



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:33 PM UTC

PDB ID : 3DLB / pdb_00003dlb
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)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

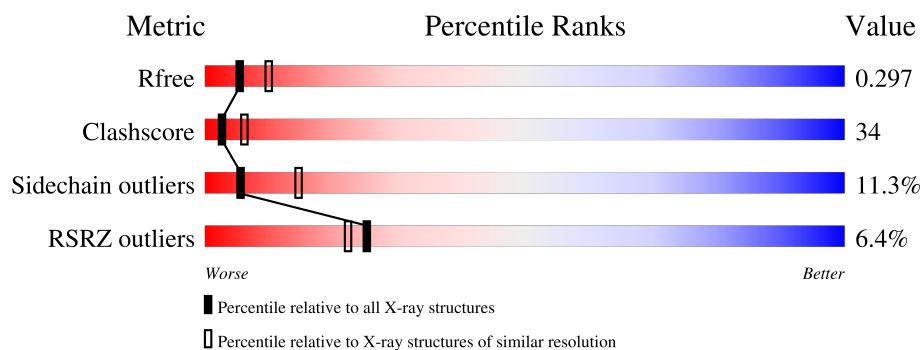
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (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 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	685	5% 51% 34% 8% 7%
1	B	685	7% 43% 38% 8% 10%
2	X	10	20% 20% 10% 50%
2	Y	10	10% 40% 10% 50%

2 Entry composition

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			

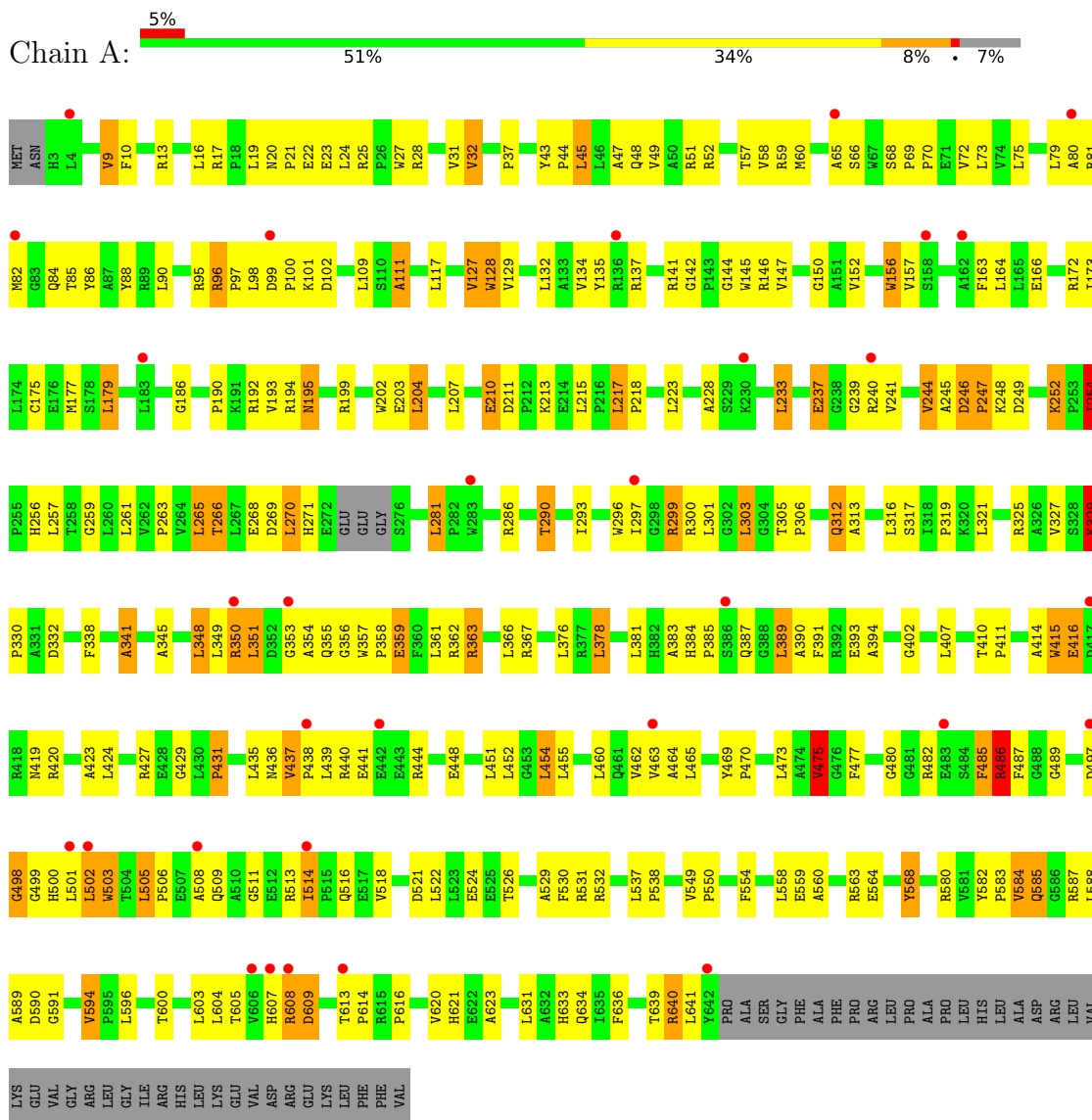
- Molecule 3 is water.

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		

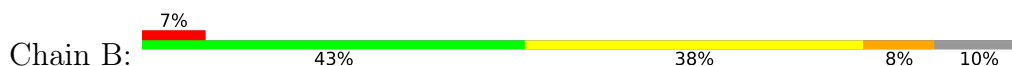
3 Residue-property plots

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

• Molecule 1: argonaute



• Molecule 1: argonaute





4 Data and refinement statistics

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 30.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.6 (30.00-2.70) 94.2 (30.00-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.86 (at 2.68Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.254 , 0.293 (Not available) , 0.297	Depositor DCC
R_{free} test set	2154 reflections (5.03%)	wwPDB-VP
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 , 42.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	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.*

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 [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	0.74	9/5009 (0.2%)	1.22	56/6817 (0.8%)
1	B	0.67	6/4780 (0.1%)	1.24	54/6509 (0.8%)
2	X	0.48	0/113	1.17	1/173 (0.6%)
2	Y	0.35	0/95	1.11	1/146 (0.7%)
All	All	0.70	15/9997 (0.2%)	1.23	112/13645 (0.8%)

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	529	ALA	C-N	-7.89	1.22	1.33
1	A	128	TRP	CB-CG	-7.86	1.25	1.50
1	A	503	TRP	CB-CG	-6.43	1.30	1.50
1	A	503	TRP	CA-C	-6.26	1.45	1.52
1	A	128	TRP	N-CA	-6.24	1.38	1.46
1	B	106	ARG	N-CA	-6.08	1.38	1.46
1	A	609	ASP	CA-C	-6.04	1.44	1.53
1	A	127	VAL	CA-CB	-5.53	1.51	1.55
1	A	355	GLN	N-CA	-5.49	1.39	1.46
1	B	100	PRO	CA-C	-5.47	1.44	1.52
1	B	640	ARG	CA-C	-5.34	1.45	1.52
1	B	102	ASP	CA-CB	-5.32	1.47	1.53
1	B	387	GLN	CA-CB	-5.24	1.46	1.53
1	A	128	TRP	CA-CB	-5.01	1.46	1.53
1	A	502	LEU	CA-C	-5.00	1.48	1.53

All (112) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	277	LEU	N-CA-C	15.05	139.69	108.53
1	A	356	GLY	N-CA-C	14.08	132.73	112.60
1	A	609	ASP	N-CA-C	11.44	125.21	109.54
1	A	608	ARG	N-CA-C	-11.43	86.45	110.80
1	B	250	PRO	N-CA-C	11.28	127.90	114.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	608	ARG	CA-C-N	-10.55	107.68	122.87
1	A	608	ARG	C-N-CA	-10.55	107.68	122.87
1	B	236	ARG	N-CA-C	-10.42	100.80	112.57
1	B	188	PRO	N-CA-CB	10.37	110.18	103.23
1	B	428	GLU	N-CA-C	-9.61	99.92	112.41
1	A	502	LEU	N-CA-C	9.30	125.86	108.65
1	B	467	GLY	N-CA-C	8.84	124.04	111.14
1	B	276	SER	N-CA-C	-8.60	96.25	109.24
1	B	250	PRO	CA-C-N	-8.26	107.49	120.88
1	B	250	PRO	C-N-CA	-8.26	107.49	120.88
1	A	246	ASP	N-CA-C	8.17	127.86	109.81
1	A	498	GLY	N-CA-C	8.10	126.29	115.59
1	B	504	THR	N-CA-C	7.92	122.12	110.17
1	A	389	LEU	N-CA-C	-7.88	103.56	113.01
1	A	355	GLN	CA-C-N	-7.81	113.38	122.83
1	A	355	GLN	C-N-CA	-7.81	113.38	122.83
1	B	277	LEU	N-CA-CB	-7.75	99.78	111.64
1	B	186	GLY	N-CA-C	7.73	131.49	113.18
1	B	531	ARG	N-CA-C	-7.61	103.46	112.89
1	B	100	PRO	CA-C-N	-7.53	110.10	122.08
1	B	100	PRO	C-N-CA	-7.53	110.10	122.08
1	A	271	HIS	N-CA-CB	7.53	123.21	110.49
1	A	137	ARG	N-CA-C	7.33	120.58	109.23
1	B	437	VAL	N-CA-C	7.32	124.69	108.88
2	Y	110	DA	C2'-C3'-O3'	7.32	122.48	111.50
1	A	437	VAL	N-CA-C	7.09	124.20	108.88
1	A	356	GLY	CA-C-O	7.08	129.13	121.90
1	B	206	ARG	CA-C-N	-7.02	112.41	122.94
1	B	206	ARG	C-N-CA	-7.02	112.41	122.94
1	B	198	ASP	N-CA-C	6.93	116.45	108.49
1	B	594	VAL	N-CA-C	6.92	115.00	107.60
1	B	323	GLY	N-CA-C	-6.86	96.93	113.18
1	B	183	LEU	N-CA-C	-6.75	104.91	113.01
1	A	129	VAL	N-CA-C	6.70	117.55	108.17
1	B	107	SER	N-CA-C	-6.60	104.16	111.82
1	B	102	ASP	N-CA-CB	-6.58	99.19	111.24
1	A	584	VAL	N-CA-C	-6.52	102.71	111.44
1	A	186	GLY	N-CA-C	6.47	123.62	115.21
1	A	128	TRP	N-CA-C	6.45	119.03	108.52
1	B	251	ARG	N-CA-CB	6.41	119.50	110.07
1	B	278	ALA	N-CA-C	6.40	124.44	110.80
1	B	214	GLU	N-CA-C	-6.33	105.33	114.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	152	VAL	N-CA-C	-6.32	100.61	109.21
1	B	469	TYR	CA-C-N	6.24	125.81	119.19
1	B	469	TYR	C-N-CA	6.24	125.81	119.19
1	B	237	GLU	N-CA-C	6.21	124.03	110.80
1	B	324	ARG	N-CA-C	-6.21	103.82	112.45
1	B	410	THR	N-CA-C	6.21	116.12	108.11
1	B	220	GLY	N-CA-C	-6.19	106.49	114.85
1	A	485	PHE	N-CA-C	6.19	119.86	112.93
1	A	47	ALA	N-CA-C	-6.12	104.60	111.28
1	B	277	LEU	CA-C-N	-6.08	109.93	121.54
1	B	277	LEU	C-N-CA	-6.08	109.93	121.54
1	B	381	LEU	N-CA-C	6.03	118.01	108.67
1	A	329	LYS	N-CA-C	5.99	115.84	108.11
1	B	472	GLU	N-CA-C	-5.94	106.03	113.28
1	B	625	ASP	N-CA-CB	-5.94	102.58	111.25
1	A	293	ILE	CB-CA-C	-5.83	104.28	112.14
1	B	42	VAL	N-CA-C	5.82	116.29	110.23
1	A	354	ALA	N-CA-C	5.81	123.17	110.80
1	B	359	GLU	N-CA-C	5.81	117.28	111.07
1	A	281	LEU	N-CA-C	5.79	117.84	109.04
1	B	100	PRO	CB-CA-C	-5.76	102.06	111.56
1	A	414	ALA	N-CA-C	-5.75	102.39	110.50
1	A	24	LEU	N-CA-C	-5.74	106.27	113.28
1	B	370	GLY	N-CA-C	-5.72	105.57	112.49
1	B	439	LEU	CA-C-N	-5.71	114.32	122.77
1	B	439	LEU	C-N-CA	-5.71	114.32	122.77
1	A	353	GLY	CA-C-N	-5.70	110.66	121.54
1	A	353	GLY	C-N-CA	-5.70	110.66	121.54
1	A	254	ILE	CA-C-N	-5.67	114.47	120.66
1	A	254	ILE	C-N-CA	-5.67	114.47	120.66
1	B	466	SER	CA-C-N	-5.62	117.10	121.82
1	B	466	SER	C-N-CA	-5.62	117.10	121.82
1	A	568	TYR	N-CA-C	5.62	116.80	108.60
1	B	424	LEU	N-CA-C	-5.60	105.33	111.82
1	A	486	ARG	N-CA-C	-5.58	102.39	111.04
1	A	270	LEU	N-CA-C	5.52	117.10	111.14
1	A	416	GLU	N-CA-C	-5.52	104.66	111.40
1	B	38	GLY	N-CA-C	-5.51	104.91	111.36
1	A	503	TRP	CA-C-N	-5.50	112.98	122.10
1	A	503	TRP	C-N-CA	-5.50	112.98	122.10
2	X	10	DA	C2'-C3'-O3'	5.47	119.71	111.50
1	A	609	ASP	O-C-N	5.46	129.38	122.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	97	PRO	N-CA-C	5.44	119.74	111.19
1	A	111	ALA	N-CA-C	-5.39	105.48	111.36
1	A	594	VAL	CA-C-N	-5.38	114.17	119.99
1	A	594	VAL	C-N-CA	-5.38	114.17	119.99
1	A	127	VAL	CA-C-N	-5.27	115.67	123.05
1	A	127	VAL	C-N-CA	-5.27	115.67	123.05
1	A	195	ASN	N-CA-C	-5.26	103.09	110.50
1	B	210	GLU	N-CA-C	5.22	117.47	109.95
1	B	207	LEU	N-CA-C	5.22	117.90	109.40
1	B	484	SER	N-CA-C	5.20	116.74	108.79
1	A	475	VAL	N-CA-C	5.18	115.59	108.12
1	A	128	TRP	N-CA-CB	-5.13	102.50	110.55
1	B	298	GLY	N-CA-C	-5.11	108.98	115.31
1	B	640	ARG	CA-CB-CG	-5.09	103.92	114.10
1	A	341	ALA	N-CA-C	5.09	118.24	110.36
1	A	508	ALA	N-CA-C	5.08	117.20	107.75
1	A	414	ALA	CA-C-N	-5.08	111.13	121.18
1	A	414	ALA	C-N-CA	-5.08	111.13	121.18
1	A	319	PRO	N-CA-C	5.07	118.45	110.80
1	A	609	ASP	CA-CB-CG	-5.05	107.55	112.60
1	B	357	TRP	N-CA-C	5.04	116.18	109.93
1	A	96	ARG	CA-C-N	5.02	124.78	119.76
1	A	96	ARG	C-N-CA	5.02	124.78	119.76

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	4891	0	4892	298	0
1	B	4668	0	4624	357	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	X	3	0	0	0	0
3	Y	1	0	0	0	0
All	All	9793	0	9621	650	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 34.

All (650) 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:O	1:B:237:GLU:HG3	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:415:TRP:CD1	1:A:415:TRP:C	2.37	1.01
1:A:482:ARG:CZ	1:A:487:PHE:HB2	1.90	1.01
1:A:101:LYS:H	1:A:101:LYS:HD2	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:600:THR:HG22	1:A:620:VAL:HG22	1.46	0.96
1:B:206:ARG:HG3	1:B:206:ARG:HH11	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:A:350:ARG:O	1:A:350:ARG:HG2	1.63	0.94
1:B:382:HIS:CD2	1:B:382:HIS:H	1.77	0.94
1:A:265:LEU:HD12	1:A:265:LEU:H	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:184:ALA:C	1:B:186:GLY:H	1.76	0.92
1:B:432:SER:H	1:B:503:TRP:HH2	1.00	0.92
1:B:574:ARG:HH11	1:B:574:ARG:HB3	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:B:440:ARG:HD3	1:B:440:ARG:C	1.95	0.89
1:A:482:ARG:NH1	1:A:487:PHE:HB2	1.88	0.87
1:B:513:ARG:HH11	1:B:513:ARG:HG2	1.39	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:198:ASP:CG	1:B:200:ARG:HD3	2.02	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:A:49:VAL:HG22	1:A:79:LEU:HD21	1.63	0.81
1:B:20:ASN:HB2	1:B:21:PRO:HD2	1.61	0.81
1:B:207:LEU:C	1:B:207:LEU:HD23	2.06	0.80
1:B:441:GLU:C	1:B:441:GLU:OE1	2.24	0.80
1:B:289:ARG:HH11	1:B:289:ARG:HA	1.45	0.80
1:B:437:VAL:O	1:B:439:LEU:N	2.15	0.80
1:B:244:VAL:HG23	1:B:254:ILE:HD12	1.63	0.80
1:B:350:ARG:HD3	1:B:354:ALA:C	2.07	0.79
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: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:97:PRO:C	1:B:98:LEU:HD12	2.09	0.78
1:A:256:HIS:CD2	1:A:257:LEU:H	2.02	0.77
1:B:293:ILE:O	1:B:297:ILE:HG22	1.83	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:128:TRP:CD1	1:A:128:TRP:C	2.62	0.77
1:A:57:THR:HG21	1:A:73:LEU:HD21	1.65	0.77
1:B:352:ASP:CG	1:B:353:GLY:H	1.92	0.77
1:B:382:HIS:H	1:B:382:HIS:HD2	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:251:ARG:O	1:B:252:LYS:C	2.28	0.76
1:A:57:THR:HG22	1:A:66:SER:OG	1.85	0.76
1:B:181:ALA:O	1:B:184:ALA:HB3	1.86	0.76
1:A:101:LYS:HD2	1:A:101:LYS:N	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:184:ALA:C	1:B:186:GLY:N	2.45	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:A:266:THR:HG23	1:A:268:GLU:H	1.54	0.73
1:B:195:ASN:HD22	1:B:200:ARG:CD	2.01	0.73
1:B:56:VAL:HG12	1:B:67:TRP:HB2	1.71	0.73
1:B:45:LEU:CD1	1:B:81:ARG:HD3	2.19	0.73
1:B:440:ARG:HA	1:B:440:ARG:NE	2.04	0.73
1:B:200:ARG:HE	1:B:200:ARG:C	1.96	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
1:A:505:LEU:HB2	1:A:506:PRO:CD	2.20	0.72
1:A:329:LYS:CB	1:A:329:LYS:NZ	2.53	0.71
1:B:200:ARG:NE	1:B:200:ARG:N	2.39	0.71
1:B:440:ARG:C	1:B:440:ARG:CD	2.62	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:HB3	1:A:252:LYS:HZ3	1.52	0.70
1:A:312:GLN:H	1:A:312:GLN:HE21	1.37	0.70
1:A:505:LEU:HB2	1:A:506:PRO:HD2	1.73	0.70
1:B:205:LEU:O	1:B:206:ARG:HB3	1.92	0.70
1:B:244:VAL:HG23	1:B:254:ILE:CD1	2.22	0.70
1:B:200:ARG:NE	1:B:200:ARG:O	2.23	0.70
1:A:256:HIS:HD2	1:A:257:LEU:H	1.37	0.70
1:B:489:GLY:O	1:B:506:PRO:HD2	1.92	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:390:ALA:O	1:B:393:GLU:HB3	1.92	0.69
1:B:440:ARG:HG3	1:B:442:GLU:HG2	1.74	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:A:203:GLU:HB3	1:A:245:ALA:HB3	1.74	0.69
1:B:198:ASP:H	1:B:200:ARG:HH12	1.38	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:HH11	1:B:206:ARG:CG	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:234:GLN:O	1:B:234:GLN:HG2	1.94	0.68
1:A:455:LEU:HD22	1:A:460:LEU:HD23	1.76	0.68
1:B:193:VAL:HG22	1:B:194:ARG:N	2.09	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:283:TRP:CD1	1:B:283:TRP:H	2.12	0.67
1:A:351:LEU:HD21	1:A:385:PRO:HB3	1.77	0.67
1:B:251:ARG:O	1:B:253:PRO:N	2.28	0.67
1:B:440:ARG:CG	1:B:442:GLU:HG2	2.25	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
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:A:28:ARG:HD2	1:A:60:MET:HE3	1.78	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:246:ASP:HB3	1:A:249:ASP:H	1.61	0.65
1:A:407:LEU:HD13	1:A:454:LEU:HG	1.77	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:A:192:ARG:HG3	1:A:202:TRP:O	1.98	0.64
1:B:251:ARG:O	1:B:253:PRO:HD3	1.97	0.64
1:B:299:ARG:HG2	1:B:300:ARG:H	1.62	0.64
1:B:506:PRO:HG2	1:B:518:VAL:HG13	1.80	0.64
1:A:437:VAL:CG1	1:A:438:PRO:HD3	2.27	0.64
1:B:198:ASP:OD2	1:B:200:ARG:NH1	2.27	0.64
1:A:141:ARG:CG	1:A:142:GLY:H	2.11	0.64
1:A:266:THR:HG22	1:A:269:ASP:H	1.61	0.64
1:A:604:LEU:HG	1:A:616:PRO:HB3	1.80	0.64
1:B:234:GLN:O	1:B:234:GLN:CG	2.45	0.64
1:B:251:ARG:O	1:B:253:PRO:CD	2.46	0.63
1:B:441:GLU:O	1:B:443:GLU:N	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:505:LEU:N	1:A:505:LEU:HD22	2.14	0.63
1:B:223:LEU:HD12	1:B:257:LEU:HD21	1.80	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:B:200:ARG:HE	1:B:200:ARG:CA	2.10	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:NZ	1:A:329:LYS:HB2	2.13	0.62
1:A:411:PRO:HG3	1:A:437:VAL:HG11	1.80	0.62
1:B:538:PRO:O	1:B:566:ILE:HD12	1.99	0.62
1:B:238:GLY:CA	1:B:259:GLY:HA3	2.29	0.62
1:B:232:ARG:HA	1:B:232:ARG:NE	2.14	0.62
1:A:363:ARG:HH11	1:A:363:ARG:HB3	1.64	0.62
1:A:639:THR:HG22	1:A:640:ARG:HE	1.64	0.62
1:B:344:THR:HG21	1:B:369:PHE:CZ	2.34	0.62
1:A:141:ARG:O	1:A:145:TRP:CE2	2.53	0.61
1:A:350:ARG:O	1:A:350:ARG:CG	2.42	0.61
1:B:198:ASP:N	1:B:200:ARG:NH1	2.48	0.61
1:A:96:ARG:HG2	1:A:96:ARG:O	2.00	0.61
1:A:265:LEU:HD12	1:A:265:LEU:N	2.09	0.61
1:B:350:ARG:HH12	1:B:358:PRO:HD3	1.64	0.61
1:B:506:PRO:HD3	1:B:522:LEU:CD2	2.18	0.61
1:B:238:GLY:HA3	1:B:259:GLY:HA3	1.83	0.61
1:A:385:PRO:O	1:A:387:GLN:N	2.33	0.61
1:B:16:LEU:HB3	1:B:303:LEU:O	1.99	0.61
1:B:316:LEU:HD22	1:B:633:HIS:CD2	2.36	0.61
1:A:194:ARG:HD3	1:A:199:ARG:HA	1.81	0.61
1:A:482:ARG:HD3	1:A:487:PHE:O	2.01	0.61
1:A:156:TRP:CZ3	1:A:164:LEU:HD23	2.35	0.60
1:A:358:PRO:HD2	1:A:361:LEU:HD12	1.82	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:B:350:ARG:HE	1:B:352:ASP:CG	2.09	0.60
1:B:452:LEU:HD22	1:B:462:VAL:HG11	1.83	0.60
1:A:363:ARG:HD2	1:A:367:ARG:HH21	1.66	0.60
1:B:238:GLY:C	1:B:259:GLY:HA3	2.25	0.60
1:A:299:ARG:HG3	1:A:299:ARG:HH11	1.66	0.60
1:B:513:ARG:HG2	1:B:513:ARG:NH1	2.09	0.60
1:B:53:ALA:O	1:B:54:GLY:O	2.19	0.60
1:B:179:LEU:HD22	1:B:263:PRO:CG	2.28	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:544:LEU:HD21	1:B:635:ILE:HD12	1.83	0.60
1:B:180:GLU:O	1:B:184:ALA:HB2	2.02	0.60
1:B:301:LEU:O	1:B:303:LEU:HD13	2.02	0.60
1:B:574:ARG:HH11	1:B:574:ARG:CB	2.12	0.60
1:B:286:ARG:HG2	1:B:582:TYR:OH	2.02	0.59
1:B:287:ARG:C	1:B:290:THR:HG22	2.26	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:28:ARG:C	1:B:29:LEU:HD12	2.27	0.59
1:B:278:ALA:O	1:B:279:LEU:C	2.45	0.59
1:B:195:ASN:ND2	1:B:202:TRP:HE1	1.99	0.59
1:A:9:VAL:HG22	1:A:582:TYR:O	2.02	0.59
1:B:329:LYS:HG2	1:B:332:ASP:OD2	2.03	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
1:B:206:ARG:CG	1:B:206:ARG:NH1	2.62	0.59
1:B:422:LYS:HZ1	1:B:503:TRP:HZ2	1.49	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:A:608:ARG:O	1:A:609:ASP:CG	2.47	0.58
1:B:193:VAL:HG22	1:B:194:ARG:H	1.66	0.58
1:B:102:ASP:O	1:B:103:PRO:C	2.46	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:509:GLN:NE2	1:B:420:ARG:HG3	2.19	0.58
1:A:559:GLU:O	1:A:563:ARG:HG3	2.03	0.58
1:B:437:VAL:C	1:B:439:LEU:N	2.61	0.58
1:A:265:LEU:H	1:A:265:LEU:CD1	2.11	0.58
1:A:424:LEU:O	1:A:427:ARG:HB3	2.03	0.58
1:B:17:ARG:NH1	1:B:303:LEU:HG	2.19	0.58
1:B:89:ARG:HG2	1:B:91:TYR:CE1	2.38	0.58
1:B:329:LYS:HB3	1:B:329:LYS:HZ3	1.67	0.58
1:B:283:TRP:HA	1:B:613:THR:CG2	2.34	0.58
1:B:99:ASP:C	1:B:101:LYS:H	2.12	0.58
1:B:440:ARG:HG2	1:B:440:ARG:NH2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:22:GLU:CD	1:A:22:GLU:H	2.13	0.56
1:B:195:ASN:CG	1:B:202:TRP:HE1	2.12	0.56
1:A:475:VAL:HG22	1:A:477:PHE:CE1	2.40	0.56
1:B:296:TRP:O	1:B:299:ARG:HB3	2.05	0.56
1:B:530:PHE:HD2	1:B:538:PRO:HD3	1.70	0.56
1:A:135:TYR:CE2	1:A:172:ARG:HB2	2.40	0.56
1:B:530:PHE:CD2	1:B:538:PRO:HD3	2.40	0.56
1:A:134:VAL:O	1:A:150:GLY:HA3	2.06	0.56
1:A:363:ARG:HD2	1:A:367:ARG:NH2	2.20	0.56
1:A:316:LEU:HD22	1:A:633:HIS:CD2	2.41	0.56
1:A:503:TRP:CZ3	1:A:505:LEU:CD1	2.88	0.56
1:B:396:ARG:HG2	1:B:396:ARG:HH11	1.71	0.56
1:B:223:LEU:C	1:B:223:LEU:HD13	2.31	0.56
1:B:327:VAL:CG2	1:B:332:ASP:HB2	2.36	0.56
1:A:299:ARG:HG3	1:A:299:ARG:NH1	2.20	0.55
1:B:58:VAL:HG21	1:B:111:ALA:HB1	1.87	0.55
1:B:184:ALA:O	1:B:186:GLY:N	2.40	0.55
1:B:208:GLY:HA3	1:B:241:VAL:HB	1.88	0.55
1:B:223:LEU:HD13	1:B:223:LEU:O	2.06	0.55
1:B:232:ARG:CZ	1:B:236:ARG:HD3	2.36	0.55
1:B:246:ASP:OD2	1:B:247:PRO:HD2	2.05	0.55
1:B:349:LEU:HA	1:B:381:LEU:HB2	1.89	0.55
1:A:489:GLY:O	1:A:506:PRO:HD3	2.06	0.55
1:B:200:ARG:HE	1:B:200:ARG:N	2.04	0.55
1:B:177:MET:O	1:B:178:SER:CB	2.54	0.55
1:B:545:ARG:NH1	1:B:549:VAL:O	2.39	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:41:GLU:O	1:B:44:PRO:HD2	2.06	0.55
1:B:537:LEU:HD12	1:B:537:LEU:N	2.21	0.55
1:A:57:THR:HG21	1:A:73:LEU:CD2	2.37	0.55
1:A:462:VAL:CG1	1:A:463:VAL:HG23	2.33	0.55
1:A:51:ARG:NE	2:X:7:DA:OP1	2.33	0.55
1:B:289:ARG:HH11	1:B:289:ARG:CA	2.19	0.55
1:A:99:ASP:OD2	1:A:102:ASP:HB3	2.07	0.55
1:B:455:LEU:HD22	1:B:460:LEU:CD1	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:341:ALA:HA	1:A:460:LEU:HD11	1.89	0.55
1:B:433:GLN:HG2	1:B:450:ALA:O	2.07	0.55
1:B:454:LEU:HD13	1:B:454:LEU:C	2.31	0.55
1:A:37:PRO:HB3	1:A:86:TYR:CE2	2.42	0.54
1:B:441:GLU:C	1:B:443:GLU:N	2.64	0.54
1:B:177:MET:O	1:B:178:SER:HB3	2.06	0.54
1:A:521:ASP:HA	1:A:524:GLU:HB3	1.90	0.54
1:B:71:GLU:H	1:B:71:GLU:CD	2.14	0.54
1:B:106:ARG:O	1:B:106:ARG:HG3	2.06	0.54
1:A:25:ARG:HB3	1:A:95:ARG:HG2	1.89	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:156:TRP:N	1:A:156:TRP:CD1	2.75	0.54
1:B:28:ARG:HG3	1:B:60:MET:HE2	1.89	0.54
1:A:128:TRP:CD1	1:A:128:TRP:O	2.61	0.54
1:A:58:VAL:HG12	1:A:59:ARG:N	2.22	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:441:GLU:C	1:B:443:GLU:H	2.15	0.53
1:A:389:LEU:HB2	1:B:564:GLU:OE2	2.09	0.53
1:B:113:ALA:O	1:B:155:LEU:HD23	2.08	0.53
1:A:223:LEU:HD11	1:A:257:LEU:HG	1.89	0.53
1:A:455:LEU:HD22	1:A:460:LEU:CD2	2.39	0.53
1:B:545:ARG:HD2	1:B:554:PHE:CE1	2.43	0.53
1:A:16:LEU:HB2	1:A:163:PHE:HB2	1.91	0.53
1:A:101:LYS:H	1:A:101:LYS:CD	2.04	0.53
1:A:266:THR:HG23	1:A:268:GLU:N	2.22	0.53
1:A:470:PRO:HD2	1:A:634:GLN:OE1	2.09	0.53
1:A:506:PRO:HD3	1:A:522:LEU:HD21	1.89	0.53
1:B:244:VAL:HG22	1:B:256:HIS:HB2	1.89	0.53
1:A:98:LEU:HD23	1:A:109:LEU:HG	1.88	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:A:501:LEU:HD11	1:A:529:ALA:C	2.33	0.53
1:A:145:TRP:CZ3	1:A:270:LEU:HD13	2.44	0.53
1:B:195:ASN:OD1	1:B:256:HIS:CE1	2.62	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:B:352:ASP:CG	1:B:353:GLY:N	2.61	0.52
1:A:329:LYS:CB	1:A:329:LYS:HZ1	2.23	0.52
1:B:434:ILE:O	1:B:434:ILE:HG22	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:395:LEU:HD22	1:B:425:LEU:HD23	1.92	0.52
1:A:58:VAL:CG1	1:A:59:ARG:N	2.72	0.52
1:B:358:PRO:HG2	1:B:361:LEU:HD12	1.91	0.52
1:A:621:HIS:CE1	1:A:623:ALA:O	2.63	0.52
1:A:363:ARG:HB3	1:A:363:ARG:NH1	2.24	0.52
1:B:179:LEU:CG	1:B:258:THR:HG22	2.39	0.52
1:A:384:HIS:C	1:A:385:PRO:O	2.52	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:114:ARG:HD2	1:B:154:ASP:OD1	2.10	0.51
1:B:200:ARG:NE	1:B:200:ARG:H	2.07	0.51
1:B:345:ALA:C	1:B:346:LEU:HD12	2.35	0.51
1:A:486:ARG:HH11	1:A:487:PHE:HZ	1.28	0.51
1:A:501:LEU:HD21	1:A:526:THR:O	2.11	0.51
1:A:600:THR:CG2	1:A:620:VAL:HG22	2.31	0.51
1:B:79:LEU:O	1:B:79:LEU:HD22	2.09	0.51
1:B:290:THR:HG23	1:B:291:ARG:N	2.26	0.51
1:B:360:PHE:CD2	1:B:441:GLU:HG2	2.44	0.51
1:A:49:VAL:CG2	1:A:79:LEU:HD21	2.38	0.51
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:A:240:ARG:HG3	1:A:241:VAL:N	2.25	0.51
1:B:200:ARG:NE	1:B:200:ARG:CA	2.74	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:A:558:LEU:HD13	1:A:568:TYR:CE2	2.46	0.50
1:B:254:ILE:HD12	1:B:254:ILE:O	2.12	0.50
1:B:345:ALA:HB3	1:B:402:GLY:O	2.11	0.50
1:B:441:GLU:OE1	1:B:441:GLU:O	2.29	0.50
1:B:444:ARG:O	1:B:445:HIS:C	2.52	0.50
1:A:25:ARG:CB	1:A:95:ARG:HD3	2.36	0.50
1:A:482:ARG:NH2	1:A:487:PHE:CD2	2.73	0.50
1:A:141:ARG:CG	1:A:142:GLY:N	2.75	0.50
1:A:312:GLN:H	1:A:312:GLN:NE2	2.08	0.50
1:A:437:VAL:HG13	1:A:438:PRO:CD	2.40	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:399:LYS:HG3	1:B:428:GLU:O	2.12	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:9:VAL:HG22	1:B:311:ALA:O	2.12	0.49
1:B:99:ASP:C	1:B:101:LYS:N	2.68	0.49
1:A:147:VAL:HG22	1:A:173:ILE:HG12	1.94	0.49
1:B:198:ASP:OD2	1:B:198:ASP:N	2.46	0.49
1:B:190:PRO:HG3	1:B:263:PRO:HB3	1.94	0.49
1:A:19:LEU:HD21	1:A:157:VAL:HG21	1.95	0.49
1:A:329:LYS:HB2	1:A:329:LYS:HZ1	1.75	0.49
1:A:587:ARG:HG2	1:A:588:LEU:H	1.76	0.49
1:B:177:MET:CB	1:B:182:TRP:HE3	2.26	0.49
1:B:420:ARG:HG3	1:B:420:ARG:HH11	1.78	0.49
1:A:338:PHE:CD1	1:A:460:LEU:HD21	2.48	0.49
1:A:286:ARG:CD	1:A:613:THR:HG21	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:B:376:LEU:HG	1:B:378:LEU:CD2	2.43	0.49
1:A:13:ARG:NH1	1:A:156:TRP:HH2	2.10	0.48
1:A:228:ALA:HA	1:A:233:LEU:HB2	1.95	0.48
1:B:130:GLU:O	1:B:130:GLU:HG3	2.12	0.48
1:A:498:GLY:C	1:A:500:HIS:H	2.21	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:CD1	1:B:477:PHE:N	2.82	0.48
1:A:99:ASP:HB2	1:A:101:LYS:CD	2.43	0.48
1:B:153:LEU:CD1	1:B:297:ILE:HD12	2.36	0.48
1:B:244:VAL:CG2	1:B:256:HIS:HB2	2.43	0.48
1:B:599:LYS:HA	1:B:628:LEU:HD11	1.95	0.48
1:A:28:ARG:HD2	1:A:60:MET:CE	2.43	0.48
1:A:415:TRP:O	1:A:415:TRP:CG	2.62	0.48
1:A:514:ILE:HD13	1:A:514:ILE:C	2.38	0.48
1:A:190:PRO:HG3	1:A:263:PRO:HB3	1.95	0.48
1:A:202:TRP:HB3	1:A:244:VAL:HG13	1.96	0.48
1:A:514:ILE:O	1:A:514:ILE:HG23	2.13	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:43:TYR:HB2	1:A:44:PRO:HD3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:384:HIS:HB3	1:A:385:PRO:CD	2.43	0.48
1:A:437:VAL:O	1:A:439:LEU:N	2.47	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: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:330:PRO:HG2	1:B:641:LEU:HA	1.96	0.48
1:B:193:VAL:CG2	1:B:194:ARG:N	2.76	0.47
1:B:422:LYS:NZ	1:B:503:TRP:HZ2	2.11	0.47
1:B:492:CYS:HA	1:B:503:TRP:HB2	1.96	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:A:590:ASP:OD2	1:A:605:THR:HA	2.14	0.47
1:B:183:LEU:HD13	1:B:183:LEU:O	2.15	0.47
1:A:514:ILE:HD12	1:A:516:GLN:HB2	1.95	0.47
1:B:321:LEU:HB3	1:B:463:VAL:HG11	1.96	0.47
1:B:195:ASN:HA	1:B:261:LEU:HD23	1.95	0.47
1:B:198:ASP:C	1:B:200:ARG:NH1	2.72	0.47
1:B:212:PRO:HD3	1:B:241:VAL:HG22	1.97	0.47
1:B:329:LYS:NZ	1:B:329:LYS:CB	2.76	0.47
1:B:382:HIS:CD2	1:B:382:HIS:N	2.59	0.47
1:B:551:GLN:HG3	1:B:622:GLU:OE1	2.14	0.47
1:A:281:LEU:N	1:A:281:LEU:HD12	2.29	0.47
1:A:317:SER:OG	1:A:633:HIS:HE1	1.97	0.47
1:A:506:PRO:CD	1:A:522:LEU:HD21	2.44	0.47
1:B:352:ASP:CG	1:B:437:VAL:HG21	2.38	0.47
1:B:455:LEU:HD22	1:B:460:LEU:HD13	1.96	0.47
1:B:601:PHE:CE1	1:B:628:LEU:HD22	2.50	0.47
1:A:135:TYR:CZ	1:A:172:ARG:HB2	2.50	0.47
1:A:296:TRP:CZ3	1:A:300:ARG:CZ	2.98	0.47
1:A:503:TRP:CZ3	1:A:505:LEU:HD11	2.49	0.47
1:A:558:LEU:HD22	1:A:568:TYR:CE2	2.50	0.47
1:B:208:GLY:H	1:B:242:ALA:HA	1.80	0.47
1:B:238:GLY:HA3	1:B:259:GLY:CA	2.43	0.47
1:B:435:LEU:HG	1:B:450:ALA:CB	2.45	0.47
1:B:475:VAL:HG13	1:B:543:LEU:HD23	1.96	0.47
1:B:590:ASP:O	1:B:605:THR:HA	2.15	0.47
1:A:560:ALA:O	1:A:564:GLU:HG2	2.15	0.47
1:B:361:LEU:HD22	1:B:451:LEU:HD11	1.95	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:116:LEU:O	1:B:117:LEU:C	2.59	0.46
1:B:259:GLY:C	1:B:260:LEU:HD12	2.41	0.46
1:B:513:ARG:HH21	1:B:521:ASP:CG	2.22	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:22:GLU:CD	1:A:22:GLU:N	2.73	0.46
1:A:31:VAL:HG22	1:A:90:LEU:HD23	1.97	0.46
1:A:427:ARG:HA	1:A:427:ARG:HD3	1.48	0.46
1:B:283:TRP:CG	1:B:284:GLU:H	2.33	0.46
1:B:440:ARG:HA	1:B:440:ARG:HE	1.78	0.46
1:A:301:LEU:HD22	1:A:303:LEU:HD22	1.98	0.46
1:A:410:THR:O	1:A:436:ASN:HA	2.16	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:179:LEU:HD22	1:A:179:LEU:O	2.16	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:173:ILE:CG2	1:A:270:LEU:HD11	2.46	0.46
1:A:325:ARG:O	1:A:327:VAL:HG23	2.16	0.46
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:456:ALA:HB1	1:B:500:HIS:CG	2.51	0.45
1:A:583:PRO:HG3	1:A:588:LEU:HB2	1.99	0.45
1:B:92:PRO:C	1:B:93:LYS:HG2	2.41	0.45
1:B:537:LEU:HD12	1:B:537:LEU:H	1.81	0.45
2:X:6:DT:H2'	2:X:6:DT:O2	2.16	0.45
1:A:31:VAL:CG1	1:A:32:VAL:N	2.80	0.45
1:A:327:VAL:HG13	1:A:332:ASP:CB	2.44	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:287:ARG:HA	1:B:290:THR:CG2	2.47	0.45
1:B:329:LYS:HB3	1:B:329:LYS:HZ2	1.81	0.45
1:B:432:SER:O	1:B:503:TRP:CZ2	2.69	0.45
1:B:626:THR:HG21	1:B:631:LEU:HD13	1.97	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:503:TRP:N	1:B:503:TRP:HE3	2.15	0.45
1:B:134:VAL:HG12	1:B:135:TYR:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:181:ALA:HA	1:B:184:ALA:HB3	1.97	0.45
1:B:234:GLN:O	1:B:234:GLN:CD	2.60	0.45
1:A:45:LEU:O	1:A:49:VAL:HG23	2.17	0.45
1:B:181:ALA:O	1:B:184:ALA:N	2.50	0.45
1:B:257:LEU:O	1:B:261:LEU:HG	2.17	0.45
1:A:117:LEU:HD23	1:A:132:LEU:HD22	1.99	0.45
1:A:415:TRP:CD1	1:A:415:TRP:O	2.68	0.45
1:B:109:LEU:HB3	1:B:157:VAL:HG21	1.98	0.45
1:B:377:ARG:C	1:B:378:LEU:HD22	2.42	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:25:ARG:O	1:A:95:ARG:CD	2.65	0.45
1:A:341:ALA:HA	1:A:460:LEU:CD1	2.47	0.45
1:A:357:TRP:CE2	1:A:378:LEU:HG	2.52	0.45
1:A:415:TRP:HD1	1:A:416:GLU:N	2.13	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:B:601:PHE:CD1	1:B:628:LEU:HD22	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:551:GLN:HG2	1:B:551:GLN:O	2.17	0.44
1:A:345:ALA:HB3	1:A:402:GLY:O	2.17	0.44
1:A:485:PHE:O	1:A:518:VAL:HG21	2.17	0.44
1:B:98:LEU:HD12	1:B:98:LEU:N	2.31	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:A:144:GLY:HA3	1:A:177:MET:CE	2.47	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:B:440:ARG:NH2	1:B:442:GLU:OE2	2.51	0.44
1:A:58:VAL:HG11	1:A:111:ALA:CB	2.48	0.44
1:A:286:ARG:O	1:A:290:THR:CG2	2.63	0.44
1:A:381:LEU:C	1:A:383:ALA:H	2.25	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:213:LYS:H	1:A:213:LYS:HG2	1.56	0.44
1:B:605:THR:O	1:B:606:VAL:CG1	2.58	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:B:564:GLU:HB2	1:B:566:ILE:HG12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:GLN:HE22	1:A:80:ALA:H	1.65	0.43
1:B:198:ASP:C	1:B:200:ARG:CZ	2.91	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:A:383:ALA:HB2	1:A:394:ALA:CB	2.49	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:420:ARG:O	1:A:423:ALA:HB3	2.18	0.43
1:A:514:ILE:HD13	1:A:516:GLN:H	1.84	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:B:418:ARG:O	1:B:419:ASN:C	2.59	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:A:452:LEU:HD23	1:A:462:VAL:HG21	2.01	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:52:ARG:HD3	2:X:7:DA:C2	2.46	0.43
1:A:79:LEU:HD12	1:A:79:LEU:N	2.34	0.43
1:A:440:ARG:O	1:A:441:GLU:C	2.61	0.43
1:A:531:ARG:CZ	1:A:532:ARG:HG2	2.48	0.43
1:B:71:GLU:CD	1:B:71:GLU:N	2.76	0.43
1:A:505:LEU:CB	1:A:506:PRO:CD	2.89	0.43
1:B:234:GLN:C	1:B:234:GLN:OE1	2.62	0.43
1:A:99:ASP:OD2	1:A:99:ASP:O	2.36	0.43
1:A:338:PHE:CE1	1:A:460:LEU:HD21	2.53	0.43
1:A:415:TRP:CH2	1:A:480:GLY:HA3	2.54	0.43
1:A:486:ARG:HG3	1:A:513:ARG:O	2.18	0.43
1:B:79:LEU:HD22	1:B:79:LEU:C	2.43	0.43
1:A:603:LEU:HD12	1:A:603:LEU:HA	1.91	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: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:294:ALA:O	1:B:306:PRO:HG2	2.19	0.42
1:B:297:ILE:HG12	1:B:297:ILE:O	2.18	0.42
1:A:329:LYS:NZ	1:A:329:LYS:HB3	2.32	0.42
1:B:422:LYS:NZ	1:B:503:TRP:CZ2	2.87	0.42
1:B:426:LEU:HD23	1:B:426:LEU:HA	1.77	0.42
1:A:17:ARG:NH2	1:A:23:GLU:OE2	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:349:LEU:C	1:A:349:LEU:HD23	2.43	0.42
1:B:81:ARG:HG2	1:B:81:ARG:NH1	2.34	0.42
1:A:211:ASP:N	1:A:211:ASP:OD2	2.47	0.42
1:A:358:PRO:O	1:A:359:GLU:C	2.61	0.42
1:A:580:ARG:NE	1:A:613:THR:CG2	2.76	0.42
1:A:81:ARG:HG2	1:A:81:ARG:HH11	1.84	0.42
1:A:469:TYR:CD2	1:A:634:GLN:HG3	2.54	0.42
1:A:641:LEU:HD12	1:A:641:LEU:O	2.19	0.42
1:B:195:ASN:OD1	1:B:202:TRP:NE1	2.50	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:343:GLU:CD	1:B:375:SER:OG	2.63	0.42
1:A:192:ARG:NH2	1:A:247:PRO:HG3	2.35	0.42
1:A:312:GLN:HE21	1:A:312:GLN:N	2.11	0.42
1:A:503:TRP:CZ3	1:A:505:LEU:HD13	2.54	0.42
1:B:48:GLN:O	1:B:52:ARG:HG2	2.19	0.42
1:B:181:ALA:O	1:B:184:ALA:CB	2.61	0.42
1:B:569:ASP:HA	1:B:623:ALA:O	2.20	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:155:LEU:HD21	1:B:163:PHE:CD2	2.55	0.42
1:A:173:ILE:HG21	1:A:270:LEU:HD11	2.02	0.42
1:B:489:GLY:H	1:B:506:PRO:HD2	1.85	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:A:237:GLU:OE2	1:A:239:GLY:HA2	2.19	0.41
1:A:254:ILE:HD12	2:X:10:DA:O4'	2.20	0.41
1:A:455:LEU:O	1:A:460:LEU:HB3	2.20	0.41
1:B:283:TRP:CG	1:B:284:GLU:N	2.87	0.41
1:B:409:LEU:HA	1:B:435:LEU:O	2.20	0.41
1:B:349:LEU:HD13	1:B:381:LEU:CD1	2.50	0.41
1:A:202:TRP:HB3	1:A:245:ALA:O	2.20	0.41
1:B:144:GLY:HA3	1:B:182:TRP:HZ3	1.85	0.41
1:B:234:GLN:O	1:B:234:GLN:OE1	2.38	0.41
1:B:302:GLY:O	1:B:303:LEU:HD12	2.20	0.41
1:A:424:LEU:O	1:A:427:ARG:CB	2.67	0.41
1:A:590:ASP:OD2	1:A:590:ASP:C	2.63	0.41
1:B:350:ARG:NH1	1:B:358:PRO:HD3	2.32	0.41
1:B:396:ARG:HG2	1:B:396:ARG:NH1	2.33	0.41
1:A:144:GLY:HA3	1:A:177:MET:HE3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:395:LEU:HB2	1:B:428:GLU:HG3	2.02	0.41
1:B:513:ARG:NH2	1:B:521:ASP:CG	2.79	0.41
1:B:545:ARG:HH11	1:B:549:VAL:HG23	1.85	0.41
1:B:617:LEU:O	1:B:619:LEU:HD12	2.20	0.41
1:A:27:TRP:O	1:A:65:ALA:HA	2.21	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:499:GLY:O	1:A:500:HIS:C	2.63	0.41
1:A:613:THR:HA	1:A:614:PRO:HD3	1.93	0.41
1:B:12:ASN:HB3	1:B:580:ARG:HB2	2.03	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:B:297:ILE:C	1:B:299:ARG:H	2.29	0.41
1:B:344:THR:CG2	1:B:376:LEU:HD13	2.51	0.41
1:B:521:ASP:O	1:B:522:LEU:C	2.62	0.41
1:A:305:THR:HA	1:A:306:PRO:HD3	1.93	0.41
1:B:505:LEU:HA	1:B:506:PRO:HD3	1.85	0.41
1:A:13:ARG:CZ	1:A:156:TRP:HH2	2.34	0.40
1:A:244:VAL:HG13	1:A:245:ALA:N	2.35	0.40
1:A:537:LEU:HD21	1:B:389:LEU:HD13	2.02	0.40
1:B:52:ARG:HA	1:B:52:ARG:HD2	1.90	0.40
1:B:440:ARG:O	1:B:441:GLU:C	2.63	0.40
1:A:210:GLU:HG3	1:A:215:LEU:HD22	2.02	0.40
1:A:505:LEU:HD22	1:A:505:LEU:H	1.84	0.40
1:B:228:ALA:HA	1:B:233:LEU:HB2	2.02	0.40
1:A:127:VAL:HG22	1:A:128:TRP:H	1.87	0.40
1:A:321:LEU:CD2	1:A:330:PRO:HD3	2.51	0.40
1:A:348:LEU:HD23	1:A:348:LEU:O	2.21	0.40
1:A:57:THR:CG2	1:A:73:LEU:HD21	2.44	0.40
1:A:359:GLU:OE1	1:A:362:ARG:NH1	2.51	0.40
1:A:501:LEU:HG	1:A:502:LEU:H	1.87	0.40
1:B:348:LEU:C	1:B:348:LEU:HD23	2.47	0.40
1:B:440:ARG:CD	1:B:442:GLU:HG2	2.51	0.40
1:A:217:LEU:HD12	1:A:217:LEU:HA	1.88	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:31:VAL:HG12	1:B:32:VAL:N	2.36	0.40
1:B:181:ALA:C	1:B:184:ALA:H	2.30	0.40
1:B:360:PHE:CE1	1:B:361:LEU:HG	2.56	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](#)

There are no protein backbone outliers to report in this entry.

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%)	429 (90%)	46 (10%)	8	20
1	B	447/549 (81%)	389 (87%)	58 (13%)	4	10
All	All	922/1098 (84%)	818 (89%)	104 (11%)	5	14

All (104) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	VAL
1	A	32	VAL
1	A	45	LEU
1	A	68	SER
1	A	82	MET
1	A	85	THR
1	A	146	ARG
1	A	156	TRP
1	A	166	GLU

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Mol	Chain	Res	Type
1	A	179	LEU
1	A	204	LEU
1	A	207	LEU
1	A	210	GLU
1	A	217	LEU
1	A	218	PRO
1	A	233	LEU
1	A	237	GLU
1	A	244	VAL
1	A	247	PRO
1	A	252	LYS
1	A	254	ILE
1	A	265	LEU
1	A	266	THR
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
1	A	419	ASN
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	514	ILE
1	A	585	GLN
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

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Mol	Chain	Res	Type
1	B	79	LEU
1	B	85	THR
1	B	99	ASP
1	B	121	LEU
1	B	122	ARG
1	B	128	TRP
1	B	139	HIS
1	B	141	ARG
1	B	146	ARG
1	B	174	LEU
1	B	179	LEU
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	241	VAL
1	B	258	THR
1	B	288	ARG
1	B	289	ARG
1	B	297	ILE
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	434	ILE
1	B	435	LEU
1	B	439	LEU
1	B	441	GLU
1	B	451	LEU
1	B	454	LEU
1	B	465	LEU
1	B	469	TYR
1	B	472	GLU
1	B	475	VAL

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Mol	Chain	Res	Type
1	B	502	LEU
1	B	503	TRP
1	B	505	LEU
1	B	506	PRO
1	B	521	ASP
1	B	556	LEU
1	B	574	ARG
1	B	584	VAL
1	B	597	GLU
1	B	631	LEU
1	B	639	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) 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	509	GLN
1	A	516	GLN
1	A	585	GLN
1	A	621	HIS
1	A	633	HIS
1	B	187	HIS
1	B	227	HIS
1	B	256	HIS
1	B	382	HIS
1	B	419	ASN
1	B	449	ASN
1	B	633	HIS

5.3.3 RNA ⓘ

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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	637/685 (92%)	0.48	31 (4%) 35 31	43, 73, 102, 115	3 (0%)
1	B	614/685 (89%)	0.60	49 (7%) 18 15	41, 78, 116, 126	14 (2%)
2	X	5/10 (50%)	-0.03	0 100 100	57, 68, 87, 117	0
2	Y	5/10 (50%)	0.07	1 (20%) 3 2	68, 72, 76, 93	0
All	All	1261/1390 (90%)	0.53	81 (6%) 25 22	41, 75, 110, 126	17 (1%)

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	201	THR	7.0
1	A	386	SER	6.0
1	B	187	HIS	5.6
1	B	625	ASP	5.1
1	B	181	ALA	5.1
1	B	180	GLU	4.2
1	A	136	ARG	4.1
1	A	442	GLU	4.0
1	B	238	GLY	3.9
1	A	501	LEU	3.7
1	B	184	ALA	3.6
1	A	417	ASP	3.5
1	B	140	ALA	3.5
1	B	275	GLY	3.5
1	B	249	ASP	3.4
1	B	378	LEU	3.3
1	A	642	TYR	3.3
1	B	185	GLN	3.3
1	B	574	ARG	3.2
1	A	613	THR	3.1
1	B	496	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	204	LEU	3.1
1	A	508	ALA	3.0
1	A	514	ILE	2.9
1	A	483	GLU	2.9
1	B	239	GLY	2.9
1	A	502	LEU	2.8
1	B	277	LEU	2.8
1	B	606	VAL	2.8
1	B	506	PRO	2.8
1	B	244	VAL	2.8
1	B	143	PRO	2.7
1	B	499	GLY	2.6
1	A	80	ALA	2.6
1	B	283	TRP	2.6
1	B	99	ASP	2.6
1	A	608	ARG	2.6
1	A	606	VAL	2.6
1	B	279	LEU	2.6
1	B	354	ALA	2.5
1	A	353	GLY	2.5
1	B	439	LEU	2.5
1	B	305	THR	2.5
1	A	497	ASP	2.5
1	B	356	GLY	2.5
1	A	230	LYS	2.4
1	A	240	ARG	2.4
1	A	4	LEU	2.4
1	B	254	ILE	2.4
2	Y	106	DT	2.4
1	B	257	LEU	2.4
1	B	500	HIS	2.4
1	B	276	SER	2.4
1	A	183	LEU	2.3
1	A	99	ASP	2.3
1	A	158	SER	2.3
1	B	186	GLY	2.3
1	B	241	VAL	2.3
1	B	262	VAL	2.3
1	B	389	LEU	2.3
1	B	437	VAL	2.3
1	A	162	ALA	2.2
1	A	438	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	460	LEU	2.2
1	B	371	ALA	2.2
1	B	297	ILE	2.2
1	A	82	MET	2.1
1	A	297	ILE	2.1
1	B	205	LEU	2.1
1	B	83	GLY	2.1
1	A	350	ARG	2.1
1	B	468	ALA	2.1
1	B	253	PRO	2.1
1	A	65	ALA	2.0
1	A	283	TRP	2.0
1	B	504	THR	2.0
1	A	463	VAL	2.0
1	B	469	TYR	2.0
1	B	73	LEU	2.0
1	A	607	HIS	2.0
1	B	642	TYR	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.