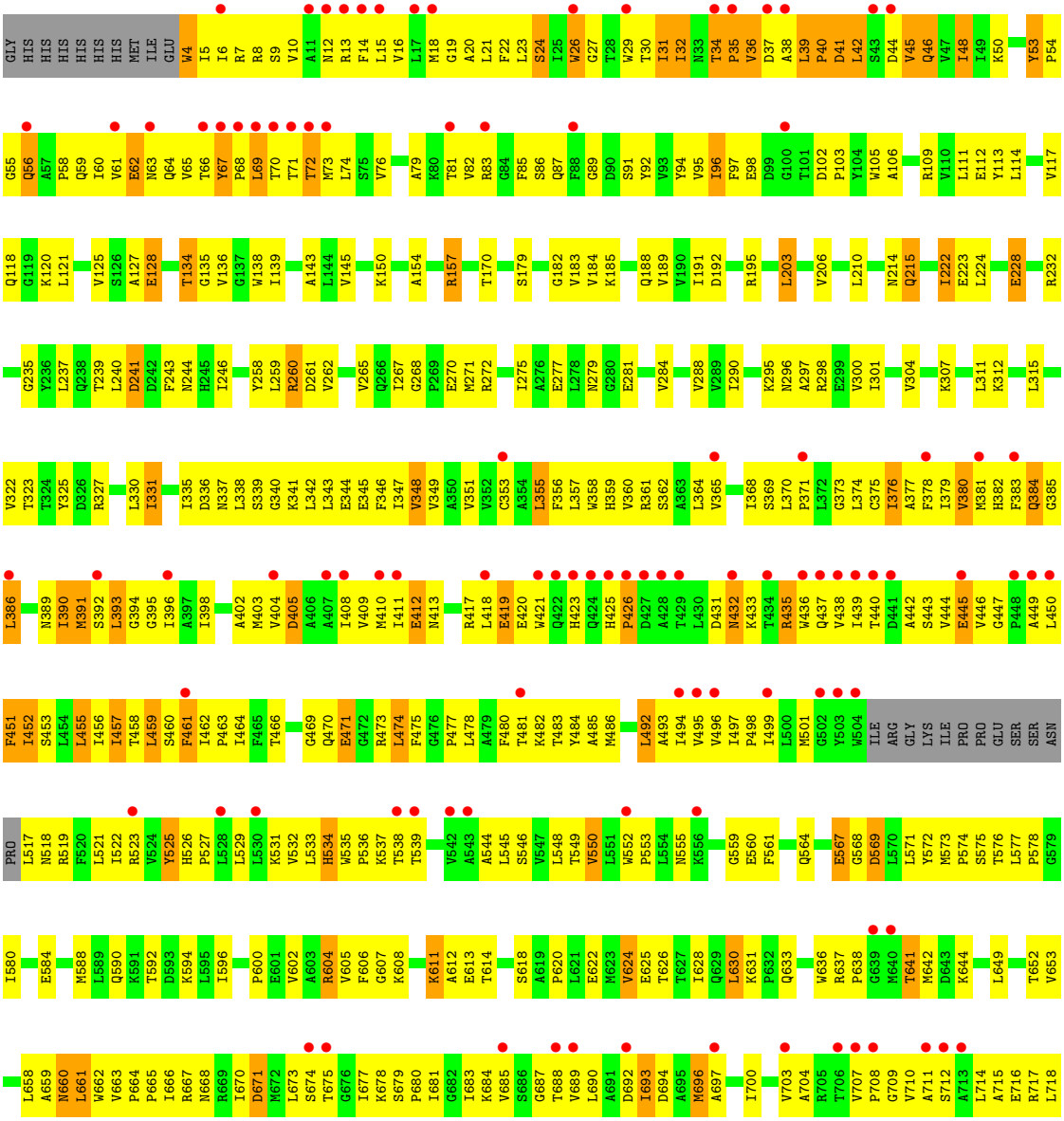
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	3	3	3	0	0
			Total	O		
4	B	4	4	4	0	0
			Total	O		
4	C	8	8	8	0	0

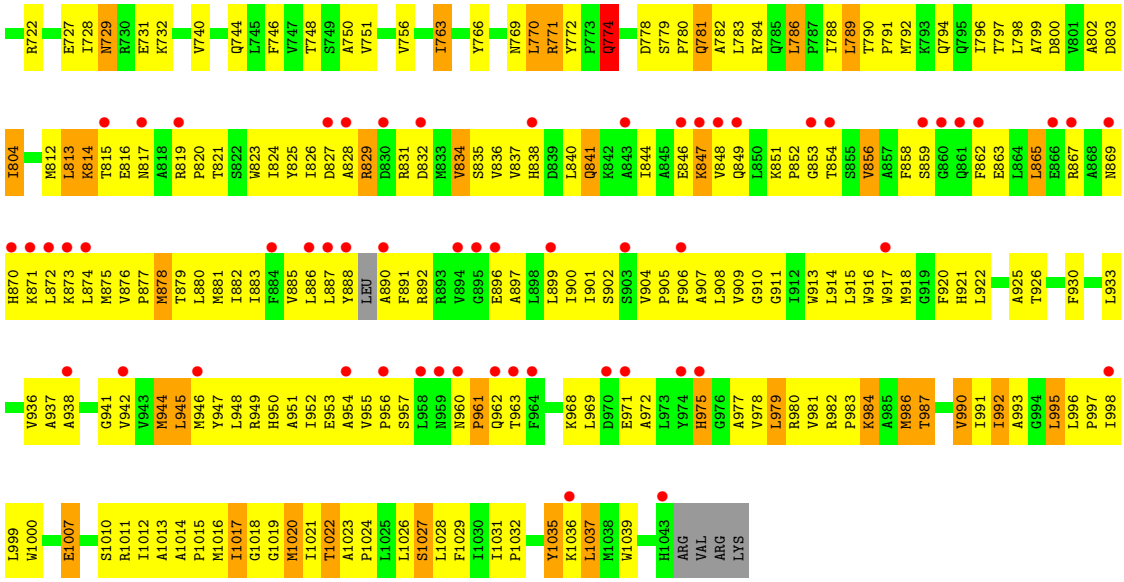
3 Residue-property plots (i)

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 CusA

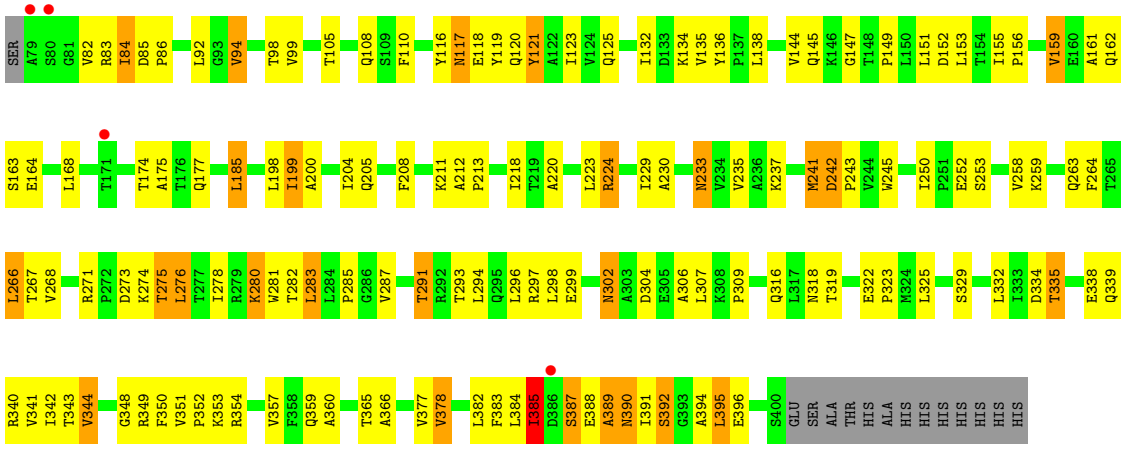
Chain A:





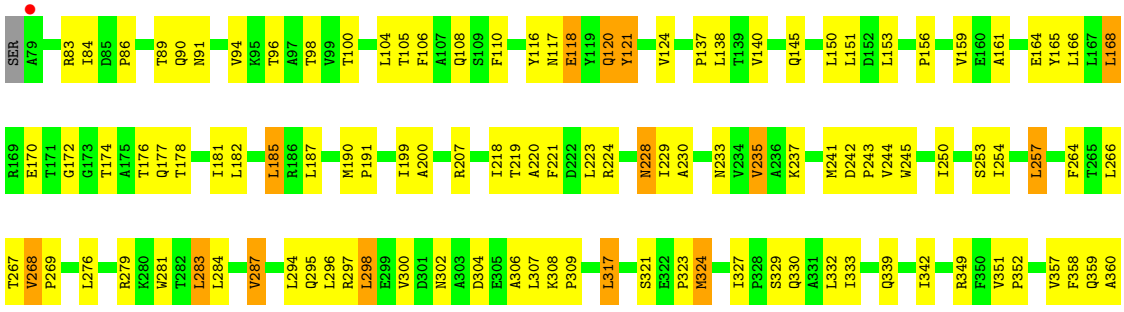
- Molecule 2: Cation efflux system protein CusB

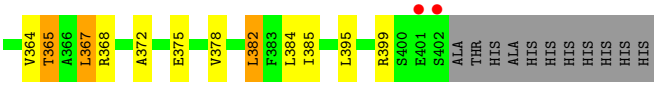
Chain B:



- Molecule 2: Cation efflux system protein CusB

Chain C:




V364
T365
A366
L367
R368
A372
E375
V378
L382
F383
L384
I385
L395
R399
S400
E401
S402
ALA
THR
HIS
ALA
HIS
HIS
HIS
HIS
HIS
HIS
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	160.12Å 160.12Å 684.95Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.25 – 3.42 49.25 – 3.42	Depositor EDS
% Data completeness (in resolution range)	88.8 (49.25-3.42) 98.7 (49.25-3.42)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.69 (at 3.40Å)	Xtriage
Refinement program	PHENIX 1.6.4_486	Depositor
R, R_{free}	0.259 , 0.294 0.259 , 0.294	Depositor DCC
R_{free} test set	2290 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	69.0	Xtriage
Anisotropy	0.130	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 76.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.85	EDS
Total number of atoms	13860	wwPDB-VP
Average B, all atoms (Å^2)	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.60% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	A	0.23	0/9093	0.44	0/12371
2	B	0.22	0/2498	0.44	0/3401
2	C	0.22	0/2513	0.44	0/3421
All	All	0.23	0/14104	0.44	0/19193

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8913	0	9201	752	0
2	B	2458	0	2522	135	0
2	C	2473	0	2533	104	0
3	A	1	0	0	0	0
4	A	3	0	0	0	0
4	B	4	0	0	0	0
4	C	8	0	0	0	0
All	All	13860	0	14256	972	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 35.

All (972) 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:A:604:ARG:HH21	1:A:604:ARG:HG3	1.11	1.16
1:A:573:MET:HE2	1:A:625:GLU:HG2	1.24	1.15
1:A:828[B]:ALA:HA	1:A:829[B]:ARG:HB2	1.27	1.09
1:A:62:GLU:HB2	1:A:86:SER:HB2	1.32	1.06
1:A:62:GLU:HA	1:A:65:VAL:HG22	1.39	1.04
1:A:380:VAL:HG21	1:A:484:TYR:HB3	1.33	1.03
2:C:254:ILE:HG23	2:C:257:LEU:HD23	1.39	1.00
1:A:660:ASN:HD22	1:A:660:ASN:H	1.08	1.00
1:A:31:ILE:HA	1:A:386:LEU:HD11	1.41	1.00
1:A:573:MET:CE	1:A:625:GLU:HG2	1.93	0.99
1:A:661:LEU:HD11	1:A:679[A]:SER:HB3	1.46	0.98
1:A:432:ASN:HA	1:A:435:ARG:HD3	1.47	0.97
1:A:535:TRP:HE1	1:A:537:LYS:HB3	1.27	0.96
1:A:552:TRP:HB3	1:A:553:PRO:HD3	1.48	0.96
1:A:87:GLN:HG2	1:A:812[A]:MET:HG3	1.50	0.94
1:A:1020:MET:O	1:A:1024:PRO:HD2	1.67	0.93
1:A:573:MET:HE2	1:A:625:GLU:CG	1.98	0.92
1:A:64:GLN:HA	1:A:67:TYR:HB3	1.51	0.91
2:B:223:LEU:HD12	2:B:235:VAL:HG12	1.54	0.90
1:A:85:PHE:HB2	1:A:92:TYR:HB2	1.52	0.90
1:A:995:LEU:HG	1:A:1017:ILE:HA	1.54	0.89
1:A:828[B]:ALA:HA	1:A:829[B]:ARG:CB	2.02	0.89
1:A:660:ASN:H	1:A:660:ASN:ND2	1.71	0.88
1:A:36:VAL:HG13	1:A:331:ILE:HG12	1.54	0.88
1:A:35:PRO:HB3	1:A:298:ARG:HB3	1.54	0.87
1:A:463:PRO:HG2	1:A:879[A]:THR:HG23	1.54	0.87
1:A:338:LEU:HB3	1:A:393:LEU:HD12	1.57	0.86
1:A:377:ALA:HB2	1:A:485:ALA:HB2	1.58	0.85
2:C:106:PHE:HE2	2:C:359:GLN:HG2	1.41	0.85
2:B:125:GLN:HE21	2:C:228:ASN:H	1.22	0.85
1:A:908:LEU:HD23	1:A:933:LEU:HD12	1.59	0.85
1:A:389:ASN:HB3	1:A:391:MET:HG2	1.57	0.84
1:A:607:GLY:HA2	1:A:626:THR:HG22	1.59	0.84
1:A:64:GLN:O	1:A:68:PRO:HD2	1.76	0.84
1:A:26:TRP:HE1	1:A:379:ILE:HG23	1.42	0.83
2:B:388:GLU:HG3	2:B:389:ALA:H	1.43	0.83
1:A:67:TYR:HB3	1:A:68:PRO:HD3	1.60	0.83
1:A:418:LEU:HG	1:A:438:VAL:HG21	1.60	0.83
1:A:24:SER:HA	1:A:375:CYS:HB3	1.61	0.82
1:A:381:MET:HE3	1:A:386:LEU:HB3	1.59	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:120:GLN:NE2	2:B:243:PRO:HD2	1.93	0.82
1:A:391:MET:HG3	1:A:474:LEU:O	1.80	0.81
1:A:960:ASN:HB2	1:A:961:PRO:HD3	1.63	0.81
1:A:572:TYR:HE1	1:A:660:ASN:HB2	1.43	0.81
1:A:652:THR:HG23	2:B:82:VAL:HG11	1.61	0.81
1:A:357:LEU:HD23	1:A:362:SER:HB3	1.61	0.81
2:C:242:ASP:HB3	2:C:243:PRO:HD3	1.63	0.81
1:A:62:GLU:CB	1:A:86:SER:HB2	2.09	0.81
1:A:66:THR:HG21	1:A:815[B]:THR:OG1	1.80	0.81
1:A:537:LYS:HB2	1:A:1037:LEU:HD11	1.62	0.80
2:B:132:ILE:HD11	2:B:223:LEU:HD13	1.62	0.80
2:C:266:LEU:HD12	2:C:300:VAL:HG21	1.61	0.80
1:A:604:ARG:HH21	1:A:604:ARG:CG	1.93	0.80
1:A:661:LEU:CD1	1:A:679[A]:SER:HB3	2.12	0.80
1:A:449:ALA:HB1	1:A:942:VAL:HG13	1.63	0.79
1:A:660:ASN:HD22	1:A:660:ASN:N	1.80	0.79
2:C:174:THR:H	2:C:177:GLN:HE21	1.29	0.79
1:A:572:TYR:HE1	1:A:660:ASN:CB	1.95	0.79
1:A:66:THR:HG22	1:A:66:THR:O	1.82	0.78
1:A:574:PRO:HA	1:A:660:ASN:HA	1.64	0.78
2:B:118:GLU:HG3	2:B:245:TRP:CZ3	2.19	0.78
1:A:30:THR:HB	1:A:382:HIS:HB2	1.64	0.78
1:A:949:ARG:O	1:A:953:GLU:HG2	1.84	0.78
1:A:977:ALA:HA	1:A:980:ARG:HD3	1.65	0.78
1:A:828[B]:ALA:HB1	1:A:831[B]:ARG:HB2	1.66	0.77
1:A:991:ILE:HG22	1:A:995:LEU:CD2	2.15	0.77
1:A:982:ARG:HB3	1:A:983:PRO:HD3	1.66	0.77
1:A:873[A]:LYS:H	1:A:873[A]:LYS:HD2	1.49	0.77
1:A:569:ASP:HB2	1:A:665[A]:PRO:HG2	1.67	0.76
1:A:661:LEU:HD11	1:A:679[A]:SER:CB	2.15	0.76
1:A:41:ASP:HB3	1:A:470:GLN:HG3	1.68	0.76
2:B:117:ASN:ND2	2:B:119:TYR:H	1.84	0.76
1:A:42:LEU:HD23	1:A:134:THR:HG21	1.68	0.76
2:B:174:THR:H	2:B:177:GLN:HE21	1.32	0.75
1:A:63:ASN:O	1:A:67:TYR:HB2	1.86	0.75
2:B:302:ASN:HD21	2:B:306:ALA:H	1.34	0.75
2:B:335:THR:HG22	2:B:391:ILE:HG21	1.69	0.75
1:A:279:ASN:ND2	1:A:605:VAL:H	1.85	0.74
1:A:390:ILE:HG13	1:A:391:MET:SD	2.26	0.74
2:B:120:GLN:HE22	2:B:242:ASP:HB3	1.51	0.74
1:A:4:TRP:CD1	1:A:4:TRP:N	2.54	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:199:ILE:HG13	2:B:200:ALA:N	2.03	0.74
1:A:535:TRP:NE1	1:A:537:LYS:HB3	2.00	0.74
1:A:65:VAL:HG21	1:A:91:SER:HB2	1.70	0.74
1:A:660:ASN:ND2	1:A:660:ASN:N	2.32	0.73
1:A:677[A]:ILE:HG22	1:A:679[A]:SER:H	1.53	0.73
1:A:784[A]:ARG:HE	1:A:804[A]:ILE:HG12	1.52	0.73
1:A:65:VAL:HA	1:A:69:LEU:HG	1.68	0.73
1:A:901:ILE:O	1:A:905:PRO:HD3	1.89	0.73
1:A:377:ALA:O	1:A:381:MET:HG2	1.88	0.73
1:A:67:TYR:HD2	1:A:68:PRO:CD	2.02	0.72
1:A:62:GLU:HB2	1:A:86:SER:CB	2.13	0.72
2:B:117:ASN:HD22	2:B:119:TYR:H	1.37	0.71
1:A:54:PRO:HA	1:A:125:VAL:HG11	1.71	0.71
1:A:604:ARG:HG3	1:A:604:ARG:NH2	1.91	0.71
1:A:680[B]:PRO:HG2	1:A:681[B]:ILE:HD12	1.71	0.71
1:A:885[A]:VAL:HA	1:A:888[A]:TYR:CE2	2.26	0.70
1:A:46:GLN:HA	1:A:95:VAL:O	1.90	0.70
1:A:763[A]:ILE:HG23	1:A:763[A]:ILE:O	1.91	0.70
1:A:31:ILE:HB	1:A:386:LEU:HD21	1.74	0.69
1:A:55:GLY:O	1:A:61:VAL:HG21	1.92	0.69
1:A:322:VAL:HG22	1:A:322:VAL:O	1.90	0.69
1:A:980:ARG:HG2	1:A:981:VAL:N	2.07	0.69
2:B:280:LYS:HE3	2:B:280:LYS:HA	1.72	0.69
2:C:118:GLU:HG3	2:C:245:TRP:CZ3	2.27	0.69
1:A:991:ILE:HG22	1:A:995:LEU:HD22	1.74	0.69
1:A:393:LEU:O	1:A:396:ILE:HG22	1.93	0.69
1:A:544:ALA:HA	1:A:906:PHE:HE1	1.56	0.69
1:A:191:ILE:HD11	1:A:206:VAL:HG11	1.75	0.69
2:B:352:PRO:HB3	2:B:395:LEU:HD13	1.75	0.69
1:A:244:ASN:O	1:A:258:TYR:HB3	1.93	0.69
1:A:545:LEU:HA	1:A:548:LEU:HD23	1.75	0.69
1:A:1018:GLY:O	1:A:1022:THR:HG22	1.92	0.68
1:A:365:VAL:HG11	1:A:501:MET:HB3	1.74	0.68
1:A:951:ALA:HB1	1:A:972:ALA:HB1	1.75	0.68
1:A:69:LEU:HD11	1:A:121:LEU:HD21	1.75	0.68
2:C:165:TYR:CE2	2:C:182:LEU:HD11	2.28	0.68
1:A:493:ALA:HA	1:A:497:ILE:HB	1.75	0.68
2:B:125:GLN:HE21	2:C:228:ASN:N	1.91	0.68
1:A:700[A]:ILE:HD13	1:A:848[A]:VAL:HG21	1.76	0.68
1:A:681[A]:ILE:HB	1:A:826[A]:ILE:HB	1.75	0.67
1:A:984:LYS:HZ3	1:A:1028:LEU:HD21	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:544:ALA:HA	1:A:906:PHE:CE1	2.28	0.67
1:A:685[B]:VAL:HG21	1:A:696[B]:MET:HB2	1.77	0.67
1:A:729[A]:ASN:ND2	1:A:732[A]:LYS:H	1.92	0.67
1:A:998:ILE:O	1:A:1010:SER:HA	1.94	0.67
2:B:291:THR:HB	2:B:293:THR:HG23	1.76	0.67
1:A:62:GLU:HA	1:A:65:VAL:CG2	2.20	0.67
1:A:536:PRO:HB2	1:A:1037:LEU:HD12	1.76	0.67
1:A:751[A]:VAL:HG23	1:A:786[A]:LEU:HD11	1.76	0.67
1:A:330:LEU:HD22	1:A:567:GLU:HG2	1.77	0.67
1:A:452:ILE:O	1:A:456:ILE:HG13	1.95	0.66
1:A:828[B]:ALA:CA	1:A:829[B]:ARG:HB2	2.15	0.66
1:A:957:SER:O	1:A:961:PRO:HD2	1.94	0.66
2:B:136:TYR:CE2	2:B:149:PRO:HB2	2.30	0.66
1:A:39:LEU:HB3	1:A:41:ASP:OD2	1.94	0.66
1:A:596:ILE:HG12	1:A:653:VAL:HG21	1.75	0.66
1:A:482:LYS:C	1:A:482:LYS:HE2	2.16	0.66
1:A:681[B]:ILE:HB	1:A:826[B]:ILE:HG12	1.76	0.66
1:A:65:VAL:O	1:A:69:LEU:HB2	1.96	0.66
1:A:993:ALA:O	1:A:997:PRO:HD3	1.96	0.66
1:A:240:LEU:HD21	1:A:267:ILE:HD11	1.76	0.66
2:C:284:LEU:HD12	2:C:295:GLN:HB3	1.78	0.66
1:A:697[B]:ALA:HB1	1:A:715[B]:ALA:HB1	1.78	0.66
1:A:97:PHE:CE1	1:A:106:ALA:HB1	2.30	0.66
1:A:39:LEU:HG	1:A:666[A]:ILE:HG21	1.78	0.66
1:A:83:ARG:HH12	1:A:674[B]:SER:HA	1.61	0.65
1:A:440:THR:O	1:A:444:VAL:HG23	1.96	0.65
1:A:847[B]:LYS:HE3	1:A:847[B]:LYS:HA	1.78	0.65
1:A:920:PHE:CE2	1:A:1010:SER:HB3	2.32	0.65
2:B:278:ILE:HG21	2:B:298:LEU:HD22	1.78	0.65
2:B:121:TYR:CD1	2:C:224:ARG:HG3	2.31	0.65
1:A:680[B]:PRO:HD2	1:A:827[B]:ASP:HA	1.78	0.65
2:B:174:THR:H	2:B:177:GLN:NE2	1.94	0.65
1:A:270:GLU:HG2	1:A:271:MET:H	1.60	0.65
1:A:21:LEU:HA	1:A:24:SER:HB3	1.78	0.65
2:B:120:GLN:HE22	2:B:243:PRO:HD2	1.60	0.65
1:A:459:LEU:HD12	1:A:462:ILE:HD11	1.78	0.65
2:C:120:GLN:OE1	2:C:243:PRO:HD2	1.97	0.65
1:A:914:LEU:HD23	1:A:1017:ILE:HB	1.78	0.65
1:A:948:LEU:HD23	1:A:1035:TYR:HD2	1.62	0.64
2:C:230:ALA:H	2:C:233:ASN:ND2	1.94	0.64
1:A:572:TYR:CE1	1:A:660:ASN:CB	2.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:GLY:O	1:A:378:PHE:HB3	1.96	0.64
1:A:980:ARG:HE	1:A:1028:LEU:HD22	1.62	0.64
2:C:137:PRO:O	2:C:138:LEU:HD12	1.97	0.64
1:A:356:PHE:O	1:A:357:LEU:HD12	1.97	0.64
2:C:138:LEU:HD23	2:C:218:ILE:HD11	1.78	0.64
1:A:578:PRO:HG3	1:A:717[A]:ARG:HB2	1.78	0.64
1:A:29:TRP:CE3	1:A:32:ILE:HG13	2.33	0.64
1:A:522:ILE:O	1:A:526:HIS:HD2	1.80	0.64
1:A:572:TYR:HD2	1:A:626:THR:HG1	1.46	0.64
1:A:23:LEU:HB3	1:A:379:ILE:HD11	1.79	0.64
1:A:535:TRP:C	1:A:535:TRP:CD1	2.70	0.64
1:A:477:PRO:O	1:A:481:THR:HG23	1.98	0.64
1:A:356:PHE:HD2	1:A:986:MET:HB3	1.61	0.64
1:A:529:LEU:O	1:A:532:VAL:HG12	1.97	0.64
1:A:907:ALA:HA	1:A:1022:THR:HG23	1.80	0.64
2:C:317:LEU:C	2:C:317:LEU:HD12	2.19	0.63
1:A:67:TYR:CD2	1:A:68:PRO:HD3	2.34	0.63
1:A:244:ASN:HB3	1:A:260:ARG:HB3	1.80	0.63
1:A:998:ILE:HB	1:A:1013:ALA:HB2	1.78	0.63
1:A:999:LEU:HD13	1:A:1017:ILE:HD12	1.81	0.63
1:A:56:GLN:HE21	1:A:56:GLN:CA	2.12	0.63
1:A:39:LEU:HD22	1:A:39:LEU:N	2.13	0.63
1:A:31:ILE:CA	1:A:386:LEU:HD11	2.23	0.63
1:A:696[A]:MET:O	1:A:700[A]:ILE:HG12	1.99	0.62
1:A:6:ILE:HD13	1:A:443:SER:HB2	1.80	0.62
2:B:340:ARG:HD2	2:B:395:LEU:HD12	1.81	0.62
1:A:48:ILE:HD12	1:A:48:ILE:H	1.64	0.62
1:A:867[B]:ARG:O	1:A:871[B]:LYS:HG2	2.00	0.62
1:A:59:GLN:O	1:A:63:ASN:HB2	1.99	0.62
1:A:70:THR:HB	1:A:82:VAL:HG11	1.82	0.62
1:A:926:THR:HG22	1:A:1011:ARG:O	1.99	0.62
1:A:980:ARG:NE	1:A:1028:LEU:HD22	2.14	0.62
1:A:61:VAL:HG12	1:A:62:GLU:HG3	1.82	0.62
1:A:76:VAL:O	1:A:79:ALA:HB2	2.00	0.62
1:A:823[B]:TRP:CD1	1:A:823[B]:TRP:N	2.68	0.62
2:B:302:ASN:HD21	2:B:306:ALA:N	1.96	0.62
1:A:876[A]:VAL:O	1:A:880[A]:LEU:HG	1.99	0.61
1:A:907:ALA:O	1:A:1019:GLY:HA2	2.00	0.61
1:A:66:THR:HA	1:A:70:THR:HG23	1.82	0.61
2:B:339:GLN:HG3	2:B:357:VAL:HG23	1.81	0.61
1:A:561:PHE:HA	1:A:865[A]:LEU:HG	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:873[A]:LYS:HD2	1:A:873[A]:LYS:N	2.16	0.61
1:A:364:LEU:O	1:A:368:ILE:HG12	2.00	0.61
1:A:452:ILE:HG21	1:A:890:ALA:HB2	1.82	0.61
2:B:223:LEU:C	2:B:224:ARG:HD2	2.20	0.61
1:A:458:THR:HB	1:A:483:THR:HG23	1.83	0.61
1:A:572:TYR:CE1	1:A:660:ASN:HB3	2.35	0.61
1:A:13:ARG:HA	1:A:499:ILE:HD13	1.83	0.61
1:A:64:GLN:O	1:A:68:PRO:CD	2.47	0.61
1:A:67:TYR:CB	1:A:68:PRO:HD3	2.30	0.61
1:A:471:GLU:CD	1:A:471:GLU:H	2.04	0.61
1:A:42:LEU:HB2	1:A:673[A]:LEU:CD2	2.30	0.60
1:A:455:LEU:O	1:A:459:LEU:HD22	2.01	0.60
1:A:553:PRO:HG2	1:A:913:TRP:CZ2	2.37	0.60
1:A:574:PRO:HG2	1:A:624:VAL:HG13	1.82	0.60
1:A:991:ILE:C	1:A:995:LEU:HD22	2.22	0.60
1:A:469:GLY:HA3	1:A:867[A]:ARG:NH2	2.17	0.60
1:A:1014:ALA:HA	1:A:1017:ILE:HG13	1.83	0.60
1:A:68:PRO:HB3	1:A:120:LYS:NZ	2.16	0.60
1:A:369:SER:HB2	1:A:497:ILE:HD11	1.83	0.60
1:A:463:PRO:HG2	1:A:879[A]:THR:CG2	2.30	0.60
1:A:38:ALA:C	1:A:39:LEU:HD13	2.21	0.60
2:B:383:PHE:C	2:B:384:LEU:HD12	2.22	0.60
2:B:388:GLU:CG	2:B:389:ALA:H	2.13	0.60
1:A:546:SER:O	1:A:549:THR:HG22	2.02	0.60
1:A:433:LYS:HD2	1:A:437:GLN:NE2	2.17	0.60
1:A:704[B]:ALA:O	1:A:707[B]:VAL:HG12	2.02	0.60
2:C:264:PHE:HE1	2:C:281:TRP:CE2	2.20	0.60
1:A:678[A]:LYS:HE2	1:A:825[A]:TYR:CD2	2.37	0.59
1:A:998:ILE:HB	1:A:1013:ALA:CB	2.31	0.59
2:B:388:GLU:OE1	2:B:388:GLU:HA	2.02	0.59
1:A:519:ARG:O	1:A:523:ARG:HG3	2.02	0.59
1:A:460:SER:HA	1:A:879[A]:THR:HG22	1.84	0.59
1:A:678[A]:LYS:HE2	1:A:825[A]:TYR:CG	2.37	0.59
1:A:887[A]:LEU:HD22	1:A:900:ILE:HG13	1.85	0.59
2:B:280:LYS:HE3	2:B:281:TRP:H	1.67	0.59
1:A:66:THR:O	1:A:66:THR:CG2	2.51	0.59
1:A:67:TYR:HD2	1:A:68:PRO:HD3	1.67	0.59
1:A:573:MET:SD	1:A:678[A]:LYS:HD2	2.43	0.59
1:A:607:GLY:CA	1:A:626:THR:HG22	2.32	0.59
1:A:272:ARG:HD2	1:A:275:ILE:HG13	1.84	0.58
1:A:763[A]:ILE:O	1:A:763[A]:ILE:CG2	2.51	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:870[A]:HIS:O	1:A:871[A]:LYS:HB2	2.02	0.58
1:A:67:TYR:CD2	1:A:68:PRO:CD	2.86	0.58
1:A:139:ILE:HG21	1:A:301:ILE:HG12	1.86	0.58
1:A:445:GLU:HG3	1:A:950:HIS:NE2	2.18	0.58
1:A:869[B]:ASN:O	1:A:873[B]:LYS:HG2	2.03	0.58
1:A:1022:THR:O	1:A:1026:LEU:HB2	2.02	0.58
2:B:302:ASN:ND2	2:B:306:ALA:H	1.99	0.58
2:C:302:ASN:ND2	2:C:307:LEU:H	2.01	0.58
1:A:86:SER:OG	1:A:813[A]:LEU:HB2	2.03	0.58
1:A:1007:GLU:CD	1:A:1007:GLU:H	2.06	0.58
1:A:214:ASN:H	1:A:215:GLN:NE2	2.00	0.58
1:A:322:VAL:O	1:A:322:VAL:CG2	2.52	0.58
1:A:342:LEU:HD11	1:A:396:ILE:HG23	1.86	0.58
1:A:828[B]:ALA:CB	1:A:831[B]:ARG:HB2	2.34	0.58
1:A:38:ALA:O	1:A:39:LEU:HD13	2.02	0.58
1:A:559:GLY:HA2	1:A:922:LEU:H	1.68	0.58
1:A:986:MET:O	1:A:990:VAL:HG12	2.03	0.58
1:A:271:MET:HG3	2:B:387:SER:HB3	1.86	0.58
2:C:174:THR:N	2:C:177:GLN:HE21	2.00	0.58
2:C:174:THR:HB	2:C:177:GLN:HG3	1.86	0.58
2:C:254:ILE:HG22	2:C:254:ILE:O	2.03	0.58
1:A:102:ASP:OD1	1:A:103:PRO:HD2	2.04	0.58
1:A:844[B]:ILE:O	1:A:848[B]:VAL:HG22	2.04	0.58
1:A:984:LYS:O	1:A:987:THR:HG22	2.04	0.58
1:A:4:TRP:N	1:A:4:TRP:HD1	2.01	0.57
1:A:696[B]:MET:HE1	1:A:851[B]:LYS:HD3	1.86	0.57
2:C:161:ALA:HB1	2:C:185:LEU:HD22	1.85	0.57
1:A:992:ILE:HD12	1:A:995:LEU:HD23	1.86	0.57
1:A:1012:ILE:HG12	1:A:1012:ILE:O	2.04	0.57
2:C:165:TYR:HB2	2:C:181:ILE:HG21	1.85	0.57
1:A:39:LEU:CG	1:A:666[A]:ILE:HG21	2.34	0.57
1:A:667[A]:ARG:O	1:A:671[A]:ASP:HB2	2.04	0.57
1:A:121:LEU:HB3	1:A:125:VAL:HG23	1.86	0.57
2:B:335:THR:HG23	2:B:338:GLU:O	2.05	0.57
1:A:297:ALA:O	1:A:301:ILE:HG13	2.04	0.57
1:A:458:THR:O	1:A:462:ILE:HG13	2.04	0.57
2:C:166:LEU:O	2:C:170:GLU:HG2	2.05	0.57
1:A:435:ARG:O	1:A:439:ILE:HD13	2.04	0.57
1:A:661:LEU:HD22	1:A:662:TRP:N	2.20	0.57
1:A:876[B]:VAL:HG23	1:A:877[B]:PRO:HD3	1.86	0.57
2:B:224:ARG:HD2	2:B:224:ARG:N	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:359:GLN:HG3	2:C:360:ALA:N	2.19	0.57
1:A:792[A]:MET:HB2	1:A:794[A]:GLN:OE1	2.04	0.57
1:A:812[A]:MET:SD	1:A:814[A]:LYS:HE2	2.44	0.56
1:A:425:HIS:HB3	1:A:426:PRO:HD2	1.86	0.56
1:A:879[A]:THR:O	1:A:883[A]:ILE:HB	2.04	0.56
1:A:920:PHE:HE2	1:A:1010:SER:HB3	1.70	0.56
2:B:250:ILE:HG21	2:B:258:VAL:HG11	1.86	0.56
1:A:53:TYR:N	1:A:89:GLY:O	2.38	0.56
1:A:380:VAL:HG21	1:A:484:TYR:CB	2.21	0.56
1:A:991:ILE:HG22	1:A:995:LEU:HD21	1.87	0.56
1:A:1023:ALA:HB3	1:A:1024:PRO:CD	2.35	0.56
1:A:390:ILE:O	1:A:394:GLY:N	2.34	0.56
1:A:692[B]:ASP:O	1:A:696[B]:MET:HG2	2.05	0.56
2:C:302:ASN:HD21	2:C:307:LEU:H	1.53	0.56
1:A:535:TRP:HD1	1:A:536:PRO:N	2.02	0.56
1:A:876[A]:VAL:N	1:A:877[A]:PRO:HD2	2.21	0.56
2:B:162:GLN:NE2	2:B:205:GLN:H	2.04	0.56
2:B:340:ARG:HB3	2:B:354:ARG:HA	1.88	0.56
2:C:283:LEU:HD23	2:C:296:LEU:HG	1.88	0.56
1:A:27:GLY:O	1:A:31:ILE:HG22	2.05	0.56
1:A:42:LEU:HB2	1:A:673[A]:LEU:HD23	1.87	0.56
1:A:74:LEU:HD11	1:A:817[B]:ASN:HA	1.87	0.56
1:A:571:LEU:HD11	1:A:573:MET:HE3	1.85	0.56
1:A:357:LEU:HD21	1:A:411:ILE:HG21	1.88	0.56
2:B:287:VAL:HG12	2:B:294:LEU:HA	1.88	0.56
1:A:64:GLN:O	1:A:67:TYR:N	2.34	0.55
1:A:596:ILE:HD13	1:A:628:ILE:HD11	1.88	0.55
1:A:402:ALA:HB3	1:A:486:MET:HE1	1.89	0.55
1:A:83:ARG:HD2	1:A:675[B]:THR:OG1	2.06	0.55
2:B:230:ALA:HB3	2:B:233:ASN:OD1	2.06	0.55
2:C:106:PHE:CE2	2:C:359:GLN:HG2	2.33	0.55
1:A:534:HIS:CD2	1:A:535:TRP:N	2.75	0.55
1:A:56:GLN:HE21	1:A:56:GLN:HA	1.71	0.55
1:A:376:ILE:O	1:A:380:VAL:HG22	2.06	0.55
2:B:332:LEU:CD2	2:B:334:ASP:HB2	2.36	0.55
1:A:359:HIS:CD2	1:A:361:ARG:H	2.25	0.55
1:A:819[B]:ARG:HH21	1:A:819[B]:ARG:HG3	1.70	0.55
1:A:243:PHE:HB3	1:A:265:VAL:HG21	1.88	0.55
1:A:461:PHE:CE1	1:A:482:LYS:HD3	2.41	0.55
1:A:1036:LYS:O	1:A:1036:LYS:HG2	2.06	0.55
2:B:245:TRP:CE3	2:B:297:ARG:HD3	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:VAL:O	1:A:96:ILE:HA	2.06	0.55
1:A:872[A]:LEU:O	1:A:876[A]:VAL:HG23	2.07	0.55
2:C:279:ARG:HH11	2:C:279:ARG:HB2	1.72	0.55
2:C:382:LEU:HD22	2:C:382:LEU:O	2.07	0.55
1:A:42:LEU:HD12	1:A:42:LEU:H	1.70	0.55
1:A:258:TYR:HB2	1:A:260:ARG:HG2	1.88	0.55
1:A:525:TYR:C	1:A:525:TYR:CD2	2.78	0.55
1:A:65:VAL:HG21	1:A:91:SER:CB	2.37	0.54
1:A:54:PRO:CA	1:A:125:VAL:HG11	2.37	0.54
1:A:311:LEU:O	1:A:315:LEU:HG	2.08	0.54
1:A:349:VAL:HG22	1:A:990:VAL:HB	1.89	0.54
1:A:594:LYS:HD2	2:B:84:ILE:HD11	1.89	0.54
1:A:784[A]:ARG:HG2	1:A:799[A]:ALA:HB2	1.88	0.54
1:A:987:THR:O	1:A:991:ILE:HG12	2.07	0.54
1:A:83:ARG:HD3	1:A:94:TYR:HB2	1.89	0.54
1:A:1023:ALA:HB3	1:A:1024:PRO:HD3	1.89	0.54
1:A:44:ASP:OD1	1:A:103:PRO:HG3	2.08	0.54
1:A:62:GLU:O	1:A:66:THR:HB	2.07	0.54
1:A:76:VAL:HA	1:A:113:TYR:CE1	2.42	0.54
1:A:941:GLY:O	1:A:945:LEU:HB2	2.07	0.54
1:A:995:LEU:O	1:A:998:ILE:HG13	2.08	0.54
2:C:174:THR:HG22	2:C:176:THR:H	1.72	0.54
1:A:900:ILE:O	1:A:904:VAL:HG23	2.07	0.54
2:C:342:ILE:HB	2:C:378:VAL:CG1	2.38	0.54
1:A:83:ARG:CD	1:A:94:TYR:HB2	2.38	0.54
1:A:223:GLU:O	1:A:224:LEU:HD23	2.08	0.54
1:A:418:LEU:HD21	1:A:438:VAL:HG11	1.89	0.54
1:A:693[B]:ILE:HD12	1:A:820[B]:PRO:O	2.07	0.54
1:A:874[A]:LEU:O	1:A:878[A]:MET:HB2	2.07	0.54
1:A:136:VAL:HG22	1:A:670[A]:ILE:HG12	1.90	0.54
1:A:714[B]:LEU:HD12	1:A:714[B]:LEU:O	2.08	0.54
1:A:829[A]:ARG:HG3	1:A:829[A]:ARG:HH21	1.73	0.54
1:A:942:VAL:O	1:A:946:MET:HG2	2.07	0.54
2:C:83:ARG:HE	2:C:349:ARG:HH21	1.56	0.54
1:A:9:SER:HB3	1:A:495:VAL:HA	1.89	0.54
1:A:50:LYS:NZ	1:A:611:LYS:HZ1	2.05	0.54
1:A:67:TYR:O	1:A:71:THR:HG23	2.08	0.54
1:A:522:ILE:HG23	1:A:526:HIS:NE2	2.23	0.54
1:A:685[A]:VAL:HG11	1:A:696[A]:MET:HB3	1.88	0.54
2:B:121:TYR:OH	2:B:237:LYS:HE2	2.08	0.53
2:B:156:PRO:O	2:B:159:VAL:HG12	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:GLN:HG2	1:A:812[A]:MET:CG	2.33	0.53
1:A:383:PHE:HB2	1:A:384:GLN:OE1	2.08	0.53
1:A:948:LEU:HD23	1:A:1035:TYR:CD2	2.44	0.53
2:B:271:ARG:CD	2:B:306:ALA:HB1	2.38	0.53
2:C:140:VAL:HG23	2:C:219:THR:HA	1.90	0.53
1:A:685[B]:VAL:HG21	1:A:696[B]:MET:CB	2.37	0.53
2:B:343:THR:HG21	2:B:353:LYS:HE3	1.90	0.53
1:A:351:VAL:HG12	1:A:351:VAL:O	2.07	0.53
1:A:494:ILE:HG23	1:A:495:VAL:HG23	1.91	0.53
1:A:559:GLY:HA2	1:A:921:HIS:HB3	1.90	0.53
1:A:774[A]:GLN:CD	2:B:391:ILE:HG12	2.29	0.53
1:A:980:ARG:HH21	1:A:1028:LEU:HB3	1.72	0.53
1:A:534:HIS:CD2	1:A:534:HIS:C	2.82	0.53
1:A:588:MET:HE2	2:C:384:LEU:HD21	1.90	0.53
1:A:786[A]:LEU:O	1:A:797[A]:THR:HA	2.08	0.53
2:B:278:ILE:HG13	2:B:298:LEU:HD22	1.90	0.53
1:A:39:LEU:HG	1:A:666[A]:ILE:CG2	2.39	0.53
1:A:421:TRP:O	1:A:425:HIS:HB2	2.08	0.53
1:A:696[B]:MET:CE	1:A:851[B]:LYS:HB2	2.39	0.53
2:B:340:ARG:HB2	2:B:353:LYS:O	2.09	0.53
2:C:165:TYR:HE2	2:C:178:THR:HG23	1.73	0.53
1:A:564:GLN:HE22	1:A:664[A]:PRO:HG2	1.73	0.53
1:A:714[B]:LEU:HG	1:A:825[B]:TYR:CE2	2.43	0.53
1:A:550:VAL:HG23	1:A:913:TRP:CD1	2.44	0.53
1:A:534:HIS:CD2	1:A:535:TRP:HB3	2.44	0.53
1:A:876[A]:VAL:H	1:A:877[A]:PRO:HD2	1.73	0.53
2:C:284:LEU:HD12	2:C:295:GLN:CB	2.39	0.53
1:A:34:THR:O	1:A:35:PRO:C	2.47	0.53
2:B:360:ALA:HB2	2:B:365:THR:HG22	1.90	0.53
1:A:469:GLY:HA3	1:A:867[A]:ARG:HH22	1.74	0.52
1:A:525:TYR:CE1	1:A:977:ALA:HB1	2.44	0.52
1:A:918:MET:HG3	1:A:999:LEU:HD11	1.92	0.52
2:C:279:ARG:HB2	2:C:279:ARG:NH1	2.24	0.52
1:A:135:GLY:O	1:A:138:TRP:CD1	2.62	0.52
1:A:395:GLY:CA	1:A:478:LEU:HG	2.40	0.52
1:A:459:LEU:HD23	1:A:886[B]:LEU:HD13	1.92	0.52
1:A:751[A]:VAL:CG2	1:A:786[A]:LEU:HD11	2.39	0.52
1:A:456:ILE:HD12	1:A:938:ALA:HB1	1.91	0.52
1:A:888[B]:TYR:CE2	1:A:892:ARG:HA	2.44	0.52
1:A:946:MET:HG3	1:A:947:TYR:N	2.25	0.52
1:A:67:TYR:HB3	1:A:68:PRO:CD	2.35	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:338:LEU:HB3	1:A:393:LEU:CD1	2.34	0.52
1:A:393:LEU:O	1:A:393:LEU:HD13	2.09	0.52
1:A:641:THR:HG23	1:A:644:LYS:HB2	1.91	0.52
1:A:696[B]:MET:HE2	1:A:854[B]:THR:HG21	1.92	0.52
1:A:24:SER:HA	1:A:375:CYS:CB	2.37	0.52
1:A:359:HIS:HB3	1:A:362:SER:OG	2.09	0.52
1:A:451:PHE:C	1:A:451:PHE:CD2	2.83	0.52
1:A:729[A]:ASN:HB3	1:A:732[A]:LYS:HB2	1.92	0.52
1:A:26:TRP:NE1	1:A:379:ILE:HG23	2.19	0.52
1:A:139:ILE:CG2	1:A:301:ILE:HG12	2.39	0.52
1:A:525:TYR:CE2	1:A:529:LEU:HB2	2.45	0.52
1:A:982:ARG:O	1:A:986:MET:HG2	2.10	0.52
1:A:404:VAL:O	1:A:408:ILE:HG12	2.09	0.52
1:A:456:ILE:CD1	1:A:938:ALA:HB1	2.39	0.52
1:A:522:ILE:HD13	1:A:978:VAL:HG23	1.91	0.52
1:A:684[B]:LYS:O	1:A:856[B]:VAL:HA	2.10	0.52
1:A:143:ALA:HB2	1:A:606:PHE:CE1	2.45	0.52
1:A:185:LYS:HB3	1:A:766[A]:TYR:CD2	2.45	0.52
1:A:588:MET:CE	2:C:384:LEU:HD21	2.40	0.52
1:A:689[A]:VAL:HG12	1:A:690[A]:LEU:N	2.25	0.52
2:B:274:LYS:O	2:B:276:LEU:HD23	2.10	0.52
1:A:70:THR:O	1:A:74:LEU:HD13	2.10	0.52
1:A:879[B]:THR:HA	1:A:882[B]:ILE:HG22	1.92	0.52
1:A:1031:ILE:HB	1:A:1032:PRO:HD3	1.90	0.52
1:A:64:GLN:HA	1:A:67:TYR:CB	2.33	0.52
1:A:409:VAL:HG11	1:A:450:LEU:HD21	1.92	0.52
1:A:522:ILE:HG23	1:A:526:HIS:CD2	2.45	0.52
2:B:94:VAL:HG12	2:B:383:PHE:CZ	2.44	0.52
2:B:117:ASN:HD22	2:B:117:ASN:C	2.14	0.52
1:A:714[B]:LEU:HG	1:A:825[B]:TYR:OH	2.10	0.51
1:A:962:GLN:HG3	1:A:963:THR:N	2.24	0.51
2:B:120:GLN:HE22	2:B:243:PRO:CD	2.22	0.51
2:C:287:VAL:HB	2:C:294:LEU:HD23	1.93	0.51
1:A:16:VAL:HG11	1:A:495:VAL:HG11	1.92	0.51
1:A:356:PHE:CD2	1:A:986:MET:HB3	2.44	0.51
1:A:729[A]:ASN:C	1:A:729[A]:ASN:HD22	2.13	0.51
1:A:60:ILE:HA	1:A:63:ASN:HB3	1.91	0.51
1:A:459:LEU:HA	1:A:462:ILE:HG13	1.92	0.51
2:C:268:VAL:HG11	2:C:307:LEU:HD11	1.92	0.51
1:A:10:VAL:O	1:A:13:ARG:HG3	2.09	0.51
1:A:307:LYS:O	1:A:311:LEU:HG	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:571:LEU:HB3	1:A:663:VAL:O	2.10	0.51
1:A:40:PRO:HD3	1:A:389:ASN:HD21	1.74	0.51
1:A:330:LEU:HD13	1:A:567:GLU:HA	1.91	0.51
1:A:526:HIS:HA	1:A:529:LEU:HB3	1.93	0.51
1:A:577:LEU:HB3	1:A:578:PRO:HD2	1.92	0.51
1:A:838[A]:HIS:HA	1:A:841[A]:GLN:OE1	2.09	0.51
2:B:220:ALA:HB3	2:B:237:LYS:CB	2.41	0.51
2:B:267:THR:HG22	2:B:275:THR:HB	1.92	0.51
2:B:220:ALA:HB3	2:B:237:LYS:HB2	1.91	0.51
2:B:360:ALA:HA	2:B:365:THR:HA	1.91	0.51
1:A:42:LEU:HB3	1:A:136:VAL:HG21	1.92	0.51
1:A:239:THR:HG22	1:A:241:ASP:H	1.76	0.51
1:A:395:GLY:O	1:A:398:ILE:HG22	2.10	0.51
1:A:925:ALA:O	1:A:1012:ILE:HG13	2.11	0.51
1:A:9:SER:CB	1:A:495:VAL:HA	2.41	0.51
1:A:391:MET:SD	1:A:391:MET:N	2.83	0.51
1:A:991:ILE:HG21	1:A:1020:MET:HG2	1.91	0.51
2:C:94:VAL:HG21	2:C:385:ILE:HD11	1.93	0.51
2:C:359:GLN:HG3	2:C:360:ALA:H	1.75	0.51
1:A:16:VAL:HG11	1:A:495:VAL:CG1	2.41	0.51
1:A:275:ILE:O	1:A:608:LYS:HA	2.11	0.51
1:A:462:ILE:HB	1:A:463:PRO:HD3	1.92	0.51
1:A:525:TYR:HE1	1:A:977:ALA:HB1	1.76	0.51
1:A:714[B]:LEU:HG	1:A:825[B]:TYR:CZ	2.45	0.51
1:A:859[A]:SER:HA	1:A:863[A]:GLU:HB2	1.92	0.51
2:C:302:ASN:HD21	2:C:306:ALA:N	2.09	0.51
1:A:83:ARG:HH22	1:A:674[B]:SER:N	2.09	0.51
1:A:729[A]:ASN:HD22	1:A:732[A]:LYS:H	1.57	0.51
2:B:116:TYR:CD2	2:B:309:PRO:HG2	2.45	0.51
2:B:242:ASP:HB3	2:B:243:PRO:CD	2.41	0.51
1:A:707[A]:VAL:HG12	1:A:709[A]:GLY:H	1.75	0.50
1:A:888[A]:TYR:O	1:A:888[A]:TYR:CD1	2.64	0.50
1:A:1035:TYR:C	1:A:1037:LEU:H	2.13	0.50
2:C:327:ILE:HD13	2:C:367:LEU:HD21	1.91	0.50
2:C:358:PHE:HD2	2:C:368:ARG:NH2	2.09	0.50
1:A:816[B]:GLU:HB3	1:A:821[B]:THR:CG2	2.41	0.50
1:A:828[B]:ALA:CA	1:A:829[B]:ARG:CB	2.82	0.50
1:A:955:VAL:HG12	1:A:956:PRO:HD3	1.93	0.50
1:A:36:VAL:HG13	1:A:331:ILE:CG1	2.35	0.50
1:A:228:GLU:O	1:A:228:GLU:HG2	2.11	0.50
1:A:751[A]:VAL:O	1:A:771[A]:ARG:HD2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:340:ARG:HD2	2:B:395:LEU:CD1	2.40	0.50
1:A:69:LEU:HD22	1:A:117:VAL:HG13	1.93	0.50
1:A:112:GLU:HB2	1:A:113:TYR:CD1	2.47	0.50
1:A:568:GLY:O	1:A:630:LEU:HD12	2.10	0.50
1:A:431:ASP:CG	1:A:432:ASN:H	2.15	0.50
1:A:270:GLU:HG2	1:A:271:MET:N	2.24	0.50
1:A:279:ASN:HD22	1:A:605:VAL:H	1.55	0.50
2:C:124:VAL:O	2:C:235:VAL:HG13	2.11	0.50
1:A:36:VAL:CG1	1:A:331:ILE:HG23	2.41	0.50
1:A:46:GLN:O	1:A:46:GLN:HG2	2.07	0.50
1:A:337:ASN:HD22	1:A:338:LEU:HD23	1.76	0.50
1:A:338:LEU:HD11	1:A:390:ILE:HD13	1.93	0.50
1:A:340:GLY:O	1:A:344:GLU:HG3	2.12	0.50
1:A:904:VAL:N	1:A:905:PRO:CD	2.75	0.50
1:A:42:LEU:H	1:A:42:LEU:CD1	2.25	0.50
1:A:342:LEU:HD11	1:A:396:ILE:CG2	2.41	0.50
2:B:153:LEU:HD23	2:B:208:PHE:O	2.11	0.50
2:B:316:GLN:HE21	2:B:318:ASN:HD21	1.58	0.50
1:A:272:ARG:HB2	2:B:385:ILE:HG13	1.93	0.50
1:A:534:HIS:HD2	1:A:535:TRP:N	2.09	0.50
1:A:35:PRO:HG2	1:A:296:ASN:HD21	1.75	0.49
1:A:138:TRP:CD1	1:A:290:ILE:HD12	2.47	0.49
1:A:301:ILE:HD11	1:A:327:ARG:HB2	1.93	0.49
1:A:408:ILE:HB	1:A:986:MET:CE	2.42	0.49
1:A:926:THR:HA	1:A:1015:PRO:HG2	1.94	0.49
2:C:108:GLN:HA	2:C:108:GLN:OE1	2.12	0.49
1:A:996:LEU:O	1:A:999:LEU:HB3	2.12	0.49
1:A:338:LEU:HD11	1:A:390:ILE:CD1	2.42	0.49
1:A:480:PHE:HB3	1:A:484:TYR:CE2	2.47	0.49
2:B:116:TYR:CE2	2:B:309:PRO:HG2	2.47	0.49
2:B:125:GLN:NE2	2:C:228:ASN:H	1.99	0.49
2:B:339:GLN:HG3	2:B:357:VAL:CG2	2.42	0.49
1:A:85:PHE:CD2	1:A:814[B]:LYS:HG2	2.47	0.49
1:A:353:CYS:O	1:A:357:LEU:HB2	2.12	0.49
1:A:359:HIS:HB3	1:A:362:SER:CB	2.42	0.49
2:C:221:PHE:HD1	2:C:224:ARG:NH1	2.09	0.49
1:A:521:LEU:HD12	1:A:522:ILE:N	2.27	0.49
1:A:979:LEU:HD13	1:A:979:LEU:O	2.12	0.49
2:B:84:ILE:HG12	2:B:85:ASP:N	2.28	0.49
1:A:260:ARG:HG3	1:A:261:ASP:N	2.27	0.49
1:A:405:ASP:HA	1:A:408:ILE:HD11	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:573:MET:CE	1:A:668[A]:ASN:HD21	2.25	0.49
1:A:972:ALA:O	1:A:975:HIS:HD2	1.96	0.49
2:C:83:ARG:HE	2:C:349:ARG:NH2	2.11	0.49
2:C:106:PHE:CE1	2:C:321:SER:HB3	2.48	0.49
2:C:165:TYR:OH	2:C:199:ILE:HG22	2.13	0.49
2:C:254:ILE:O	2:C:254:ILE:CG2	2.60	0.49
2:C:352:PRO:HG3	2:C:395:LEU:HD12	1.94	0.49
1:A:402:ALA:HB3	1:A:486:MET:CE	2.43	0.49
1:A:602:VAL:HA	1:A:630:LEU:HA	1.94	0.49
1:A:788[A]:ILE:HB	1:A:796[A]:ILE:HG13	1.95	0.49
1:A:952:ILE:O	1:A:952:ILE:HG22	2.13	0.49
1:A:999:LEU:HB2	1:A:1017:ILE:CD1	2.43	0.49
2:B:384:LEU:O	2:B:385:ILE:C	2.50	0.49
1:A:456:ILE:HG12	1:A:886[A]:LEU:HD12	1.94	0.49
1:A:596:ILE:CG1	1:A:653:VAL:HG21	2.41	0.49
2:B:242:ASP:CB	2:B:243:PRO:HD3	2.42	0.49
2:C:323:PRO:C	2:C:324:MET:HG2	2.33	0.49
1:A:71:THR:HA	1:A:74:LEU:HD22	1.94	0.49
1:A:700[B]:ILE:O	1:A:703[B]:VAL:HG22	2.12	0.49
1:A:851[A]:LYS:HB3	1:A:852[A]:PRO:HD2	1.95	0.49
1:A:955:VAL:CG1	1:A:956:PRO:HD3	2.42	0.49
2:C:242:ASP:HB3	2:C:243:PRO:CD	2.37	0.49
1:A:210:LEU:HD23	1:A:770[A]:LEU:HD11	1.94	0.49
1:A:463:PRO:CB	1:A:875[A]:MET:HG3	2.43	0.49
1:A:68:PRO:HB3	1:A:120:LYS:HZ1	1.79	0.48
1:A:370:LEU:HB2	1:A:371:PRO:HD3	1.94	0.48
1:A:995:LEU:HA	1:A:998:ILE:HD11	1.93	0.48
2:C:268:VAL:CG1	2:C:276:LEU:HD11	2.43	0.48
1:A:29:TRP:HA	1:A:32:ILE:HG13	1.95	0.48
1:A:136:VAL:CG2	1:A:670[A]:ILE:HG12	2.43	0.48
1:A:521:LEU:HD12	1:A:522:ILE:HG13	1.93	0.48
1:A:576:THR:HG23	1:A:622:GLU:HB2	1.95	0.48
2:B:283:LEU:HD21	2:C:308:LYS:HE2	1.95	0.48
1:A:38:ALA:HB3	1:A:39:LEU:HD22	1.95	0.48
1:A:580:ILE:HD11	1:A:584:GLU:HG3	1.95	0.48
2:C:327:ILE:CD1	2:C:367:LEU:HD21	2.44	0.48
1:A:685[B]:VAL:HG13	1:A:685[B]:VAL:O	2.12	0.48
2:B:110:PHE:CE1	2:B:250:ILE:HG23	2.49	0.48
2:C:230:ALA:HB3	2:C:233:ASN:OD1	2.14	0.48
1:A:349:VAL:HG11	1:A:404:VAL:HG21	1.94	0.48
1:A:697[A]:ALA:HA	1:A:824[A]:ILE:HD11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:245:TRP:CD1	2:B:299:GLU:HG2	2.48	0.48
2:B:384:LEU:HD23	2:B:394:ALA:HB3	1.96	0.48
1:A:14:PHE:CE2	1:A:18:MET:HG3	2.48	0.48
1:A:54:PRO:HG2	1:A:61:VAL:HG22	1.96	0.48
1:A:378:PHE:O	1:A:381:MET:HB2	2.13	0.48
1:A:436:TRP:CD1	1:A:436:TRP:C	2.87	0.48
1:A:574:PRO:HB2	1:A:658:LEU:HD11	1.94	0.48
1:A:740[A]:VAL:O	1:A:744[A]:GLN:HG3	2.13	0.48
1:A:905:PRO:HA	1:A:908:LEU:HG	1.95	0.48
2:B:162:GLN:HE22	2:B:205:GLN:H	1.60	0.48
2:B:390:ASN:HD22	2:B:392:SER:H	1.62	0.48
1:A:590:GLN:HG2	1:A:594:LYS:HE3	1.96	0.48
1:A:840[A]:LEU:O	1:A:844[A]:ILE:HG13	2.13	0.48
2:B:242:ASP:HB3	2:B:243:PRO:HD3	1.95	0.48
1:A:376:ILE:HA	1:A:379:ILE:HD12	1.95	0.48
1:A:707[B]:VAL:HG11	1:A:840[B]:LEU:HD21	1.95	0.48
1:A:728[A]:ILE:HA	1:A:802[A]:ALA:HB2	1.96	0.48
1:A:42:LEU:HB2	1:A:673[A]:LEU:HD21	1.96	0.48
1:A:281:GLU:O	2:B:92:LEU:HD13	2.14	0.48
1:A:420:GLU:HG3	1:A:421:TRP:N	2.29	0.48
1:A:572:TYR:CE1	1:A:660:ASN:HB2	2.35	0.48
2:B:223:LEU:HD11	2:B:229:ILE:HG13	1.95	0.48
2:B:242:ASP:CG	2:B:243:PRO:HD3	2.34	0.48
2:B:329:SER:HA	2:B:365:THR:HG23	1.94	0.48
2:C:156:PRO:O	2:C:159:VAL:HG22	2.13	0.48
2:C:342:ILE:O	2:C:378:VAL:HG12	2.13	0.48
1:A:40:PRO:HD3	1:A:389:ASN:ND2	2.29	0.47
1:A:58:PRO:HA	1:A:62:GLU:CD	2.34	0.47
1:A:457:ILE:HG13	1:A:482:LYS:NZ	2.29	0.47
2:B:332:LEU:HD21	2:B:334:ASP:HB2	1.96	0.47
1:A:83:ARG:HB2	1:A:815[A]:THR:O	2.14	0.47
1:A:275:ILE:N	1:A:275:ILE:HD12	2.29	0.47
1:A:883[B]:ILE:O	1:A:887[B]:LEU:HG	2.14	0.47
2:B:94:VAL:HG11	2:B:350:PHE:HZ	1.79	0.47
1:A:533:LEU:HB3	1:A:1036:LYS:NZ	2.29	0.47
2:B:266:LEU:HD23	2:B:267:THR:H	1.79	0.47
1:A:210:LEU:HA	1:A:246:ILE:HD13	1.96	0.47
1:A:681[B]:ILE:HB	1:A:826[B]:ILE:CG1	2.43	0.47
1:A:831[A]:ARG:HG2	1:A:832[A]:ASP:N	2.30	0.47
2:C:164:GLU:O	2:C:168:LEU:HD22	2.14	0.47
1:A:359:HIS:HB3	1:A:362:SER:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:780[A]:PRO:O	1:A:804[A]:ILE:HD11	2.13	0.47
1:A:829[A]:ARG:HG3	1:A:829[A]:ARG:NH2	2.28	0.47
1:A:862[B]:PHE:HA	1:A:865[B]:LEU:HB3	1.96	0.47
2:C:110:PHE:HE2	2:C:317:LEU:HD23	1.79	0.47
1:A:718[A]:LEU:C	1:A:718[A]:LEU:HD23	2.35	0.47
1:A:837[A]:VAL:O	1:A:841[A]:GLN:HG3	2.15	0.47
1:A:888[B]:TYR:CD2	1:A:892:ARG:HA	2.50	0.47
1:A:992:ILE:O	1:A:996:LEU:HG	2.14	0.47
1:A:1007:GLU:O	1:A:1011:ARG:HD3	2.15	0.47
1:A:1014:ALA:N	1:A:1015:PRO:HD2	2.30	0.47
2:B:108:GLN:O	2:B:316:GLN:HG3	2.15	0.47
1:A:157:ARG:HG2	1:A:182:GLY:HA3	1.96	0.47
1:A:195:ARG:HD2	1:A:261:ASP:O	2.15	0.47
1:A:325:TYR:HE1	1:A:327:ARG:HG2	1.79	0.47
1:A:361:ARG:O	1:A:365:VAL:HG23	2.14	0.47
1:A:814[A]:LYS:O	1:A:820[A]:PRO:HA	2.14	0.47
1:A:848[A]:VAL:O	1:A:849[A]:GLN:HB2	2.14	0.47
1:A:888[A]:TYR:O	1:A:888[A]:TYR:CG	2.67	0.47
1:A:891:PHE:HB3	1:A:896:GLU:OE2	2.13	0.47
1:A:916:TRP:CZ3	1:A:917:TRP:HE3	2.33	0.47
1:A:984:LYS:NZ	1:A:1028:LEU:HD21	2.29	0.47
1:A:991:ILE:O	1:A:995:LEU:HD22	2.15	0.47
2:B:162:GLN:HG2	2:B:198:LEU:HD22	1.95	0.47
2:C:329:SER:HA	2:C:365:THR:HG22	1.95	0.47
1:A:443:SER:O	1:A:447:GLY:HA3	2.14	0.47
1:A:771[A]:ARG:HG3	1:A:772[A]:TYR:N	2.28	0.47
1:A:872[A]:LEU:HA	1:A:875[A]:MET:HB2	1.97	0.47
1:A:992:ILE:HA	1:A:995:LEU:CD2	2.44	0.47
1:A:574:PRO:CA	1:A:660:ASN:HA	2.42	0.47
2:B:110:PHE:CD1	2:B:250:ILE:HG12	2.50	0.47
2:C:199:ILE:HD12	2:C:200:ALA:N	2.28	0.47
2:C:281:TRP:HB2	2:C:298:LEU:HD23	1.96	0.47
1:A:154:ALA:HA	1:A:183:VAL:HG12	1.96	0.47
1:A:534:HIS:HD2	1:A:535:TRP:HB3	1.80	0.47
1:A:876[B]:VAL:N	1:A:877[B]:PRO:HD2	2.30	0.47
1:A:348:VAL:HG11	1:A:993:ALA:CB	2.45	0.46
1:A:348:VAL:HG11	1:A:993:ALA:HB1	1.97	0.46
1:A:461:PHE:CD1	1:A:482:LYS:HD3	2.50	0.46
1:A:572:TYR:HD2	1:A:626:THR:OG1	1.97	0.46
1:A:891:PHE:CZ	1:A:945:LEU:HB3	2.50	0.46
1:A:930:PHE:O	1:A:933:LEU:HB3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:LEU:HD23	1:A:15:LEU:N	2.29	0.46
1:A:23:LEU:HB3	1:A:379:ILE:CD1	2.43	0.46
1:A:550:VAL:HG21	1:A:909:VAL:HA	1.97	0.46
1:A:992:ILE:HD12	1:A:995:LEU:CD2	2.45	0.46
2:B:117:ASN:HD22	2:B:118:GLU:N	2.14	0.46
2:B:120:GLN:HE21	2:B:243:PRO:HD2	1.78	0.46
1:A:189:VAL:HG13	1:A:259:LEU:HD11	1.98	0.46
1:A:346:PHE:CD2	1:A:370:LEU:HD13	2.50	0.46
2:B:162:GLN:HE21	2:B:204:ILE:HG23	1.81	0.46
1:A:40:PRO:HD2	1:A:41:ASP:OD1	2.16	0.46
1:A:482:LYS:HE3	1:A:486:MET:HG3	1.97	0.46
1:A:876[A]:VAL:N	1:A:877[A]:PRO:CD	2.77	0.46
1:A:877[B]:PRO:O	1:A:881[B]:MET:HG2	2.16	0.46
1:A:381:MET:CE	1:A:392:SER:HB2	2.46	0.46
2:C:333:ILE:HG13	2:C:382:LEU:HD11	1.98	0.46
1:A:69:LEU:N	1:A:69:LEU:HD23	2.30	0.46
1:A:911:GLY:O	1:A:915:LEU:HG	2.15	0.46
1:A:980:ARG:NH2	1:A:1028:LEU:HB3	2.31	0.46
2:C:283:LEU:HD22	2:C:283:LEU:HA	1.71	0.46
1:A:29:TRP:C	1:A:31:ILE:N	2.69	0.46
1:A:779[A]:SER:OG	1:A:781[A]:GLN:HG2	2.16	0.46
2:B:252:GLU:HG3	2:B:253:SER:N	2.30	0.46
2:B:342:ILE:HB	2:B:378:VAL:HG13	1.98	0.46
1:A:360:VAL:O	1:A:364:LEU:HG	2.16	0.46
2:B:325:LEU:O	2:B:366:ALA:HA	2.16	0.46
2:C:268:VAL:HA	2:C:269:PRO:HD3	1.81	0.46
1:A:23:LEU:HD12	1:A:379:ILE:HD13	1.98	0.45
1:A:29:TRP:C	1:A:31:ILE:H	2.17	0.45
1:A:53:TYR:HA	1:A:89:GLY:O	2.15	0.45
1:A:61:VAL:O	1:A:65:VAL:HG13	2.16	0.45
1:A:69:LEU:HD13	1:A:117:VAL:HG11	1.97	0.45
1:A:183:VAL:HG11	2:B:382:LEU:HD22	1.97	0.45
1:A:421:TRP:HE1	1:A:425:HIS:CE1	2.34	0.45
1:A:600:PRO:O	1:A:631:LYS:HD2	2.16	0.45
1:A:746[A]:PHE:O	1:A:750[A]:ALA:HB3	2.16	0.45
2:B:117:ASN:HD22	2:B:119:TYR:N	2.10	0.45
2:C:84:ILE:HG21	2:C:89:THR:HG23	1.97	0.45
1:A:369:SER:CB	1:A:497:ILE:HD11	2.45	0.45
1:A:870[A]:HIS:O	1:A:871[A]:LYS:CB	2.64	0.45
1:A:947:TYR:HE1	1:A:980:ARG:HA	1.81	0.45
1:A:955:VAL:N	1:A:956:PRO:CD	2.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:339:GLN:HG3	2:C:357:VAL:HG23	1.97	0.45
1:A:69:LEU:HD22	1:A:117:VAL:CG1	2.46	0.45
1:A:215:GLN:O	1:A:235:GLY:HA3	2.17	0.45
1:A:519:ARG:HG2	1:A:523:ARG:HD2	1.97	0.45
1:A:553:PRO:C	1:A:555:ASN:H	2.20	0.45
1:A:904:VAL:HG22	1:A:937:ALA:HB1	1.97	0.45
1:A:572:TYR:HB3	1:A:626:THR:OG1	2.17	0.45
1:A:823[B]:TRP:N	1:A:823[B]:TRP:HD1	2.13	0.45
1:A:1014:ALA:N	1:A:1015:PRO:CD	2.79	0.45
2:C:250:ILE:O	2:C:294:LEU:N	2.49	0.45
1:A:435:ARG:HA	1:A:438:VAL:HG12	1.98	0.45
1:A:535:TRP:CD2	1:A:538:THR:HB	2.52	0.45
1:A:816[A]:GLU:O	1:A:817[A]:ASN:HB2	2.17	0.45
1:A:917:TRP:HD1	1:A:918:MET:HE2	1.81	0.45
1:A:998:ILE:HD12	1:A:1013:ALA:HB1	1.98	0.45
2:C:116:TYR:CE2	2:C:309:PRO:HG2	2.51	0.45
2:C:245:TRP:CE3	2:C:297:ARG:HD3	2.51	0.45
1:A:375:CYS:O	1:A:379:ILE:HG13	2.16	0.45
1:A:453:SER:HA	1:A:456:ILE:HD12	1.98	0.45
1:A:790[A]:THR:HB	1:A:791[A]:PRO:HD2	1.99	0.45
1:A:834[A]:VAL:HA	1:A:837[A]:VAL:HG22	1.98	0.45
1:A:1029:PHE:N	1:A:1029:PHE:CD2	2.81	0.45
1:A:237:LEU:HD23	1:A:243:PHE:CZ	2.52	0.45
1:A:774[A]:GLN:HE21	1:A:774[A]:GLN:HB2	1.55	0.45
1:A:67:TYR:CB	1:A:68:PRO:CD	2.95	0.45
1:A:463:PRO:HB2	1:A:875[A]:MET:HG3	1.99	0.45
1:A:816[B]:GLU:HB3	1:A:821[B]:THR:HG21	1.97	0.45
1:A:902:SER:O	1:A:905:PRO:HD2	2.17	0.45
1:A:474:LEU:O	1:A:474:LEU:HD12	2.18	0.45
1:A:930:PHE:CD2	1:A:1015:PRO:HB3	2.52	0.45
1:A:960:ASN:C	1:A:962:GLN:H	2.20	0.45
1:A:1016:MET:HB2	1:A:1016:MET:HE3	1.68	0.45
2:C:86:PRO:O	2:C:90:GLN:HG3	2.17	0.45
1:A:21:LEU:HD12	1:A:22:PHE:HD2	1.82	0.44
1:A:34:THR:HG22	1:A:35:PRO:O	2.18	0.44
1:A:64:GLN:C	1:A:67:TYR:H	2.17	0.44
2:B:344:VAL:O	2:B:344:VAL:HG12	2.17	0.44
1:A:418:LEU:CG	1:A:438:VAL:HG21	2.40	0.44
1:A:620:PRO:HB2	1:A:622:GLU:OE2	2.18	0.44
1:A:786[A]:LEU:HD23	1:A:786[A]:LEU:HA	1.86	0.44
1:A:836[B]:VAL:O	1:A:840[B]:LEU:HG	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:VAL:O	1:A:355:LEU:HB2	2.17	0.44
1:A:377:ALA:O	1:A:380:VAL:HG23	2.16	0.44
1:A:696[B]:MET:HE1	1:A:851[B]:LYS:HB2	1.99	0.44
2:B:110:PHE:CG	2:B:250:ILE:HG12	2.52	0.44
2:B:136:TYR:CD2	2:B:149:PRO:HB2	2.52	0.44
2:B:174:THR:HG22	2:B:175:ALA:N	2.32	0.44
2:B:223:LEU:O	2:B:224:ARG:HD2	2.17	0.44
1:A:56:GLN:HE21	1:A:56:GLN:C	2.20	0.44
1:A:689[A]:VAL:HG12	1:A:690[A]:LEU:H	1.80	0.44
2:B:134:LYS:HG2	2:B:152:ASP:HB2	1.98	0.44
1:A:349:VAL:CG1	1:A:404:VAL:HG21	2.48	0.44
1:A:526:HIS:CD2	1:A:526:HIS:H	2.36	0.44
1:A:685[B]:VAL:HG22	1:A:693[B]:ILE:HG22	1.99	0.44
1:A:690[A]:LEU:HD13	1:A:718[A]:LEU:HD21	2.00	0.44
1:A:696[B]:MET:HE3	1:A:851[B]:LYS:HB2	1.99	0.44
1:A:67:TYR:HD2	1:A:68:PRO:CG	2.31	0.44
1:A:195:ARG:HB3	1:A:262:VAL:HA	2.00	0.44
1:A:996:LEU:N	1:A:997:PRO:CD	2.80	0.44
2:B:322:GLU:HG3	2:B:323:PRO:HD2	1.99	0.44
2:C:117:ASN:HB3	2:C:120:GLN:HG3	2.00	0.44
1:A:18:MET:HA	1:A:21:LEU:HG	1.98	0.44
1:A:72:THR:HG22	1:A:113:TYR:HD2	1.83	0.44
1:A:797[A]:THR:O	1:A:800[A]:ASP:HB2	2.17	0.44
1:A:847[B]:LYS:HG3	1:A:847[B]:LYS:O	2.17	0.44
1:A:683[B]:ILE:HB	1:A:824[B]:ILE:HB	1.99	0.44
1:A:879[B]:THR:O	1:A:883[B]:ILE:HG12	2.18	0.44
2:B:153:LEU:HD23	2:B:153:LEU:H	1.83	0.44
2:C:266:LEU:HB3	2:C:276:LEU:HD12	2.00	0.44
1:A:128:GLU:HA	1:A:128:GLU:OE1	2.18	0.44
1:A:157:ARG:HG3	1:A:183:VAL:N	2.32	0.44
1:A:380:VAL:HB	1:A:484:TYR:CD2	2.52	0.44
1:A:492:LEU:O	1:A:496:VAL:N	2.48	0.44
1:A:572:TYR:CE2	1:A:574:PRO:HG3	2.53	0.44
1:A:846[B]:GLU:O	1:A:847[B]:LYS:HB3	2.18	0.44
1:A:910:GLY:HA3	1:A:1022:THR:HG21	2.00	0.44
2:B:242:ASP:CB	2:B:243:PRO:CD	2.96	0.44
1:A:42:LEU:CD1	1:A:42:LEU:N	2.81	0.43
1:A:846[B]:GLU:O	1:A:847[B]:LYS:CB	2.66	0.43
1:A:1000:TRP:CE3	1:A:1000:TRP:HA	2.52	0.43
2:B:153:LEU:HD23	2:B:153:LEU:N	2.33	0.43
2:C:223:LEU:HD11	2:C:229:ILE:HG13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356:PHE:HD2	1:A:986:MET:CB	2.30	0.43
1:A:419:GLU:O	1:A:423:HIS:HD2	2.01	0.43
1:A:545:LEU:HA	1:A:548:LEU:CD2	2.46	0.43
1:A:633:GLN:HG2	1:A:636:TRP:CZ2	2.52	0.43
1:A:661:LEU:HD13	1:A:663:VAL:CG2	2.48	0.43
1:A:573:MET:HA	1:A:624:VAL:O	2.18	0.43
1:A:707[B]:VAL:HG22	1:A:708[B]:PRO:HD2	2.00	0.43
2:B:85:ASP:HA	2:B:86:PRO:HD3	1.81	0.43
2:B:144:VAL:HG11	2:B:218:ILE:HD11	2.00	0.43
2:B:287:VAL:CG1	2:B:294:LEU:HD23	2.48	0.43
1:A:395:GLY:HA3	1:A:478:LEU:HG	2.00	0.43
1:A:413:ASN:O	1:A:417:ARG:HB2	2.18	0.43
1:A:906:PHE:O	1:A:909:VAL:HB	2.18	0.43
1:A:987:THR:O	1:A:990:VAL:HG13	2.18	0.43
2:B:147:GLY:O	2:B:211:LYS:HD3	2.17	0.43
2:B:266:LEU:HD23	2:B:267:THR:N	2.33	0.43
1:A:27:GLY:HA2	1:A:30:THR:OG1	2.19	0.43
1:A:373:GLY:O	1:A:376:ILE:HG22	2.17	0.43
1:A:716[B]:GLU:O	1:A:717[B]:ARG:C	2.57	0.43
1:A:887[B]:LEU:HD13	1:A:897:ALA:HB1	1.99	0.43
1:A:999:LEU:HB2	1:A:1017:ILE:HD11	2.01	0.43
1:A:335:ILE:HD13	1:A:335:ILE:HA	1.88	0.43
1:A:936:VAL:HG11	1:A:1020:MET:SD	2.58	0.43
1:A:23:LEU:O	1:A:379:ILE:HD11	2.19	0.43
1:A:68:PRO:O	1:A:72:THR:OG1	2.36	0.43
1:A:121:LEU:HB3	1:A:125:VAL:CG2	2.49	0.43
1:A:210:LEU:O	1:A:210:LEU:HD12	2.18	0.43
1:A:576:THR:HG22	1:A:622:GLU:O	2.19	0.43
1:A:837[A]:VAL:HG21	1:A:862[A]:PHE:CD2	2.53	0.43
1:A:871[B]:LYS:HD3	1:A:871[B]:LYS:N	2.33	0.43
1:A:1000:TRP:HA	1:A:1000:TRP:HE3	1.84	0.43
2:B:161:ALA:HB3	2:B:185:LEU:HD11	2.00	0.43
1:A:36:VAL:O	1:A:331:ILE:HD11	2.19	0.43
1:A:573:MET:HE3	1:A:668[A]:ASN:HD21	1.83	0.43
1:A:826[B]:ILE:HG12	1:A:826[B]:ILE:O	2.19	0.43
1:A:948:LEU:HD12	1:A:948:LEU:HA	1.86	0.43
2:C:121:TYR:OH	2:C:237:LYS:HD3	2.19	0.43
2:C:333:ILE:CG1	2:C:382:LEU:HD11	2.48	0.43
1:A:40:PRO:CD	1:A:389:ASN:HD21	2.32	0.43
1:A:611:LYS:HE3	1:A:612:ALA:O	2.19	0.43
2:C:165:TYR:CE2	2:C:178:THR:HG23	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:VAL:HG12	1:A:284:VAL:HG11	2.01	0.42
2:B:241:MET:O	2:B:242:ASP:C	2.56	0.42
2:C:332:LEU:C	2:C:332:LEU:HD23	2.40	0.42
1:A:97:PHE:CZ	1:A:106:ALA:HB1	2.54	0.42
1:A:341:LYS:O	1:A:345:GLU:HG3	2.18	0.42
1:A:446:VAL:O	1:A:450:LEU:HG	2.19	0.42
1:A:482:LYS:C	1:A:484:TYR:H	2.21	0.42
1:A:666[B]:ILE:N	1:A:666[B]:ILE:HD12	2.34	0.42
2:B:285:PRO:HA	2:C:308:LYS:HE3	2.00	0.42
2:B:388:GLU:O	2:B:389:ALA:HB3	2.18	0.42
2:C:94:VAL:CG2	2:C:385:ILE:HD11	2.49	0.42
2:C:257:LEU:HD13	2:C:257:LEU:HA	1.69	0.42
2:C:372:ALA:O	2:C:375:GLU:HB2	2.19	0.42
1:A:29:TRP:HA	1:A:32:ILE:CG1	2.50	0.42
1:A:564:GLN:HE22	1:A:664[B]:PRO:HG2	1.83	0.42
1:A:874[B]:LEU:HD13	1:A:874[B]:LEU:O	2.20	0.42
1:A:1023:ALA:O	1:A:1027:SER:N	2.53	0.42
2:B:245:TRP:CZ3	2:B:297:ARG:HD3	2.54	0.42
1:A:348:VAL:HG12	1:A:349:VAL:N	2.35	0.42
1:A:464:ILE:HG12	1:A:875[A]:MET:CE	2.49	0.42
2:B:388:GLU:CG	2:B:389:ALA:N	2.82	0.42
2:C:190:MET:HA	2:C:191:PRO:HD3	1.91	0.42
1:A:35:PRO:HG2	1:A:296:ASN:ND2	2.33	0.42
1:A:203:LEU:HD23	1:A:203:LEU:HA	1.82	0.42
1:A:325:TYR:CE1	1:A:327:ARG:HG2	2.54	0.42
1:A:442:ALA:O	1:A:446:VAL:HG12	2.20	0.42
1:A:779[A]:SER:H	1:A:782[A]:ALA:HB3	1.85	0.42
1:A:876[B]:VAL:CG2	1:A:877[B]:PRO:HD3	2.49	0.42
1:A:969:LEU:HD12	1:A:969:LEU:C	2.40	0.42
1:A:195:ARG:CB	1:A:262:VAL:HA	2.49	0.42
1:A:873[A]:LYS:C	1:A:874[A]:LEU:HD12	2.40	0.42
2:C:220:ALA:HB3	2:C:237:LYS:HB2	2.01	0.42
1:A:121:LEU:HD11	1:A:127:ALA:HB2	2.01	0.42
1:A:410:MET:SD	1:A:498:PRO:HG3	2.59	0.42
1:A:483:THR:O	1:A:483:THR:HG22	2.20	0.42
1:A:517:LEU:C	1:A:519:ARG:H	2.23	0.42
1:A:559:GLY:HA2	1:A:922:LEU:N	2.35	0.42
1:A:693[A]:ILE:HG12	1:A:694[A]:ASP:N	2.34	0.42
1:A:704[A]:ALA:O	1:A:710[A]:VAL:HG21	2.19	0.42
1:A:800[A]:ASP:OD2	2:C:253:SER:HB2	2.20	0.42
1:A:841[A]:GLN:HB3	1:A:858[A]:PHE:CE1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:992:ILE:O	1:A:995:LEU:HB2	2.19	0.42
2:B:83:ARG:HD3	2:C:90:GLN:OE1	2.20	0.42
2:B:212:ALA:HA	2:B:213:PRO:HD3	1.80	0.42
2:C:223:LEU:C	2:C:224:ARG:HD2	2.39	0.42
1:A:67:TYR:CD2	1:A:68:PRO:N	2.87	0.42
1:A:535:TRP:C	1:A:535:TRP:HD1	2.18	0.42
1:A:944:MET:SD	1:A:980:ARG:HD2	2.60	0.42
1:A:980:ARG:O	1:A:983:PRO:HD2	2.19	0.42
2:B:123:ILE:HD11	2:B:237:LYS:HE3	2.02	0.42
2:B:164:GLU:O	2:B:168:LEU:HB2	2.20	0.42
2:C:110:PHE:CE2	2:C:317:LEU:HD23	2.55	0.42
1:A:19:GLY:O	1:A:23:LEU:HD23	2.20	0.42
1:A:885[B]:VAL:HG12	1:A:885[B]:VAL:O	2.20	0.42
1:A:188:GLN:NE2	1:A:268:GLY:HA3	2.34	0.42
1:A:525:TYR:OH	1:A:980:ARG:NH2	2.53	0.42
1:A:675[A]:THR:HB	1:A:859[A]:SER:OG	2.19	0.42
1:A:841[A]:GLN:HG3	1:A:841[A]:GLN:H	1.55	0.42
1:A:1013:ALA:C	1:A:1015:PRO:HD2	2.40	0.42
1:A:300:VAL:O	1:A:304:VAL:HG23	2.20	0.41
1:A:612:ALA:O	1:A:614:THR:N	2.46	0.41
1:A:687[A]:GLY:O	1:A:820[A]:PRO:HB2	2.19	0.41
1:A:947:TYR:CE1	1:A:980:ARG:HA	2.55	0.41
1:A:982:ARG:CB	1:A:983:PRO:HD3	2.42	0.41
2:B:332:LEU:HA	2:B:341:VAL:HG12	2.02	0.41
1:A:412:GLU:HG3	1:A:982:ARG:HG2	2.02	0.41
1:A:907:ALA:CB	1:A:933:LEU:HD11	2.50	0.41
2:B:84:ILE:HG22	2:C:91:ASN:CG	2.41	0.41
2:B:264:PHE:CE1	2:B:296:LEU:HD11	2.55	0.41
2:B:307:LEU:HD12	2:B:307:LEU:H	1.84	0.41
1:A:20:ALA:O	1:A:24:SER:HB3	2.21	0.41
1:A:40:PRO:O	1:A:473:ARG:HD2	2.20	0.41
1:A:243:PHE:O	1:A:246:ILE:HG13	2.20	0.41
1:A:553:PRO:C	1:A:555:ASN:N	2.73	0.41
1:A:575:SER:N	1:A:659:ALA:O	2.53	0.41
1:A:1014:ALA:HA	1:A:1017:ILE:CG1	2.47	0.41
1:A:39:LEU:HG	1:A:666[B]:ILE:HG21	2.01	0.41
1:A:535:TRP:O	1:A:539:THR:HG23	2.20	0.41
1:A:834[A]:VAL:HG13	1:A:838[A]:HIS:HD2	1.86	0.41
1:A:61:VAL:HG12	1:A:62:GLU:N	2.35	0.41
1:A:191:ILE:CD1	1:A:206:VAL:HG11	2.47	0.41
1:A:445:GLU:OE1	1:A:445:GLU:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:456:ILE:HG12	1:A:886[A]:LEU:HB3	2.02	0.41
1:A:466:THR:O	1:A:871[A]:LYS:HE2	2.20	0.41
1:A:531:LYS:HB2	1:A:531:LYS:HE3	1.85	0.41
2:C:330:GLN:CD	2:C:330:GLN:H	2.24	0.41
2:C:395:LEU:O	2:C:399:ARG:HG3	2.21	0.41
1:A:348:VAL:HG21	1:A:993:ALA:HB1	2.01	0.41
1:A:683[A]:ILE:HB	1:A:824[A]:ILE:HB	2.02	0.41
1:A:690[A]:LEU:HD23	1:A:690[A]:LEU:HA	1.87	0.41
1:A:786[A]:LEU:HD12	1:A:798[A]:LEU:HD22	2.02	0.41
2:B:174:THR:HB	2:B:177:GLN:H	1.85	0.41
2:B:259:LYS:HE3	2:B:259:LYS:HB2	1.86	0.41
2:B:266:LEU:HB2	2:B:278:ILE:HG12	2.03	0.41
1:A:54:PRO:HG2	1:A:61:VAL:HG13	2.02	0.41
1:A:114:LEU:O	1:A:118:GLN:HG2	2.20	0.41
1:A:277:GLU:OE2	1:A:590:GLN:HG3	2.20	0.41
1:A:495:VAL:HG12	1:A:495:VAL:O	2.20	0.41
1:A:522:ILE:O	1:A:526:HIS:CD2	2.68	0.41
1:A:874[B]:LEU:C	1:A:877[B]:PRO:HD2	2.41	0.41
1:A:39:LEU:N	1:A:39:LEU:CD2	2.83	0.41
1:A:519:ARG:CG	1:A:523:ARG:HD2	2.51	0.41
1:A:840[B]:LEU:O	1:A:844[B]:ILE:HG13	2.21	0.41
1:A:911:GLY:HA3	1:A:930:PHE:HE2	1.86	0.41
2:B:162:GLN:NE2	2:B:204:ILE:HG23	2.36	0.41
2:B:223:LEU:HD23	2:B:223:LEU:HA	1.82	0.41
1:A:157:ARG:CG	1:A:182:GLY:HA3	2.51	0.41
1:A:179:SER:O	1:A:612:ALA:HB1	2.21	0.41
1:A:192:ASP:HB3	1:A:195:ARG:CG	2.51	0.41
1:A:395:GLY:HA2	1:A:398:ILE:HG22	2.02	0.41
1:A:532:VAL:HG21	1:A:1029:PHE:HB3	2.02	0.41
1:A:572:TYR:HE2	1:A:592:THR:HG21	1.86	0.41
1:A:700[A]:ILE:HD12	1:A:844[A]:ILE:HG12	2.02	0.41
1:A:789[A]:LEU:HA	1:A:789[A]:LEU:HD23	1.84	0.41
1:A:1029:PHE:C	1:A:1032:PRO:HD2	2.41	0.41
2:B:334:ASP:OD2	2:B:335:THR:O	2.38	0.41
2:C:84:ILE:CG2	2:C:89:THR:HG23	2.51	0.41
2:C:241:MET:O	2:C:244:VAL:HB	2.20	0.41
2:C:317:LEU:C	2:C:317:LEU:CD1	2.89	0.41
1:A:412:GLU:CG	1:A:982:ARG:HG2	2.50	0.41
1:A:779[A]:SER:HB2	1:A:780[A]:PRO:HD2	2.03	0.41
1:A:836[A]:VAL:O	1:A:840[A]:LEU:HG	2.22	0.41
1:A:852[A]:PRO:HB2	1:A:853[A]:GLY:H	1.66	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:155:ILE:HA	2:B:156:PRO:HD3	1.83	0.41
2:B:390:ASN:O	2:B:391:ILE:C	2.58	0.41
2:C:153:LEU:HD12	2:C:229:ILE:HG21	2.01	0.41
1:A:451:PHE:C	1:A:451:PHE:HD2	2.24	0.40
1:A:874[A]:LEU:HD12	1:A:874[A]:LEU:N	2.36	0.40
1:A:991:ILE:HG21	1:A:1020:MET:CG	2.51	0.40
1:A:992:ILE:HA	1:A:995:LEU:HD22	2.02	0.40
1:A:36:VAL:CG2	1:A:37:ASP:N	2.84	0.40
1:A:357:LEU:HD21	1:A:411:ILE:CG2	2.51	0.40
1:A:461:PHE:HD2	1:A:461:PHE:HA	1.71	0.40
1:A:526:HIS:N	1:A:527:PRO:CD	2.84	0.40
1:A:714[B]:LEU:HB2	1:A:717[B]:ARG:HB2	2.03	0.40
1:A:960:ASN:CB	1:A:961:PRO:HD3	2.41	0.40
2:C:266:LEU:HD11	2:C:298:LEU:HD12	2.02	0.40
1:A:50:LYS:NZ	1:A:611:LYS:NZ	2.68	0.40
1:A:661:LEU:CD2	1:A:827[A]:ASP:HB2	2.52	0.40
1:A:971:GLU:O	1:A:975:HIS:HB3	2.21	0.40
2:C:151:LEU:C	2:C:151:LEU:HD12	2.42	0.40
1:A:56:GLN:CA	1:A:56:GLN:NE2	2.83	0.40
1:A:102:ASP:O	1:A:105:TRP:HB3	2.20	0.40
1:A:358:TRP:CH2	1:A:518:ASN:ND2	2.89	0.40
1:A:381:MET:HE2	1:A:386:LEU:HD23	2.02	0.40
1:A:392:SER:HA	1:A:481:THR:HG21	2.04	0.40
2:C:137:PRO:C	2:C:138:LEU:HD12	2.40	0.40
1:A:109:ARG:HA	1:A:109:ARG:HD3	1.76	0.40
1:A:150:LYS:HE3	1:A:150:LYS:HB2	1.88	0.40
1:A:272:ARG:HE	2:B:385:ILE:HB	1.86	0.40
1:A:368:ILE:O	1:A:371:PRO:HD2	2.22	0.40
1:A:954:ALA:HB3	1:A:956:PRO:HD2	2.03	0.40
2:B:185:LEU:HD12	2:B:185:LEU:HA	1.75	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	A	1149/1054 (109%)	1003 (87%)	119 (10%)	27 (2%)	6 34
2	B	320/336 (95%)	279 (87%)	35 (11%)	6 (2%)	8 37
2	C	322/336 (96%)	293 (91%)	28 (9%)	1 (0%)	41 74
All	All	1791/1726 (104%)	1575 (88%)	182 (10%)	34 (2%)	9 37

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	35	PRO
1	A	67	TYR
1	A	638	PRO
1	A	813[A]	LEU
1	A	814[A]	LYS
1	A	814[B]	LYS
1	A	829[A]	ARG
1	A	829[B]	ARG
1	A	847[A]	LYS
1	A	847[B]	LYS
2	B	385	ILE
2	C	172	GLY
1	A	36	VAL
1	A	295	LYS
2	B	99	VAL
2	B	387	SER
1	A	40	PRO
1	A	385	GLY
1	A	774[A]	GLN
1	A	1027	SER
2	B	242	ASP
2	B	348	GLY
2	B	389	ALA
1	A	34	THR
1	A	426	PRO
1	A	613	GLU
1	A	711[A]	ALA
1	A	711[B]	ALA
1	A	835[A]	SER
1	A	835[B]	SER
1	A	45	VAL

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Mol	Chain	Res	Type
1	A	222	ILE
1	A	961	PRO
1	A	1017	ILE

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	A	956/871 (110%)	811 (85%)	145 (15%)	3 15
2	B	263/275 (96%)	221 (84%)	42 (16%)	2 13
2	C	265/275 (96%)	235 (89%)	30 (11%)	6 25
All	All	1484/1421 (104%)	1267 (85%)	217 (15%)	3 16

All (217) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	TRP
1	A	5	ILE
1	A	7	ARG
1	A	8	ARG
1	A	12	ASN
1	A	24	SER
1	A	26	TRP
1	A	31	ILE
1	A	32	ILE
1	A	39	LEU
1	A	41	ASP
1	A	42	LEU
1	A	46	GLN
1	A	48	ILE
1	A	53	TYR
1	A	56	GLN
1	A	62	GLU
1	A	69	LEU
1	A	72	THR

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Mol	Chain	Res	Type
1	A	73	MET
1	A	81	THR
1	A	96	ILE
1	A	98	GLU
1	A	111	LEU
1	A	128	GLU
1	A	134	THR
1	A	157	ARG
1	A	170	THR
1	A	184	VAL
1	A	203	LEU
1	A	215	GLN
1	A	222	ILE
1	A	228	GLU
1	A	232	ARG
1	A	241	ASP
1	A	260	ARG
1	A	288	VAL
1	A	312	LYS
1	A	323	THR
1	A	331	ILE
1	A	336	ASP
1	A	339	SER
1	A	343	LEU
1	A	347	ILE
1	A	348	VAL
1	A	355	LEU
1	A	374	LEU
1	A	376	ILE
1	A	380	VAL
1	A	384	GLN
1	A	386	LEU
1	A	390	ILE
1	A	391	MET
1	A	393	LEU
1	A	403	MET
1	A	405	ASP
1	A	412	GLU
1	A	419	GLU
1	A	432	ASN
1	A	435	ARG
1	A	445	GLU

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Mol	Chain	Res	Type
1	A	451	PHE
1	A	452	ILE
1	A	455	LEU
1	A	457	ILE
1	A	459	LEU
1	A	461	PHE
1	A	471	GLU
1	A	474	LEU
1	A	475	PHE
1	A	492	LEU
1	A	525	TYR
1	A	534	HIS
1	A	550	VAL
1	A	560	GLU
1	A	567	GLU
1	A	569	ASP
1	A	604	ARG
1	A	611	LYS
1	A	618	SER
1	A	624	VAL
1	A	630	LEU
1	A	637	ARG
1	A	641	THR
1	A	642	MET
1	A	649	LEU
1	A	660	ASN
1	A	661	LEU
1	A	671[A]	ASP
1	A	671[B]	ASP
1	A	688[A]	THR
1	A	688[B]	THR
1	A	693[A]	ILE
1	A	693[B]	ILE
1	A	696[A]	MET
1	A	696[B]	MET
1	A	712[A]	SER
1	A	712[B]	SER
1	A	722[A]	ARG
1	A	727[A]	GLU
1	A	729[A]	ASN
1	A	731[A]	GLU
1	A	748[A]	THR

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Mol	Chain	Res	Type
1	A	756[A]	VAL
1	A	763[A]	ILE
1	A	769[A]	ASN
1	A	770[A]	LEU
1	A	771[A]	ARG
1	A	774[A]	GLN
1	A	778[A]	ASP
1	A	781[A]	GLN
1	A	783[A]	LEU
1	A	786[A]	LEU
1	A	789[A]	LEU
1	A	803[A]	ASP
1	A	804[A]	ILE
1	A	834[A]	VAL
1	A	834[B]	VAL
1	A	841[A]	GLN
1	A	841[B]	GLN
1	A	856[A]	VAL
1	A	856[B]	VAL
1	A	865[A]	LEU
1	A	865[B]	LEU
1	A	878[A]	MET
1	A	878[B]	MET
1	A	899	LEU
1	A	944	MET
1	A	945	LEU
1	A	968	LYS
1	A	975	HIS
1	A	979	LEU
1	A	984	LYS
1	A	986	MET
1	A	987	THR
1	A	990	VAL
1	A	992	ILE
1	A	995	LEU
1	A	1007	GLU
1	A	1020	MET
1	A	1021	ILE
1	A	1022	THR
1	A	1035	TYR
1	A	1037	LEU
1	A	1039	TRP

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Mol	Chain	Res	Type
2	B	84	ILE
2	B	94	VAL
2	B	98	THR
2	B	105	THR
2	B	117	ASN
2	B	121	TYR
2	B	135	VAL
2	B	138	LEU
2	B	145	GLN
2	B	151	LEU
2	B	159	VAL
2	B	163	SER
2	B	185	LEU
2	B	199	ILE
2	B	224	ARG
2	B	233	ASN
2	B	241	MET
2	B	263	GLN
2	B	266	LEU
2	B	268	VAL
2	B	273	ASP
2	B	275	THR
2	B	276	LEU
2	B	280	LYS
2	B	282	THR
2	B	283	LEU
2	B	291	THR
2	B	302	ASN
2	B	304	ASP
2	B	319	THR
2	B	335	THR
2	B	344	VAL
2	B	349	ARG
2	B	351	VAL
2	B	359	GLN
2	B	377	VAL
2	B	378	VAL
2	B	385	ILE
2	B	390	ASN
2	B	392	SER
2	B	395	LEU
2	B	396	GLU

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Mol	Chain	Res	Type
2	C	96	THR
2	C	98	THR
2	C	100	THR
2	C	104	LEU
2	C	105	THR
2	C	118	GLU
2	C	120	GLN
2	C	121	TYR
2	C	145	GLN
2	C	150	LEU
2	C	168	LEU
2	C	185	LEU
2	C	187	LEU
2	C	207	ARG
2	C	228	ASN
2	C	235	VAL
2	C	257	LEU
2	C	267	THR
2	C	268	VAL
2	C	283	LEU
2	C	287	VAL
2	C	298	LEU
2	C	304	ASP
2	C	317	LEU
2	C	324	MET
2	C	351	VAL
2	C	364	VAL
2	C	365	THR
2	C	367	LEU
2	C	382	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	GLN
1	A	115	ASN
1	A	194	GLN
1	A	215	GLN
1	A	238	GLN
1	A	279	ASN
1	A	329	GLN
1	A	337	ASN

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Mol	Chain	Res	Type
1	A	359	HIS
1	A	389	ASN
1	A	413	ASN
1	A	423	HIS
1	A	470	GLN
1	A	526	HIS
1	A	534	HIS
1	A	564	GLN
1	A	566	ASN
1	A	629	GLN
1	A	635	GLN
1	A	660	ASN
1	A	729[A]	ASN
1	A	744[A]	GLN
1	A	769[A]	ASN
1	A	795[A]	GLN
1	A	975	HIS
2	B	90	GLN
2	B	108	GLN
2	B	117	ASN
2	B	120	GLN
2	B	125	GLN
2	B	177	GLN
2	B	302	ASN
2	B	316	GLN
2	B	330	GLN
2	B	359	GLN
2	B	390	ASN
2	C	145	GLN
2	C	177	GLN
2	C	228	ASN
2	C	233	ASN
2	C	263	GLN
2	C	302	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides 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 (i)

6.1 Protein, DNA and RNA chains (i)

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	A	1027/1054 (97%)	0.63	158 (15%)	2	3	2, 106, 283, 420	96 (9%)
2	B	322/336 (95%)	-0.22	4 (1%)	79	77	2, 33, 92, 166	0
2	C	324/336 (96%)	-0.20	3 (0%)	84	83	2, 33, 81, 209	0
All	All	1673/1726 (96%)	0.31	165 (9%)	7	10	2, 54, 257, 420	96 (5%)

All (165) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	539	THR	9.7
1	A	386	LEU	8.0
1	A	438	VAL	7.8
2	C	402	SER	7.7
1	A	890	ALA	7.7
1	A	392	SER	7.5
1	A	68	PRO	7.2
1	A	423	HIS	6.5
1	A	1043	HIS	6.1
1	A	14	PHE	5.8
1	A	428	ALA	5.6
1	A	552	TRP	5.6
1	A	495	VAL	5.5
1	A	481	THR	5.4
1	A	441	ASP	5.4
1	A	956	PRO	5.2
1	A	895	GLY	5.2
1	A	815[A]	THR	5.1
1	A	445	GLU	5.1
1	A	12	ASN	5.0
1	A	847[A]	LYS	4.9
1	A	494	ILE	4.9
1	A	862[A]	PHE	4.7

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Mol	Chain	Res	Type	RSRZ
1	A	903	SER	4.6
1	A	69	LEU	4.5
1	A	896	GLU	4.4
1	A	873[A]	LYS	4.4
1	A	407	ALA	4.3
1	A	496	VAL	4.3
1	A	426	PRO	4.3
1	A	437	GLN	4.3
2	B	79	ALA	4.2
1	A	422	GLN	4.1
1	A	429	THR	4.0
1	A	449	ALA	3.9
1	A	35	PRO	3.9
1	A	418	LEU	3.9
1	A	712[A]	SER	3.9
1	A	434	THR	3.8
1	A	81	THR	3.8
1	A	44	ASP	3.7
1	A	817[A]	ASN	3.7
1	A	827[A]	ASP	3.7
1	A	832[A]	ASP	3.6
1	A	425	HIS	3.6
1	A	848[A]	VAL	3.5
1	A	639	GLY	3.4
1	A	556	LYS	3.4
1	A	962	GLN	3.4
1	A	13	ARG	3.4
1	A	436	TRP	3.3
1	A	67	TYR	3.3
1	A	964	PHE	3.3
2	C	401	GLU	3.3
1	A	938	ALA	3.3
1	A	26	TRP	3.2
1	A	18	MET	3.2
1	A	963	THR	3.2
1	A	866[A]	GLU	3.2
2	C	79	ALA	3.2
1	A	503	TYR	3.2
1	A	849[A]	GLN	3.1
1	A	543	ALA	3.1
1	A	427	ASP	3.1
2	B	80	SER	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	942	VAL	3.1
1	A	959	ASN	3.1
1	A	872[A]	LEU	3.0
1	A	43	SER	3.0
1	A	504	TRP	3.0
1	A	640	MET	3.0
1	A	63	ASN	3.0
1	A	708[A]	PRO	3.0
1	A	975	HIS	3.0
1	A	61	VAL	3.0
1	A	450	LEU	2.9
1	A	871[A]	LYS	2.9
1	A	502	GLY	2.9
1	A	404	VAL	2.9
1	A	870[A]	HIS	2.9
1	A	378	PHE	2.9
1	A	538	THR	2.8
1	A	448	PRO	2.8
1	A	29	TRP	2.8
1	A	675[A]	THR	2.8
1	A	974	TYR	2.8
1	A	960	ASN	2.8
1	A	917	TRP	2.8
1	A	523	ARG	2.8
1	A	703[A]	VAL	2.8
1	A	854[A]	THR	2.8
1	A	884[A]	PHE	2.7
1	A	439	ILE	2.7
1	A	461	PHE	2.7
1	A	874[A]	LEU	2.7
1	A	886[A]	LEU	2.7
1	A	530	LEU	2.7
1	A	899	LEU	2.7
1	A	819[A]	ARG	2.6
1	A	830[A]	ASP	2.6
1	A	371	PRO	2.6
1	A	843[A]	ALA	2.6
1	A	73	MET	2.6
1	A	66	THR	2.6
1	A	860[A]	GLY	2.6
1	A	828[A]	ALA	2.6
1	A	970	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	353	CYS	2.6
1	A	421	TRP	2.5
1	A	888[A]	TYR	2.5
1	A	411	ILE	2.5
1	A	56	GLN	2.5
1	A	689[A]	VAL	2.5
1	A	37	ASP	2.5
1	A	894	VAL	2.5
1	A	861[A]	GLN	2.5
1	A	410	MET	2.5
1	A	688[A]	THR	2.5
1	A	11	ALA	2.5
1	A	859[A]	SER	2.5
1	A	542	VAL	2.4
1	A	432	ASN	2.4
1	A	15	LEU	2.4
1	A	711[A]	ALA	2.4
1	A	440	THR	2.4
1	A	71	THR	2.4
1	A	34	THR	2.4
1	A	853[A]	GLY	2.4
1	A	17	LEU	2.4
1	A	70	THR	2.3
1	A	869[A]	ASN	2.3
1	A	408	ILE	2.3
1	A	846[A]	GLU	2.3
1	A	100	GLY	2.3
1	A	867[A]	ARG	2.3
1	A	38	ALA	2.3
1	A	971	GLU	2.3
1	A	1036	LYS	2.3
2	B	386	ASP	2.3
1	A	6	ILE	2.3
1	A	697[A]	ALA	2.2
1	A	88	PHE	2.2
1	A	706[A]	THR	2.2
1	A	674[A]	SER	2.2
1	A	72	THR	2.2
1	A	707[A]	VAL	2.2
1	A	838[A]	HIS	2.2
1	A	906	PHE	2.2
1	A	381	MET	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	499	ILE	2.1
1	A	83	ARG	2.1
1	A	998	ILE	2.1
1	A	958	LEU	2.1
1	A	396	ILE	2.1
2	B	171	THR	2.1
1	A	528	LEU	2.1
1	A	954	ALA	2.1
1	A	946	MET	2.1
1	A	713[A]	ALA	2.1
1	A	887[A]	LEU	2.1
1	A	383	PHE	2.0
1	A	365	VAL	2.0
1	A	424	GLN	2.0
1	A	692[A]	ASP	2.0
1	A	685[A]	VAL	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides 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	1048	1/1	0.78	1.16	478,478,478,478	0

6.5 Other polymers (i)

There are no such residues in this entry.