



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 01:47 AM UTC

PDB ID : 3T56 / pdb_00003t56
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 ⓘ symbol.

The types of validation reports are described at

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

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

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

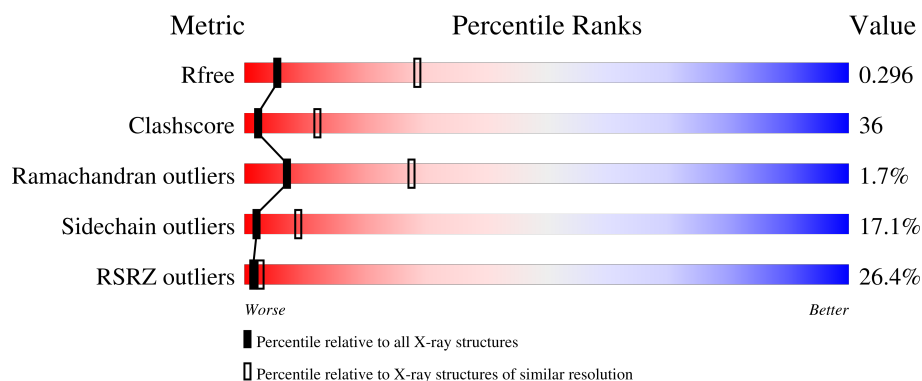
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.42 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}	180053	1210 (3.48-3.36)
Clashscore	190562	1234 (3.48-3.36)
Ramachandran outliers	187476	1222 (3.48-3.36)
Sidechain outliers	187428	1222 (3.48-3.36)
RSRZ outliers	180081	1210 (3.48-3.36)

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	A	1054	40% 37% 48% 12% .
2	B	336	5% 51% 37% 7% . .
2	C	336	% 57% 32% 7% .

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

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
1	A	1027	Total	C	N	O	S	0	225	0
			8913	5754	1502	1615	42			

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
2	B	322	Total	C	N	O	S	0	0	0
			2458	1555	428	469	6			
2	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

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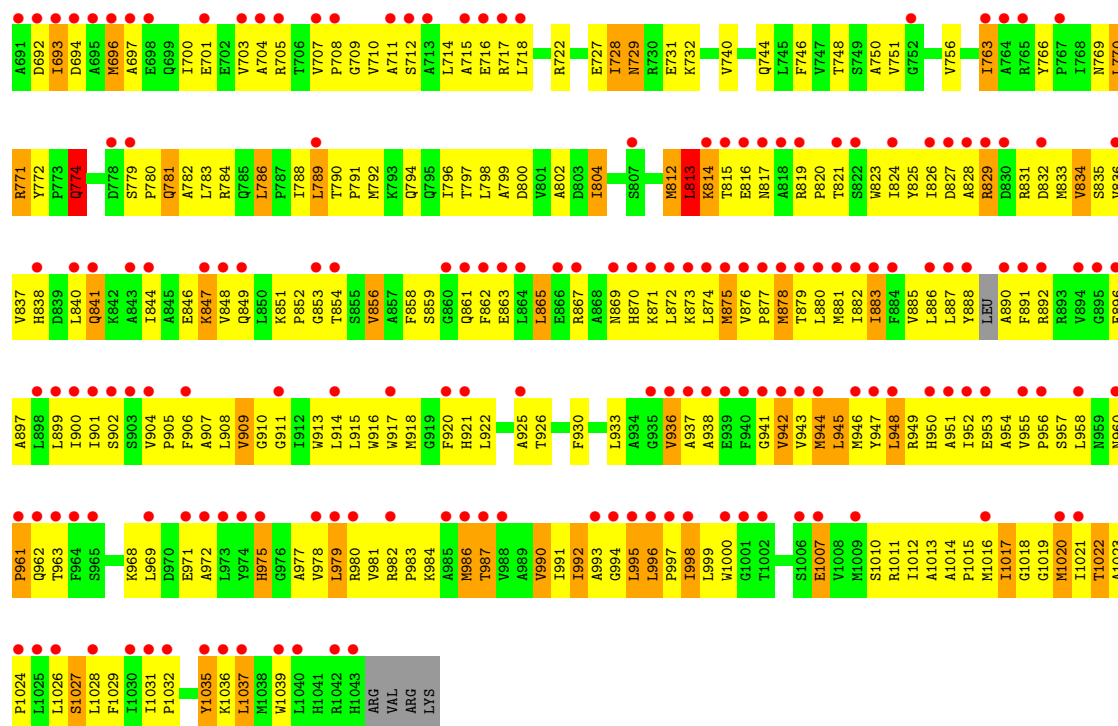
Chain	Residue	Modelled	Actual	Comment	Reference
C	409	HIS	-	expression tag	UNP P77239
C	410	HIS	-	expression tag	UNP P77239
C	411	HIS	-	expression tag	UNP P77239
C	412	HIS	-	expression tag	UNP P77239
C	413	HIS	-	expression tag	UNP P77239

- Molecule 3 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

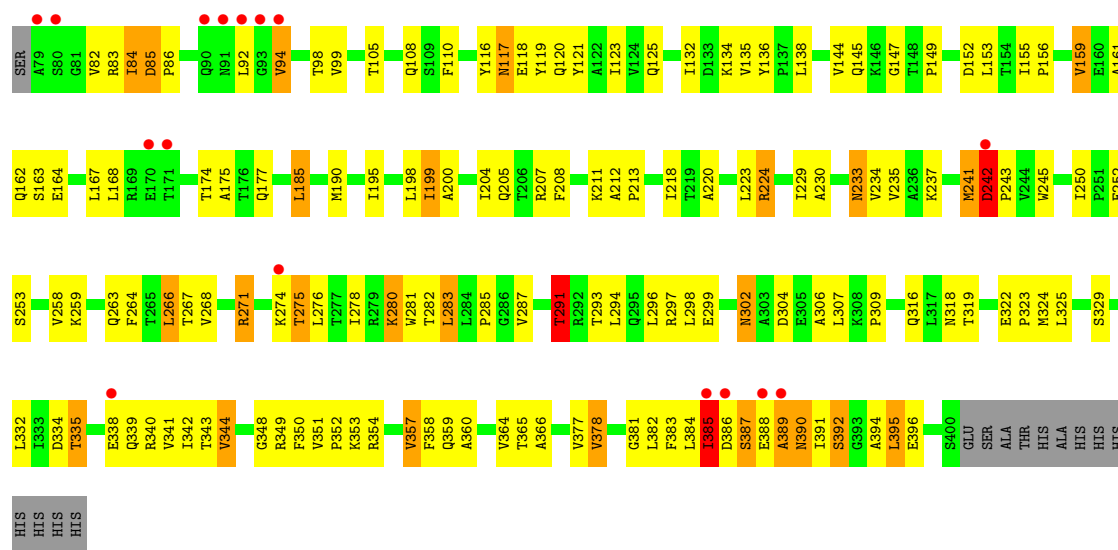
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Cu 1 1	0	0

- Molecule 4 is water.

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



• Molecule 2: Cation efflux system protein CusB



• Molecule 2: Cation efflux system protein CusB





4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ ¹	1.69 (at 3.40Å)	Xtriage
Refinement program	PHENIX 1.6.4_486	Depositor
R, R_{free}	0.259 , 0.294 0.262 , 0.296	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)	0.29 , 93.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.30	0/9093	0.75	6/12371 (0.0%)
2	B	0.30	0/2498	0.78	8/3401 (0.2%)
2	C	0.29	0/2513	0.77	4/3421 (0.1%)
All	All	0.30	0/14104	0.76	18/19193 (0.1%)

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	381	GLY	N-CA-C	-6.76	104.44	115.46
1	A	554	LEU	N-CA-C	-6.50	105.21	113.01
1	A	521	LEU	N-CA-C	-5.71	108.11	114.62
2	C	284	LEU	CA-C-N	5.70	126.97	119.84
2	C	284	LEU	C-N-CA	5.70	126.97	119.84
2	B	271	ARG	CA-C-N	5.54	126.27	120.12
2	B	271	ARG	C-N-CA	5.54	126.27	120.12
1	A	599	VAL	CA-C-N	5.53	125.36	119.28
1	A	599	VAL	C-N-CA	5.53	125.36	119.28
2	B	85	ASP	CA-C-N	5.41	124.75	118.85
2	B	85	ASP	C-N-CA	5.41	124.75	118.85
2	B	291	THR	N-CA-C	-5.39	103.58	110.53
2	C	190	MET	CA-C-N	5.20	125.19	119.89
2	C	190	MET	C-N-CA	5.20	125.19	119.89
1	A	994	GLY	N-CA-C	-5.20	108.51	115.32
1	A	958	LEU	N-CA-C	-5.16	106.83	113.02
2	B	242	ASP	CA-C-N	-5.12	113.44	119.84
2	B	242	ASP	C-N-CA	-5.12	113.44	119.84

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	A	8913	0	9201	789	0
2	B	2458	0	2522	140	0
2	C	2473	0	2533	108	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	1018	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 36.

All (1018) 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:828[B]:ALA:HA	1:A:829[B]:ARG:HB2	1.27	1.09
1:A:573:MET:HE2	1:A:625:GLU:HG2	1.30	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:402:ALA:HB3	1:A:486:MET:HE1	1.48	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	1.99	0.91
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:696[B]:MET:HE1	1:A:851[B]:LYS:HB2	1.53	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: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:660:ASN:H	1:A:660:ASN:ND2	1.71	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:381:MET:HE3	1:A:386:LEU:HB3	1.57	0.84
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:381:MET:HE1	1:A:392:SER:HB2	1.66	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:680[B]:PRO:HB2	1:A:833[B]:MET:HE1	1.68	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
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:408:ILE:HB	1:A:986:MET:HE1	1.69	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
1:A:466:THR:HG21	1:A:875[B]:MET:HE2	1.71	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:482:LYS:C	1:A:482:LYS:HE2	2.16	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
2:C:317:LEU:C	2:C:317:LEU:HD12	2.19	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
1:A:535:TRP:C	1:A:535:TRP:CD1	2.70	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
2:B:223:LEU:C	2:B:224:ARG:HD2	2.20	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
1:A:991:ILE:C	1:A:995:LEU:HD22	2.22	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
2:B:383:PHE:C	2:B:384:LEU:HD12	2.22	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:471:GLU:CD	1:A:471:GLU:H	2.04	0.64
1:A:572:TYR:CE1	1:A:660:ASN:CB	2.80	0.64
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:23:LEU:HB3	1:A:379:ILE:HD11	1.79	0.64
1:A:38:ALA:C	1:A:39:LEU:HD13	2.21	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:1007:GLU:CD	1:A:1007:GLU:H	2.06	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
1:A:571:LEU:HD11	1:A:573:MET:HE3	1.82	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
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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:411:ILE:HA	1:A:501:MET:HE1	1.83	0.60
1:A:463:PRO:HG2	1:A:879[A]:THR:CG2	2.30	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
1:A:519:ARG:O	1:A:523:ARG:HG3	2.02	0.59
1:A:525:TYR:C	1:A:525:TYR:CD2	2.78	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
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
2:B:388:GLU:OE1	2:B:388:GLU:HA	2.02	0.58
1:A:86:SER:OG	1:A:813[A]:LEU:HB2	2.03	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:774[A]:GLN:CD	2:B:391:ILE:HG12	2.29	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
1:A:534:HIS:C	1:A:534:HIS:CD2	2.82	0.58
2:B:190:MET:HE2	2:B:195:ILE:HA	1.84	0.58
2:C:174:THR:HB	2:C:177:GLN:HG3	1.86	0.58
2:C:174:THR:N	2:C:177:GLN:HE21	2.00	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
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:34:THR:O	1:A:35:PRO:C	2.47	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
1:A:1020:MET:HE3	1:A:1020:MET:HA	1.86	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
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:833[A]:MET:HE1	1:A:861[A]:GLN:OE1	2.04	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:241:MET:HE3	2:B:309:PRO:CD	2.36	0.56
1:A:390:ILE:O	1:A:394:GLY:N	2.34	0.56
1:A:729[A]:ASN:C	1:A:729[A]:ASN:HD22	2.13	0.56
2:B:117:ASN:HD22	2:B:117:ASN:C	2.14	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:696[B]:MET:HE1	1:A:851[B]:LYS:CB	2.29	0.56
1:A:876[A]:VAL:N	1:A:877[A]:PRO:HD2	2.21	0.56
1:A:984:LYS:HZ3	1:A:1028:LEU:HD21	1.70	0.56
2:B:162:GLN:NE2	2:B:205:GLN:H	2.04	0.56
2:B:241:MET:HE3	2:B:309:PRO:HD3	1.87	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:357:LEU:HD21	1:A:411:ILE:HG21	1.88	0.56
1:A:451:PHE:C	1:A:451:PHE:CD2	2.83	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: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:1035:TYR:C	1:A:1037:LEU:H	2.13	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:431:ASP:CG	1:A:432:ASN:H	2.15	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:384:LEU:O	2:B:385:ILE:C	2.50	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: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:C:323:PRO:C	2:C:324:MET:HG2	2.33	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:980:ARG:HH21	1:A:1028:LEU:HB3	1.72	0.53
1:A:672[B]:MET:HA	1:A:672[B]:MET:HE2	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
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:436:TRP:CD1	1:A:436:TRP:C	2.87	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
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:B:242:ASP:CG	2:B:243:PRO:HD3	2.34	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:58:PRO:HA	1:A:62:GLU:CD	2.34	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:67:TYR:HB3	1:A:68:PRO:CD	2.35	0.52
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:24:SER:HA	1:A:375:CYS:CB	2.37	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:359:HIS:HB3	1:A:362:SER:OG	2.09	0.52
1:A:535:TRP:C	1:A:535:TRP:HD1	2.18	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
1:A:718[A]:LEU:C	1:A:718[A]:LEU:HD23	2.35	0.52
1:A:946:MET:HG3	1:A:947:TYR: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:457:ILE:HG13	1:A:482:LYS:HZ2	1.75	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
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:324:MET:HE1	2:B:358:PHE:CG	2.46	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
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:642:MET:HA	1:A:642:MET:HE3	1.94	0.50
1:A:816[B]:GLU:HB3	1:A:821[B]:THR:CG2	2.41	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:751[A]:VAL:O	1:A:771[A]:ARG:HD2	2.11	0.50
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:918:MET:HE3	1:A:999:LEU:HD21	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:TRP:C	1:A:31:ILE:H	2.17	0.50
1:A:56:GLN:HE21	1:A:56:GLN:C	2.20	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: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
1:A:553:PRO:C	1:A:555:ASN:H	2.20	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:49:ILE:HD13	1:A:73:MET:HE2	1.93	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: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
1:A:960:ASN:C	1:A:962:GLN:H	2.20	0.49
2:C:221:PHE:HD1	2:C:224:ARG:NH1	2.09	0.49
1:A:64:GLN:C	1:A:67:TYR:H	2.17	0.49
1:A:228:GLU:O	1:A:228:GLU:HG2	2.11	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:29:TRP:C	1:A:31:ILE:N	2.69	0.49
1:A:46:GLN:O	1:A:46:GLN:HG2	2.07	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
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
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
2:B:245:TRP:CD1	2:B:299:GLU:HG2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:716[B]:GLU:O	1:A:717[B]:ARG:C	2.57	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:588:MET:HE2	2:C:384:LEU:HD21	1.96	0.48
1:A:680[B]:PRO:CB	1:A:833[B]:MET:HE1	2.41	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:398:ILE:CG1	1:A:1016:MET:HE1	2.44	0.48
1:A:420:GLU:HG3	1:A:421:TRP:N	2.29	0.48
1:A:482:LYS:C	1:A:484:TYR:H	2.21	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: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:457:ILE:HG13	1:A:482:LYS:NZ	2.29	0.47
1:A:833[B]:MET:HE3	1:A:862[B]:PHE:HB3	1.96	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:241:MET:O	2:B:242:ASP:C	2.56	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:381:MET:HE3	1:A:386:LEU:HD23	1.95	0.47
1:A:814[A]:LYS:O	1:A:820[A]:PRO:HA	2.14	0.47
1:A:831[A]:ARG:HG2	1:A:832[A]:ASP:N	2.30	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:969:LEU:HD12	1:A:969:LEU:C	2.40	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:873[A]:LYS:C	1:A:874[A]:LEU:HD12	2.40	0.47
1:A:992:ILE:HA	1:A:995:LEU:CD2	2.44	0.47
2:C:223:LEU:C	2:C:224:ARG:HD2	2.39	0.47
2:C:332:LEU:C	2:C:332:LEU:HD23	2.40	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:A:517:LEU:C	1:A:519:ARG:H	2.23	0.46
1:A:1029:PHE:C	1:A:1032:PRO:HD2	2.41	0.46
2:B:84:ILE:HG22	2:C:91:ASN:CG	2.41	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:553:PRO:C	1:A:555:ASN:N	2.73	0.46
1:A:1013:ALA:C	1:A:1015:PRO:HD2	2.40	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:451:PHE:C	1:A:451:PHE:HD2	2.24	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:779[A]:SER:OG	1:A:781[A]:GLN:HG2	2.16	0.46
1:A:874[B]:LEU:C	1:A:877[B]:PRO:HD2	2.41	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:904:VAL:HG22	1:A:937:ALA:HB1	1.97	0.45
2:B:390:ASN:O	2:B:391:ILE:C	2.58	0.45
2:C:137:PRO:C	2:C:138:LEU:HD12	2.40	0.45
1:A:410:MET:HE1	1:A:493:ALA:O	2.15	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: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
2:C:330:GLN:CD	2:C:330:GLN:H	2.24	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:B:344:VAL:O	2:B:344:VAL:HG12	2.17	0.44
2:C:151:LEU:C	2:C:151:LEU:HD12	2.42	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
2:C:189:GLY:O	2:C:190:MET:C	2.60	0.44
1:A:351:VAL:O	1:A:355:LEU:HB2	2.17	0.44
1:A:374:LEU:HD13	1:A:374:LEU:C	2.42	0.44
1:A:377:ALA:O	1:A:380:VAL:HG23	2.16	0.44
1:A:696[B]:MET:HE3	1:A:854[B]:THR:HG21	1.98	0.44
1:A:870[B]:HIS:HD1	1:A:870[B]:HIS:C	2.25	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
2:B:386:ASP:C	2:B:388:GLU:H	2.25	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:451:PHE:O	1:A:452:ILE:C	2.61	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: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:368:ILE:C	1:A:371:PRO:HD2	2.43	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:C:179:GLU:C	2:C:181:ILE:H	2.27	0.43
1:A:573:MET:HA	1:A:624:VAL:O	2.18	0.43
1:A:701[A]:GLU:CD	1:A:705[A]:ARG:HH12	2.27	0.43
1:A:707[B]:VAL:HG22	1:A:708[B]:PRO:HD2	2.00	0.43
1:A:933:LEU:HD13	1:A:933:LEU:C	2.43	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:408:ILE:HB	1:A:986:MET:CE	2.42	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:464:ILE:HA	1:A:875[A]:MET:HE3	2.01	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:214:ASN:C	1:A:215:GLN:HG3	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:540:LEU:HD23	1:A:540:LEU:C	2.43	0.43
1:A:826[B]:ILE:HG12	1:A:826[B]:ILE:O	2.19	0.43
1:A:902:SER:C	1:A:905:PRO:HD2	2.44	0.43
1:A:944:MET:HE2	1:A:1028:LEU:HA	2.01	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
1:A:145:VAL:HG12	1:A:284:VAL:HG11	2.01	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:525:TYR:C	1:A:527:PRO:HD2	2.44	0.42
1:A:666[B]:ILE:N	1:A:666[B]:ILE:HD12	2.34	0.42
1:A:729[A]:ASN:ND2	1:A:729[A]:ASN:C	2.77	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:571:LEU:C	1:A:571:LEU:HD13	2.45	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:390:ILE:C	1:A:390:ILE:HD12	2.44	0.42
1:A:464:ILE:HG12	1:A:875[A]:MET:CE	2.49	0.42
1:A:1026:LEU:C	1:A:1028:LEU:H	2.28	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:195:ARG:CB	1:A:262:VAL:HA	2.49	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:541:LEU:HD13	1:A:541:LEU:C	2.45	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
1:A:952:ILE:C	1:A:957:SER:HB2	2.45	0.42
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
1:A:35:PRO:C	1:A:36:VAL:HG12	2.44	0.42
1:A:50:LYS:NZ	1:A:611:LYS:NZ	2.68	0.42
1:A:67:TYR:CD2	1:A:68:PRO:N	2.87	0.42
1:A:535:TRP:CD1	1:A:537:LYS:H	2.38	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:MET:HE3	1:A:21:LEU:HD21	2.01	0.41
1:A:95:VAL:C	1:A:96:ILE:HG12	2.45	0.41
1:A:223:GLU:C	1:A:224:LEU:HD23	2.45	0.41
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
2:C:199:ILE:HD12	2:C:199:ILE:C	2.45	0.41
1:A:225:ALA:C	1:A:227:ALA:H	2.28	0.41
1:A:412:GLU:HG3	1:A:982:ARG:HG2	2.02	0.41
1:A:517:LEU:C	1:A:519:ARG:N	2.78	0.41
1:A:907:ALA:CB	1:A:933:LEU:HD11	2.50	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
2:C:171:THR:O	2:C:172:GLY:C	2.62	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: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:633:GLN:C	1:A:635:GLN:H	2.28	0.41
1:A:834[A]:VAL:HG13	1:A:838[A]:HIS:HD2	1.86	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:GLN:CD	1:A:215:GLN:N	2.78	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:519:ARG:C	1:A:521:LEU:H	2.28	0.41
1:A:522:ILE:O	1:A:526:HIS:CD2	2.68	0.41
1:A:917:TRP:HD1	1:A:918:MET:HE2	1.86	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
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
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
2:B:155:ILE:HA	2:B:156:PRO:HD3	1.83	0.41
2:C:153:LEU:HD12	2:C:229:ILE:HG21	2.01	0.41
1:A:530:LEU:C	1:A:530:LEU:HD12	2.46	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:61:VAL:HG12	1:A:62:GLU:N	2.35	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:ILE:HG12	1:A:1016:MET:HE1	2.04	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
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:392:SER:HA	1:A:481:THR:HG21	2.04	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
2:C:317:LEU:C	2:C:317:LEU:CD1	2.89	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%)	5	23
2	B	320/336 (95%)	279 (87%)	35 (11%)	6 (2%)	6	26
2	C	322/336 (96%)	293 (91%)	28 (9%)	1 (0%)	36	65
All	All	1791/1726 (104%)	1575 (88%)	182 (10%)	34 (2%)	7	26

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	35	PRO
1	A	67	TYR
1	A	638	PRO

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

5.3.2 Protein sidechains ⓘ

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

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	956/871 (110%)	791 (83%)	165 (17%)	2	8
2	B	263/275 (96%)	220 (84%)	43 (16%)	2	10
2	C	265/275 (96%)	226 (85%)	39 (15%)	3	12
All	All	1484/1421 (104%)	1237 (83%)	247 (17%)	2	10

All (247) 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	12	ASN
1	A	24	SER
1	A	26	TRP
1	A	31	ILE
1	A	32	ILE
1	A	36	VAL
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	61	VAL
1	A	62	GLU
1	A	69	LEU
1	A	72	THR
1	A	73	MET
1	A	74	LEU
1	A	81	THR
1	A	95	VAL
1	A	96	ILE
1	A	98	GLU
1	A	111	LEU
1	A	117	VAL
1	A	128	GLU
1	A	134	THR
1	A	139	ILE

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Mol	Chain	Res	Type
1	A	144	LEU
1	A	170	THR
1	A	183	VAL
1	A	184	VAL
1	A	203	LEU
1	A	215	GLN
1	A	222	ILE
1	A	228	GLU
1	A	237	LEU
1	A	241	ASP
1	A	259	LEU
1	A	260	ARG
1	A	288	VAL
1	A	312	LYS
1	A	322	VAL
1	A	323	THR
1	A	331	ILE
1	A	336	ASP
1	A	338	LEU
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	411	ILE
1	A	412	GLU
1	A	419	GLU
1	A	432	ASN
1	A	435	ARG
1	A	437	GLN
1	A	445	GLU
1	A	452	ILE
1	A	455	LEU

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Mol	Chain	Res	Type
1	A	457	ILE
1	A	459	LEU
1	A	461	PHE
1	A	471	GLU
1	A	474	LEU
1	A	482	LYS
1	A	492	LEU
1	A	534	HIS
1	A	550	VAL
1	A	560	GLU
1	A	567	GLU
1	A	569	ASP
1	A	592	THR
1	A	602	VAL
1	A	604	ARG
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	728[A]	ILE
1	A	729[A]	ASN
1	A	731[A]	GLU
1	A	748[A]	THR
1	A	756[A]	VAL
1	A	763[A]	ILE

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Mol	Chain	Res	Type
1	A	769[A]	ASN
1	A	770[A]	LEU
1	A	771[A]	ARG
1	A	774[A]	GLN
1	A	781[A]	GLN
1	A	783[A]	LEU
1	A	786[A]	LEU
1	A	789[A]	LEU
1	A	804[A]	ILE
1	A	812[A]	MET
1	A	813[A]	LEU
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	875[A]	MET
1	A	875[B]	MET
1	A	878[A]	MET
1	A	878[B]	MET
1	A	883[A]	ILE
1	A	883[B]	ILE
1	A	899	LEU
1	A	909	VAL
1	A	936	VAL
1	A	942	VAL
1	A	943	VAL
1	A	944	MET
1	A	945	LEU
1	A	948	LEU
1	A	968	LYS
1	A	975	HIS
1	A	979	LEU
1	A	986	MET
1	A	987	THR
1	A	990	VAL
1	A	992	ILE
1	A	995	LEU
1	A	996	LEU

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Mol	Chain	Res	Type
1	A	998	ILE
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
2	B	84	ILE
2	B	94	VAL
2	B	98	THR
2	B	105	THR
2	B	117	ASN
2	B	135	VAL
2	B	138	LEU
2	B	145	GLN
2	B	159	VAL
2	B	163	SER
2	B	167	LEU
2	B	185	LEU
2	B	199	ILE
2	B	207	ARG
2	B	224	ARG
2	B	233	ASN
2	B	234	VAL
2	B	241	MET
2	B	263	GLN
2	B	266	LEU
2	B	268	VAL
2	B	275	THR
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	357	VAL

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Mol	Chain	Res	Type
2	B	359	GLN
2	B	364	VAL
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
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	134	LYS
2	C	145	GLN
2	C	150	LEU
2	C	168	LEU
2	C	178	THR
2	C	181	ILE
2	C	185	LEU
2	C	187	LEU
2	C	207	ARG
2	C	228	ASN
2	C	234	VAL
2	C	235	VAL
2	C	250	ILE
2	C	257	LEU
2	C	258	VAL
2	C	267	THR
2	C	268	VAL
2	C	271	ARG
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	357	VAL

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Mol	Chain	Res	Type
2	C	364	VAL
2	C	365	THR
2	C	367	LEU
2	C	373	GLU
2	C	378	VAL
2	C	382	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	GLN
1	A	115	ASN
1	A	188	GLN
1	A	194	GLN
1	A	238	GLN
1	A	279	ASN
1	A	329	GLN
1	A	337	ASN
1	A	359	HIS
1	A	389	ASN
1	A	413	ASN
1	A	415	HIS
1	A	423	HIS
1	A	470	GLN
1	A	518	ASN
1	A	526	HIS
1	A	534	HIS
1	A	564	GLN
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	774[A]	GLN
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

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Mol	Chain	Res	Type
2	B	177	GLN
2	B	302	ASN
2	B	318	ASN
2	B	330	GLN
2	B	359	GLN
2	B	390	ASN
2	C	125	GLN
2	C	145	GLN
2	C	177	GLN
2	C	228	ASN
2	C	233	ASN
2	C	239	GLN
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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1027/1054 (97%)	1.92	420 (40%) 0 1	1, 86, 279, 420	225 (21%)
2	B	322/336 (95%)	0.14	16 (4%) 34 25	2, 33, 92, 166	0
2	C	324/336 (96%)	-0.02	5 (1%) 72 58	2, 33, 81, 209	0
All	All	1673/1726 (96%)	1.20	441 (26%) 1 2	1, 52, 254, 420	225 (13%)

All (441) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	494	ILE	11.6
1	A	40	PRO	10.8
1	A	44	ASP	10.5
1	A	903	SER	10.1
1	A	450	LEU	9.4
1	A	495	VAL	9.3
1	A	61	VAL	8.6
1	A	539	THR	8.5
1	A	815[A]	THR	8.4
1	A	563	PRO	8.4
1	A	68	PRO	8.3
1	A	66	THR	8.3
1	A	38	ALA	7.9
1	A	39	LEU	7.8
1	A	88	PHE	7.7
1	A	998	ILE	7.4
1	A	887[A]	LEU	7.3
1	A	69	LEU	7.1
1	A	888[A]	TYR	7.1
1	A	994	GLY	7.0
1	A	496	VAL	6.7
1	A	15	LEU	6.7
1	A	942	VAL	6.6

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Mol	Chain	Res	Type	RSRZ
1	A	899	LEU	6.6
1	A	827[A]	ASP	6.5
1	A	712[A]	SER	6.5
1	A	1036	LYS	6.5
1	A	552	TRP	6.5
1	A	438	VAL	6.5
1	A	392	SER	6.4
1	A	67	TYR	6.4
1	A	886[A]	LEU	6.4
1	A	470	GLN	6.4
1	A	943	VAL	6.3
2	B	386	ASP	6.3
1	A	1000	TRP	6.2
1	A	55	GLY	6.2
1	A	63	ASN	6.0
1	A	404	VAL	6.0
2	B	242	ASP	5.9
1	A	817[A]	ASN	5.9
1	A	37	ASP	5.9
1	A	41	ASP	5.9
1	A	11	ALA	5.9
1	A	538	THR	5.8
1	A	56	GLN	5.7
1	A	939	GLU	5.7
1	A	814[A]	LYS	5.6
1	A	407	ALA	5.6
1	A	406	ALA	5.6
1	A	449	ALA	5.6
1	A	872[A]	LEU	5.6
1	A	73	MET	5.5
1	A	12	ASN	5.5
1	A	410	MET	5.5
1	A	895	GLY	5.5
1	A	83	ARG	5.5
1	A	17	LEU	5.5
1	A	894	VAL	5.4
1	A	72	THR	5.4
1	A	995	LEU	5.3
1	A	35	PRO	5.2
1	A	671[A]	ASP	5.2
1	A	711[A]	ALA	5.2
1	A	673[A]	LEU	5.2

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Mol	Chain	Res	Type	RSRZ
1	A	388	ALA	5.1
1	A	697[A]	ALA	5.1
1	A	99	ASP	5.1
1	A	568	GLY	5.0
1	A	972	ALA	5.0
1	A	689[A]	VAL	5.0
1	A	6	ILE	5.0
1	A	871[A]	LYS	5.0
1	A	896	GLU	5.0
1	A	938	ALA	5.0
1	A	1020	MET	5.0
1	A	400	VAL	4.9
1	A	70	THR	4.9
1	A	14	PHE	4.8
1	A	639	GLY	4.8
1	A	948	LEU	4.8
1	A	59	GLN	4.8
1	A	1024	PRO	4.7
1	A	996	LEU	4.7
1	A	870[A]	HIS	4.7
1	A	97	PHE	4.6
1	A	115	ASN	4.6
1	A	875[A]	MET	4.6
1	A	57	ALA	4.6
1	A	542	VAL	4.6
1	A	501	MET	4.6
1	A	900	ILE	4.5
1	A	1031	ILE	4.5
1	A	692[A]	ASP	4.5
1	A	81	THR	4.5
1	A	819[A]	ARG	4.4
1	A	543	ALA	4.4
1	A	890	ALA	4.4
1	A	386	LEU	4.4
1	A	874[A]	LEU	4.4
1	A	863[A]	GLU	4.4
1	A	396	ILE	4.4
1	A	116	GLN	4.3
1	A	763[A]	ILE	4.3
2	B	93	GLY	4.3
1	A	821[A]	THR	4.3
1	A	46	GLN	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	694[A]	ASP	4.3
1	A	866[A]	GLU	4.3
1	A	390	ILE	4.2
1	A	481	THR	4.2
1	A	862[A]	PHE	4.2
1	A	980	ARG	4.2
1	A	670[A]	ILE	4.2
1	A	540	LEU	4.2
1	A	675[A]	THR	4.2
1	A	963	THR	4.2
2	C	176	THR	4.2
1	A	690[A]	LEU	4.2
1	A	880[A]	LEU	4.2
1	A	816[A]	GLU	4.1
1	A	843[A]	ALA	4.1
1	A	378	PHE	4.1
1	A	42	LEU	4.1
1	A	74	LEU	4.1
2	B	388	GLU	4.1
1	A	940	PHE	4.1
1	A	548	LEU	4.0
1	A	881[A]	MET	4.0
1	A	528	LEU	4.0
1	A	532	VAL	4.0
1	A	838[A]	HIS	4.0
1	A	941	GLY	3.9
1	A	447	GLY	3.9
1	A	718[A]	LEU	3.9
1	A	408	ILE	3.9
1	A	717[A]	ARG	3.9
1	A	135	GLY	3.9
1	A	674[A]	SER	3.9
1	A	891	PHE	3.9
1	A	1026	LEU	3.9
1	A	100	GLY	3.9
1	A	569	ASP	3.9
1	A	418	LEU	3.9
1	A	5	ILE	3.8
1	A	520	PHE	3.8
1	A	564	GLN	3.8
1	A	950	HIS	3.8
1	A	951	ALA	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	946	MET	3.8
1	A	411	ILE	3.8
1	A	491	LEU	3.8
1	A	444	VAL	3.8
1	A	504	TRP	3.8
1	A	1035	TYR	3.8
1	A	473	ARG	3.8
1	A	906	PHE	3.8
1	A	854[A]	THR	3.8
1	A	43	SER	3.7
1	A	686[A]	SER	3.7
1	A	879[A]	THR	3.7
1	A	545	LEU	3.7
1	A	752[A]	GLY	3.7
1	A	884[A]	PHE	3.7
1	A	98	GLU	3.7
1	A	1025	LEU	3.7
1	A	71	THR	3.7
1	A	383	PHE	3.7
1	A	448	PRO	3.6
1	A	53	TYR	3.6
1	A	445	GLU	3.6
1	A	867[A]	ARG	3.6
1	A	688[A]	THR	3.6
1	A	883[A]	ILE	3.6
1	A	962	GLN	3.6
1	A	441	ASP	3.6
1	A	464	ILE	3.6
1	A	853[A]	GLY	3.6
1	A	765[A]	ARG	3.6
1	A	389	ASN	3.6
1	A	462	ILE	3.6
1	A	530	LEU	3.6
1	A	360	VAL	3.6
1	A	18	MET	3.6
1	A	898	LEU	3.6
1	A	439	ILE	3.6
1	A	901	ILE	3.6
1	A	902	SER	3.6
1	A	667[A]	ARG	3.5
1	A	371	PRO	3.5
1	A	533	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	716[A]	GLU	3.5
1	A	484	TYR	3.5
1	A	960	ASN	3.5
1	A	436	TRP	3.5
1	A	882[A]	ILE	3.5
1	A	860[A]	GLY	3.5
2	B	389	ALA	3.5
1	A	921	HIS	3.5
1	A	978	VAL	3.5
1	A	562	LEU	3.5
1	A	34	THR	3.4
1	A	181	GLY	3.4
1	A	551	LEU	3.4
1	A	997	PRO	3.4
1	A	1021	ILE	3.4
1	A	26	TRP	3.4
1	A	62	GLU	3.4
1	A	446	VAL	3.4
1	A	979	LEU	3.4
1	A	403	MET	3.4
1	A	826[A]	ILE	3.4
1	A	475	PHE	3.4
1	A	65	VAL	3.4
1	A	969	LEU	3.4
1	A	368	ILE	3.4
1	A	465	PHE	3.4
1	A	84	GLY	3.4
1	A	947	TYR	3.3
1	A	366	ALA	3.3
1	A	499	ILE	3.3
1	A	553	PRO	3.3
1	A	58	PRO	3.3
1	A	841[A]	GLN	3.3
1	A	861[A]	GLN	3.3
1	A	85	PHE	3.3
1	A	358	TRP	3.3
1	A	434	THR	3.3
2	B	94	VAL	3.3
1	A	4	TRP	3.2
1	A	60	ILE	3.2
1	A	708[A]	PRO	3.2
1	A	430	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	840[A]	LEU	3.2
1	A	64	GLN	3.2
1	A	554	LEU	3.2
1	A	1040	LEU	3.2
1	A	503	TYR	3.2
1	A	457	ILE	3.2
1	A	487	ALA	3.2
1	A	610	GLY	3.1
1	A	682[A]	GLY	3.1
1	A	387	ASN	3.1
1	A	703[A]	VAL	3.1
1	A	1032	PRO	3.1
1	A	96	ILE	3.1
1	A	7	ARG	3.1
1	A	460	SER	3.1
1	A	500	LEU	3.1
1	A	937	ALA	3.1
1	A	1028	LEU	3.1
1	A	828[A]	ALA	3.1
1	A	982	ARG	3.1
1	A	547	VAL	3.1
1	A	557	VAL	3.1
1	A	952	ILE	3.1
1	A	956	PRO	3.1
1	A	393	LEU	3.0
1	A	698[A]	GLU	3.0
1	A	1039	TRP	3.0
1	A	873[A]	LYS	3.0
1	A	987	THR	3.0
1	A	779[A]	SER	3.0
1	A	353	CYS	3.0
1	A	29	TRP	3.0
1	A	32	ILE	3.0
2	B	79	ALA	3.0
1	A	36	VAL	3.0
1	A	971	GLU	3.0
1	A	428	ALA	3.0
1	A	974	TYR	3.0
1	A	385	GLY	3.0
1	A	451	PHE	2.9
1	A	822[A]	SER	2.9
1	A	425	HIS	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	975	HIS	2.9
1	A	467	LEU	2.9
1	A	490	ALA	2.9
1	A	695[A]	ALA	2.9
1	A	45	VAL	2.9
1	A	482	LYS	2.9
1	A	522	ILE	2.9
1	A	565	ILE	2.9
1	A	878[A]	MET	2.9
1	A	485	ALA	2.8
1	A	917	TRP	2.8
1	A	402	ALA	2.8
1	A	345	GLU	2.8
1	A	409	VAL	2.8
1	A	502	GLY	2.8
1	A	993	ALA	2.8
1	A	10	VAL	2.8
1	A	421	TRP	2.8
1	A	379	ILE	2.8
1	A	33	ASN	2.8
1	A	329	GLN	2.8
1	A	961	PRO	2.8
1	A	973	LEU	2.8
1	A	560	GLU	2.8
1	A	944	MET	2.7
2	C	242	ASP	2.7
1	A	273	ARG	2.7
1	A	985	ALA	2.7
1	A	876[A]	VAL	2.7
2	B	171	THR	2.7
1	A	691[A]	ALA	2.7
1	A	836[A]	VAL	2.7
2	B	92	LEU	2.7
1	A	22	PHE	2.7
1	A	715[A]	ALA	2.7
1	A	384	GLN	2.7
2	B	80	SER	2.7
1	A	474	LEU	2.7
1	A	541	LEU	2.7
1	A	331	ILE	2.6
1	A	704[A]	ALA	2.6
1	A	914	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	367	ILE	2.6
1	A	401	GLY	2.6
1	A	685[A]	VAL	2.6
1	A	94	TYR	2.6
1	A	626	THR	2.6
1	A	1042	ARG	2.6
2	B	170	GLU	2.6
1	A	1009	MET	2.6
1	A	911	GLY	2.6
1	A	707[A]	VAL	2.6
1	A	426	PRO	2.5
1	A	497	ILE	2.5
1	A	696[A]	MET	2.5
1	A	701[A]	GLU	2.5
1	A	381	MET	2.5
1	A	395	GLY	2.5
1	A	112	GLU	2.5
1	A	376	ILE	2.5
1	A	338	LEU	2.5
1	A	864[A]	LEU	2.5
1	A	848[A]	VAL	2.5
1	A	1016	MET	2.5
1	A	30	THR	2.5
1	A	1043	HIS	2.5
1	A	680[A]	PRO	2.4
1	A	1001	GLY	2.4
1	A	416	LYS	2.4
1	A	778[A]	ASP	2.4
1	A	461	PHE	2.4
1	A	869[A]	ASN	2.4
1	A	25	ILE	2.4
1	A	544	ALA	2.4
1	A	964	PHE	2.4
1	A	75	SER	2.4
1	A	965	SER	2.4
1	A	382	HIS	2.4
1	A	521	LEU	2.4
2	C	402	SER	2.4
1	A	79	ALA	2.3
1	A	452	ILE	2.3
1	A	705[A]	ARG	2.3
1	A	498	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	676[A]	GLY	2.3
1	A	693[A]	ILE	2.3
1	A	764[A]	ALA	2.3
1	A	986	MET	2.3
1	A	459	LEU	2.3
1	A	47	VAL	2.3
1	A	556	LYS	2.3
1	A	561	PHE	2.3
1	A	394	GLY	2.3
1	A	440	THR	2.3
1	A	398	ILE	2.3
1	A	877[A]	PRO	2.3
2	B	385	ILE	2.3
1	A	429	THR	2.3
1	A	369	SER	2.3
1	A	1006	SER	2.3
1	A	405	ASP	2.3
1	A	832[A]	ASP	2.3
1	A	925	ALA	2.2
1	A	849[A]	GLN	2.2
2	B	338	GLU	2.2
1	A	661	LEU	2.2
1	A	818[A]	ALA	2.2
1	A	1002	THR	2.2
1	A	523	ARG	2.2
1	A	362	SER	2.2
1	A	117	VAL	2.2
1	A	437	GLN	2.2
1	A	343	LEU	2.2
1	A	958	LEU	2.2
2	C	347	ASP	2.2
1	A	354	ALA	2.2
1	A	847[A]	LYS	2.2
1	A	13	ARG	2.2
1	A	892	ARG	2.2
1	A	423	HIS	2.2
1	A	325	TYR	2.2
1	A	988	VAL	2.2
1	A	1030	ILE	2.2
1	A	570	LEU	2.2
1	A	789[A]	LEU	2.2
1	A	953	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	294	GLY	2.2
2	B	90	GLN	2.2
1	A	123	ALA	2.2
1	A	713[A]	ALA	2.2
1	A	550	VAL	2.1
1	A	955	VAL	2.1
1	A	844[A]	ILE	2.1
1	A	432	ASN	2.1
2	B	91	ASN	2.1
1	A	431	ASP	2.1
1	A	101	THR	2.1
1	A	627	THR	2.1
2	C	97	ALA	2.1
1	A	463	PRO	2.1
1	A	322	VAL	2.1
1	A	904	VAL	2.1
1	A	374	LEU	2.1
2	B	274	LYS	2.1
1	A	361	ARG	2.1
1	A	767[A]	PRO	2.1
1	A	105	TRP	2.1
1	A	1037	LEU	2.1
1	A	293	SER	2.1
1	A	298	ARG	2.1
1	A	78	GLY	2.1
1	A	77	PRO	2.1
1	A	936	VAL	2.0
1	A	31	ILE	2.0
1	A	829[A]	ARG	2.0
1	A	414	ALA	2.0
1	A	830[A]	ASP	2.0
1	A	920	PHE	2.0
1	A	678[A]	LYS	2.0
1	A	1007	GLU	2.0
1	A	807[A]	SER	2.0
1	A	356	PHE	2.0
1	A	935	GLY	2.0
1	A	524	VAL	2.0
1	A	517	LEU	2.0
1	A	824[A]	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CU	A	1048	1/1	0.66	0.49	478,478,478,478	0

6.5 Other polymers [i](#)

There are no such residues in this entry.