W O R L D W I D E
wwPDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:10 AM GMT

PDB ID : 3DLB
Title : Crystal structure of the guide-strand-containing Argonaute protein silencing complex
Authors : Wang, Y.; Sheng, G.; Patel, D.J.
Deposited on : 2008-06-26
Resolution : 2.70 Å(reported)

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 2.70 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.
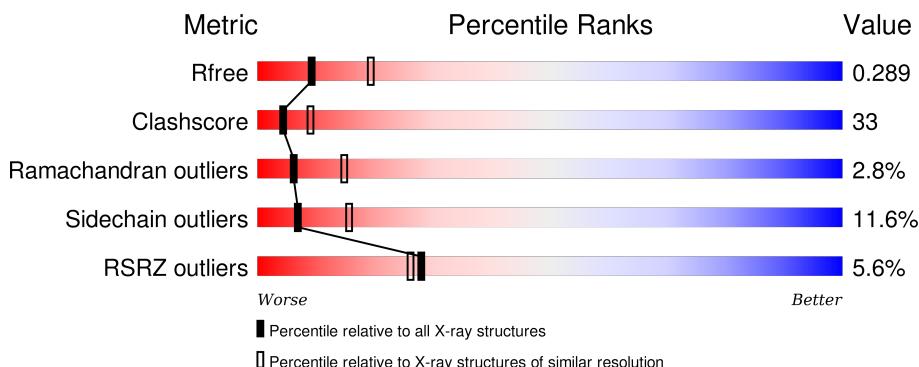
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	685	
1	B	685	
2	X	10	
2	Y	10	
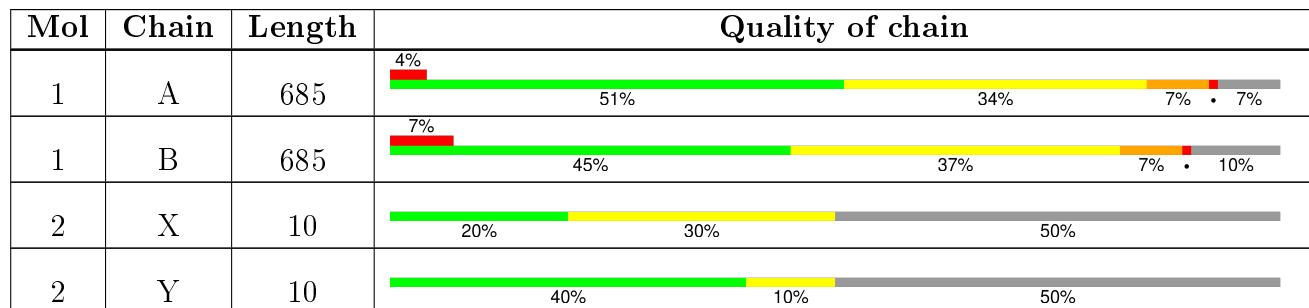
2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 9793 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 argonaute.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	637	Total	C	N	O	S	9	0	0
			4891	3125	913	846	7			
1	B	614	Total	C	N	O	S	34	0	0
			4668	2983	873	806	6			

- Molecule 2 is a DNA chain called DNA (5'-D(*DTP*DGP*DAP*DGP*DGP*DTP*DAP* DGP*DTP*DA)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	X	5	Total	C	N	O	P	0	0	0
			101	50	19	28	4			
2	Y	5	Total	C	N	O	P	0	0	1
			85	40	17	24	4			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	25	Total	O	0	0
			25	25		
3	B	19	Total	O	0	0
			19	19		
3	X	3	Total	O	0	0
			3	3		
3	Y	1	Total	O	0	0
			1	1		

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: argonaute

- Molecule 1: argonaute

• Molecule 2: DNA (5'-D(*DTP*DGP*DAP*DGP*DGP*DTP*DAP*DGP*DTP*DA)-3')

Chain X:

• Molecule 2: DNA (5'-D(*DTP*DGP*DAP*DGP*DGP*DTP*DAP*DGP*DTP*DA)-3')

Chain Y:
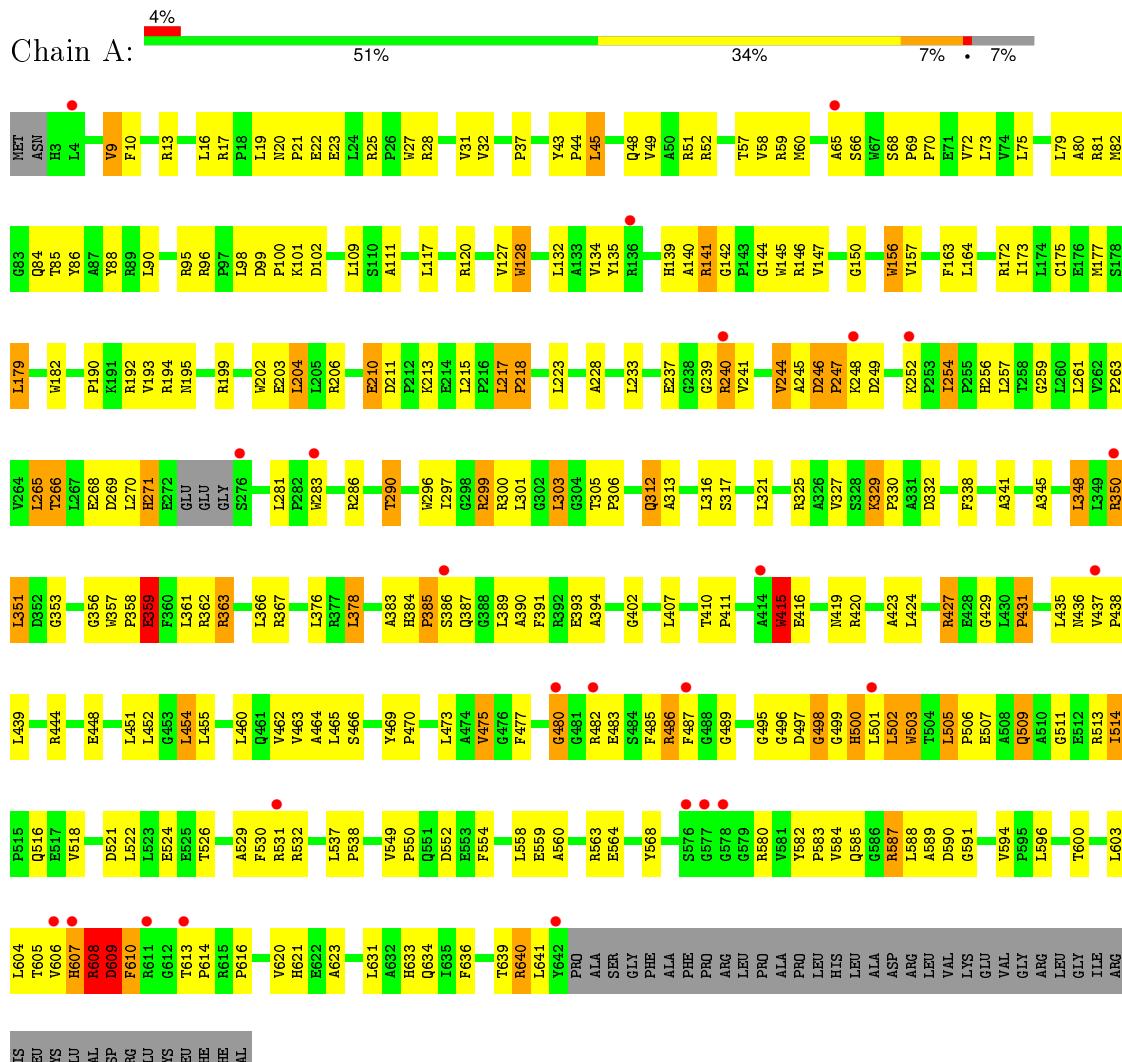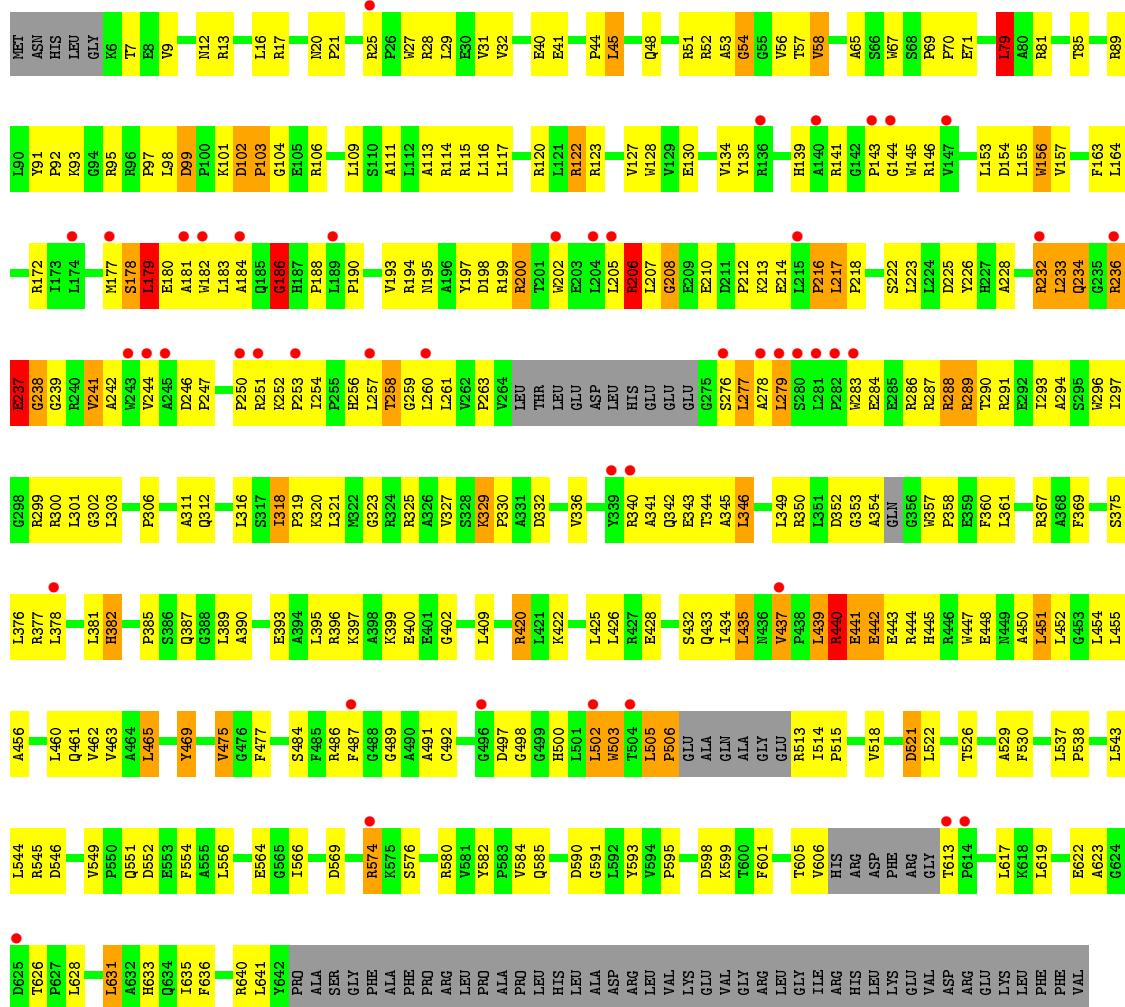
4   Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	77.85Å 123.40Å 84.91Å 90.00° 95.70° 90.00°	Depositor
Resolution (Å)	30.00 – 2.70 32.82 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.6 (30.00-2.70) 94.2 (32.82-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	1.86 (at 2.68Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.254 , 0.293 0.254 , 0.289	Depositor DCC
R_{free} test set	2153 reflections (5.48%)	DCC
Wilson B-factor (Å^2)	77.0	Xtriage
Anisotropy	0.149	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 50.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Outliers	0 of 42792 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	9793	wwPDB-VP
Average B, all atoms (Å^2)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.40% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

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	0.61	3/5009 (0.1%)	0.86	12/6817 (0.2%)
1	B	0.52	4/4780 (0.1%)	0.86	14/6509 (0.2%)
2	X	0.93	0/113	1.19	0/173
2	Y	0.55	0/95	0.95	0/146
All	All	0.57	7/9997 (0.1%)	0.86	26/13645 (0.2%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	128	TRP	CB-CG	-13.53	1.25	1.50
1	A	503	TRP	CB-CG	-11.07	1.30	1.50
1	A	415	TRP	CB-CG	-5.93	1.39	1.50
1	B	640	ARG	CB-CG	-5.35	1.38	1.52
1	B	387	GLN	CB-CG	-5.31	1.38	1.52
1	B	237	GLU	CB-CG	5.15	1.61	1.52
1	B	529	ALA	C-N	-5.08	1.22	1.34

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	277	LEU	N-CA-C	10.63	139.69	111.00
1	A	608	ARG	N-CA-C	-9.09	86.45	111.00
1	A	609	ASP	CB-CG-OD2	-8.72	110.45	118.30
1	A	356	GLY	N-CA-C	7.85	132.73	113.10
1	B	102	ASP	CB-CG-OD1	-7.66	111.41	118.30
1	B	186	GLY	N-CA-C	7.36	131.49	113.10
1	A	271	HIS	N-CA-CB	7.00	123.21	110.60
1	B	440	ARG	NE-CZ-NH2	-6.55	117.02	120.30
1	B	323	GLY	N-CA-C	-6.47	96.93	113.10
1	A	609	ASP	CA-C-N	-6.36	103.22	117.20
1	B	102	ASP	N-CA-CB	-6.34	99.19	110.60
1	A	246	ASP	N-CA-C	6.25	127.86	111.00
1	A	609	ASP	CB-CG-OD1	6.11	123.80	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	250	PRO	N-CA-C	6.08	127.90	112.10
1	B	188	PRO	N-CA-CB	5.73	110.18	103.30
1	B	250	PRO	C-N-CA	-5.68	107.49	121.70
1	A	608	ARG	C-N-CA	-5.61	107.68	121.70
1	A	502	LEU	N-CA-C	5.50	125.86	111.00
1	B	276	SER	N-CA-C	-5.46	96.25	111.00
1	B	277	LEU	N-CA-CB	-5.31	99.78	110.40
1	A	498	GLY	N-CA-C	5.28	126.29	113.10
1	A	609	ASP	N-CA-C	5.26	125.21	111.00
1	B	102	ASP	C-N-CD	-5.17	109.22	120.60
1	A	356	GLY	CA-C-N	-5.14	105.89	117.20
1	B	437	VAL	N-CA-C	5.07	124.69	111.00
1	B	79	LEU	CA-CB-CG	5.01	126.82	115.30

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	4891	0	4892	292	0
1	B	4668	0	4624	345	0
2	X	101	0	59	7	0
2	Y	85	0	46	1	0
3	A	25	0	0	0	0
3	B	19	0	0	0	0
3	X	3	0	0	0	0
3	Y	1	0	0	0	0
All	All	9793	0	9621	632	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 33.

All (632) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:506:PRO:HD3	1:B:522:LEU:HD21	1.28	1.12
1:A:175:CYS:HB2	1:A:265:LEU:HD11	1.28	1.08
1:B:237:GLU:HG3	1:B:237:GLU:O	1.51	1.08
1:B:349:LEU:HB2	1:B:381:LEU:HD12	1.38	1.05
1:B:440:ARG:HD3	1:B:441:GLU:N	1.71	1.03
1:A:482:ARG:CZ	1:A:487:PHE:HB2	1.90	1.01
1:B:237:GLU:O	1:B:238:GLY:C	1.98	1.01
1:A:101:LYS:HD2	1:A:101:LYS:H	1.22	0.99
1:A:486:ARG:NH1	1:A:487:PHE:CZ	2.32	0.97
1:B:195:ASN:HB2	1:B:200:ARG:NH1	1.78	0.97
1:B:288:ARG:HH11	1:B:289:ARG:HH12	1.08	0.96
1:A:415:TRP:C	1:A:415:TRP:CD1	2.37	0.96
1:A:600:THR:HG22	1:A:620:VAL:HG22	1.46	0.96
1:B:206:ARG:HH11	1:B:206:ARG:HG3	1.29	0.96
1:B:179:LEU:HD22	1:B:263:PRO:HG3	1.49	0.95
1:B:350:ARG:HG2	1:B:352:ASP:OD1	1.65	0.95
1:B:382:HIS:CD2	1:B:382:HIS:H	1.77	0.94
1:A:350:ARG:O	1:A:350:ARG:HG2	1.63	0.94
1:A:265:LEU:H	1:A:265:LEU:HD12	1.28	0.94
1:B:195:ASN:ND2	1:B:200:ARG:HD2	1.82	0.93
1:B:195:ASN:HD22	1:B:200:ARG:HD2	1.31	0.93
1:B:432:SER:H	1:B:503:TRP:HH2	1.00	0.92
1:B:574:ARG:HB3	1:B:574:ARG:HH11	1.36	0.91
1:B:318:ILE:HD12	1:B:319:PRO:HD2	1.51	0.91
1:B:153:LEU:HD13	1:B:297:ILE:HD12	1.53	0.90
1:B:352:ASP:OD2	1:B:437:VAL:HG21	1.70	0.90
1:A:75:LEU:HA	1:A:90:LEU:HD12	1.52	0.90
1:A:486:ARG:NH1	1:A:487:PHE:HZ	1.68	0.89
1:A:482:ARG:NH1	1:A:487:PHE:HB2	1.88	0.87
1:B:513:ARG:HG2	1:B:513:ARG:HH11	1.39	0.87
1:B:184:ALA:C	1:B:186:GLY:H	1.76	0.87
1:B:605:THR:O	1:B:606:VAL:HG12	1.74	0.87
1:A:462:VAL:HG12	1:A:463:VAL:HG23	1.57	0.87
1:B:198:ASP:OD2	1:B:200:ARG:HD3	1.76	0.86
1:B:340:ARG:HB2	1:B:461:GLN:HB2	1.58	0.85
1:B:350:ARG:CG	1:B:352:ASP:OD1	2.24	0.85
1:B:198:ASP:H	1:B:200:ARG:NH1	1.78	0.81
1:B:195:ASN:HB2	1:B:200:ARG:CZ	2.10	0.81
1:B:20:ASN:HB2	1:B:21:PRO:HD2	1.61	0.81
1:A:49:VAL:HG22	1:A:79:LEU:HD21	1.63	0.81
1:B:198:ASP:CG	1:B:200:ARG:HD3	2.02	0.81
1:B:437:VAL:O	1:B:439:LEU:N	2.15	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:289:ARG:HA	1:B:289:ARG:HH11	1.45	0.80
1:B:244:VAL:HG23	1:B:254:ILE:HD12	1.63	0.80
1:A:25:ARG:HB3	1:A:95:ARG:HD3	1.63	0.79
1:A:156:TRP:CH2	1:A:164:LEU:HD23	2.17	0.79
1:B:440:ARG:HD3	1:B:440:ARG:C	1.95	0.79
1:A:252:LYS:NZ	1:A:252:LYS:HB3	1.98	0.79
1:A:389:LEU:HD23	1:B:564:GLU:OE2	1.83	0.79
1:B:256:HIS:CD2	1:B:257:LEU:H	2.01	0.78
1:B:293:ILE:O	1:B:297:ILE:HG22	1.83	0.77
1:A:256:HIS:CD2	1:A:257:LEU:H	2.02	0.77
1:B:506:PRO:CD	1:B:522:LEU:HD21	2.13	0.77
1:B:352:ASP:OD1	1:B:353:GLY:N	2.17	0.77
1:A:57:THR:HG21	1:A:73:LEU:HD21	1.65	0.77
1:B:382:HIS:HD2	1:B:382:HIS:H	1.25	0.77
1:A:286:ARG:O	1:A:290:THR:HG22	1.85	0.76
1:A:411:PRO:HA	1:A:437:VAL:HG12	1.67	0.76
1:B:462:VAL:HG12	1:B:463:VAL:HG23	1.66	0.76
1:B:574:ARG:HD3	1:B:576:SER:O	1.85	0.76
1:B:181:ALA:O	1:B:184:ALA:HB3	1.86	0.76
1:A:57:THR:HG22	1:A:66:SER:OG	1.85	0.76
1:B:207:LEU:HD23	1:B:207:LEU:C	2.06	0.76
1:B:441:GLU:OE1	1:B:441:GLU:C	2.24	0.75
1:B:350:ARG:HD3	1:B:354:ALA:C	2.07	0.75
1:A:101:LYS:N	1:A:101:LYS:HD2	2.01	0.74
1:A:580:ARG:HE	1:A:613:THR:CG2	2.00	0.74
1:A:452:LEU:HD22	1:A:462:VAL:HG11	1.69	0.74
1:B:102:ASP:O	1:B:104:GLY:N	2.20	0.74
1:B:288:ARG:NH1	1:B:289:ARG:HH12	1.85	0.74
1:B:432:SER:N	1:B:503:TRP:HH2	1.82	0.74
1:A:482:ARG:NH2	1:A:487:PHE:HD2	1.86	0.74
1:B:299:ARG:HG2	1:B:300:ARG:N	2.02	0.74
1:B:329:LYS:NZ	1:B:329:LYS:HB3	2.02	0.73
1:B:195:ASN:HD22	1:B:200:ARG:CD	2.01	0.73
1:A:266:THR:HG23	1:A:268:GLU:H	1.54	0.73
1:B:97:PRO:C	1:B:98:LEU:HD12	2.09	0.73
1:B:56:VAL:HG12	1:B:67:TRP:HB2	1.71	0.73
1:B:440:ARG:NE	1:B:440:ARG:HA	2.04	0.73
1:B:45:LEU:CD1	1:B:81:ARG:HD3	2.19	0.73
1:A:128:TRP:C	1:A:128:TRP:CD1	2.62	0.72
1:B:360:PHE:CE2	1:B:441:GLU:HG2	2.23	0.72
1:A:437:VAL:HG13	1:A:438:PRO:HD3	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:352:ASP:CG	1:B:353:GLY:H	1.92	0.72
1:A:505:LEU:HB2	1:A:506:PRO:CD	2.20	0.72
1:B:200:ARG:N	1:B:200:ARG:NE	2.39	0.71
1:B:251:ARG:O	1:B:252:LYS:C	2.28	0.71
1:A:329:LYS:CB	1:A:329:LYS:NZ	2.53	0.71
1:A:25:ARG:HB3	1:A:95:ARG:CD	2.21	0.71
1:B:232:ARG:HE	1:B:232:ARG:HA	1.54	0.70
1:A:252:LYS:HZ3	1:A:252:LYS:HB3	1.52	0.70
1:A:312:GLN:HE21	1:A:312:GLN:H	1.37	0.70
1:A:505:LEU:HB2	1:A:506:PRO:HD2	1.73	0.70
1:B:244:VAL:HG23	1:B:254:ILE:CD1	2.22	0.70
1:B:205:LEU:O	1:B:206:ARG:HB3	1.92	0.70
1:B:200:ARG:O	1:B:200:ARG:NE	2.23	0.70
1:B:489:GLY:O	1:B:506:PRO:HD2	1.92	0.70
1:A:256:HIS:HD2	1:A:257:LEU:H	1.37	0.70
1:A:193:VAL:HG11	1:A:261:LEU:HB3	1.74	0.70
1:A:580:ARG:HE	1:A:613:THR:HG21	1.56	0.69
1:B:440:ARG:HG3	1:B:442:GLU:HG2	1.74	0.69
1:B:390:ALA:O	1:B:393:GLU:HB3	1.92	0.69
1:A:194:ARG:HD2	1:A:195:ASN:O	1.91	0.69
1:A:175:CYS:CB	1:A:265:LEU:HD11	2.15	0.69
1:B:198:ASP:H	1:B:200:ARG:HH12	1.38	0.69
1:A:203:GLU:HB3	1:A:245:ALA:HB3	1.74	0.69
1:B:45:LEU:HD13	1:B:81:ARG:HD3	1.75	0.69
1:B:156:TRP:CZ3	1:B:164:LEU:HD23	2.29	0.69
1:B:206:ARG:CG	1:B:206:ARG:HH11	2.04	0.68
1:B:546:ASP:O	1:B:549:VAL:HG22	1.93	0.68
1:B:194:ARG:HG2	1:B:200:ARG:HH21	1.58	0.68
1:B:234:GLN:O	1:B:234:GLN:HG2	1.94	0.68
1:B:200:ARG:HE	1:B:200:ARG:C	1.96	0.68
1:B:193:VAL:HG22	1:B:194:ARG:N	2.09	0.68
1:A:455:LEU:HD22	1:A:460:LEU:HD23	1.76	0.68
1:A:25:ARG:HB3	1:A:95:ARG:CG	2.23	0.67
1:A:193:VAL:CG1	1:A:261:LEU:HB3	2.24	0.67
1:A:549:VAL:HG13	1:A:550:PRO:HD2	1.77	0.67
1:B:440:ARG:CG	1:B:442:GLU:HG2	2.25	0.67
1:B:251:ARG:O	1:B:253:PRO:N	2.28	0.67
1:A:351:LEU:HD21	1:A:385:PRO:HB3	1.77	0.67
1:A:52:ARG:HD3	2:X:7:DA:H2	1.59	0.67
1:A:327:VAL:HG13	1:A:332:ASP:HB2	1.77	0.67
1:B:352:ASP:OD2	1:B:437:VAL:CG2	2.43	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:210:GLU:O	1:B:241:VAL:HG21	1.95	0.66
1:A:452:LEU:CD2	1:A:462:VAL:HG11	2.25	0.66
1:A:237:GLU:O	1:A:259:GLY:HA3	1.96	0.66
1:A:327:VAL:CG1	1:A:332:ASP:HB2	2.25	0.66
1:B:206:ARG:HG3	1:B:206:ARG:NH1	2.04	0.65
1:A:607:HIS:O	1:A:608:ARG:CB	2.43	0.65
1:B:127:VAL:HG13	1:B:135:TYR:O	1.95	0.65
1:A:327:VAL:HG12	1:A:329:LYS:H	1.62	0.65
1:A:407:LEU:HD13	1:A:454:LEU:HG	1.77	0.65
1:A:246:ASP:HB3	1:A:249:ASP:H	1.61	0.65
1:A:482:ARG:NH1	1:A:482:ARG:HB3	2.12	0.65
1:B:122:ARG:HG2	1:B:123:ARG:N	2.11	0.64
1:A:25:ARG:O	1:A:95:ARG:HG3	1.97	0.64
1:B:346:LEU:HG	1:B:454:LEU:HD11	1.79	0.64
1:B:179:LEU:HG	1:B:258:THR:HG22	1.79	0.64
1:B:251:ARG:O	1:B:253:PRO:HD3	1.97	0.64
1:A:192:ARG:HG3	1:A:202:TRP:O	1.98	0.64
1:B:506:PRO:HG2	1:B:518:VAL:HG13	1.80	0.64
1:B:299:ARG:HG2	1:B:300:ARG:H	1.62	0.64
1:B:198:ASP:OD2	1:B:200:ARG:NH1	2.27	0.64
1:A:437:VAL:CG1	1:A:438:PRO:HD3	2.27	0.64
1:A:266:THR:HG22	1:A:269:ASP:H	1.61	0.64
1:B:234:GLN:O	1:B:234:GLN:CG	2.45	0.64
1:A:141:ARG:CG	1:A:142:GLY:H	2.11	0.64
1:A:604:LEU:HG	1:A:616:PRO:HB3	1.80	0.64
1:B:441:GLU:O	1:B:443:GLU:N	2.31	0.63
1:B:251:ARG:O	1:B:253:PRO:CD	2.46	0.63
1:B:223:LEU:HD12	1:B:257:LEU:HD21	1.80	0.63
1:A:505:LEU:N	1:A:505:LEU:HD22	2.14	0.63
1:B:200:ARG:CA	1:B:200:ARG:HE	2.10	0.63
1:B:256:HIS:HD2	1:B:257:LEU:H	1.45	0.63
1:A:444:ARG:O	1:A:448:GLU:HG3	1.99	0.63
1:A:530:PHE:CD2	1:A:538:PRO:HD3	2.33	0.63
1:A:415:TRP:CD1	1:A:416:GLU:N	2.67	0.63
1:A:501:LEU:HD21	1:A:529:ALA:HB3	1.80	0.63
1:A:329:LYS:HB2	1:A:329:LYS:NZ	2.13	0.62
1:B:538:PRO:O	1:B:566:ILE:HD12	1.99	0.62
1:A:411:PRO:HG3	1:A:437:VAL:HG11	1.80	0.62
1:B:238:GLY:CA	1:B:259:GLY:HA3	2.29	0.62
1:B:232:ARG:NE	1:B:232:ARG:HA	2.14	0.62
1:A:363:ARG:HB3	1:A:363:ARG:HH11	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:344:THR:HG21	1:B:369:PHE:CZ	2.34	0.62
1:A:639:THR:HG22	1:A:640:ARG:HE	1.64	0.62
1:B:236:ARG:O	1:B:238:GLY:N	2.32	0.62
1:A:141:ARG:O	1:A:145:TRP:CE2	2.53	0.61
1:B:198:ASP:N	1:B:200:ARG:NH1	2.48	0.61
1:A:350:ARG:O	1:A:350:ARG:CG	2.42	0.61
1:B:237:GLU:O	1:B:238:GLY:O	2.18	0.61
1:A:96:ARG:HG2	1:A:96:ARG:O	2.00	0.61
1:A:265:LEU:N	1:A:265:LEU:HD12	2.09	0.61
1:B:506:PRO:HD3	1:B:522:LEU:CD2	2.18	0.61
1:B:350:ARG:HH12	1:B:358:PRO:HD3	1.64	0.61
1:B:238:GLY:HA3	1:B:259:GLY:HA3	1.83	0.61
1:B:16:LEU:HB3	1:B:303:LEU:O	1.99	0.61
1:A:385:PRO:O	1:A:387:GLN:N	2.33	0.61
1:B:316:LEU:HD22	1:B:633:HIS:CD2	2.36	0.61
1:A:482:ARG:HD3	1:A:487:PHE:O	2.01	0.61
1:A:194:ARG:HD3	1:A:199:ARG:HA	1.81	0.61
1:A:156:TRP:CZ3	1:A:164:LEU:HD23	2.35	0.60
1:B:156:TRP:CH2	1:B:164:LEU:HD23	2.36	0.60
1:B:212:PRO:HB3	1:B:241:VAL:HG13	1.82	0.60
1:A:358:PRO:HD2	1:A:361:LEU:HD12	1.82	0.60
1:B:452:LEU:HD22	1:B:462:VAL:HG11	1.83	0.60
1:B:184:ALA:C	1:B:186:GLY:N	2.45	0.60
1:A:363:ARG:HD2	1:A:367:ARG:HH21	1.66	0.60
1:B:513:ARG:NH1	1:B:513:ARG:HG2	2.09	0.60
1:A:299:ARG:HH11	1:A:299:ARG:HG3	1.66	0.60
1:B:179:LEU:HD22	1:B:263:PRO:CG	2.28	0.60
1:B:422:LYS:HZ1	1:B:503:TRP:HZ2	1.48	0.60
1:B:53:ALA:O	1:B:54:GLY:O	2.19	0.60
1:B:544:LEU:HD21	1:B:635:ILE:HD12	1.83	0.60
1:B:574:ARG:CB	1:B:574:ARG:HH11	2.12	0.60
1:B:301:LEU:O	1:B:303:LEU:HD13	2.02	0.60
1:B:180:GLU:O	1:B:184:ALA:HB2	2.02	0.60
1:B:286:ARG:HG2	1:B:582:TYR:OH	2.02	0.59
1:A:564:GLU:OE1	1:B:389:LEU:HD12	2.02	0.59
1:A:100:PRO:HD2	1:A:101:LYS:NZ	2.17	0.59
1:B:195:ASN:ND2	1:B:202:TRP:HE1	1.99	0.59
1:B:329:LYS:HG2	1:B:332:ASP:OD2	2.03	0.59
1:A:9:VAL:HG22	1:A:582:TYR:O	2.02	0.59
1:B:143:PRO:HD2	1:B:145:TRP:CH2	2.37	0.59
1:A:327:VAL:HG12	1:A:329:LYS:N	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:206:ARG:CG	1:B:206:ARG:NH1	2.62	0.59
1:B:222:SER:OG	1:B:225:ASP:HB2	2.02	0.58
1:A:31:VAL:HG12	1:A:32:VAL:N	2.17	0.58
1:B:299:ARG:CG	1:B:300:ARG:N	2.66	0.58
1:B:341:ALA:O	1:B:342:GLN:HG3	2.03	0.58
1:B:193:VAL:HG22	1:B:194:ARG:H	1.66	0.58
1:B:223:LEU:HD11	1:B:257:LEU:HG	1.84	0.58
1:A:141:ARG:HG3	1:A:142:GLY:H	1.66	0.58
1:A:559:GLU:O	1:A:563:ARG:HG3	2.03	0.58
1:A:509:GLN:NE2	1:B:420:ARG:HG3	2.19	0.58
1:A:265:LEU:CD1	1:A:265:LEU:H	2.11	0.58
1:B:17:ARG:NH1	1:B:303:LEU:HG	2.19	0.58
1:B:329:LYS:HB3	1:B:329:LYS:HZ3	1.67	0.58
1:A:424:LEU:O	1:A:427:ARG:HB3	2.03	0.58
1:B:89:ARG:HG2	1:B:91:TYR:CE1	2.38	0.58
1:B:283:TRP:HA	1:B:613:THR:CG2	2.34	0.58
1:B:440:ARG:NH2	1:B:440:ARG:HG2	2.17	0.58
1:B:606:VAL:HG13	1:B:606:VAL:O	2.03	0.57
1:A:435:LEU:HD21	1:A:439:LEU:HD22	1.87	0.57
1:B:544:LEU:HD21	1:B:635:ILE:CD1	2.33	0.57
1:B:237:GLU:O	1:B:239:GLY:N	2.37	0.57
1:B:641:LEU:HD12	1:B:641:LEU:O	2.03	0.57
1:B:506:PRO:HG3	1:B:522:LEU:HG	1.86	0.57
1:A:99:ASP:HB2	1:A:101:LYS:HD3	1.86	0.57
1:B:530:PHE:HD2	1:B:538:PRO:HD3	1.70	0.56
1:B:296:TRP:O	1:B:299:ARG:HB3	2.05	0.56
1:A:475:VAL:HG22	1:A:477:PHE:CE1	2.40	0.56
1:B:238:GLY:C	1:B:259:GLY:HA3	2.25	0.56
1:B:530:PHE:CD2	1:B:538:PRO:HD3	2.40	0.56
1:A:135:TYR:CE2	1:A:172:ARG:HB2	2.40	0.56
1:A:134:VAL:O	1:A:150:GLY:HA3	2.06	0.56
1:B:350:ARG:HE	1:B:352:ASP:CG	2.09	0.56
1:A:363:ARG:HD2	1:A:367:ARG:NH2	2.20	0.56
1:A:503:TRP:CZ3	1:A:505:LEU:CD1	2.88	0.56
1:A:316:LEU:HD22	1:A:633:HIS:CD2	2.41	0.56
1:B:396:ARG:HG2	1:B:396:ARG:HH11	1.71	0.56
1:B:327:VAL:CG2	1:B:332:ASP:HB2	2.36	0.56
1:B:184:ALA:O	1:B:186:GLY:N	2.40	0.55
1:A:299:ARG:NH1	1:A:299:ARG:HG3	2.20	0.55
1:B:58:VAL:HG21	1:B:111:ALA:HB1	1.87	0.55
1:B:232:ARG:CZ	1:B:236:ARG:HD3	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:349:LEU:HA	1:B:381:LEU:HB2	1.89	0.55
1:B:223:LEU:HD13	1:B:223:LEU:O	2.06	0.55
1:B:208:GLY:HA3	1:B:241:VAL:HB	1.88	0.55
1:B:246:ASP:OD2	1:B:247:PRO:HD2	2.05	0.55
1:B:200:ARG:HE	1:B:200:ARG:N	2.04	0.55
1:A:489:GLY:O	1:A:506:PRO:HD3	2.06	0.55
1:B:545:ARG:NH1	1:B:549:VAL:O	2.39	0.55
1:B:177:MET:O	1:B:178:SER:CB	2.54	0.55
1:A:482:ARG:CZ	1:A:487:PHE:CB	2.77	0.55
1:B:283:TRP:HA	1:B:613:THR:HG23	1.87	0.55
1:A:141:ARG:O	1:A:145:TRP:CD2	2.59	0.55
1:A:145:TRP:CD2	1:A:270:LEU:HD22	2.41	0.55
1:B:287:ARG:C	1:B:290:THR:HG22	2.26	0.55
1:B:41:GLU:O	1:B:44:PRO:HD2	2.06	0.55
1:B:537:LEU:N	1:B:537:LEU:HD12	2.21	0.55
1:A:462:VAL:CG1	1:A:463:VAL:HG23	2.33	0.55
1:A:57:THR:HG21	1:A:73:LEU:CD2	2.37	0.55
1:B:289:ARG:CA	1:B:289:ARG:HH11	2.19	0.55
1:A:51:ARG:NE	2:X:7:DA:OP1	2.33	0.55
1:B:455:LEU:HD22	1:B:460:LEU:CD1	2.36	0.55
1:A:99:ASP:OD2	1:A:102:ASP:HB3	2.07	0.55
1:A:58:VAL:HG12	1:A:59:ARG:N	2.22	0.55
1:A:341:ALA:HA	1:A:460:LEU:HD11	1.89	0.55
1:B:28:ARG:C	1:B:29:LEU:HD12	2.27	0.55
1:B:433:GLN:HG2	1:B:450:ALA:O	2.07	0.55
1:B:278:ALA:O	1:B:279:LEU:C	2.45	0.55
1:A:37:PRO:HB3	1:A:86:TYR:CE2	2.42	0.54
1:B:177:MET:O	1:B:178:SER:HB3	2.06	0.54
1:B:106:ARG:HG3	1:B:106:ARG:O	2.06	0.54
1:A:521:ASP:HA	1:A:524:GLU:HB3	1.90	0.54
1:B:349:LEU:HD13	1:B:381:LEU:HD13	1.88	0.54
1:B:440:ARG:HG2	1:B:440:ARG:HH21	1.72	0.54
1:A:25:ARG:HB3	1:A:95:ARG:HG2	1.89	0.54
1:A:156:TRP:N	1:A:156:TRP:CD1	2.75	0.54
1:A:128:TRP:CD1	1:A:128:TRP:O	2.61	0.54
1:B:352:ASP:CG	1:B:353:GLY:N	2.61	0.54
1:A:608:ARG:O	1:A:609:ASP:CG	2.47	0.54
1:B:16:LEU:HB2	1:B:163:PHE:HB2	1.90	0.54
1:B:153:LEU:HD13	1:B:297:ILE:CD1	2.30	0.53
1:B:102:ASP:O	1:B:103:PRO:C	2.46	0.53
1:B:437:VAL:C	1:B:439:LEU:N	2.61	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:113:ALA:O	1:B:155:LEU:HD23	2.08	0.53
1:A:389:LEU:HB2	1:B:564:GLU:OE2	2.09	0.53
1:A:223:LEU:HD11	1:A:257:LEU:HG	1.89	0.53
1:B:545:ARG:HD2	1:B:554:PHE:CE1	2.43	0.53
1:A:455:LEU:HD22	1:A:460:LEU:CD2	2.39	0.53
1:A:101:LYS:CD	1:A:101:LYS:H	2.04	0.53
1:B:244:VAL:HG22	1:B:256:HIS:HB2	1.89	0.53
1:A:266:THR:HG23	1:A:268:GLU:N	2.22	0.53
1:A:506:PRO:HD3	1:A:522:LEU:HD21	1.89	0.53
1:A:470:PRO:HD2	1:A:634:GLN:OE1	2.09	0.53
1:A:16:LEU:HB2	1:A:163:PHE:HB2	1.91	0.53
1:A:98:LEU:HD23	1:A:109:LEU:HG	1.88	0.53
1:B:99:ASP:C	1:B:101:LYS:H	2.12	0.53
1:B:514:ILE:HG23	1:B:515:PRO:HD2	1.91	0.53
1:A:51:ARG:HE	2:X:7:DA:P	2.31	0.53
1:B:195:ASN:CG	1:B:202:TRP:HE1	2.12	0.53
1:B:195:ASN:OD1	1:B:256:HIS:CE1	2.62	0.53
1:A:145:TRP:CZ3	1:A:270:LEU:HD13	2.44	0.53
1:A:48:GLN:HG3	2:X:7:DA:O4'	2.08	0.52
1:A:69:PRO:HG2	1:A:72:VAL:CG2	2.40	0.52
1:A:329:LYS:CB	1:A:329:LYS:HZ1	2.23	0.52
1:B:434:ILE:HG22	1:B:434:ILE:O	2.08	0.52
1:B:395:LEU:HD22	1:B:425:LEU:HD23	1.92	0.52
1:B:358:PRO:HG2	1:B:361:LEU:HD12	1.91	0.52
1:A:58:VAL:CG1	1:A:59:ARG:N	2.72	0.52
1:A:22:GLU:H	1:A:22:GLU:CD	2.13	0.52
1:A:621:HIS:CE1	1:A:623:ALA:O	2.63	0.52
1:B:179:LEU:CG	1:B:258:THR:HG22	2.39	0.52
1:A:363:ARG:NH1	1:A:363:ARG:HB3	2.24	0.52
1:B:232:ARG:NH2	1:B:236:ARG:HD3	2.24	0.52
1:A:462:VAL:HG12	1:A:463:VAL:N	2.24	0.51
1:B:195:ASN:HD21	1:B:202:TRP:HE1	1.58	0.51
1:B:200:ARG:NE	1:B:200:ARG:H	2.07	0.51
1:B:114:ARG:HD2	1:B:154:ASP:OD1	2.10	0.51
1:A:486:ARG:HH11	1:A:487:PHE:HZ	1.28	0.51
1:B:360:PHE:CD2	1:B:441:GLU:HG2	2.44	0.51
1:A:600:THR:CG2	1:A:620:VAL:HG22	2.31	0.51
1:A:501:LEU:HD21	1:A:526:THR:O	2.11	0.51
1:B:290:THR:HG23	1:B:291:ARG:N	2.26	0.51
1:B:79:LEU:O	1:B:79:LEU:HD22	2.09	0.51
1:A:49:VAL:CG2	1:A:79:LEU:HD21	2.38	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:344:THR:OG1	1:B:346:LEU:HD11	2.11	0.51
1:B:484:SER:OG	1:B:486:ARG:HG3	2.11	0.51
1:B:200:ARG:CA	1:B:200:ARG:NE	2.74	0.51
1:B:223:LEU:C	1:B:223:LEU:HD13	2.31	0.51
1:A:240:ARG:HG3	1:A:241:VAL:N	2.25	0.51
1:B:13:ARG:NH1	1:B:156:TRP:HH2	2.09	0.51
1:A:99:ASP:OD2	1:A:102:ASP:CB	2.59	0.51
1:B:287:ARG:HA	1:B:290:THR:HG22	1.93	0.51
1:A:463:VAL:HG12	1:A:464:ALA:N	2.25	0.50
1:B:254:ILE:HD12	1:B:254:ILE:O	2.12	0.50
1:A:558:LEU:HD13	1:A:568:TYR:CE2	2.46	0.50
1:B:441:GLU:C	1:B:443:GLU:N	2.64	0.50
1:B:441:GLU:O	1:B:441:GLU:OE1	2.29	0.50
1:B:345:ALA:HB3	1:B:402:GLY:O	2.11	0.50
1:A:482:ARG:NH2	1:A:487:PHE:CD2	2.73	0.50
1:A:25:ARG:CB	1:A:95:ARG:HD3	2.36	0.50
1:A:437:VAL:HG13	1:A:438:PRO:CD	2.40	0.50
1:A:312:GLN:NE2	1:A:312:GLN:H	2.08	0.50
1:B:454:LEU:HD13	1:B:454:LEU:C	2.31	0.50
1:A:141:ARG:CG	1:A:142:GLY:N	2.75	0.50
1:A:79:LEU:HD11	1:A:88:TYR:HD1	1.76	0.50
1:B:444:ARG:HA	1:B:447:TRP:NE1	2.27	0.50
1:A:473:LEU:HD23	1:A:538:PRO:HG3	1.94	0.49
1:B:399:LYS:HG3	1:B:428:GLU:O	2.12	0.49
1:B:25:ARG:HG2	1:B:95:ARG:HB3	1.93	0.49
1:B:51:ARG:NH2	1:B:115:ARG:CZ	2.75	0.49
1:B:584:VAL:HG12	1:B:585:GLN:N	2.27	0.49
1:B:297:ILE:HG12	1:B:301:LEU:CD1	2.42	0.49
1:B:452:LEU:CD2	1:B:462:VAL:HG11	2.40	0.49
1:B:71:GLU:CD	1:B:71:GLU:H	2.14	0.49
1:B:9:VAL:HG22	1:B:311:ALA:O	2.12	0.49
1:B:198:ASP:N	1:B:198:ASP:OD2	2.46	0.49
1:A:147:VAL:HG22	1:A:173:ILE:HG12	1.94	0.49
1:B:190:PRO:HG3	1:B:263:PRO:HB3	1.94	0.49
1:A:329:LYS:HB2	1:A:329:LYS:HZ1	1.75	0.49
1:A:19:LEU:HD21	1:A:157:VAL:HG21	1.95	0.49
1:B:441:GLU:C	1:B:443:GLU:H	2.15	0.49
1:B:420:ARG:HH11	1:B:420:ARG:HG3	1.78	0.49
1:B:177:MET:CB	1:B:182:TRP:HE3	2.26	0.49
1:A:587:ARG:HG2	1:A:588:LEU:H	1.76	0.49
1:A:338:PHE:CD1	1:A:460:LEU:HD21	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:ARG:CD	1:A:613:THR:HG21	2.43	0.49
1:B:376:LEU:HG	1:B:378:LEU:CD2	2.43	0.49
1:A:498:GLY:O	1:A:500:HIS:N	2.38	0.49
1:A:584:VAL:O	1:A:585:GLN:HG3	2.13	0.49
1:A:13:ARG:NH1	1:A:156:TRP:HH2	2.10	0.48
1:B:130:GLU:HG3	1:B:130:GLU:O	2.12	0.48
1:A:228:ALA:HA	1:A:233:LEU:HB2	1.95	0.48
1:B:369:PHE:CD1	1:B:376:LEU:HD22	2.48	0.48
1:B:102:ASP:O	1:B:102:ASP:OD2	2.32	0.48
1:B:477:PHE:N	1:B:477:PHE:CD1	2.82	0.48
1:A:99:ASP:HB2	1:A:101:LYS:CD	2.43	0.48
1:B:244:VAL:CG2	1:B:256:HIS:HB2	2.43	0.48
1:B:153:LEU:CD1	1:B:297:ILE:HD12	2.36	0.48
1:A:501:LEU:HD11	1:A:529:ALA:C	2.33	0.48
1:B:599:LYS:HA	1:B:628:LEU:HD11	1.95	0.48
1:A:415:TRP:CG	1:A:415:TRP:O	2.62	0.48
1:A:28:ARG:HD2	1:A:60:MET:CE	2.43	0.48
1:A:202:TRP:HB3	1:A:244:VAL:HG13	1.96	0.48
1:A:190:PRO:HG3	1:A:263:PRO:HB3	1.95	0.48
1:B:345:ALA:O	1:B:346:LEU:HD12	2.14	0.48
1:B:465:LEU:HD12	1:B:469:TYR:OH	2.14	0.48
1:A:514:ILE:HG23	1:A:514:ILE:O	2.13	0.48
1:A:482:ARG:CZ	1:A:482:ARG:HB3	2.44	0.48
1:B:297:ILE:CD1	1:B:301:LEU:HD11	2.44	0.48
1:A:437:VAL:O	1:A:439:LEU:N	2.47	0.48
1:A:384:HIS:HB3	1:A:385:PRO:CD	2.43	0.48
1:A:28:ARG:HD2	1:A:60:MET:HE1	1.95	0.48
1:A:43:TYR:HB2	1:A:44:PRO:HD3	1.96	0.48
1:B:330:PRO:HG2	1:B:641:LEU:HA	1.96	0.48
1:A:384:HIS:HB3	1:A:385:PRO:HD2	1.96	0.48
1:B:214:GLU:O	1:B:216:PRO:HD3	2.14	0.48
1:B:193:VAL:CG2	1:B:194:ARG:N	2.76	0.47
1:B:492:CYS:HA	1:B:503:TRP:HB2	1.96	0.47
1:B:422:LYS:NZ	1:B:503:TRP:HZ2	2.11	0.47
1:B:631:LEU:O	1:B:635:ILE:HG12	2.14	0.47
1:A:463:VAL:CG1	1:A:464:ALA:N	2.76	0.47
1:B:183:LEU:HD13	1:B:183:LEU:O	2.15	0.47
1:A:590:ASP:OD2	1:A:605:THR:HA	2.14	0.47
1:B:321:LEU:HB3	1:B:463:VAL:HG11	1.96	0.47
1:A:514:ILE:HD12	1:A:516:GLN:HB2	1.95	0.47
1:B:195:ASN:HA	1:B:261:LEU:HD23	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:382:HIS:CD2	1:B:382:HIS:N	2.59	0.47
1:B:329:LYS:CB	1:B:329:LYS:NZ	2.76	0.47
1:B:212:PRO:HD3	1:B:241:VAL:HG22	1.97	0.47
1:B:551:GLN:HG3	1:B:622:GLU:OE1	2.14	0.47
1:B:455:LEU:HD22	1:B:460:LEU:HD13	1.96	0.47
1:A:506:PRO:CD	1:A:522:LEU:HD21	2.44	0.47
1:A:317:SER:OG	1:A:633:HIS:HE1	1.97	0.47
1:B:601:PHE:CE1	1:B:628:LEU:HD22	2.50	0.47
1:A:281:LEU:N	1:A:281:LEU:HD12	2.29	0.47
1:B:238:GLY:HA3	1:B:259:GLY:CA	2.43	0.47
1:B:590:ASP:O	1:B:605:THR:HA	2.15	0.47
1:A:503:TRP:CZ3	1:A:505:LEU:HD11	2.49	0.47
1:A:384:HIS:C	1:A:385:PRO:O	2.52	0.47
1:B:208:GLY:H	1:B:242:ALA:HA	1.80	0.47
1:B:345:ALA:C	1:B:346:LEU:HD12	2.35	0.47
1:A:135:TYR:CZ	1:A:172:ARG:HB2	2.50	0.47
1:B:435:LEU:HG	1:B:450:ALA:CB	2.45	0.47
1:A:558:LEU:HD22	1:A:568:TYR:CE2	2.50	0.47
1:B:475:VAL:HG13	1:B:543:LEU:HD23	1.96	0.47
1:A:296:TRP:CZ3	1:A:300:ARG:CZ	2.98	0.47
1:B:361:LEU:HD22	1:B:451:LEU:HD11	1.95	0.47
1:A:560:ALA:O	1:A:564:GLU:HG2	2.15	0.47
1:B:357:TRP:CZ2	1:B:378:LEU:HD12	2.50	0.47
1:A:195:ASN:OD1	1:A:256:HIS:HE1	1.98	0.47
1:A:503:TRP:CH2	1:A:505:LEU:CD1	2.98	0.47
1:B:325:ARG:NH2	1:B:336:VAL:HG13	2.29	0.47
1:A:20:ASN:HB2	1:A:21:PRO:HD2	1.97	0.46
1:A:25:ARG:O	1:A:95:ARG:CG	2.62	0.46
1:A:588:LEU:HD23	1:A:589:ALA:O	2.15	0.46
1:A:31:VAL:HG22	1:A:90:LEU:HD23	1.97	0.46
1:A:427:ARG:HD3	1:A:427:ARG:HA	1.48	0.46
1:B:440:ARG:HE	1:B:440:ARG:HA	1.78	0.46
1:A:410:THR:O	1:A:436:ASN:HA	2.16	0.46
1:A:301:LEU:HD22	1:A:303:LEU:HD22	1.98	0.46
1:A:531:ARG:NH1	1:A:532:ARG:HG2	2.31	0.46
1:B:81:ARG:HG2	1:B:81:ARG:HH11	1.79	0.46
1:A:246:ASP:HB3	1:A:248:LYS:N	2.30	0.46
1:A:390:ALA:O	1:A:393:GLU:HB3	2.16	0.46
1:A:179:LEU:HD22	1:A:179:LEU:O	2.16	0.46
1:A:325:ARG:O	1:A:327:VAL:HG23	2.16	0.46
1:A:173:ILE:CG2	1:A:270:LEU:HD11	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:193:VAL:CG2	1:B:194:ARG:H	2.29	0.45
1:B:198:ASP:HB2	1:B:199:ARG:H	1.64	0.45
1:B:444:ARG:O	1:B:445:HIS:C	2.52	0.45
1:B:456:ALA:HB1	1:B:500:HIS:CG	2.51	0.45
1:B:134:VAL:HG12	1:B:135:TYR:N	2.31	0.45
1:B:537:LEU:H	1:B:537:LEU:HD12	1.81	0.45
1:A:583:PRO:HG3	1:A:588:LEU:HB2	1.99	0.45
2:X:6:DT:H2'	2:X:6:DT:O2	2.16	0.45
1:B:432:SER:O	1:B:503:TRP:CZ2	2.69	0.45
1:A:31:VAL:CG1	1:A:32:VAL:N	2.80	0.45
1:B:329:LYS:HB3	1:B:329:LYS:HZ2	1.81	0.45
1:A:327:VAL:HG13	1:A:332:ASP:CB	2.44	0.45
1:B:626:THR:HG21	1:B:631:LEU:HD13	1.97	0.45
1:B:287:ARG:HA	1:B:290:THR:CG2	2.47	0.45
1:A:558:LEU:HD22	1:A:568:TYR:CD2	2.52	0.45
1:A:594:VAL:HG12	1:A:596:LEU:CD1	2.47	0.45
1:B:503:TRP:N	1:B:503:TRP:HE3	2.15	0.45
1:B:325:ARG:CZ	1:B:336:VAL:HG13	2.46	0.45
1:B:397:LYS:O	1:B:400:GLU:HB2	2.17	0.45
1:B:181:ALA:HA	1:B:184:ALA:HB3	1.97	0.45
1:B:257:LEU:O	1:B:261:LEU:HG	2.17	0.45
1:B:181:ALA:O	1:B:184:ALA:N	2.50	0.45
1:A:45:LEU:O	1:A:49:VAL:HG23	2.17	0.45
1:A:415:TRP:CD1	1:A:415:TRP:O	2.68	0.45
1:A:117:LEU:HD23	1:A:132:LEU:HD22	1.99	0.45
1:B:109:LEU:HB3	1:B:157:VAL:HG21	1.98	0.45
1:B:277:LEU:O	1:B:279:LEU:N	2.49	0.45
1:A:193:VAL:HG23	1:A:204:LEU:HB2	1.98	0.45
1:A:415:TRP:HD1	1:A:416:GLU:N	2.13	0.45
1:A:25:ARG:O	1:A:95:ARG:CD	2.65	0.45
1:B:48:GLN:OE1	1:B:81:ARG:HD2	2.17	0.45
1:B:545:ARG:NH1	1:B:549:VAL:HG23	2.31	0.45
1:A:341:ALA:HA	1:A:460:LEU:CD1	2.47	0.45
1:B:601:PHE:CD1	1:B:628:LEU:HD22	2.52	0.45
1:A:357:TRP:CE2	1:A:378:LEU:HG	2.52	0.45
1:B:522:LEU:O	1:B:526:THR:HG23	2.17	0.44
1:A:435:LEU:CD2	1:A:439:LEU:HD22	2.47	0.44
1:B:99:ASP:C	1:B:101:LYS:N	2.68	0.44
1:B:551:GLN:HG2	1:B:551:GLN:O	2.17	0.44
1:B:98:LEU:N	1:B:98:LEU:HD12	2.31	0.44
1:A:485:PHE:O	1:A:518:VAL:HG21	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:345:ALA:HB3	1:A:402:GLY:O	2.17	0.44
1:A:296:TRP:CZ3	1:A:300:ARG:NH2	2.85	0.44
1:B:343:GLU:OE1	1:B:375:SER:OG	2.32	0.44
1:B:440:ARG:C	1:B:440:ARG:CD	2.62	0.44
1:B:20:ASN:HB2	1:B:21:PRO:CD	2.42	0.44
1:B:56:VAL:HG12	1:B:56:VAL:O	2.18	0.44
1:B:99:ASP:O	1:B:101:LYS:N	2.50	0.44
1:A:144:GLY:HA3	1:A:177:MET:CE	2.47	0.44
1:B:440:ARG:NH2	1:B:442:GLU:OE2	2.51	0.44
1:B:451:LEU:O	1:B:455:LEU:HG	2.18	0.44
1:B:491:ALA:O	1:B:503:TRP:HB2	2.18	0.44
1:A:286:ARG:O	1:A:290:THR:CG2	2.63	0.44
1:A:58:VAL:HG11	1:A:111:ALA:CB	2.48	0.44
1:B:605:THR:O	1:B:606:VAL:CG1	2.58	0.44
1:A:213:LYS:HG2	1:A:213:LYS:H	1.56	0.44
1:B:564:GLU:HB2	1:B:566:ILE:HG12	1.99	0.44
1:A:329:LYS:HB2	1:A:329:LYS:HE3	1.70	0.44
1:A:465:LEU:HB2	1:A:497:ASP:HA	2.00	0.44
1:A:48:GLN:HE22	1:A:80:ALA:H	1.65	0.43
1:B:287:ARG:CA	1:B:290:THR:HG22	2.47	0.43
1:B:195:ASN:OD1	1:B:256:HIS:HE1	2.01	0.43
1:B:489:GLY:O	1:B:506:PRO:CD	2.62	0.43
1:B:626:THR:CG2	1:B:631:LEU:HD13	2.49	0.43
1:A:514:ILE:C	1:A:514:ILE:HD13	2.38	0.43
1:A:383:ALA:HB2	1:A:394:ALA:CB	2.49	0.43
1:A:514:ILE:HD13	1:A:516:GLN:H	1.84	0.43
1:A:420:ARG:O	1:A:423:ALA:HB3	2.18	0.43
1:B:297:ILE:O	1:B:297:ILE:HG12	2.18	0.43
1:A:80:ALA:HA	1:A:84:GLN:O	2.18	0.43
1:A:511:GLY:HA2	1:B:487:PHE:O	2.17	0.43
1:A:452:LEU:HD23	1:A:462:VAL:HG21	2.01	0.43
1:A:69:PRO:HG2	1:A:72:VAL:HG23	2.00	0.43
1:A:297:ILE:HD12	1:A:297:ILE:HA	1.94	0.43
1:B:591:GLY:HA3	1:B:636:PHE:CZ	2.52	0.43
1:A:31:VAL:HG22	1:A:90:LEU:CD2	2.49	0.43
1:A:79:LEU:N	1:A:79:LEU:HD12	2.34	0.43
1:A:52:ARG:HD3	2:X:7:DA:C2	2.46	0.43
1:A:531:ARG:CZ	1:A:532:ARG:HG2	2.48	0.43
1:A:505:LEU:CB	1:A:506:PRO:CD	2.89	0.43
1:A:486:ARG:HG3	1:A:513:ARG:O	2.18	0.43
1:A:99:ASP:O	1:A:99:ASP:OD2	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:415:TRP:CH2	1:A:480:GLY:HA3	2.54	0.43
1:A:338:PHE:CE1	1:A:460:LEU:HD21	2.53	0.43
1:B:232:ARG:HH22	1:B:236:ARG:NE	2.16	0.43
1:B:330:PRO:HA	1:B:463:VAL:HG21	2.00	0.43
1:B:444:ARG:O	1:B:448:GLU:HG3	2.19	0.43
1:A:603:LEU:HD12	1:A:603:LEU:HA	1.91	0.43
1:A:127:VAL:HG22	1:A:128:TRP:N	2.34	0.42
1:B:143:PRO:HD2	1:B:145:TRP:CZ2	2.54	0.42
1:B:283:TRP:CG	1:B:284:GLU:N	2.87	0.42
1:B:294:ALA:O	1:B:306:PRO:HG2	2.19	0.42
1:B:198:ASP:C	1:B:200:ARG:NH1	2.72	0.42
1:B:422:LYS:NZ	1:B:503:TRP:CZ2	2.87	0.42
1:A:329:LYS:HB3	1:A:329:LYS:NZ	2.32	0.42
1:B:426:LEU:HD23	1:B:426:LEU:HA	1.77	0.42
1:B:81:ARG:HG2	1:B:81:ARG:NH1	2.34	0.42
1:A:17:ARG:NH2	1:A:23:GLU:OE2	2.51	0.42
1:A:580:ARG:NE	1:A:613:THR:CG2	2.76	0.42
1:A:211:ASP:OD2	1:A:211:ASP:N	2.47	0.42
1:B:195:ASN:OD1	1:B:202:TRP:NE1	2.50	0.42
1:A:469:TYR:CD2	1:A:634:GLN:HG3	2.54	0.42
1:A:81:ARG:HG2	1:A:81:ARG:HH11	1.84	0.42
1:A:641:LEU:O	1:A:641:LEU:HD12	2.19	0.42
1:A:391:PHE:HE2	1:A:424:LEU:HD23	1.84	0.42
1:B:69:PRO:HA	1:B:70:PRO:HD3	1.84	0.42
1:B:181:ALA:O	1:B:184:ALA:CB	2.61	0.42
1:B:48:GLN:O	1:B:52:ARG:HG2	2.19	0.42
1:A:503:TRP:CZ3	1:A:505:LEU:HD13	2.54	0.42
1:A:312:GLN:HE21	1:A:312:GLN:N	2.11	0.42
1:A:192:ARG:NH2	1:A:247:PRO:HG3	2.35	0.42
1:B:569:ASP:HA	1:B:623:ALA:O	2.20	0.42
1:B:155:LEU:HD21	1:B:163:PHE:CD2	2.55	0.42
1:B:513:ARG:HH21	1:B:521:ASP:CG	2.22	0.42
1:A:549:VAL:CG1	1:A:550:PRO:HD2	2.46	0.42
1:B:27:TRP:O	1:B:65:ALA:HA	2.20	0.42
1:B:489:GLY:H	1:B:506:PRO:HD2	1.85	0.42
1:A:173:ILE:HG21	1:A:270:LEU:HD11	2.02	0.42
1:B:259:GLY:C	1:B:260:LEU:HD12	2.41	0.42
1:A:192:ARG:NH1	1:A:203:GLU:HG3	2.35	0.42
1:A:296:TRP:CD1	1:A:297:ILE:N	2.88	0.42
1:A:591:GLY:HA3	1:A:636:PHE:CZ	2.55	0.42
1:B:116:LEU:O	1:B:117:LEU:C	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:455:LEU:O	1:A:460:LEU:HB3	2.20	0.41
1:A:237:GLU:OE2	1:A:239:GLY:HA2	2.19	0.41
1:B:409:LEU:HA	1:B:435:LEU:O	2.20	0.41
1:A:254:ILE:HD12	2:X:10:DA:O4'	2.20	0.41
1:B:349:LEU:HD13	1:B:381:LEU:CD1	2.50	0.41
1:B:302:GLY:O	1:B:303:LEU:HD12	2.20	0.41
1:A:202:TRP:HB3	1:A:245:ALA:O	2.20	0.41
1:B:234:GLN:O	1:B:234:GLN:OE1	2.38	0.41
1:B:144:GLY:HA3	1:B:182:TRP:HZ3	1.85	0.41
1:A:22:GLU:N	1:A:22:GLU:CD	2.73	0.41
1:B:350:ARG:NH1	1:B:358:PRO:HD3	2.32	0.41
1:A:424:LEU:O	1:A:427:ARG:CB	2.67	0.41
1:B:396:ARG:HG2	1:B:396:ARG:NH1	2.33	0.41
1:A:313:ALA:CB	1:A:594:VAL:HG22	2.50	0.41
1:A:429:GLY:O	1:A:431:PRO:HD3	2.20	0.41
1:A:10:PHE:CD2	1:A:584:VAL:HG22	2.55	0.41
1:A:554:PHE:CD1	1:A:554:PHE:N	2.89	0.41
1:B:545:ARG:HH11	1:B:549:VAL:HG23	1.85	0.41
1:B:395:LEU:HB2	1:B:428:GLU:HG3	2.02	0.41
1:B:617:LEU:O	1:B:619:LEU:HD12	2.20	0.41
1:A:362:ARG:O	1:A:366:LEU:HG	2.21	0.41
1:B:226:TYR:CE2	2:Y:110:DA:H2'	2.56	0.41
1:B:217:LEU:CD2	1:B:223:LEU:HA	2.51	0.41
1:B:297:ILE:HG12	1:B:301:LEU:HD11	2.03	0.41
1:A:613:THR:HA	1:A:614:PRO:HD3	1.93	0.41
1:B:344:THR:CG2	1:B:376:LEU:HD13	2.51	0.41
1:A:69:PRO:HA	1:A:70:PRO:HD3	1.95	0.41
1:A:296:TRP:CH2	1:A:300:ARG:NE	2.89	0.41
1:A:376:LEU:HD21	1:A:378:LEU:HD13	2.03	0.41
1:A:27:TRP:O	1:A:65:ALA:HA	2.21	0.41
1:B:12:ASN:HB3	1:B:580:ARG:HB2	2.03	0.41
1:B:505:LEU:HA	1:B:506:PRO:HD3	1.85	0.41
1:A:244:VAL:HG13	1:A:245:ALA:N	2.35	0.41
1:A:305:THR:HA	1:A:306:PRO:HD3	1.93	0.41
1:B:92:PRO:C	1:B:93:LYS:HG2	2.41	0.41
1:B:441:GLU:OE1	1:B:441:GLU:CA	2.67	0.40
1:A:13:ARG:CZ	1:A:156:TRP:HH2	2.34	0.40
1:B:52:ARG:HD2	1:B:52:ARG:HA	1.90	0.40
1:A:537:LEU:HD21	1:B:389:LEU:HD13	2.02	0.40
1:A:505:LEU:H	1:A:505:LEU:HD22	1.84	0.40
1:B:234:GLN:O	1:B:234:GLN:CD	2.60	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:498:GLY:C	1:A:500:HIS:H	2.21	0.40
1:B:228:ALA:HA	1:B:233:LEU:HB2	2.02	0.40
1:A:210:GLU:HG3	1:A:215:LEU:HD22	2.02	0.40
1:A:127:VAL:HG22	1:A:128:TRP:H	1.87	0.40
1:A:348:LEU:HD23	1:A:348:LEU:O	2.21	0.40
1:A:321:LEU:CD2	1:A:330:PRO:HD3	2.51	0.40
1:B:440:ARG:CD	1:B:442:GLU:HG2	2.51	0.40
1:A:57:THR:CG2	1:A:73:LEU:HD21	2.44	0.40
1:B:377:ARG:C	1:B:378:LEU:HD22	2.42	0.40
1:A:501:LEU:HG	1:A:502:LEU:H	1.87	0.40
1:A:359:GLU:OE1	1:A:362:ARG:NH1	2.51	0.40
1:A:139:HIS:O	1:A:140:ALA:HB2	2.21	0.40
1:B:360:PHE:CE1	1:B:361:LEU:HG	2.56	0.40
1:B:31:VAL:HG12	1:B:32:VAL:N	2.36	0.40
1:A:217:LEU:HD12	1:A:217:LEU:HA	1.88	0.40
1:B:593:TYR:CZ	1:B:595:PRO:HG3	2.56	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	633/685 (92%)	554 (88%)	61 (10%)	18 (3%)	6	15
1	B	604/685 (88%)	530 (88%)	57 (9%)	17 (3%)	6	15
All	All	1237/1370 (90%)	1084 (88%)	118 (10%)	35 (3%)	6	15

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	466	SER
1	A	507	GLU

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Mol	Chain	Res	Type
1	A	606	VAL
1	A	607	HIS
1	A	608	ARG
1	B	103	PRO
1	B	186	GLY
1	B	237	GLU
1	A	480	GLY
1	A	610	PHE
1	B	54	GLY
1	B	172	ARG
1	B	213	LYS
1	B	238	GLY
1	B	279	LEU
1	B	442	GLU
1	A	218	PRO
1	A	386	SER
1	A	500	HIS
1	B	178	SER
1	B	502	LEU
1	B	598	ASP
1	A	271	HIS
1	A	353	GLY
1	A	483	GLU
1	B	206	ARG
1	A	359	GLU
1	A	496	GLY
1	B	179	LEU
1	B	208	GLY
1	A	385	PRO
1	A	495	GLY
1	B	498	GLY
1	B	385	PRO
1	A	499	GLY

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	475/549 (86%)	424 (89%)	51 (11%)	8	19
1	B	447/549 (81%)	391 (88%)	56 (12%)	6	13
All	All	922/1098 (84%)	815 (88%)	107 (12%)	7	16

All (107) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	VAL
1	A	45	LEU
1	A	68	SER
1	A	82	MET
1	A	85	THR
1	A	120	ARG
1	A	141	ARG
1	A	146	ARG
1	A	156	TRP
1	A	179	LEU
1	A	182	TRP
1	A	204	LEU
1	A	206	ARG
1	A	210	GLU
1	A	217	LEU
1	A	218	PRO
1	A	240	ARG
1	A	244	VAL
1	A	247	PRO
1	A	254	ILE
1	A	265	LEU
1	A	266	THR
1	A	283	TRP
1	A	290	THR
1	A	299	ARG
1	A	303	LEU
1	A	312	GLN
1	A	329	LYS
1	A	348	LEU
1	A	350	ARG
1	A	351	LEU
1	A	359	GLU
1	A	363	ARG
1	A	378	LEU
1	A	415	TRP

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Mol	Chain	Res	Type
1	A	419	ASN
1	A	427	ARG
1	A	431	PRO
1	A	451	LEU
1	A	454	LEU
1	A	475	VAL
1	A	486	ARG
1	A	505	LEU
1	A	509	GLN
1	A	514	ILE
1	A	552	ASP
1	A	587	ARG
1	A	609	ASP
1	A	610	PHE
1	A	631	LEU
1	A	640	ARG
1	B	7	THR
1	B	40	GLU
1	B	45	LEU
1	B	57	THR
1	B	58	VAL
1	B	79	LEU
1	B	85	THR
1	B	99	ASP
1	B	120	ARG
1	B	122	ARG
1	B	128	TRP
1	B	139	HIS
1	B	141	ARG
1	B	146	ARG
1	B	156	TRP
1	B	179	LEU
1	B	197	TYR
1	B	200	ARG
1	B	206	ARG
1	B	216	PRO
1	B	217	LEU
1	B	218	PRO
1	B	232	ARG
1	B	233	LEU
1	B	234	GLN
1	B	236	ARG

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Mol	Chain	Res	Type
1	B	241	VAL
1	B	258	THR
1	B	288	ARG
1	B	289	ARG
1	B	312	GLN
1	B	318	ILE
1	B	320	LYS
1	B	329	LYS
1	B	346	LEU
1	B	367	ARG
1	B	382	HIS
1	B	420	ARG
1	B	435	LEU
1	B	439	LEU
1	B	440	ARG
1	B	441	GLU
1	B	451	LEU
1	B	465	LEU
1	B	469	TYR
1	B	475	VAL
1	B	497	ASP
1	B	502	LEU
1	B	503	TRP
1	B	505	LEU
1	B	506	PRO
1	B	521	ASP
1	B	552	ASP
1	B	556	LEU
1	B	574	ARG
1	B	631	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	GLN
1	A	84	GLN
1	A	256	HIS
1	A	312	GLN
1	A	387	GLN
1	A	500	HIS
1	A	516	GLN
1	A	585	GLN

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Mol	Chain	Res	Type
1	A	621	HIS
1	A	633	HIS
1	B	227	HIS
1	B	256	HIS
1	B	382	HIS
1	B	419	ASN
1	B	445	HIS
1	B	633	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (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(Å²)	Q<0.9
1	A	637/685 (92%)	0.26	25 (3%)	43	43	43, 74, 102, 115	3 (0%)
1	B	614/685 (89%)	0.37	45 (7%)	18	16	46, 78, 116, 126	14 (2%)
2	X	5/10 (50%)	-0.10	0	100	100	57, 68, 87, 117	0
2	Y	5/10 (50%)	-0.30	0	100	100	68, 72, 76, 93	0
All	All	1261/1390 (90%)	0.31	70 (5%)	28	26	43, 76, 112, 126	17 (1%)

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	177	MET	5.6
1	A	607	HIS	5.0
1	A	437	VAL	4.8
1	B	143	PRO	4.4
1	B	144	GLY	4.1
1	B	253	PRO	4.0
1	A	613	THR	4.0
1	A	487	PHE	3.4
1	B	437	VAL	3.4
1	B	204	LEU	3.4
1	A	276	SER	3.3
1	B	182	TRP	3.3
1	A	606	VAL	3.3
1	B	140	ALA	3.2
1	B	184	ALA	3.2
1	A	386	SER	3.2
1	B	174	LEU	3.1
1	A	283	TRP	3.1
1	A	642	TYR	3.0
1	A	4	LEU	3.0
1	B	245	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	244	VAL	3.0
1	A	240	ARG	2.9
1	B	496	GLY	2.9
1	A	611	ARG	2.9
1	B	279	LEU	2.9
1	B	243	TRP	2.8
1	B	278	ALA	2.8
1	A	501	LEU	2.7
1	B	25	ARG	2.7
1	B	260	LEU	2.7
1	B	257	LEU	2.7
1	B	181	ALA	2.7
1	A	576	SER	2.7
1	B	189	LEU	2.6
1	B	136	ARG	2.6
1	B	250	PRO	2.6
1	B	378	LEU	2.6
1	B	574	ARG	2.5
1	B	625	ASP	2.5
1	A	136	ARG	2.5
1	B	280	SER	2.4
1	B	340	ARG	2.4
1	A	414	ALA	2.4
1	A	480	GLY	2.4
1	A	531	ARG	2.4
1	B	614	PRO	2.4
1	B	276	SER	2.4
1	B	283	TRP	2.4
1	A	248	LYS	2.3
1	A	482	ARG	2.3
1	B	232	ARG	2.3
1	B	487	PHE	2.3
1	B	205	LEU	2.3
1	B	282	PRO	2.3
1	B	251	ARG	2.3
1	A	578	GLY	2.3
1	A	252	LYS	2.2
1	B	215	LEU	2.2
1	B	339	TYR	2.2
1	A	350	ARG	2.2
1	B	502	LEU	2.2
1	B	236	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	202	TRP	2.1
1	B	281	LEU	2.1
1	B	613	THR	2.1
1	A	65	ALA	2.1
1	B	504	THR	2.1
1	A	577	GLY	2.1
1	B	147	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 carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.