



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 08:55 am BST

PDB ID : 5XQ2
Title : Crystal structure of T. thermophilus Argonaute protein complexed with a bulge 5A6 on the guide strand
Authors : Sheng, G.; Gogakos, T.; Wang, J.; Zhao, H.; Serganov, A.; Juranek, S.; Tuschl, T.; Patel, D.; Wang, Y.
Deposited on : 2017-06-06
Resolution : 3.33 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

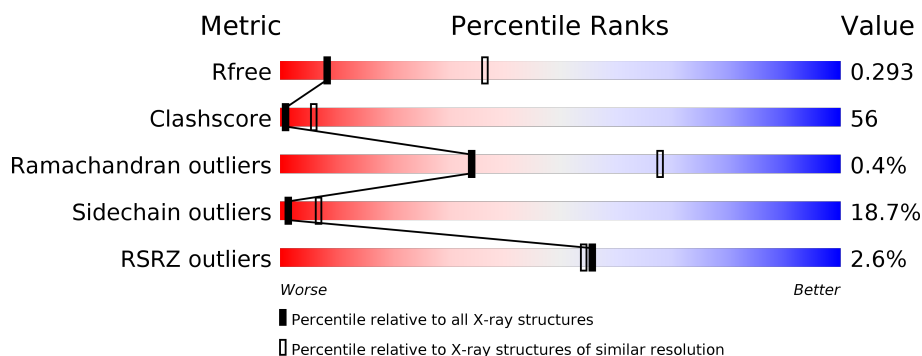
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.33 Å.

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





Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1060 (3.38-3.30)
Clashscore	141614	1111 (3.38-3.30)
Ramachandran outliers	138981	1090 (3.38-3.30)
Sidechain outliers	138945	1089 (3.38-3.30)
RSRZ outliers	127900	1028 (3.38-3.30)

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 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	<div> <div>2%</div> <div>41%</div> <div>44%</div> <div>13%</div> <div>..</div> </div>
1	B	685	<div> <div>3%</div> <div>41%</div> <div>46%</div> <div>12%</div> <div>.</div> </div>
2	E	22	<div> <div>5%</div> <div>36%</div> <div>36%</div> <div>23%</div> </div>
2	X	22	<div> <div>5%</div> <div>45%</div> <div>27%</div> <div>23%</div> </div>
3	F	19	<div> <div>11%</div> <div>68%</div> <div>5%</div> <div>16%</div> </div>
3	Y	19	<div> <div>11%</div> <div>58%</div> <div>16%</div> <div>16%</div> </div>

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Mol	Chain	Length	Quality of chain
4	C	3	 67%33%
4	D	3	 67%33%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 11844 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 TtAgo (D546N).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	679	Total	C	N	O	S	0	0	0
			5184	3317	967	895	5			
1	B	679	Total	C	N	O	S	0	0	0
			5185	3318	968	893	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	546	ASN	ASP	engineered mutation	UNP Q746M7
B	546	ASN	ASP	engineered mutation	UNP Q746M7

- Molecule 2 is a DNA chain called DNA (5'-D(P*TP*GP*AP*AP*GP*AP*TP*AP*GP*TP*AP*GP*GP*TP*TP*GP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	X	17	Total	C	N	O	P	0	0	0
			359	170	67	105	17			
2	E	17	Total	C	N	O	P	0	0	0
			359	170	67	105	17			

- Molecule 3 is a DNA chain called DNA (5'-D(*AP*CP*AP*AP*CP*CP*TP*AP*CP*TP*AP*CP*CP*TP*CP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	Y	16	Total	C	N	O	P	0	0	0
			317	153	57	92	15			
3	F	16	Total	C	N	O	P	0	0	0
			317	153	57	92	15			

- Molecule 4 is a DNA chain called DNA (5'-D(*AP*GP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	C	3	Total	C	N	O	P	0	0	0
			59	30	12	15	2			
4	D	3	Total	C	N	O	P	0	0	0
			59	30	12	15	2			

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	X	1	Total	Mg	0	0
			1	1		
5	E	1	Total	Mg	0	0
			1	1		

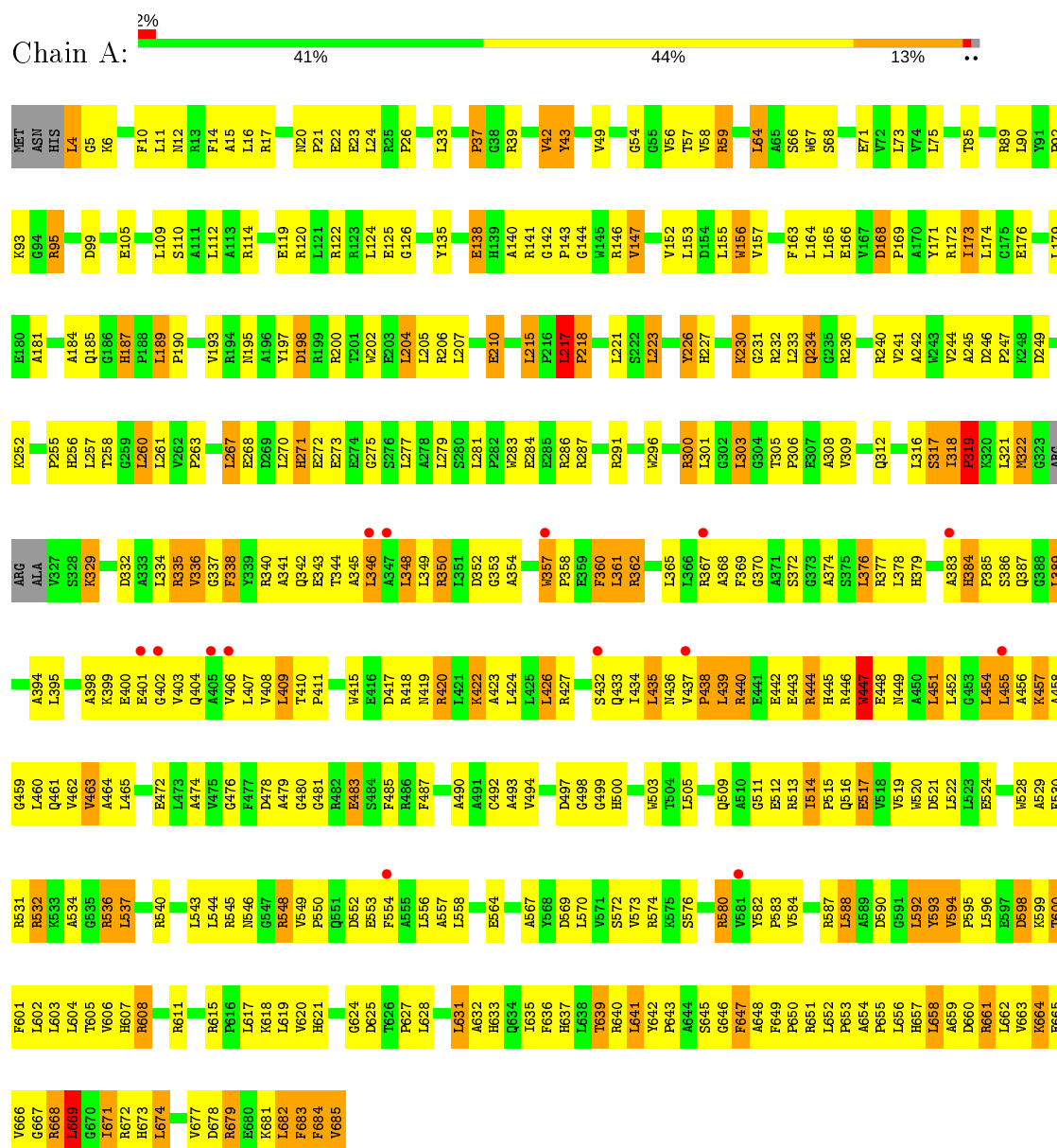
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	O	0	0
			1	1		
6	B	2	Total	O	0	0
			2	2		

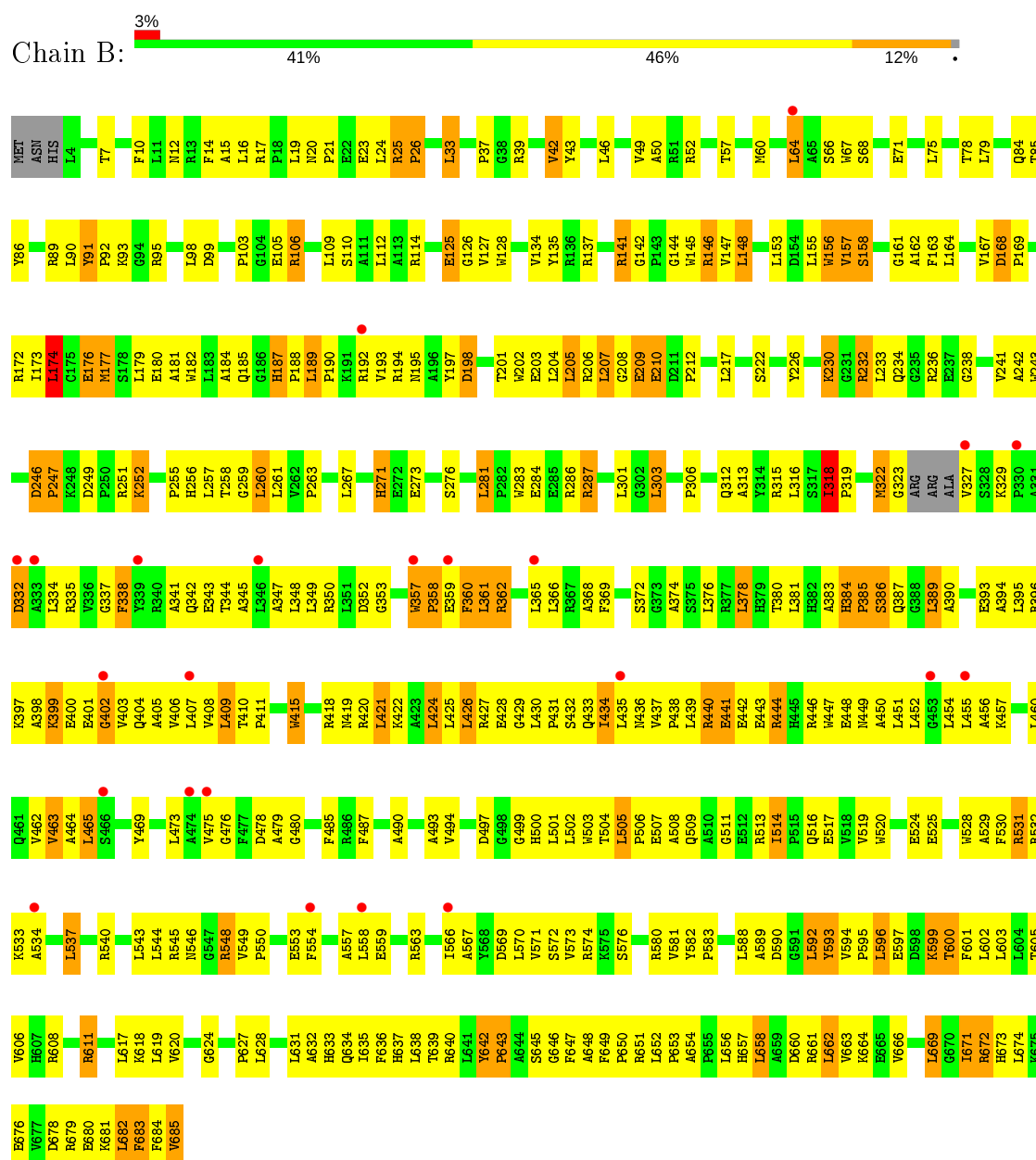
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

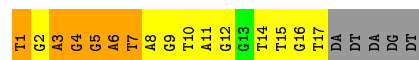
• Molecule 1: TtAgo (D546N)



• Molecule 1: TtAgo (D546N)




- Molecule 2: DNA (5'-D(P*TP*GP*AP*AP*GP*AP*TP*AP*GP*TP*AP*GP*GP*TP*TP*G P*T)-3')



- Molecule 2: DNA (5'-D(P*TP*GP*AP*AP*GP*AP*TP*AP*GP*TP*AP*GP*GP*TP*TP*G P*T)-3')

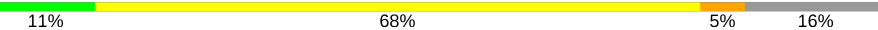


- Molecule 3: DNA (5'-D(*AP*CP*AP*AP*CP*CP*TP*AP*CP*TP*AP*CP*CP*TP*CP*G)-3')

Chain Y: 



- Molecule 3: DNA (5'-D(*AP*CP*AP*AP*CP*CP*TP*AP*CP*TP*AP*CP*CP*TP*CP*G)-3')

Chain F: 



- Molecule 4: DNA (5'-D(*AP*GP*T)-3')

Chain C: 



- Molecule 4: DNA (5'-D(*AP*GP*T)-3')

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, α , β , γ	201.84Å 201.84Å 201.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.95 – 3.33 48.95 – 3.32	Depositor EDS
% Data completeness (in resolution range)	92.1 (48.95-3.33) 92.2 (48.95-3.32)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.65 (at 3.33Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.252 , 0.294 0.253 , 0.293	Depositor DCC
R_{free} test set	1846 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	47.8	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 24.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.459 for l,-k,h	Xtriage
F_o, F_c correlation	0.82	EDS
Total number of atoms	11844	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.82% 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: MG

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	0.64	4/5312 (0.1%)	0.84	20/7233 (0.3%)
1	B	0.61	6/5312 (0.1%)	0.83	23/7229 (0.3%)
2	E	1.53	7/403 (1.7%)	1.30	4/621 (0.6%)
2	X	1.56	6/403 (1.5%)	1.31	3/621 (0.5%)
3	F	1.32	1/354 (0.3%)	1.17	3/542 (0.6%)
3	Y	1.28	1/354 (0.3%)	1.19	2/542 (0.4%)
4	C	1.02	0/66	1.11	0/101
4	D	1.17	0/66	1.14	0/101
All	All	0.78	25/12270 (0.2%)	0.90	55/16990 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	2

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	X	1	DT	OP3-P	-11.29	1.47	1.61
2	E	1	DT	OP3-P	-11.19	1.47	1.61
2	X	17	DT	C1'-N1	8.05	1.59	1.49
2	E	17	DT	C1'-N1	7.96	1.59	1.49
2	E	5	DG	O3'-P	-7.51	1.52	1.61
2	X	5	DG	O3'-P	-7.27	1.52	1.61
2	X	3	DA	O3'-P	-6.87	1.52	1.61
3	F	15	DC	C1'-N1	6.41	1.57	1.49
2	E	3	DA	O3'-P	-6.20	1.53	1.61
2	E	7	DT	C3'-O3'	-6.17	1.35	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	X	4	DG	O3'-P	-6.13	1.53	1.61
2	E	4	DG	O3'-P	-5.57	1.54	1.61
2	X	7	DT	C3'-O3'	-5.33	1.37	1.44
2	E	8	DA	C3'-O3'	-5.31	1.37	1.44
1	B	643	PRO	N-CD	5.19	1.55	1.47
1	A	218	PRO	N-CD	5.18	1.55	1.47
1	B	92	PRO	N-CD	5.16	1.55	1.47
3	Y	19	DG	C2-N2	-5.16	1.29	1.34
1	A	319	PRO	N-CD	5.14	1.55	1.47
1	B	247	PRO	N-CD	5.12	1.55	1.47
1	B	188	PRO	N-CD	5.12	1.55	1.47
1	B	385	PRO	N-CD	5.10	1.54	1.47
1	B	26	PRO	N-CD	5.09	1.54	1.47
1	A	411	PRO	N-CD	5.03	1.54	1.47
1	A	438	PRO	N-CD	5.01	1.54	1.47

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	505	LEU	C-N-CD	-11.60	95.09	120.60
2	X	6	DA	O5'-P-OP2	-9.12	97.49	105.70
1	B	174	LEU	CA-CB-CG	8.54	134.95	115.30
1	B	669	LEU	CA-CB-CG	7.90	133.48	115.30
1	B	126	GLY	N-CA-C	-7.21	95.08	113.10
1	A	669	LEU	CA-CB-CG	7.17	131.79	115.30
2	X	7	DT	N3-C4-O4	6.47	123.78	119.90
1	B	402	GLY	N-CA-C	6.44	129.21	113.10
1	A	124	LEU	CA-CB-CG	6.44	130.11	115.30
1	B	357	TRP	C-N-CD	6.31	141.65	128.40
1	A	642	TYR	C-N-CD	6.22	141.46	128.40
1	A	142	GLY	C-N-CD	6.18	141.39	128.40
1	A	384	HIS	C-N-CD	6.14	141.30	128.40
1	B	549	VAL	C-N-CD	6.12	141.25	128.40
2	E	1	DT	O5'-P-OP2	-6.10	100.21	105.70
1	A	318	ILE	C-N-CD	6.05	141.11	128.40
1	A	411	PRO	C-N-CD	5.99	140.98	128.40
1	B	318	ILE	C-N-CD	5.98	140.95	128.40
1	B	168	ASP	C-N-CD	5.97	140.94	128.40
1	A	252	LYS	C-N-CD	5.94	140.87	128.40
1	B	249	ASP	C-N-CD	5.93	140.86	128.40
3	Y	17	DT	N3-C4-O4	5.93	123.46	119.90
1	B	252	LYS	C-N-CD	5.89	140.77	128.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	514	ILE	C-N-CD	5.89	140.76	128.40
1	A	168	ASP	C-N-CD	5.87	140.73	128.40
1	A	594	VAL	C-N-CD	5.81	140.60	128.40
1	A	187	HIS	C-N-CD	5.80	140.58	128.40
1	A	249	ASP	C-N-CD	5.80	140.58	128.40
1	B	384	HIS	C-N-CD	5.78	140.54	128.40
1	A	447	TRP	CA-CB-CG	5.78	124.69	113.70
1	B	187	HIS	C-N-CD	5.76	140.50	128.40
1	B	148	LEU	CA-CB-CG	5.76	128.55	115.30
3	Y	9	DC	O4'-C4'-C3'	-5.75	102.20	104.50
1	A	410	THR	C-N-CD	5.74	140.44	128.40
1	A	126	GLY	N-CA-C	-5.72	98.79	113.10
2	E	7	DT	N3-C4-O4	5.72	123.33	119.90
1	A	217	LEU	C-N-CD	5.71	140.39	128.40
1	B	25	ARG	C-N-CD	5.70	140.36	128.40
1	B	246	ASP	C-N-CD	5.68	140.33	128.40
1	B	642	TYR	C-N-CD	5.62	140.21	128.40
1	B	43	TYR	CA-CB-CG	5.58	123.99	113.40
1	B	303	LEU	CB-CG-CD2	-5.56	101.56	111.00
3	F	13	DT	O5'-P-OP1	-5.54	100.72	105.70
1	A	454	LEU	CB-CG-CD1	-5.52	101.61	111.00
1	B	91	TYR	C-N-CD	5.50	139.94	128.40
3	F	17	DT	N3-C4-O4	5.49	123.19	119.90
1	A	43	TYR	CA-CB-CG	5.42	123.69	113.40
2	E	15	DT	O5'-P-OP1	5.37	117.14	110.70
1	B	611	ARG	NE-CZ-NH2	-5.31	117.64	120.30
1	A	588	LEU	CB-CG-CD1	-5.31	101.98	111.00
1	B	332	ASP	CB-CG-OD2	5.20	122.98	118.30
1	B	207	LEU	CA-CB-CG	5.14	127.12	115.30
2	X	7	DT	C5-C4-O4	-5.13	121.31	124.90
3	F	5	DC	O4'-C1'-N1	5.07	111.55	108.00
2	E	10	DT	N3-C4-O4	5.01	122.91	119.90

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	125	GLU	Peptide
1	B	203	GLU	Peptide

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	5184	0	5154	624	2
1	B	5185	0	5161	627	0
2	E	359	0	194	28	0
2	X	359	0	194	25	0
3	F	317	0	181	15	0
3	Y	317	0	179	23	0
4	C	59	0	33	11	0
4	D	59	0	33	1	0
5	E	1	0	0	0	0
5	X	1	0	0	0	0
6	A	1	0	0	0	0
6	B	2	0	0	0	0
All	All	11844	0	11129	1278	2

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 56.

All (1278) 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:319:PRO:HB3	1:A:637:HIS:CD2	1.25	1.65
1:B:455:LEU:HD22	1:B:460:LEU:CD2	1.18	1.60
1:B:455:LEU:CD2	1:B:460:LEU:HD23	1.15	1.56
1:A:426:LEU:HD11	1:A:677:VAL:CG2	1.47	1.43
1:B:658:LEU:HD12	1:B:684:PHE:CE2	1.53	1.42
1:B:348:LEU:HD22	1:B:357:TRP:CE3	1.55	1.40
1:A:439:LEU:HD12	1:A:440:ARG:N	1.35	1.39
1:A:437:VAL:CG1	1:A:438:PRO:HA	1.50	1.38
1:B:369:PHE:CD2	1:B:376:LEU:HD13	1.60	1.35
1:A:658:LEU:HD12	1:A:684:PHE:CE2	1.64	1.31
1:B:447:TRP:CZ3	1:B:448:GLU:HG2	1.65	1.31
1:B:600:THR:CG2	1:B:620:VAL:HG22	1.60	1.29
1:A:345:ALA:C	1:A:346:LEU:HD23	1.52	1.27
1:A:319:PRO:CB	1:A:637:HIS:CD2	2.16	1.27
1:A:230:LYS:HE3	1:A:232:ARG:CG	1.63	1.27

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:ARG:NH1	1:A:367:ARG:NE	1.80	1.27
1:A:362:ARG:HG2	1:A:378:LEU:CD1	1.66	1.25
1:A:335:ARG:CG	1:A:367:ARG:HD2	1.68	1.24
1:A:514:ILE:HG22	1:A:519:VAL:CG2	1.69	1.22
1:A:544:LEU:CD1	1:A:656:LEU:HD21	1.70	1.21
1:A:661:ARG:NH1	2:X:4:DG:OP1	1.73	1.21
1:B:360:PHE:CE2	1:B:441:GLU:HB2	1.76	1.20
1:A:658:LEU:HD21	1:A:682:LEU:HD21	1.24	1.19
1:A:365:LEU:O	1:A:369:PHE:HD2	1.25	1.18
1:B:476:GLY:HA2	1:B:544:LEU:HD11	1.26	1.18
1:A:335:ARG:HG2	1:A:367:ARG:CD	1.72	1.17
1:A:476:GLY:HA2	1:A:544:LEU:HD11	1.20	1.17
1:A:514:ILE:CG2	1:A:519:VAL:HG22	1.73	1.16
1:A:544:LEU:HD13	1:A:656:LEU:CD2	1.75	1.15
1:A:658:LEU:HD11	1:A:682:LEU:CD2	1.76	1.15
1:B:505:LEU:HD11	1:B:671:ILE:HD11	1.28	1.15
1:B:236:ARG:HD2	1:B:260:LEU:HD23	1.28	1.14
1:B:357:TRP:CD1	1:B:362:ARG:HD2	1.82	1.14
1:A:335:ARG:HH12	1:A:367:ARG:NE	1.42	1.11
1:A:365:LEU:O	1:A:369:PHE:CD2	2.02	1.11
1:B:387:GLN:CB	1:B:389:LEU:HD11	1.80	1.11
1:A:230:LYS:HE3	1:A:232:ARG:HG2	1.27	1.10
1:A:335:ARG:O	1:A:368:ALA:HA	1.51	1.10
1:B:658:LEU:CD1	1:B:684:PHE:CE2	2.34	1.09
1:A:530:PHE:O	1:A:534:ALA:HB3	1.52	1.09
1:A:426:LEU:CD1	1:A:677:VAL:CG2	2.31	1.08
1:B:348:LEU:CD2	1:B:357:TRP:CE3	2.37	1.08
1:B:230:LYS:HE3	1:B:232:ARG:HG3	1.28	1.07
1:B:357:TRP:NE1	1:B:362:ARG:HD2	1.69	1.07
1:B:447:TRP:CZ3	1:B:448:GLU:CG	2.37	1.07
1:A:628:LEU:HA	1:A:631:LEU:HD12	1.30	1.07
1:A:530:PHE:O	1:A:534:ALA:CB	2.03	1.06
1:B:600:THR:CG2	1:B:620:VAL:CG2	2.34	1.06
1:B:168:ASP:OD1	1:B:580:ARG:NH1	1.89	1.06
1:B:398:ALA:HB1	1:B:403:VAL:HG21	1.35	1.05
1:B:600:THR:CG2	1:B:620:VAL:HA	1.87	1.04
1:A:342:GLN:O	1:A:344:THR:HG23	1.54	1.04
1:B:422:LYS:HG2	1:B:425:LEU:HD12	1.36	1.04
1:B:600:THR:HG21	1:B:620:VAL:HG22	1.05	1.04
1:A:345:ALA:O	1:A:346:LEU:HD23	1.55	1.04
1:B:404:GLN:O	1:B:681:LYS:HE2	1.58	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:PHE:CD2	1:A:303:LEU:HD13	1.93	1.03
1:A:230:LYS:HE3	1:A:232:ARG:HG3	1.41	1.03
1:B:369:PHE:CD2	1:B:376:LEU:CD1	2.42	1.03
1:A:231:GLY:HA2	1:A:234:GLN:HE22	1.24	1.02
1:A:349:LEU:CD1	1:A:383:ALA:HB2	1.88	1.02
1:A:409:LEU:HB3	1:A:435:LEU:HD13	1.40	1.02
1:B:342:GLN:O	1:B:344:THR:HG23	1.59	1.02
1:B:358:PRO:HD2	1:B:361:LEU:CD1	1.89	1.02
1:B:658:LEU:HD11	1:B:682:LEU:CD2	1.88	1.02
1:B:600:THR:CG2	1:B:620:VAL:CA	2.38	1.01
1:B:389:LEU:H	1:B:389:LEU:HD12	1.23	1.01
1:B:358:PRO:CD	1:B:361:LEU:HD11	1.90	1.01
1:A:163:PHE:CD2	1:A:303:LEU:CD1	2.44	1.00
1:B:233:LEU:CD2	1:B:260:LEU:HD21	1.92	1.00
1:A:147:VAL:HG23	1:A:173:ILE:HA	1.44	1.00
1:A:514:ILE:HG21	1:A:519:VAL:HG22	1.43	1.00
1:A:437:VAL:HG13	1:A:438:PRO:HA	1.05	1.00
1:A:658:LEU:CD1	1:A:684:PHE:CE2	2.45	1.00
1:B:398:ALA:HB1	1:B:403:VAL:CG2	1.90	0.99
1:A:514:ILE:HG22	1:A:519:VAL:HG23	1.42	0.99
1:B:457:LYS:HE3	1:B:685:VAL:HG23	1.45	0.99
1:B:168:ASP:OD2	1:B:580:ARG:NH1	1.95	0.99
1:A:207:LEU:O	1:A:241:VAL:O	1.81	0.98
1:B:360:PHE:CD2	1:B:441:GLU:HB2	1.97	0.98
1:A:605:THR:HB	1:A:639:THR:HG21	1.44	0.98
1:A:435:LEU:H	1:A:435:LEU:HD12	1.22	0.98
1:A:514:ILE:CG2	1:A:519:VAL:CG2	2.38	0.98
1:A:437:VAL:CG1	1:A:438:PRO:CA	2.41	0.98
1:B:168:ASP:CG	1:B:580:ARG:NH1	2.17	0.98
1:B:600:THR:HG22	1:B:619:LEU:C	1.84	0.97
1:B:658:LEU:HD11	1:B:682:LEU:HD21	1.45	0.97
1:A:658:LEU:CD2	1:A:682:LEU:HD21	1.94	0.97
1:B:233:LEU:HD23	1:B:260:LEU:HD21	1.46	0.97
1:B:230:LYS:HE3	1:B:232:ARG:CG	1.95	0.96
1:A:426:LEU:CD1	1:A:677:VAL:HG21	1.95	0.96
1:B:505:LEU:HD11	1:B:671:ILE:CD1	1.95	0.96
1:B:658:LEU:HD12	1:B:684:PHE:HE2	0.90	0.96
1:A:362:ARG:CD	1:A:378:LEU:HD12	1.96	0.95
1:B:348:LEU:HD22	1:B:357:TRP:HE3	1.27	0.95
1:B:505:LEU:CD1	1:B:671:ILE:HD11	1.96	0.95
1:A:236:ARG:HD2	1:A:260:LEU:HD23	1.46	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:PRO:HB3	1:A:637:HIS:CG	2.01	0.95
1:A:437:VAL:HG12	1:A:438:PRO:HA	1.46	0.95
1:A:426:LEU:HD11	1:A:677:VAL:HG21	0.99	0.95
1:B:583:PRO:HG3	1:B:588:LEU:HD12	1.46	0.95
1:B:600:THR:HG22	1:B:620:VAL:CA	1.96	0.95
1:A:335:ARG:HH11	1:A:367:ARG:CD	1.79	0.94
1:A:439:LEU:CD1	1:A:440:ARG:N	2.29	0.94
1:B:345:ALA:HB1	1:B:402:GLY:HA2	1.49	0.94
1:B:661:ARG:HH12	2:E:4:DG:P	1.89	0.94
1:B:318:ILE:H	1:B:318:ILE:HD12	1.32	0.94
1:B:49:VAL:HG12	1:B:64:LEU:HD21	1.48	0.94
1:B:360:PHE:CE2	1:B:441:GLU:CB	2.50	0.94
1:A:521:ASP:OD2	1:B:673:HIS:NE2	2.01	0.94
1:A:628:LEU:HA	1:A:631:LEU:CD1	1.98	0.93
1:A:335:ARG:O	1:A:368:ALA:CA	2.15	0.93
1:B:600:THR:HG23	1:B:620:VAL:CB	1.98	0.93
1:B:645:SER:OG	1:B:648:ALA:O	1.85	0.93
1:A:349:LEU:HD11	1:A:383:ALA:HB2	1.49	0.93
1:B:600:THR:HG23	1:B:620:VAL:HA	1.51	0.93
1:A:43:TYR:HD2	1:A:59:ARG:NH1	1.67	0.93
1:A:335:ARG:NH1	1:A:367:ARG:HE	1.67	0.92
1:A:335:ARG:HH11	1:A:335:ARG:HG2	1.32	0.92
1:B:444:ARG:HD3	1:B:448:GLU:CD	1.89	0.92
1:A:43:TYR:HD2	1:A:59:ARG:HH12	0.97	0.92
1:A:517:GLU:OE1	1:A:517:GLU:N	2.02	0.92
1:A:409:LEU:HB3	1:A:435:LEU:CD1	2.00	0.92
1:B:447:TRP:HZ3	1:B:448:GLU:HG2	1.29	0.92
1:A:362:ARG:CG	1:A:378:LEU:CD1	2.48	0.92
1:B:599:LYS:HA	1:B:599:LYS:HZ2	1.35	0.92
1:A:464:ALA:HB1	1:A:499:GLY:H	1.35	0.91
1:B:369:PHE:CG	1:B:376:LEU:HD13	2.05	0.91
1:B:349:LEU:HD22	1:B:350:ARG:H	1.32	0.91
1:B:658:LEU:HD21	1:B:682:LEU:HD21	1.50	0.91
1:A:528:TRP:HB3	1:A:532:ARG:HH22	1.34	0.91
1:A:335:ARG:NH1	1:A:367:ARG:CD	2.32	0.91
1:A:514:ILE:HB	1:A:553:GLU:OE2	1.71	0.90
1:B:349:LEU:HD22	1:B:350:ARG:N	1.85	0.90
1:A:636:PHE:O	1:A:639:THR:OG1	1.88	0.90
1:B:544:LEU:HD13	1:B:656:LEU:HD21	1.53	0.90
1:A:362:ARG:CG	1:A:378:LEU:HD12	2.02	0.90
1:B:319:PRO:HG3	1:B:640:ARG:HG3	1.54	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:358:PRO:HG2	1:B:360:PHE:HE1	1.33	0.90
1:B:600:THR:HG23	1:B:620:VAL:CA	2.02	0.90
1:A:628:LEU:CA	1:A:631:LEU:HD12	2.02	0.89
1:A:650:PRO:HB3	1:A:657:HIS:ND1	1.86	0.89
1:A:54:GLY:O	1:A:73:LEU:CD2	2.20	0.89
1:A:439:LEU:HD12	1:A:440:ARG:H	1.08	0.89
1:B:345:ALA:CB	1:B:402:GLY:HA2	2.03	0.89
1:A:230:LYS:HG3	1:A:232:ARG:HE	1.34	0.89
1:B:348:LEU:HD22	1:B:357:TRP:CZ3	2.06	0.89
1:A:658:LEU:HD11	1:A:682:LEU:HD21	1.54	0.88
1:B:600:THR:HG21	1:B:620:VAL:CG2	1.99	0.88
1:B:600:THR:HG22	1:B:620:VAL:N	1.87	0.88
1:A:531:ARG:HG2	1:A:536:ARG:O	1.73	0.88
1:B:352:ASP:N	1:B:353:GLY:HA2	1.85	0.88
1:B:360:PHE:HE2	1:B:441:GLU:HB2	1.34	0.88
1:B:365:LEU:O	1:B:369:PHE:HD2	1.57	0.88
1:B:449:ASN:OD1	1:B:646:GLY:HA3	1.74	0.88
1:A:361:LEU:H	1:A:361:LEU:HD22	1.39	0.87
1:A:362:ARG:HG2	1:A:378:LEU:HD12	1.54	0.87
1:A:437:VAL:HG13	1:A:438:PRO:CA	2.00	0.87
1:A:358:PRO:HB2	1:A:360:PHE:CE1	2.08	0.87
1:A:521:ASP:OD1	1:B:672:ARG:NH1	2.06	0.87
1:B:679:ARG:HH11	1:B:679:ARG:HG3	1.38	0.87
1:B:600:THR:HG22	1:B:619:LEU:O	1.73	0.87
1:A:335:ARG:HH12	1:A:367:ARG:CZ	1.87	0.87
1:B:460:LEU:HD11	1:B:462:VAL:CG1	2.04	0.87
1:B:661:ARG:NH1	2:E:4:DG:OP2	2.08	0.87
1:A:234:GLN:OE1	1:A:234:GLN:N	2.08	0.87
1:A:207:LEU:HD21	1:A:240:ARG:HD2	1.55	0.86
1:A:360:PHE:CD1	1:A:361:LEU:HD22	2.08	0.86
1:B:322:MET:CG	1:B:323:GLY:HA3	2.05	0.86
1:B:232:ARG:O	1:B:236:ARG:NH1	2.07	0.86
1:B:110:SER:HB3	1:B:114:ARG:HH12	1.39	0.86
1:B:315:ARG:NH1	1:B:589:ALA:CB	2.38	0.86
1:B:460:LEU:HD11	1:B:462:VAL:HG12	1.56	0.86
1:B:480:GLY:O	1:B:487:PHE:HB2	1.76	0.86
1:B:344:THR:HG22	1:B:404:GLN:OE1	1.76	0.85
1:B:661:ARG:NH1	2:E:4:DG:P	2.49	0.85
1:A:455:LEU:O	1:A:458:ALA:O	1.94	0.85
1:B:590:ASP:CB	3:F:19:DG:H22	1.89	0.85
1:A:110:SER:HB3	1:A:114:ARG:HH12	1.40	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:SER:O	1:A:637:HIS:NE2	2.09	0.85
1:A:544:LEU:HD13	1:A:656:LEU:HD21	0.87	0.85
1:A:138:GLU:HB2	1:A:141:ARG:HE	1.41	0.85
1:B:502:LEU:CD2	1:B:680:GLU:HA	2.06	0.85
1:A:658:LEU:HD12	1:A:684:PHE:HE2	1.09	0.84
1:A:226:TYR:OH	4:C:21:DT:OP2	1.95	0.84
1:B:662:LEU:O	1:B:662:LEU:HD12	1.77	0.84
1:A:358:PRO:O	1:A:361:LEU:HD23	1.77	0.84
1:B:17:ARG:NH2	1:B:23:GLU:OE1	2.10	0.84
1:B:348:LEU:CD2	1:B:357:TRP:HE3	1.81	0.84
1:A:387:GLN:HB3	1:A:389:LEU:CD2	2.07	0.84
1:B:190:PRO:HG3	1:B:263:PRO:HB3	1.57	0.84
1:B:395:LEU:O	1:B:399:LYS:HB2	1.77	0.84
1:A:531:ARG:NH1	1:A:537:LEU:CD2	2.41	0.84
1:A:316:LEU:HD11	1:A:632:ALA:HB1	1.59	0.84
1:B:449:ASN:OD1	1:B:646:GLY:CA	2.26	0.84
1:B:358:PRO:HG2	1:B:360:PHE:CE1	2.12	0.84
1:B:348:LEU:O	1:B:381:LEU:HB2	1.78	0.84
1:A:387:GLN:HE21	1:A:389:LEU:CD2	1.89	0.83
1:A:460:LEU:CB	1:A:462:VAL:HG22	2.08	0.83
1:B:650:PRO:HB3	1:B:657:HIS:ND1	1.93	0.83
1:A:369:PHE:CZ	1:A:376:LEU:CD1	2.61	0.83
1:A:334:LEU:O	1:A:334:LEU:HD12	1.77	0.83
1:A:226:TYR:CE2	4:C:21:DT:H71	2.14	0.83
1:A:232:ARG:O	1:A:236:ARG:NH1	2.11	0.83
1:B:347:ALA:HB1	1:B:381:LEU:CD1	2.09	0.83
1:B:520:TRP:NE1	1:B:524:GLU:OE1	2.12	0.82
1:B:573:VAL:HG21	1:B:656:LEU:CD1	2.09	0.82
1:A:350:ARG:HH21	1:A:350:ARG:HG3	1.43	0.82
1:A:358:PRO:HD2	1:A:361:LEU:HD21	1.59	0.82
1:A:521:ASP:CG	1:B:673:HIS:HE2	1.82	0.81
1:A:147:VAL:HG22	1:A:172:ARG:O	1.80	0.81
1:B:234:GLN:OE1	1:B:234:GLN:N	2.14	0.81
1:B:322:MET:N	1:B:463:VAL:HG12	1.89	0.81
1:A:335:ARG:HG2	1:A:367:ARG:HD2	0.84	0.81
1:A:43:TYR:CD2	1:A:59:ARG:NH1	2.45	0.80
1:B:583:PRO:CG	1:B:588:LEU:HD12	2.10	0.80
1:B:194:ARG:HG3	1:B:201:THR:HG22	1.64	0.80
1:B:236:ARG:CD	1:B:260:LEU:HD23	2.11	0.80
1:B:544:LEU:CD1	1:B:656:LEU:HD21	2.12	0.80
1:A:661:ARG:NH1	2:X:4:DG:P	2.54	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:358:PRO:CG	1:B:360:PHE:HE1	1.95	0.80
1:B:422:LYS:HA	1:B:425:LEU:HD12	1.64	0.80
1:B:271:HIS:HB2	1:B:276:SER:HB3	1.63	0.79
1:A:494:VAL:O	1:A:499:GLY:HA2	1.82	0.79
1:B:387:GLN:CB	1:B:389:LEU:CD1	2.59	0.79
1:A:197:TYR:CE1	1:A:230:LYS:NZ	2.50	0.79
1:A:197:TYR:CZ	1:A:230:LYS:NZ	2.51	0.79
1:A:319:PRO:HB3	1:A:637:HIS:HD2	0.96	0.79
1:B:600:THR:HG23	1:B:620:VAL:HG13	1.64	0.79
1:B:449:ASN:OD1	1:B:646:GLY:N	2.15	0.79
1:A:439:LEU:CD1	1:A:440:ARG:H	1.90	0.79
1:B:422:LYS:HZ3	1:B:432:SER:HB2	1.48	0.79
1:B:513:ARG:NH2	2:E:16:DG:OP2	2.14	0.78
1:B:544:LEU:HD13	1:B:656:LEU:CD2	2.13	0.78
1:B:529:ALA:HA	1:B:532:ARG:CZ	2.13	0.78
1:A:640:ARG:HD2	1:A:649:PHE:CE2	2.19	0.78
1:B:462:VAL:HG23	1:B:463:VAL:HG22	1.66	0.78
1:B:671:ILE:HD13	1:B:671:ILE:O	1.84	0.78
1:B:334:LEU:O	1:B:368:ALA:HB2	1.84	0.77
1:A:361:LEU:H	1:A:361:LEU:CD2	1.97	0.77
1:B:384:HIS:CE1	1:B:387:GLN:H	2.02	0.77
1:A:362:ARG:HG2	1:A:378:LEU:HD11	1.63	0.77
1:B:478:ASP:OD1	1:B:479:ALA:N	2.17	0.77
1:B:600:THR:HG23	1:B:620:VAL:CG1	2.14	0.77
1:A:437:VAL:HG12	1:A:438:PRO:CA	2.10	0.77
1:A:43:TYR:HB3	1:A:59:ARG:NH1	1.98	0.77
1:A:658:LEU:CD1	1:A:682:LEU:HD21	2.14	0.77
1:B:502:LEU:HD22	1:B:679:ARG:O	1.85	0.77
1:A:223:LEU:HD11	1:A:255:PRO:HB2	1.66	0.76
1:A:426:LEU:HD11	1:A:677:VAL:HG22	1.63	0.76
1:A:509:GLN:NE2	1:A:511:GLY:O	2.15	0.76
1:B:425:LEU:O	1:B:430:LEU:HB2	1.85	0.76
1:B:600:THR:CG2	1:B:620:VAL:CB	2.59	0.76
1:B:449:ASN:CG	1:B:646:GLY:H	1.89	0.76
1:B:433:GLN:NE2	1:B:434:ILE:O	2.19	0.76
1:B:501:LEU:CD1	1:B:643:PRO:HD3	2.16	0.76
1:B:476:GLY:CA	1:B:544:LEU:HD11	2.11	0.76
1:B:590:ASP:CB	3:F:19:DG:N2	2.48	0.76
1:A:665:GLU:HA	1:A:668:ARG:HD2	1.67	0.76
1:B:464:ALA:HB1	1:B:499:GLY:H	1.50	0.75
1:A:349:LEU:HD11	1:A:383:ALA:CB	2.16	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:ASP:OD2	1:A:580:ARG:NH1	2.20	0.75
1:B:322:MET:HG2	1:B:323:GLY:HA3	1.67	0.75
1:B:357:TRP:CD1	1:B:362:ARG:CD	2.68	0.75
1:A:230:LYS:CE	1:A:232:ARG:HG2	2.10	0.75
1:B:608:ARG:HB2	1:B:611:ARG:HG2	1.68	0.75
1:B:197:TYR:CE2	1:B:230:LYS:NZ	2.51	0.74
1:A:387:GLN:HE21	1:A:389:LEU:HD21	1.52	0.74
1:A:479:ALA:HA	1:A:487:PHE:O	1.87	0.74
1:B:529:ALA:HA	1:B:532:ARG:NH2	2.03	0.74
1:A:661:ARG:HH12	2:X:4:DG:P	2.10	0.74
1:A:640:ARG:HD2	1:A:649:PHE:CD2	2.23	0.74
1:B:628:LEU:HA	1:B:631:LEU:HD12	1.69	0.74
1:A:345:ALA:HB3	1:A:402:GLY:C	2.09	0.74
1:A:335:ARG:NH1	1:A:335:ARG:HG2	2.00	0.74
1:B:600:THR:HG22	1:B:620:VAL:HA	1.60	0.73
1:A:350:ARG:NH2	1:A:350:ARG:HG3	1.99	0.73
1:A:319:PRO:CB	1:A:637:HIS:HD2	1.77	0.73
1:A:362:ARG:HG2	1:A:378:LEU:HD13	1.70	0.73
1:A:545:ARG:O	1:A:573:VAL:HG22	1.88	0.73
1:A:138:GLU:HB2	1:A:141:ARG:NE	2.04	0.73
1:B:394:ALA:O	1:B:398:ALA:N	2.17	0.73
1:A:465:LEU:O	1:A:497:ASP:O	2.06	0.73
1:A:515:PRO:O	1:A:519:VAL:HG23	1.89	0.73
1:B:334:LEU:O	1:B:334:LEU:HD12	1.89	0.73
1:B:455:LEU:CG	1:B:460:LEU:HD23	2.15	0.73
1:B:424:LEU:N	1:B:424:LEU:HD23	2.04	0.73
1:B:529:ALA:O	1:B:532:ARG:HG3	1.88	0.73
1:A:344:THR:HG22	1:A:404:GLN:OE1	1.87	0.73
1:B:422:LYS:NZ	1:B:432:SER:HB2	2.04	0.73
1:B:447:TRP:CE3	1:B:448:GLU:HG2	2.24	0.73
1:B:464:ALA:CB	1:B:499:GLY:H	2.02	0.73
1:A:226:TYR:HE2	4:C:21:DT:H71	1.54	0.73
1:B:599:LYS:HA	1:B:599:LYS:NZ	2.03	0.73
1:B:449:ASN:ND2	1:B:646:GLY:H	1.87	0.73
1:A:358:PRO:HB2	1:A:360:PHE:HE1	1.49	0.72
1:A:531:ARG:NH1	1:A:537:LEU:HD23	2.03	0.72
1:B:422:LYS:HG2	1:B:425:LEU:CD1	2.16	0.72
1:A:520:TRP:NE1	1:A:524:GLU:OE1	2.22	0.72
1:B:658:LEU:CD1	1:B:682:LEU:HD21	2.17	0.72
1:B:357:TRP:NE1	1:B:362:ARG:CD	2.51	0.72
1:B:369:PHE:HD2	1:B:376:LEU:HD13	1.49	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:345:ALA:O	1:A:346:LEU:CD2	2.37	0.72
1:B:360:PHE:HE2	1:B:441:GLU:CB	1.94	0.72
1:B:505:LEU:HD11	1:B:671:ILE:CG1	2.20	0.72
1:A:190:PRO:HG3	1:A:263:PRO:HB3	1.71	0.72
1:B:208:GLY:H	1:B:243:TRP:HD1	1.37	0.72
1:B:455:LEU:HD22	1:B:460:LEU:CG	2.17	0.72
1:A:531:ARG:NH1	1:A:537:LEU:HD22	2.03	0.71
1:B:52:ARG:NH1	1:B:78:THR:O	2.23	0.71
1:A:365:LEU:CD1	1:A:378:LEU:HD21	2.19	0.71
1:A:605:THR:CB	1:A:639:THR:HG21	2.20	0.71
1:B:418:ARG:NH1	1:B:419:ASN:OD1	2.23	0.71
1:B:168:ASP:CG	1:B:580:ARG:HH12	1.87	0.71
1:B:318:ILE:N	1:B:318:ILE:HD12	2.04	0.71
1:A:369:PHE:CZ	1:A:376:LEU:HD13	2.23	0.71
1:A:394:ALA:O	1:A:398:ALA:N	2.16	0.71
1:B:181:ALA:O	1:B:184:ALA:HB3	1.90	0.71
1:A:530:PHE:O	1:A:534:ALA:HB2	1.89	0.71
1:A:476:GLY:CA	1:A:544:LEU:HD11	2.12	0.71
1:A:658:LEU:HD21	1:A:682:LEU:CD2	2.14	0.71
1:B:529:ALA:HB2	1:B:532:ARG:NH1	2.04	0.71
1:A:169:PRO:O	1:A:286:ARG:NH2	2.23	0.71
1:B:14:PHE:HD2	1:B:306:PRO:HB2	1.56	0.71
1:A:37:PRO:HG2	1:A:42:VAL:HG23	1.73	0.71
1:A:231:GLY:HA2	1:A:234:GLN:NE2	2.03	0.70
1:A:345:ALA:CB	1:A:402:GLY:H	2.04	0.70
1:B:212:PRO:HG3	1:B:241:VAL:HG23	1.72	0.70
1:B:389:LEU:HD12	1:B:389:LEU:N	2.03	0.70
1:A:599:LYS:O	1:A:621:HIS:N	2.15	0.70
1:B:271:HIS:HB2	1:B:276:SER:CB	2.22	0.70
1:B:156:TRP:CD1	1:B:164:LEU:HB2	2.26	0.70
1:B:369:PHE:HB3	1:B:374:ALA:O	1.90	0.70
1:A:608:ARG:HB2	1:A:611:ARG:HG3	1.72	0.70
1:A:573:VAL:HG21	1:A:656:LEU:CD1	2.22	0.70
1:A:147:VAL:HG23	1:A:173:ILE:CA	2.20	0.70
1:A:335:ARG:HH11	1:A:367:ARG:HD2	1.53	0.69
2:E:9:DG:H2''	2:E:10:DT:H5'	1.73	0.69
1:A:657:HIS:HE1	2:X:4:DG:H5''	1.57	0.69
1:B:504:THR:O	1:B:506:PRO:HD3	1.92	0.69
1:A:345:ALA:HB2	1:A:402:GLY:H	1.56	0.69
1:B:349:LEU:HD21	1:B:383:ALA:HB3	1.74	0.69
1:B:358:PRO:HD2	1:B:361:LEU:HD11	0.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:431:PRO:HG3	1:B:681:LYS:HG3	1.75	0.69
1:A:223:LEU:HD23	1:A:257:LEU:CD2	2.22	0.69
1:A:312:GLN:O	1:A:594:VAL:HG13	1.93	0.69
1:A:346:LEU:HD23	1:A:346:LEU:N	2.03	0.69
1:A:334:LEU:O	1:A:368:ALA:HB2	1.93	0.69
1:A:529:ALA:HA	1:A:532:ARG:CZ	2.23	0.69
1:B:658:LEU:CD2	1:B:682:LEU:HD21	2.22	0.69
1:B:358:PRO:HB2	1:B:360:PHE:CE1	2.27	0.69
1:B:395:LEU:HA	1:B:398:ALA:HB3	1.74	0.69
1:B:532:ARG:O	1:B:533:LYS:HD3	1.93	0.69
1:B:661:ARG:NH1	2:E:4:DG:OP1	2.25	0.69
1:A:387:GLN:HB3	1:A:389:LEU:HD23	1.73	0.69
1:B:177:MET:HE3	1:B:182:TRP:HE3	1.57	0.69
1:B:462:VAL:HG23	1:B:463:VAL:CG2	2.23	0.69
1:B:360:PHE:H	1:B:360:PHE:HD1	1.41	0.68
1:A:119:GLU:OE1	1:A:122:ARG:NH1	2.26	0.68
1:A:284:GLU:OE2	1:A:587:ARG:NH2	2.26	0.68
1:A:365:LEU:HD13	1:A:378:LEU:HD21	1.74	0.68
1:A:387:GLN:HB3	1:A:389:LEU:HD21	1.74	0.68
1:B:476:GLY:HA2	1:B:544:LEU:CD1	2.16	0.68
1:B:192:ARG:NH2	1:B:201:THR:OG1	2.27	0.68
1:B:15:ALA:O	1:B:306:PRO:HA	1.93	0.68
1:B:347:ALA:HB1	1:B:381:LEU:HD11	1.75	0.68
1:A:267:LEU:HD12	1:A:279:LEU:HD12	1.76	0.68
1:B:349:LEU:O	1:B:408:VAL:HA	1.94	0.68
1:B:573:VAL:HG21	1:B:656:LEU:HD11	1.76	0.68
1:B:502:LEU:HD22	1:B:680:GLU:HA	1.75	0.68
1:B:662:LEU:O	1:B:666:VAL:HG23	1.94	0.68
1:A:156:TRP:HE1	1:A:164:LEU:HD12	1.58	0.68
1:A:548:ARG:HH21	3:Y:7:DA:H1'	1.58	0.67
1:B:362:ARG:CG	1:B:378:LEU:HD13	2.24	0.67
1:B:661:ARG:HH21	1:B:685:VAL:HG12	1.58	0.67
1:A:17:ARG:HB2	1:A:303:LEU:O	1.95	0.67
1:A:138:GLU:CG	1:A:141:ARG:HH21	2.07	0.67
1:A:427:ARG:HA	1:A:673:HIS:HB3	1.77	0.67
1:B:158:SER:OG	1:B:162:ALA:O	2.13	0.67
2:X:5:DG:H2'	2:X:6:DA:C8	2.30	0.67
1:A:529:ALA:HA	1:A:532:ARG:NE	2.09	0.67
1:B:384:HIS:HE1	1:B:386:SER:CB	2.08	0.67
1:A:684:PHE:C	1:A:685:VAL:HG22	2.15	0.67
1:B:349:LEU:HD13	1:B:349:LEU:C	2.15	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:362:ARG:HG2	1:B:378:LEU:HD13	1.75	0.67
1:B:684:PHE:C	1:B:685:VAL:HG22	2.15	0.67
1:A:424:LEU:HD23	1:A:427:ARG:HH11	1.60	0.67
1:B:322:MET:N	1:B:463:VAL:CG1	2.57	0.67
1:A:319:PRO:CA	1:A:637:HIS:CD2	2.78	0.67
1:B:502:LEU:HD21	1:B:680:GLU:HA	1.76	0.67
1:A:365:LEU:HB3	1:A:369:PHE:HE2	1.61	0.66
1:A:439:LEU:HD12	1:A:440:ARG:CA	2.24	0.66
1:A:658:LEU:HD11	1:A:682:LEU:HD23	1.73	0.66
1:B:545:ARG:O	1:B:573:VAL:HG22	1.96	0.66
1:B:684:PHE:O	1:B:685:VAL:HG13	1.96	0.66
1:A:349:LEU:C	1:A:349:LEU:HD23	2.15	0.66
1:A:605:THR:OG1	1:A:651:ARG:HG3	1.94	0.66
1:B:365:LEU:HD12	1:B:378:LEU:HD21	1.76	0.66
1:B:684:PHE:O	1:B:685:VAL:HG22	1.96	0.66
1:A:337:GLY:HA2	1:A:372:SER:HB2	1.78	0.66
1:A:322:MET:H	1:A:463:VAL:HG12	1.59	0.66
1:A:684:PHE:O	1:A:685:VAL:HG13	1.96	0.66
1:B:146:ARG:NH2	1:B:148:LEU:HD13	2.11	0.66
1:B:662:LEU:HD12	1:B:662:LEU:C	2.16	0.66
1:B:109:LEU:CB	1:B:157:VAL:HG21	2.26	0.66
1:B:444:ARG:CG	1:B:444:ARG:HH11	2.09	0.66
1:A:554:PHE:HB3	1:A:558:LEU:HD13	1.78	0.66
1:A:350:ARG:HG2	1:A:409:LEU:CD1	2.26	0.66
1:A:352:ASP:N	1:A:353:GLY:HA2	2.10	0.66
1:A:590:ASP:CB	3:Y:19:DG:N2	2.59	0.66
1:B:444:ARG:HG2	1:B:444:ARG:HH11	1.61	0.65
1:A:57:THR:HG22	1:A:66:SER:OG	1.97	0.65
1:B:447:TRP:CE3	1:B:448:GLU:CG	2.80	0.65
1:B:531:ARG:O	1:B:531:ARG:HG3	1.96	0.65
1:B:404:GLN:O	1:B:681:LYS:CE	2.41	0.65
1:A:322:MET:N	1:A:463:VAL:HG12	2.12	0.65
1:B:457:LYS:HE3	1:B:685:VAL:CG2	2.23	0.65
1:A:358:PRO:HB2	1:A:360:PHE:CD1	2.31	0.65
1:B:315:ARG:NH1	1:B:589:ALA:HB1	2.12	0.65
2:E:7:DT:H2'	2:E:8:DA:H5''	1.79	0.65
1:A:345:ALA:C	1:A:346:LEU:CD2	2.48	0.65
1:A:474:ALA:HB3	1:A:493:ALA:HB3	1.79	0.65
1:B:177:MET:HE3	1:B:182:TRP:HB2	1.78	0.65
1:B:365:LEU:O	1:B:369:PHE:CD2	2.47	0.65
1:B:460:LEU:HD12	1:B:460:LEU:C	2.16	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:576:SER:HB3	3:F:9:DC:OP2	1.97	0.64
1:A:43:TYR:CB	1:A:59:ARG:NH1	2.60	0.64
2:X:9:DG:H2"	2:X:10:DT:H5'	1.80	0.64
1:A:163:PHE:CE2	1:A:303:LEU:CD1	2.81	0.64
1:B:596:LEU:HD22	1:B:602:LEU:HG	1.80	0.64
1:A:357:TRP:HE1	1:A:362:ARG:HG3	1.63	0.64
1:A:655:PRO:O	1:A:659:ALA:HB2	1.97	0.64
1:B:657:HIS:HE1	2:E:4:DG:H5"	1.63	0.64
1:A:230:LYS:HG2	1:A:232:ARG:HG2	1.79	0.64
1:A:230:LYS:CE	1:A:232:ARG:HG3	2.22	0.64
1:B:514:ILE:N	1:B:553:GLU:OE2	2.29	0.64
1:B:635:ILE:HA	1:B:638:LEU:HD12	1.80	0.64
1:A:138:GLU:HG3	1:A:141:ARG:HH21	1.63	0.64
1:A:362:ARG:HD3	1:A:378:LEU:HD12	1.80	0.64
1:A:361:LEU:N	1:A:361:LEU:HD22	2.13	0.63
1:B:407:LEU:HB2	1:B:454:LEU:HD22	1.78	0.63
1:B:583:PRO:HD3	1:B:588:LEU:CD1	2.28	0.63
1:A:531:ARG:HD3	1:A:537:LEU:HD23	1.79	0.63
1:B:494:VAL:CG2	1:B:500:HIS:HB3	2.28	0.63
1:B:663:VAL:HG23	1:B:664:LYS:N	2.14	0.63
1:A:422:LYS:NZ	1:A:432:SER:HB2	2.13	0.63
1:B:460:LEU:HD11	1:B:462:VAL:HG13	1.80	0.63
1:A:345:ALA:CB	1:A:402:GLY:CA	2.77	0.63
1:A:350:ARG:HB3	1:A:409:LEU:H	1.62	0.63
1:A:350:ARG:HB2	1:A:409:LEU:O	1.98	0.63
1:A:436:ASN:ND2	2:X:1:DT:H2"	2.13	0.63
1:A:349:LEU:CG	1:A:383:ALA:HB2	2.29	0.63
1:A:668:ARG:HG2	1:A:669:LEU:HD23	1.81	0.63
1:B:447:TRP:CZ3	1:B:448:GLU:HG3	2.33	0.63
1:A:544:LEU:CD1	1:A:656:LEU:CD2	2.53	0.63
1:A:684:PHE:O	1:A:685:VAL:HG22	1.98	0.63
1:B:395:LEU:O	1:B:399:LYS:N	2.31	0.63
1:B:267:LEU:O	1:B:271:HIS:HB3	1.98	0.63
1:A:583:PRO:HD3	1:A:588:LEU:HD13	1.81	0.63
1:A:531:ARG:HG2	1:A:536:ARG:C	2.19	0.62
1:A:531:ARG:CZ	1:A:537:LEU:HD23	2.29	0.62
1:A:658:LEU:CG	1:A:682:LEU:HD21	2.28	0.62
1:B:406:VAL:O	1:B:454:LEU:CD1	2.47	0.62
1:A:230:LYS:CE	1:A:232:ARG:CG	2.58	0.62
1:B:135:TYR:CE2	1:B:172:ARG:HB2	2.34	0.62
1:B:316:LEU:HD21	1:B:632:ALA:HB1	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:679:ARG:HH11	1:B:679:ARG:CG	2.09	0.62
1:A:156:TRP:CD1	1:A:164:LEU:HB2	2.34	0.62
1:A:33:LEU:HD11	1:A:37:PRO:HD3	1.81	0.62
1:A:409:LEU:HB2	1:A:437:VAL:CG2	2.29	0.62
1:A:544:LEU:HD12	1:A:544:LEU:O	1.98	0.62
1:B:195:ASN:OD1	1:B:202:TRP:NE1	2.32	0.62
1:A:531:ARG:CG	1:A:536:ARG:O	2.47	0.62
1:A:143:PRO:HG2	1:A:144:GLY:H	1.64	0.62
1:A:163:PHE:CE2	1:A:303:LEU:HD13	2.34	0.62
1:B:352:ASP:N	1:B:353:GLY:CA	2.60	0.62
1:B:517:GLU:OE1	1:B:517:GLU:N	2.33	0.62
1:B:174:LEU:HD11	1:B:176:GLU:OE2	1.99	0.62
1:B:197:TYR:CG	1:B:232:ARG:HD2	2.35	0.62
1:A:365:LEU:HB3	1:A:376:LEU:HD21	1.79	0.61
1:A:358:PRO:CB	1:A:360:PHE:HE1	2.11	0.61
1:A:57:THR:HG22	1:A:66:SER:CB	2.30	0.61
1:B:177:MET:CE	1:B:182:TRP:HB2	2.30	0.61
1:B:359:GLU:HG2	1:B:359:GLU:O	2.00	0.61
1:A:217:LEU:HB2	1:A:221:LEU:O	2.01	0.61
1:B:357:TRP:NE1	1:B:361:LEU:HD12	2.16	0.61
1:B:631:LEU:C	1:B:635:ILE:HD12	2.21	0.61
1:A:147:VAL:CG2	1:A:172:ARG:O	2.48	0.61
1:B:365:LEU:CD1	1:B:378:LEU:HD21	2.31	0.61
1:B:398:ALA:HB1	1:B:403:VAL:HG23	1.77	0.61
1:A:573:VAL:HG21	1:A:656:LEU:HD11	1.83	0.61
1:A:573:VAL:HG12	1:A:619:LEU:HD22	1.82	0.61
1:B:436:ASN:ND2	2:E:1:DT:H2''	2.16	0.61
1:A:99:ASP:N	1:A:105:GLU:OE1	2.24	0.61
1:A:516:GLN:OE1	1:A:556:LEU:HB2	2.00	0.61
1:A:611:ARG:NH2	2:X:5:DG:H4'	2.16	0.61
1:B:358:PRO:CB	1:B:360:PHE:HE1	2.13	0.61
1:A:426:LEU:CD1	1:A:677:VAL:HG22	2.26	0.61
1:A:345:ALA:CB	1:A:402:GLY:C	2.69	0.61
1:A:350:ARG:HG2	1:A:409:LEU:HG	1.83	0.61
1:A:532:ARG:CG	1:A:532:ARG:HH21	2.14	0.61
1:A:532:ARG:HG3	1:A:532:ARG:NH2	2.15	0.61
1:B:519:VAL:HG21	1:B:553:GLU:HG2	1.82	0.61
1:B:660:ASP:O	1:B:664:LYS:HG3	2.00	0.61
1:A:242:ALA:HB2	1:A:258:THR:HG22	1.83	0.60
1:A:407:LEU:HD12	1:A:408:VAL:H	1.65	0.60
1:A:227:HIS:CE1	4:C:21:DT:HO3'	2.18	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:505:LEU:HD11	1:A:671:ILE:HD13	1.83	0.60
1:A:640:ARG:CD	1:A:649:PHE:CD2	2.84	0.60
1:B:349:LEU:CD2	1:B:383:ALA:HB3	2.31	0.60
1:B:421:LEU:O	1:B:425:LEU:HG	2.00	0.60
1:B:109:LEU:C	1:B:157:VAL:CG2	2.70	0.60
1:B:460:LEU:HD12	1:B:460:LEU:O	2.01	0.60
1:A:514:ILE:CB	1:A:553:GLU:OE2	2.47	0.60
1:B:480:GLY:HA3	1:B:663:VAL:HG21	1.82	0.60
1:B:494:VAL:HB	1:B:500:HIS:HB3	1.83	0.60
1:B:531:ARG:HA	1:B:534:ALA:HB3	1.83	0.60
2:E:8:DA:H1'	2:E:9:DG:H5'	1.84	0.60
1:B:271:HIS:HB2	1:B:276:SER:HA	1.84	0.60
1:A:358:PRO:HD2	1:A:361:LEU:CD2	2.29	0.60
1:B:358:PRO:HB2	1:B:360:PHE:HE1	1.66	0.60
1:A:271:HIS:HB2	1:A:275:GLY:O	2.01	0.60
1:B:365:LEU:HD12	1:B:378:LEU:CD2	2.31	0.60
2:X:7:DT:H2'	2:X:8:DA:H5''	1.84	0.60
1:A:600:THR:HG22	1:A:620:VAL:HG13	1.83	0.60
1:B:600:THR:HG23	1:B:620:VAL:CG2	2.17	0.60
1:A:409:LEU:HB2	1:A:437:VAL:HG23	1.84	0.59
1:B:444:ARG:HG2	1:B:444:ARG:NH1	2.15	0.59
1:A:207:LEU:CD2	1:A:240:ARG:HD2	2.30	0.59
1:A:606:VAL:HG21	1:A:649:PHE:O	2.02	0.59
1:B:611:ARG:NH2	2:E:5:DG:H4'	2.18	0.59
1:A:205:LEU:HD11	1:A:245:ALA:CB	2.32	0.59
1:A:658:LEU:CD1	1:A:682:LEU:CD2	2.63	0.59
1:B:233:LEU:HD21	1:B:260:LEU:HD21	1.80	0.59
2:E:7:DT:C2'	2:E:8:DA:H5''	2.32	0.59
1:A:476:GLY:O	1:A:490:ALA:HA	2.02	0.59
1:A:360:PHE:CE1	1:A:361:LEU:CD2	2.86	0.59
1:A:43:TYR:CB	1:A:59:ARG:HH12	2.16	0.59
1:A:548:ARG:NH2	3:Y:7:DA:H1'	2.16	0.59
1:A:109:LEU:HB2	1:A:157:VAL:HG21	1.85	0.59
1:A:395:LEU:O	1:A:399:LYS:N	2.35	0.59
1:A:433:GLN:HB2	1:A:457:LYS:HE2	1.85	0.59
1:B:271:HIS:HA	1:B:276:SER:HA	1.85	0.59
1:B:554:PHE:HB3	1:B:558:LEU:HD13	1.83	0.59
1:B:197:TYR:OH	4:D:21:DT:OP1	2.15	0.59
1:B:14:PHE:CD2	1:B:306:PRO:HB2	2.37	0.58
1:B:457:LYS:HA	1:B:681:LYS:O	2.02	0.58
1:A:20:ASN:N	1:A:23:GLU:OE2	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:440:ARG:NH1	1:A:443:GLU:HB2	2.17	0.58
1:A:54:GLY:O	1:A:73:LEU:HD22	2.03	0.58
1:B:384:HIS:CE1	1:B:386:SER:CB	2.86	0.58
1:B:422:LYS:HA	1:B:425:LEU:CD1	2.33	0.58
1:A:20:ASN:HB2	1:A:21:PRO:HD2	1.85	0.58
1:A:464:ALA:CB	1:A:499:GLY:H	2.11	0.58
1:A:636:PHE:HE1	1:A:640:ARG:HH21	1.51	0.58
1:A:636:PHE:CE1	1:A:640:ARG:NH2	2.71	0.58
1:B:286:ARG:HH12	2:E:7:DT:P	2.26	0.58
1:A:476:GLY:HA2	1:A:544:LEU:CD1	2.13	0.58
1:A:16:LEU:HD11	1:A:165:LEU:HB2	1.86	0.58
1:A:516:GLN:HG2	1:A:553:GLU:O	2.02	0.58
1:A:660:ASP:O	1:A:664:LYS:HG2	2.03	0.58
1:B:596:LEU:CD2	1:B:602:LEU:HG	2.34	0.58
1:A:509:GLN:NE2	1:A:513:ARG:O	2.37	0.58
1:B:654:ALA:O	1:B:658:LEU:HB2	2.04	0.58
1:B:345:ALA:CB	1:B:402:GLY:O	2.52	0.58
1:B:606:VAL:HG21	1:B:649:PHE:O	2.04	0.58
1:B:352:ASP:CB	1:B:353:GLY:HA2	2.32	0.58
1:B:406:VAL:O	1:B:454:LEU:CD2	2.52	0.58
1:B:573:VAL:HG12	1:B:619:LEU:HD22	1.84	0.58
1:A:439:LEU:HD12	1:A:439:LEU:C	2.16	0.58
1:A:406:VAL:O	1:A:454:LEU:HD11	2.04	0.58
1:B:230:LYS:HE3	1:B:232:ARG:CD	2.34	0.58
1:B:599:LYS:HB2	1:B:599:LYS:HZ3	1.68	0.58
1:A:223:LEU:HD23	1:A:257:LEU:HD21	1.86	0.57
1:A:334:LEU:C	1:A:334:LEU:HD12	2.23	0.57
1:A:528:TRP:CB	1:A:532:ARG:HH22	2.11	0.57
1:B:177:MET:HE3	1:B:182:TRP:CE3	2.38	0.57
2:E:5:DG:C6	2:E:6:DA:C6	2.92	0.57
1:B:20:ASN:HB2	1:B:21:PRO:HD2	1.86	0.57
1:B:652:LEU:HD13	1:B:656:LEU:HB3	1.86	0.57
1:A:335:ARG:NH1	1:A:367:ARG:HD2	2.16	0.57
1:A:522:LEU:CD2	1:B:672:ARG:NH2	2.67	0.57
1:B:360:PHE:N	1:B:360:PHE:HD1	2.03	0.57
1:A:352:ASP:HB2	1:A:353:GLY:HA2	1.85	0.57
1:A:531:ARG:HH11	1:A:537:LEU:HA	1.70	0.57
1:A:540:ARG:HG3	1:A:567:ALA:HB3	1.86	0.57
1:A:573:VAL:HG23	1:A:573:VAL:O	2.02	0.57
1:A:195:ASN:ND2	1:A:197:TYR:CZ	2.73	0.57
1:A:424:LEU:HA	1:A:427:ARG:CD	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:336:VAL:HG23	1:A:337:GLY:N	2.20	0.57
1:B:315:ARG:HH12	1:B:589:ALA:CB	2.14	0.57
1:A:409:LEU:HD13	1:A:437:VAL:HG21	1.87	0.57
1:A:345:ALA:HB3	1:A:402:GLY:CA	2.35	0.57
1:A:522:LEU:HD21	1:B:672:ARG:CZ	2.34	0.57
1:B:60:MET:HG2	1:B:60:MET:O	2.03	0.57
1:A:350:ARG:CG	1:A:350:ARG:HH21	2.14	0.57
1:A:439:LEU:CD1	1:A:440:ARG:O	2.53	0.57
1:B:195:ASN:ND2	1:B:197:TYR:CZ	2.73	0.57
1:B:360:PHE:N	1:B:360:PHE:CD1	2.73	0.57
1:B:444:ARG:HD3	1:B:448:GLU:OE2	2.04	0.57
1:A:522:LEU:CD2	1:B:672:ARG:CZ	2.82	0.57
1:A:360:PHE:CD1	1:A:361:LEU:CD2	2.86	0.56
1:A:168:ASP:CG	1:A:580:ARG:HH11	2.09	0.56
1:A:345:ALA:CB	1:A:402:GLY:N	2.68	0.56
1:A:636:PHE:HE1	1:A:640:ARG:NH2	2.02	0.56
1:A:683:PHE:CD1	1:A:684:PHE:HD1	2.23	0.56
1:B:16:LEU:HB2	1:B:163:PHE:O	2.04	0.56
1:B:406:VAL:HG12	1:B:407:LEU:N	2.20	0.56
1:B:574:ARG:NH1	3:F:8:DC:OP1	2.38	0.56
1:B:480:GLY:HA3	1:B:663:VAL:CG2	2.35	0.56
3:Y:17:DT:C2	3:Y:18:DC:C5	2.94	0.56
1:A:531:ARG:CZ	1:A:537:LEU:CD2	2.83	0.56
1:B:23:GLU:HB3	1:B:67:TRP:CZ2	2.41	0.56
1:A:369:PHE:CE1	1:A:376:LEU:HD13	2.40	0.56
1:B:194:ARG:NH1	1:B:198:ASP:O	2.38	0.56
1:A:658:LEU:O	1:A:684:PHE:CE2	2.59	0.56
1:A:435:LEU:N	1:A:435:LEU:HD12	2.02	0.56
1:B:550:PRO:HD2	1:B:553:GLU:OE1	2.05	0.56
1:B:544:LEU:HD13	1:B:656:LEU:CG	2.36	0.56
1:A:233:LEU:HD12	1:A:233:LEU:O	2.06	0.56
1:A:544:LEU:HD12	1:A:544:LEU:C	2.26	0.56
1:B:256:HIS:CD2	1:B:261:LEU:HD21	2.41	0.56
1:B:345:ALA:HB1	1:B:402:GLY:CA	2.27	0.56
1:B:531:ARG:HH21	1:B:537:LEU:HA	1.69	0.56
1:A:369:PHE:CG	1:A:376:LEU:HB2	2.41	0.56
1:A:684:PHE:N	1:A:684:PHE:CD1	2.73	0.56
1:A:267:LEU:O	1:A:271:HIS:HB3	2.06	0.56
1:A:464:ALA:HB1	1:A:499:GLY:N	2.13	0.56
1:A:532:ARG:HH21	1:A:532:ARG:HG3	1.71	0.56
1:A:654:ALA:O	1:A:658:LEU:HB2	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:583:PRO:HD3	1:B:588:LEU:HD13	1.88	0.56
1:B:661:ARG:NH2	1:B:685:VAL:HG12	2.19	0.56
1:A:67:TRP:CE2	1:A:112:LEU:HD23	2.41	0.56
1:A:362:ARG:NE	1:A:378:LEU:HD12	2.21	0.56
1:B:318:ILE:CD1	1:B:318:ILE:H	2.11	0.56
1:B:405:ALA:HB2	1:B:457:LYS:O	2.06	0.56
1:A:573:VAL:HG12	1:A:619:LEU:CD2	2.35	0.55
1:B:286:ARG:NH1	2:E:7:DT:OP1	2.39	0.55
3:F:17:DT:C2	3:F:18:DC:C5	2.94	0.55
1:B:514:ILE:HG13	1:B:553:GLU:OE2	2.06	0.55
1:A:464:ALA:HB1	1:A:498:GLY:HA2	1.89	0.55
1:B:344:THR:CG2	1:B:404:GLN:OE1	2.53	0.55
1:B:444:ARG:CD	1:B:448:GLU:CD	2.69	0.55
1:B:357:TRP:CZ2	1:B:378:LEU:HD22	2.42	0.55
1:A:168:ASP:CG	1:A:580:ARG:NH1	2.60	0.55
1:A:321:LEU:CB	1:A:463:VAL:HG11	2.37	0.55
1:A:433:GLN:NE2	1:A:685:VAL:OXT	2.37	0.55
1:A:633:HIS:HD2	1:A:633:HIS:O	1.90	0.55
1:B:19:LEU:HD13	1:B:161:GLY:O	2.07	0.55
2:E:14:DT:H2"	2:E:15:DT:C6	2.42	0.55
1:A:198:ASP:OD1	1:A:200:ARG:N	2.33	0.55
1:B:501:LEU:HD12	1:B:643:PRO:HD3	1.89	0.55
1:B:529:ALA:CA	1:B:532:ARG:CZ	2.85	0.55
1:A:231:GLY:CA	1:A:234:GLN:HE22	2.07	0.55
1:B:369:PHE:HD2	1:B:376:LEU:CD1	2.13	0.55
1:B:651:ARG:HB2	2:E:5:DG:H5"	1.89	0.55
1:A:349:LEU:O	1:A:349:LEU:HD23	2.05	0.55
1:A:529:ALA:CA	1:A:532:ARG:CZ	2.85	0.55
1:B:109:LEU:C	1:B:157:VAL:HG21	2.27	0.55
1:B:433:GLN:HG2	1:B:450:ALA:O	2.07	0.55
1:B:545:ARG:NH1	1:B:546:ASN:O	2.40	0.55
1:B:631:LEU:O	1:B:635:ILE:HD12	2.07	0.55
1:B:147:VAL:HG22	1:B:173:ILE:HA	1.88	0.54
1:B:494:VAL:HB	1:B:500:HIS:CB	2.37	0.54
1:B:529:ALA:HA	1:B:532:ARG:HG3	1.89	0.54
1:B:544:LEU:C	1:B:544:LEU:HD12	2.27	0.54
1:A:358:PRO:CB	1:A:360:PHE:CE1	2.86	0.54
1:B:146:ARG:HH22	1:B:148:LEU:HD13	1.71	0.54
1:B:599:LYS:HG3	1:B:599:LYS:O	2.07	0.54
1:A:360:PHE:CE1	1:A:361:LEU:HD22	2.41	0.54
1:A:424:LEU:HA	1:A:427:ARG:HD2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:544:LEU:CD1	1:B:656:LEU:CD2	2.80	0.54
1:A:193:VAL:HG22	1:A:261:LEU:HB3	1.89	0.54
1:B:384:HIS:HE1	1:B:386:SER:HB3	1.70	0.54
1:B:469:TYR:OH	1:B:637:HIS:ND1	2.38	0.54
2:X:3:DA:H61	3:Y:16:DC:H42	1.53	0.54
1:A:358:PRO:CD	1:A:361:LEU:HD21	2.35	0.54
1:A:407:LEU:HD12	1:A:408:VAL:N	2.23	0.54
1:A:444:ARG:HG3	1:A:445:HIS:N	2.21	0.54
1:A:517:GLU:H	1:A:517:GLU:CD	1.97	0.54
1:A:26:PRO:C	1:A:95:ARG:HB3	2.28	0.54
1:B:271:HIS:HB2	1:B:276:SER:CA	2.37	0.54
1:B:592:LEU:O	1:B:603:LEU:HD12	2.08	0.54
1:A:435:LEU:H	1:A:435:LEU:CD1	2.05	0.54
1:B:319:PRO:HA	1:B:637:HIS:CE1	2.42	0.54
1:B:37:PRO:HG2	1:B:42:VAL:HG23	1.89	0.54
1:B:473:LEU:HD12	1:B:493:ALA:O	2.06	0.54
1:A:205:LEU:CD1	1:A:245:ALA:HB2	2.38	0.54
1:B:110:SER:N	1:B:157:VAL:CG2	2.70	0.54
1:B:455:LEU:CD2	1:B:460:LEU:CD2	2.11	0.54
1:B:457:LYS:HE2	1:B:683:PHE:O	2.08	0.54
1:A:345:ALA:HB2	1:A:402:GLY:N	2.23	0.54
1:B:357:TRP:HB3	1:B:362:ARG:NH2	2.23	0.54
1:B:33:LEU:HD13	1:B:37:PRO:HD3	1.90	0.54
1:A:230:LYS:CG	1:A:232:ARG:HG2	2.37	0.54
1:A:516:GLN:NE2	1:A:552:ASP:O	2.41	0.54
1:B:177:MET:CE	1:B:182:TRP:HE3	2.19	0.54
1:A:215:LEU:HD22	1:A:223:LEU:HD13	1.90	0.54
1:A:439:LEU:HA	1:A:446:ARG:NH2	2.23	0.54
1:A:658:LEU:O	1:A:684:PHE:HE2	1.91	0.54
1:B:606:VAL:HG13	3:F:19:DG:O6	2.08	0.54
1:A:205:LEU:HD11	1:A:245:ALA:HB2	1.90	0.53
1:A:545:ARG:NH1	1:A:546:ASN:O	2.40	0.53
1:B:168:ASP:CG	1:B:580:ARG:HH11	1.94	0.53
1:A:465:LEU:HG	1:A:641:LEU:HD11	1.91	0.53
1:B:634:GLN:HG2	1:B:638:LEU:HD11	1.90	0.53
1:B:230:LYS:HZ2	1:B:232:ARG:NH1	2.06	0.53
1:B:128:TRP:CZ3	1:B:172:ARG:HG2	2.43	0.53
1:A:23:GLU:HB3	1:A:67:TRP:CZ2	2.44	0.53
1:B:343:GLU:C	1:B:344:THR:HG23	2.28	0.53
1:A:218:PRO:HD2	4:C:21:DT:C4	2.44	0.53
1:A:440:ARG:HD2	1:A:442:GLU:HB3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:544:LEU:HD12	1:B:544:LEU:O	2.08	0.53
1:A:10:PHE:CZ	1:A:291:ARG:NH2	2.76	0.53
1:A:573:VAL:HA	1:A:619:LEU:CD2	2.38	0.53
1:B:462:VAL:HG23	1:B:463:VAL:N	2.23	0.53
1:B:144:GLY:HA3	1:B:177:MET:HE1	1.89	0.53
1:B:347:ALA:CB	1:B:381:LEU:HD11	2.37	0.53
1:B:509:GLN:NE2	1:B:511:GLY:O	2.31	0.53
1:A:543:LEU:HB3	1:A:570:LEU:HD12	1.91	0.52
1:B:395:LEU:O	1:B:399:LYS:CB	2.55	0.52
1:B:684:PHE:CD1	1:B:684:PHE:N	2.75	0.52
1:A:456:ALA:CB	1:A:643:PRO:HG2	2.40	0.52
1:B:313:ALA:HB2	1:B:594:VAL:HG22	1.90	0.52
2:X:7:DT:C2'	2:X:8:DA:H5''	2.40	0.52
1:A:485:PHE:HB2	1:A:509:GLN:O	2.09	0.52
1:B:233:LEU:HD23	1:B:260:LEU:CD2	2.30	0.52
1:B:601:PHE:N	1:B:619:LEU:O	2.36	0.52
1:A:230:LYS:CG	1:A:232:ARG:HE	2.14	0.52
1:A:592:LEU:O	1:A:603:LEU:HD12	2.09	0.52
1:B:109:LEU:HB2	1:B:157:VAL:HG21	1.90	0.52
1:B:169:PRO:O	1:B:286:ARG:NH2	2.36	0.52
1:B:599:LYS:NZ	1:B:599:LYS:CB	2.73	0.52
1:A:440:ARG:NH1	1:A:443:GLU:CB	2.73	0.52
1:B:212:PRO:HB3	1:B:257:LEU:HD21	1.92	0.52
1:B:342:GLN:C	1:B:344:THR:HG23	2.29	0.52
1:A:352:ASP:N	1:A:353:GLY:CA	2.73	0.52
1:A:418:ARG:NH1	1:A:419:ASN:OD1	2.42	0.52
1:A:426:LEU:CD1	1:A:677:VAL:HG23	2.36	0.52
1:A:514:ILE:O	1:A:553:GLU:HG3	2.09	0.52
1:B:509:GLN:NE2	1:B:513:ARG:O	2.43	0.52
1:A:360:PHE:CE1	1:A:361:LEU:HD21	2.45	0.52
1:B:352:ASP:H	1:B:353:GLY:HA2	1.70	0.52
1:B:365:LEU:CD1	1:B:378:LEU:CD2	2.87	0.52
1:B:648:ALA:CB	2:E:4:DG:H1'	2.40	0.52
1:A:15:ALA:O	1:A:306:PRO:HA	2.09	0.52
1:A:223:LEU:HD23	1:A:257:LEU:HD23	1.92	0.52
1:A:316:LEU:HD12	1:A:636:PHE:HB2	1.92	0.52
1:A:645:SER:OG	1:A:648:ALA:O	2.15	0.52
1:B:476:GLY:O	1:B:490:ALA:HA	2.09	0.52
1:B:657:HIS:HE1	2:E:4:DG:C5'	2.22	0.52
1:A:360:PHE:HD1	1:A:360:PHE:H	1.57	0.51
1:A:666:VAL:HG13	1:A:671:ILE:HG22	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:455:LEU:CG	1:B:460:LEU:CD2	2.84	0.51
1:B:415:TRP:CH2	3:F:12:DC:H5'	2.45	0.51
1:B:236:ARG:HD2	1:B:260:LEU:CD2	2.20	0.51
1:B:600:THR:HG23	1:B:620:VAL:HG22	1.68	0.51
1:B:642:TYR:OH	1:B:661:ARG:NH2	2.43	0.51
2:X:16:DG:N2	3:Y:5:DC:O2	2.30	0.51
1:A:227:HIS:NE2	4:C:21:DT:O3'	2.32	0.51
1:A:655:PRO:O	1:A:659:ALA:CB	2.58	0.51
1:B:540:ARG:HG3	1:B:567:ALA:HB3	1.93	0.51
1:B:357:TRP:CG	1:B:362:ARG:NH2	2.79	0.51
1:B:478:ASP:OD2	1:B:546:ASN:ND2	2.42	0.51
1:B:348:LEU:HD23	1:B:357:TRP:HE3	1.70	0.51
1:B:530:PHE:O	1:B:534:ALA:HB2	2.10	0.51
1:B:531:ARG:NH2	1:B:537:LEU:HD23	2.26	0.51
3:F:16:DC:H2'	3:F:17:DT:C6	2.46	0.51
1:A:140:ALA:C	1:A:141:ARG:HD3	2.31	0.51
1:B:514:ILE:CB	1:B:553:GLU:OE2	2.59	0.51
1:A:548:ARG:NH2	3:Y:7:DA:N3	2.57	0.51
1:A:4:LEU:CD1	1:A:5:GLY:H	2.24	0.51
1:A:532:ARG:CG	1:A:532:ARG:NH2	2.73	0.51
1:A:618:LYS:O	1:A:619:LEU:HD23	2.10	0.51
1:A:600:THR:HA	1:A:620:VAL:HA	1.91	0.51
1:B:357:TRP:NE1	1:B:361:LEU:CD1	2.73	0.51
1:B:599:LYS:CB	1:B:599:LYS:HZ3	2.24	0.51
1:B:648:ALA:HB3	2:E:4:DG:H1'	1.93	0.51
1:A:451:LEU:O	1:A:454:LEU:N	2.43	0.51
1:B:531:ARG:HH21	1:B:537:LEU:HD23	1.75	0.51
1:A:657:HIS:CE1	2:X:4:DG:H5''	2.43	0.51
1:B:187:HIS:NE2	1:B:273:GLU:OE2	2.37	0.50
1:B:362:ARG:HG3	1:B:378:LEU:HD13	1.93	0.50
1:B:403:VAL:O	1:B:403:VAL:HG12	2.12	0.50
1:B:406:VAL:O	1:B:454:LEU:HD11	2.11	0.50
1:A:350:ARG:C	1:A:350:ARG:HD2	2.30	0.50
1:B:283:TRP:HZ3	1:B:287:ARG:NH2	2.09	0.50
1:B:529:ALA:CA	1:B:532:ARG:NH2	2.73	0.50
1:A:54:GLY:O	1:A:73:LEU:HD21	2.09	0.50
1:A:573:VAL:HA	1:A:619:LEU:HD23	1.93	0.50
1:B:581:VAL:O	1:B:581:VAL:HG23	2.11	0.50
1:B:633:HIS:HD2	1:B:633:HIS:O	1.94	0.50
1:A:218:PRO:HD2	4:C:21:DT:O4	2.11	0.50
1:A:338:PHE:HD2	1:A:341:ALA:HB2	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:554:PHE:O	1:A:557:ALA:N	2.45	0.50
1:A:256:HIS:CD2	1:A:261:LEU:HD21	2.47	0.50
1:A:426:LEU:HD12	1:A:426:LEU:O	2.11	0.50
1:A:478:ASP:CG	1:A:479:ALA:H	2.15	0.50
1:A:531:ARG:HD3	1:A:537:LEU:N	2.26	0.50
1:B:146:ARG:HH21	1:B:148:LEU:HB2	1.77	0.50
1:B:424:LEU:N	1:B:424:LEU:CD2	2.73	0.50
1:B:494:VAL:CB	1:B:500:HIS:HB3	2.41	0.50
1:A:606:VAL:HG13	3:Y:19:DG:O6	2.11	0.50
1:A:217:LEU:HD21	4:C:21:DT:H72	1.93	0.50
1:A:350:ARG:HG2	1:A:409:LEU:CG	2.41	0.50
1:B:99:ASP:N	1:B:105:GLU:OE1	2.27	0.50
1:B:342:GLN:O	1:B:344:THR:CG2	2.45	0.50
1:B:572:SER:O	1:B:619:LEU:HA	2.12	0.50
2:X:8:DA:H1'	2:X:9:DG:H5'	1.94	0.50
1:A:329:LYS:HG2	1:A:332:ASP:HB2	1.93	0.50
1:B:559:GLU:O	1:B:563:ARG:HG3	2.12	0.50
1:B:427:ARG:HG2	1:B:673:HIS:CD2	2.46	0.50
1:A:226:TYR:CE2	4:C:21:DT:C7	2.93	0.50
1:A:349:LEU:HG	1:A:383:ALA:HB2	1.93	0.50
1:A:422:LYS:HZ3	1:A:432:SER:HB2	1.76	0.50
1:A:460:LEU:CB	1:A:462:VAL:CG2	2.86	0.50
1:A:674:LEU:HD23	1:A:677:VAL:HB	1.93	0.50
1:A:296:TRP:NE1	1:A:300:ARG:NH2	2.54	0.49
1:A:321:LEU:CB	1:A:463:VAL:HB	2.42	0.49
1:A:387:GLN:CB	1:A:389:LEU:HD21	2.41	0.49
3:F:14:DA:OP2	3:F:14:DA:H2'	2.12	0.49
1:A:226:TYR:C	1:A:226:TYR:CD1	2.85	0.49
1:A:296:TRP:HE1	1:A:300:ARG:HH22	1.59	0.49
1:A:335:ARG:CG	1:A:335:ARG:NH1	2.73	0.49
1:B:380:THR:HG22	1:B:381:LEU:N	2.27	0.49
3:F:4:DA:HO5'	3:F:4:DA:H8	1.59	0.49
1:A:545:ARG:O	1:A:573:VAL:CG2	2.58	0.49
1:B:389:LEU:H	1:B:389:LEU:CD1	1.97	0.49
1:B:583:PRO:CG	1:B:588:LEU:CD1	2.88	0.49
1:A:11:LEU:HB2	1:A:309:VAL:HG13	1.95	0.49
1:A:357:TRP:NE1	1:A:362:ARG:HG3	2.26	0.49
1:A:605:THR:CG2	1:A:639:THR:HG21	2.42	0.49
1:B:197:TYR:CD2	1:B:232:ARG:HD2	2.48	0.49
1:B:212:PRO:HG3	1:B:241:VAL:CG2	2.39	0.49
2:X:14:DT:H2''	2:X:15:DT:C6	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:465:LEU:O	1:B:497:ASP:O	2.31	0.49
1:A:10:PHE:N	1:A:582:TYR:O	2.39	0.49
1:A:494:VAL:HB	1:A:500:HIS:HB3	1.95	0.49
1:B:573:VAL:HA	1:B:619:LEU:HD23	1.95	0.49
1:B:548:ARG:NH2	3:F:7:DA:H1'	2.27	0.49
1:A:286:ARG:HH12	2:X:7:DT:P	2.34	0.49
1:A:384:HIS:C	1:A:384:HIS:CD2	2.85	0.49
1:A:395:LEU:HA	1:A:398:ALA:HB3	1.95	0.49
1:B:345:ALA:CB	1:B:402:GLY:CA	2.83	0.49
1:B:418:ARG:O	1:B:418:ARG:HD2	2.13	0.49
1:B:10:PHE:N	1:B:582:TYR:O	2.40	0.49
1:B:658:LEU:O	1:B:684:PHE:CE2	2.66	0.49
1:A:110:SER:HB3	1:A:114:ARG:NH1	2.19	0.49
1:A:633:HIS:CD2	1:A:633:HIS:C	2.85	0.49
1:B:600:THR:CG2	1:B:619:LEU:O	2.53	0.49
1:A:528:TRP:O	1:A:532:ARG:HG3	2.12	0.49
1:A:529:ALA:N	1:A:532:ARG:NH1	2.60	0.49
1:B:169:PRO:HD2	1:B:286:ARG:HE	1.78	0.49
1:B:39:ARG:O	1:B:39:ARG:HG2	2.13	0.49
1:B:469:TYR:HH	1:B:637:HIS:HD1	1.53	0.49
1:A:14:PHE:HD2	1:A:306:PRO:HB2	1.78	0.48
1:A:334:LEU:O	1:A:368:ALA:CB	2.59	0.48
1:B:384:HIS:CE1	1:B:387:GLN:N	2.76	0.48
1:B:50:ALA:HA	1:B:64:LEU:HD22	1.93	0.48
1:A:169:PRO:HD2	1:A:286:ARG:HE	1.78	0.48
1:B:327:VAL:HG13	1:B:332:ASP:HB2	1.94	0.48
1:B:42:VAL:O	1:B:46:LEU:HD12	2.14	0.48
1:A:195:ASN:OD1	1:A:202:TRP:NE1	2.46	0.48
1:A:24:LEU:O	1:A:26:PRO:HD3	2.13	0.48
1:A:335:ARG:O	1:A:368:ALA:N	2.44	0.48
1:A:606:VAL:HG12	1:A:611:ARG:HH22	1.77	0.48
1:A:685:VAL:OXT	2:X:1:DT:P	2.72	0.48
1:B:322:MET:HG2	1:B:323:GLY:CA	2.40	0.48
1:B:347:ALA:HB1	1:B:381:LEU:HD12	1.94	0.48
1:B:599:LYS:NZ	1:B:599:LYS:CA	2.73	0.48
1:A:135:TYR:CE1	1:A:172:ARG:HB2	2.48	0.48
1:B:366:LEU:HA	1:B:376:LEU:HD11	1.95	0.48
1:B:345:ALA:HB1	1:B:402:GLY:O	2.13	0.48
2:E:2:DG:H2''	2:E:3:DA:C8	2.48	0.48
1:A:505:LEU:HD23	1:B:672:ARG:HA	1.94	0.48
1:B:179:LEU:O	1:B:179:LEU:HD12	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:426:LEU:O	1:B:429:GLY:N	2.39	0.48
1:A:514:ILE:N	1:A:553:GLU:OE2	2.45	0.48
1:A:668:ARG:NH2	3:Y:12:DC:OP2	2.45	0.48
1:A:672:ARG:NH2	1:B:525:GLU:HG2	2.28	0.48
1:B:514:ILE:CG1	1:B:553:GLU:OE2	2.61	0.48
1:A:666:VAL:HG13	1:A:671:ILE:CG2	2.44	0.48
1:B:460:LEU:CD1	1:B:462:VAL:CG1	2.85	0.48
1:B:516:GLN:HG2	1:B:553:GLU:O	2.14	0.48
1:B:618:LYS:O	1:B:619:LEU:HD23	2.14	0.48
1:A:576:SER:CB	3:Y:9:DC:OP2	2.61	0.48
1:B:465:LEU:HD22	1:B:637:HIS:HB3	1.95	0.48
1:A:56:VAL:O	1:A:56:VAL:HG12	2.14	0.48
1:A:606:VAL:CG1	1:A:611:ARG:HH22	2.27	0.48
1:A:647:PHE:CD1	1:A:647:PHE:N	2.82	0.48
1:A:403:VAL:HG13	1:A:403:VAL:O	2.13	0.47
1:A:322:MET:O	1:A:463:VAL:HG12	2.13	0.47
1:B:663:VAL:CG2	1:B:664:LYS:N	2.77	0.47
1:B:679:ARG:CG	1:B:679:ARG:NH1	2.73	0.47
1:A:268:GLU:HB2	3:Y:14:DA:O3'	2.14	0.47
1:B:322:MET:CB	1:B:323:GLY:HA3	2.38	0.47
1:B:485:PHE:CD1	1:B:485:PHE:C	2.88	0.47
1:B:633:HIS:CD2	1:B:633:HIS:C	2.86	0.47
1:B:449:ASN:HD21	1:B:646:GLY:H	1.60	0.47
1:A:440:ARG:HB2	1:A:442:GLU:H	1.80	0.47
1:A:231:GLY:CA	1:A:234:GLN:NE2	2.71	0.47
1:A:455:LEU:HD13	1:A:461:GLN:CB	2.44	0.47
1:A:631:LEU:O	1:A:635:ILE:HG13	2.15	0.47
1:B:571:VAL:HG11	1:B:631:LEU:HD22	1.96	0.47
1:B:84:GLN:O	1:B:86:TYR:CE1	2.67	0.47
1:A:321:LEU:CB	1:A:463:VAL:CB	2.93	0.47
1:A:529:ALA:N	1:A:532:ARG:CZ	2.78	0.47
1:B:242:ALA:HB2	1:B:258:THR:HG22	1.95	0.47
1:B:548:ARG:HH21	3:F:7:DA:H1'	1.78	0.47
2:X:11:DA:H2''	2:X:12:DG:O5'	2.15	0.47
1:A:649:PHE:HB2	3:Y:19:DG:O6	2.15	0.47
1:A:179:LEU:HD23	1:A:258:THR:HG22	1.96	0.47
1:A:281:LEU:HA	1:A:281:LEU:HD12	1.61	0.47
1:A:640:ARG:HA	1:A:640:ARG:HD3	1.73	0.47
1:A:658:LEU:HD11	1:A:682:LEU:HD22	1.83	0.47
1:A:522:LEU:HD21	1:B:672:ARG:NE	2.29	0.47
1:A:417:ASP:OD1	1:A:420:ARG:NH1	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:506:PRO:HG2	1:B:666:VAL:HG21	1.97	0.47
1:B:509:GLN:OE1	1:B:514:ILE:HG23	2.14	0.47
1:B:257:LEU:HB2	1:B:260:LEU:HD12	1.96	0.47
1:A:522:LEU:HD23	1:B:672:ARG:NH2	2.28	0.47
1:A:181:ALA:O	1:A:184:ALA:HB3	2.14	0.47
1:A:350:ARG:O	1:A:350:ARG:HD2	2.15	0.47
1:A:472:GLU:OE1	1:A:530:PHE:HZ	1.98	0.47
1:A:481:GLY:HA2	1:A:667:GLY:HA3	1.97	0.47
1:B:531:ARG:HH21	1:B:537:LEU:CD2	2.28	0.47
2:X:2:DG:C2	2:X:3:DA:N3	2.83	0.47
1:A:360:PHE:HD1	1:A:360:PHE:N	2.13	0.47
1:A:378:LEU:O	1:A:379:HIS:CG	2.67	0.47
1:B:189:LEU:HG	1:B:189:LEU:H	1.53	0.47
1:B:338:PHE:HD1	1:B:341:ALA:HB2	1.79	0.47
1:A:522:LEU:HD23	1:B:672:ARG:CZ	2.45	0.47
1:B:89:ARG:HD3	1:B:91:TYR:CZ	2.50	0.47
1:A:267:LEU:HD12	1:A:279:LEU:CD1	2.44	0.46
1:A:163:PHE:CE2	1:A:303:LEU:HD11	2.50	0.46
1:A:595:PRO:O	1:A:596:LEU:HB2	2.15	0.46
1:B:193:VAL:HG22	1:B:261:LEU:HB3	1.97	0.46
1:B:424:LEU:H	1:B:424:LEU:HD23	1.78	0.46
3:Y:4:DA:HO5'	3:Y:4:DA:H8	1.60	0.46
1:A:400:GLU:HA	1:A:401:GLU:HA	1.70	0.46
1:A:439:LEU:HA	1:A:446:ARG:HH21	1.78	0.46
1:A:668:ARG:HG2	1:A:669:LEU:N	2.29	0.46
1:B:446:ARG:O	1:B:450:ALA:HB2	2.14	0.46
1:B:531:ARG:NH2	1:B:537:LEU:CD2	2.79	0.46
1:A:193:VAL:CG2	1:A:261:LEU:HB3	2.45	0.46
1:B:142:GLY:HA3	1:B:145:TRP:CE2	2.49	0.46
1:B:155:LEU:HD11	1:B:163:PHE:HB3	1.98	0.46
1:B:286:ARG:NH1	2:E:7:DT:P	2.88	0.46
1:A:165:LEU:HD12	1:A:166:GLU:N	2.30	0.46
1:A:223:LEU:CD1	1:A:255:PRO:HB2	2.43	0.46
1:A:316:LEU:HD23	1:A:316:LEU:N	2.30	0.46
1:A:531:ARG:CD	1:A:537:LEU:HD23	2.45	0.46
1:A:449:ASN:OD1	1:A:646:GLY:N	2.48	0.46
1:B:246:ASP:OD1	1:B:247:PRO:HD2	2.15	0.46
1:A:257:LEU:HB2	1:A:260:LEU:HD12	1.96	0.46
1:A:449:ASN:ND2	1:A:646:GLY:H	2.12	0.46
1:B:573:VAL:HG21	1:B:656:LEU:HD13	1.96	0.46
1:B:502:LEU:CD2	1:B:679:ARG:O	2.62	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:283:TRP:CE2	1:B:284:GLU:HG3	2.50	0.46
1:A:423:ALA:O	1:A:427:ARG:HG3	2.16	0.46
1:A:639:THR:HA	1:A:653:PRO:HA	1.98	0.46
1:B:349:LEU:HD13	1:B:350:ARG:N	2.31	0.46
3:F:4:DA:O5'	3:F:4:DA:H8	1.98	0.46
1:B:408:VAL:HG22	1:B:409:LEU:N	2.30	0.46
1:B:605:THR:HB	1:B:639:THR:HG21	1.98	0.46
1:B:658:LEU:O	1:B:684:PHE:HE2	1.99	0.46
1:A:163:PHE:CG	1:A:303:LEU:CD1	2.95	0.46
1:A:457:LYS:HA	1:A:681:LYS:O	2.16	0.46
1:A:521:ASP:CG	1:B:673:HIS:NE2	2.60	0.46
1:A:545:ARG:CB	1:A:549:VAL:HG22	2.46	0.46
1:B:642:TYR:OH	1:B:685:VAL:HG12	2.16	0.46
1:A:143:PRO:HG2	1:A:144:GLY:N	2.29	0.45
1:B:67:TRP:CG	1:B:112:LEU:HD13	2.51	0.45
1:B:376:LEU:HD23	1:B:376:LEU:N	2.31	0.45
1:B:529:ALA:HA	1:B:532:ARG:CG	2.45	0.45
1:B:89:ARG:O	1:B:90:LEU:HD23	2.16	0.45
1:A:217:LEU:CD2	4:C:21:DT:H72	2.46	0.45
1:A:365:LEU:HB3	1:A:369:PHE:CE2	2.45	0.45
1:A:520:TRP:HB2	1:A:557:ALA:HA	1.99	0.45
1:B:230:LYS:CE	1:B:232:ARG:HG3	2.21	0.45
1:A:165:LEU:HD12	1:A:166:GLU:H	1.81	0.45
1:A:204:LEU:HD12	1:A:205:LEU:N	2.31	0.45
1:B:312:GLN:O	1:B:594:VAL:HG13	2.17	0.45
1:B:422:LYS:CG	1:B:425:LEU:HD12	2.26	0.45
1:B:50:ALA:HB2	1:B:64:LEU:HD23	1.97	0.45
2:E:11:DA:H2''	2:E:12:DG:O5'	2.15	0.45
1:A:155:LEU:HD12	1:A:164:LEU:O	2.17	0.45
1:A:283:TRP:CZ3	1:A:287:ARG:HD2	2.51	0.45
1:A:376:LEU:HD12	1:A:377:ARG:N	2.31	0.45
1:A:409:LEU:HB2	1:A:437:VAL:HG21	1.98	0.45
1:A:569:ASP:HA	1:A:624:GLY:HA3	1.98	0.45
1:B:352:ASP:CB	1:B:353:GLY:CA	2.94	0.45
1:B:531:ARG:HH11	1:B:531:ARG:HG2	1.81	0.45
1:B:638:LEU:HB2	1:B:653:PRO:HB3	1.99	0.45
1:A:422:LYS:HZ1	1:A:432:SER:HB2	1.79	0.45
1:B:103:PRO:HA	1:B:106:ARG:HG2	1.99	0.45
1:B:197:TYR:HB3	1:B:232:ARG:HD3	1.98	0.45
1:B:566:ILE:HG22	1:B:567:ALA:O	2.17	0.45
1:A:360:PHE:CD1	1:A:360:PHE:N	2.83	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:401:GLU:HA	1:A:402:GLY:HA2	1.65	0.45
1:B:12:ASN:O	1:B:14:PHE:CE1	2.70	0.45
1:B:485:PHE:HE1	1:B:487:PHE:CE1	2.34	0.45
1:B:636:PHE:O	1:B:639:THR:OG1	2.26	0.45
1:B:436:ASN:CG	2:E:1:DT:H2"	2.37	0.45
2:X:2:DG:H2"	2:X:3:DA:C8	2.52	0.45
1:A:12:ASN:O	1:A:14:PHE:CE1	2.70	0.45
1:A:659:ALA:O	1:A:663:VAL:HG22	2.17	0.45
1:B:50:ALA:HA	1:B:64:LEU:CD2	2.47	0.45
1:A:147:VAL:HG23	1:A:173:ILE:HG23	1.99	0.45
1:A:459:GLY:HA2	1:A:460:LEU:HA	1.71	0.45
1:A:661:ARG:HB2	1:A:684:PHE:HD2	1.81	0.45
1:B:14:PHE:HB3	1:B:306:PRO:HB2	1.99	0.45
1:B:441:GLU:O	1:B:442:GLU:C	2.52	0.45
1:B:660:ASP:O	1:B:663:VAL:HG22	2.17	0.45
2:E:5:DG:H2'	2:E:6:DA:C8	2.51	0.45
1:A:197:TYR:CB	1:A:232:ARG:HD2	2.46	0.45
1:A:598:ASP:HB3	1:A:599:LYS:H	1.54	0.45
1:B:238:GLY:O	1:B:259:GLY:N	2.45	0.45
1:B:20:ASN:N	1:B:23:GLU:OE2	2.50	0.45
1:B:39:ARG:HH11	1:B:39:ARG:HG3	1.82	0.45
1:B:501:LEU:CD1	1:B:643:PRO:CD	2.91	0.45
2:E:8:DA:H2"	2:E:9:DG:O5'	2.16	0.45
1:A:171:TYR:HD2	1:A:279:LEU:HD23	1.82	0.45
1:B:406:VAL:O	1:B:454:LEU:HD22	2.17	0.45
1:B:440:ARG:HB3	1:B:440:ARG:CZ	2.47	0.45
1:B:602:LEU:HA	1:B:617:LEU:O	2.17	0.45
3:Y:11:DA:H2"	3:Y:12:DC:O5'	2.16	0.45
1:A:283:TRP:HZ3	1:A:287:ARG:HD2	1.82	0.44
1:B:141:ARG:HH11	1:B:146:ARG:HG2	1.81	0.44
1:B:658:LEU:CG	1:B:682:LEU:HD21	2.47	0.44
1:B:684:PHE:C	1:B:685:VAL:CG2	2.85	0.44
1:A:57:THR:HG22	1:A:66:SER:HB2	1.99	0.44
1:B:315:ARG:NH1	1:B:589:ALA:HB2	2.27	0.44
1:A:338:PHE:HB2	1:A:340:ARG:O	2.17	0.44
1:A:478:ASP:CG	1:A:479:ALA:N	2.71	0.44
1:A:627:PRO:O	1:A:631:LEU:HD12	2.18	0.44
1:A:648:ALA:CB	2:X:4:DG:H1'	2.46	0.44
1:B:57:THR:HG22	1:B:66:SER:OG	2.17	0.44
1:B:601:PHE:CE2	1:B:619:LEU:HD12	2.52	0.44
1:A:217:LEU:HD21	4:C:21:DT:C5	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:316:LEU:HD21	1:A:593:TYR:HB3	2.00	0.44
1:A:595:PRO:O	1:A:600:THR:O	2.36	0.44
1:A:663:VAL:HG23	1:A:664:LYS:N	2.32	0.44
1:B:410:THR:HG23	1:B:411:PRO:HD2	2.00	0.44
1:B:554:PHE:O	1:B:557:ALA:N	2.50	0.44
1:A:503:TRP:CE2	1:A:679:ARG:HA	2.53	0.44
1:B:397:LYS:O	1:B:400:GLU:O	2.35	0.44
1:B:505:LEU:HD12	1:B:506:PRO:HD2	1.99	0.44
1:B:573:VAL:HG12	1:B:619:LEU:CD2	2.46	0.44
3:Y:16:DC:H2'	3:Y:17:DT:C6	2.52	0.44
1:A:16:LEU:HB2	1:A:163:PHE:O	2.17	0.44
1:A:437:VAL:HG12	1:A:438:PRO:N	2.30	0.44
1:B:454:LEU:HD12	1:B:454:LEU:HA	1.71	0.44
1:B:661:ARG:CZ	2:E:4:DG:OP1	2.66	0.44
1:A:684:PHE:C	1:A:685:VAL:CG2	2.85	0.44
1:B:210:GLU:H	1:B:210:GLU:HG2	1.26	0.44
1:B:400:GLU:HA	1:B:401:GLU:HA	1.57	0.44
2:X:5:DG:C6	2:X:6:DA:C6	3.06	0.44
3:Y:6:DA:H2''	3:Y:7:DA:C8	2.52	0.44
1:A:342:GLN:C	1:A:344:THR:HG23	2.30	0.44
1:A:615:ARG:HH21	1:A:651:ARG:NH2	2.16	0.44
1:B:67:TRP:CD2	1:B:112:LEU:HD13	2.53	0.44
1:B:517:GLU:H	1:B:517:GLU:CD	2.13	0.44
1:B:475:VAL:O	1:B:544:LEU:HG	2.18	0.44
1:B:583:PRO:CD	1:B:588:LEU:CD1	2.94	0.44
3:Y:8:DC:H2'	3:Y:9:DC:O4'	2.18	0.44
1:A:164:LEU:HA	1:A:164:LEU:HD23	1.63	0.44
1:A:189:LEU:H	1:A:189:LEU:HG	1.65	0.44
1:A:439:LEU:HD12	1:A:440:ARG:O	2.18	0.44
1:B:380:THR:CG2	1:B:381:LEU:N	2.81	0.44
1:B:658:LEU:CD1	1:B:684:PHE:CZ	2.94	0.44
1:B:649:PHE:HD2	3:F:19:DG:C6	2.36	0.44
1:A:464:ALA:CB	1:A:498:GLY:HA2	2.48	0.43
1:A:654:ALA:O	1:A:658:LEU:CB	2.65	0.43
1:A:71:GLU:N	1:A:71:GLU:OE1	2.43	0.43
1:B:109:LEU:HB3	1:B:157:VAL:HG21	1.99	0.43
1:B:194:ARG:CG	1:B:201:THR:HG22	2.43	0.43
1:B:230:LYS:CG	1:B:232:ARG:HG2	2.48	0.43
1:B:427:ARG:HG2	1:B:673:HIS:HD2	1.82	0.43
1:B:633:HIS:CD2	1:B:633:HIS:O	2.70	0.43
1:A:318:ILE:C	1:A:637:HIS:HE2	2.22	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:657:HIS:O	1:A:657:HIS:HD2	2.00	0.43
1:B:193:VAL:CG2	1:B:261:LEU:HB3	2.48	0.43
1:B:428:GLU:HA	1:B:428:GLU:OE1	2.17	0.43
1:B:507:GLU:HG3	1:B:508:ALA:N	2.33	0.43
1:A:12:ASN:O	1:A:14:PHE:CD1	2.70	0.43
1:A:369:PHE:HB3	1:A:374:ALA:O	2.18	0.43
1:A:387:GLN:HE21	1:A:389:LEU:HD22	1.78	0.43
1:A:398:ALA:O	1:A:403:VAL:HB	2.18	0.43
1:A:58:VAL:HG22	1:A:112:LEU:HD13	2.00	0.43
1:B:197:TYR:CB	1:B:232:ARG:HD3	2.48	0.43
2:E:2:DG:C2	2:E:3:DA:N3	2.85	0.43
1:A:286:ARG:NH1	2:X:7:DT:P	2.91	0.43
1:A:168:ASP:OD1	1:A:580:ARG:NH1	2.40	0.43
1:A:242:ALA:HB2	1:A:258:THR:CG2	2.48	0.43
1:A:316:LEU:HB2	1:A:636:PHE:CD2	2.54	0.43
1:B:543:LEU:HB3	1:B:570:LEU:CD1	2.48	0.43
1:B:57:THR:HG22	1:B:66:SER:CB	2.48	0.43
1:B:640:ARG:HD3	1:B:649:PHE:CG	2.54	0.43
1:A:343:GLU:C	1:A:344:THR:HG23	2.39	0.43
1:A:503:TRP:NE1	1:A:679:ARG:HA	2.33	0.43
1:B:334:LEU:HD12	1:B:334:LEU:C	2.38	0.43
1:B:514:ILE:CA	1:B:553:GLU:OE2	2.67	0.43
1:B:606:VAL:CG1	1:B:611:ARG:HH22	2.32	0.43
1:B:642:TYR:OH	1:B:685:VAL:CG1	2.66	0.43
1:A:365:LEU:C	1:A:369:PHE:HD2	2.09	0.43
1:B:456:ALA:HB1	1:B:643:PRO:HG3	2.01	0.43
1:A:14:PHE:CD2	1:A:306:PRO:HB2	2.53	0.43
1:A:316:LEU:HD12	1:A:636:PHE:CB	2.48	0.43
1:A:529:ALA:HB2	1:A:532:ARG:HH11	1.83	0.43
1:B:217:LEU:HA	1:B:217:LEU:HD12	1.78	0.43
1:B:366:LEU:HD23	1:B:376:LEU:HD21	2.00	0.43
1:B:390:ALA:O	1:B:393:GLU:N	2.52	0.43
1:B:460:LEU:CD1	1:B:462:VAL:HG12	2.38	0.43
1:A:439:LEU:HD11	1:A:440:ARG:O	2.19	0.43
1:B:444:ARG:HD3	1:B:448:GLU:CG	2.48	0.43
1:B:573:VAL:HA	1:B:619:LEU:CD2	2.48	0.43
1:B:676:GLU:N	1:B:676:GLU:OE1	2.51	0.43
3:F:11:DA:H2''	3:F:12:DC:O5'	2.18	0.43
1:A:531:ARG:HH11	1:A:537:LEU:CA	2.31	0.43
1:A:529:ALA:O	1:A:532:ARG:HB2	2.19	0.43
1:A:531:ARG:CG	1:A:536:ARG:C	2.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:PHE:CG	1:A:303:LEU:HD12	2.54	0.43
1:A:301:LEU:HA	1:A:301:LEU:HD12	1.81	0.43
1:A:342:GLN:O	1:A:344:THR:CG2	2.44	0.43
1:B:26:PRO:HG3	1:B:98:LEU:HD11	2.01	0.43
1:B:322:MET:H	1:B:463:VAL:HG12	1.79	0.43
1:A:109:LEU:CB	1:A:157:VAL:HG21	2.49	0.42
1:A:283:TRP:CE2	1:A:284:GLU:HG2	2.53	0.42
1:A:344:THR:CG2	1:A:404:GLN:OE1	2.62	0.42
1:B:110:SER:N	1:B:157:VAL:HG23	2.33	0.42
1:B:544:LEU:HD13	1:B:656:LEU:HG	2.01	0.42
1:A:652:LEU:HD13	1:A:656:LEU:HB3	2.01	0.42
1:A:152:VAL:C	1:A:153:LEU:HD23	2.39	0.42
1:A:195:ASN:ND2	1:A:197:TYR:OH	2.53	0.42
1:A:322:MET:N	1:A:463:VAL:CG1	2.81	0.42
1:A:350:ARG:CG	1:A:409:LEU:HG	2.48	0.42
1:A:576:SER:HB2	3:Y:9:DC:OP2	2.19	0.42
1:A:596:LEU:HD23	1:A:596:LEU:HA	1.84	0.42
1:A:602:LEU:HA	1:A:617:LEU:O	2.20	0.42
1:A:633:HIS:CD2	1:A:633:HIS:O	2.70	0.42
1:B:384:HIS:C	1:B:384:HIS:ND1	2.73	0.42
3:Y:4:DA:H2''	3:Y:5:DC:O5'	2.18	0.42
1:A:528:TRP:C	1:A:532:ARG:NH2	2.73	0.42
1:A:10:PHE:CE1	1:A:308:ALA:HB3	2.55	0.42
1:A:588:LEU:HD23	1:A:607:HIS:CD2	2.54	0.42
1:A:572:SER:O	1:A:619:LEU:HA	2.19	0.42
1:B:177:MET:HE3	1:B:182:TRP:CB	2.47	0.42
1:B:514:ILE:O	1:B:553:GLU:HG3	2.19	0.42
1:A:22:GLU:CD	1:A:95:ARG:HH12	2.23	0.42
1:A:92:PRO:O	1:A:93:LYS:HG2	2.20	0.42
1:B:127:VAL:HG11	1:B:134:VAL:CG2	2.50	0.42
1:B:24:LEU:O	1:B:26:PRO:HD3	2.19	0.42
1:B:444:ARG:HB2	1:B:447:TRP:CZ2	2.54	0.42
1:A:187:HIS:NE2	1:A:273:GLU:OE2	2.44	0.42
1:B:179:LEU:HD13	1:B:263:PRO:HG3	2.02	0.42
1:A:232:ARG:HD3	1:A:232:ARG:HA	1.71	0.42
1:A:267:LEU:H	1:A:267:LEU:HD22	1.84	0.42
1:B:230:LYS:HG2	1:B:232:ARG:HG2	2.01	0.42
1:B:533:LYS:HA	1:B:533:LYS:HD3	1.74	0.42
1:B:627:PRO:O	1:B:631:LEU:HD12	2.18	0.42
1:B:465:LEU:CD2	1:B:637:HIS:HB3	2.50	0.42
1:B:501:LEU:HD11	1:B:643:PRO:HD3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:431:PRO:CG	1:B:681:LYS:HG3	2.48	0.42
1:A:14:PHE:HB2	1:A:165:LEU:HB3	2.01	0.42
1:A:210:GLU:HB2	1:A:215:LEU:HD12	2.02	0.42
1:A:350:ARG:N	1:A:350:ARG:HD2	2.34	0.42
1:A:353:GLY:HA2	1:A:354:ALA:HA	1.87	0.42
1:A:10:PHE:CE2	1:A:584:VAL:HG13	2.55	0.42
1:B:156:TRP:HE1	1:B:164:LEU:CD1	2.32	0.42
1:B:531:ARG:HH21	1:B:537:LEU:CA	2.31	0.42
1:B:600:THR:HA	1:B:620:VAL:HA	2.01	0.42
1:A:435:LEU:HD22	1:A:439:LEU:HD23	2.02	0.42
1:A:492:CYS:SG	1:A:492:CYS:O	2.78	0.42
1:A:607:HIS:CE1	1:A:608:ARG:O	2.73	0.42
1:A:640:ARG:CD	1:A:649:PHE:CG	3.03	0.42
1:B:217:LEU:HD22	1:B:226:TYR:HB2	2.02	0.42
1:B:79:LEU:O	1:B:79:LEU:HD12	2.20	0.42
1:A:365:LEU:HB3	1:A:376:LEU:CD2	2.47	0.41
1:A:449:ASN:CG	1:A:646:GLY:H	2.23	0.41
1:A:550:PRO:HD2	1:A:553:GLU:OE1	2.20	0.41
1:B:505:LEU:HD11	1:B:671:ILE:HG13	1.99	0.41
1:B:503:TRP:HB2	1:B:662:LEU:HD22	2.01	0.41
1:B:242:ALA:HB2	1:B:258:THR:CG2	2.50	0.41
1:B:312:GLN:O	1:B:595:PRO:HD2	2.20	0.41
1:B:447:TRP:CE3	1:B:448:GLU:N	2.88	0.41
1:A:204:LEU:HD12	1:A:205:LEU:H	1.84	0.41
1:A:352:ASP:CB	1:A:353:GLY:HA2	2.47	0.41
1:B:163:PHE:CD2	1:B:303:LEU:HD13	2.55	0.41
1:B:204:LEU:HD12	1:B:204:LEU:O	2.20	0.41
1:B:358:PRO:HG2	1:B:361:LEU:HD21	2.02	0.41
1:B:337:GLY:HA2	1:B:372:SER:HB2	2.02	0.41
1:B:439:LEU:HA	1:B:446:ARG:NH2	2.35	0.41
1:B:440:ARG:O	1:B:441:GLU:C	2.57	0.41
1:A:439:LEU:HD12	1:A:440:ARG:C	2.41	0.41
1:A:440:ARG:HD3	1:A:442:GLU:OE1	2.20	0.41
1:A:447:TRP:CE3	1:A:448:GLU:N	2.89	0.41
1:A:480:GLY:O	1:A:487:PHE:HB2	2.20	0.41
1:A:4:LEU:HD22	1:A:316:LEU:HA	2.01	0.41
1:A:434:ILE:HB	2:X:1:DT:H4'	2.01	0.41
1:B:156:TRP:HD1	1:B:164:LEU:HB2	1.81	0.41
1:B:422:LYS:HA	1:B:425:LEU:CG	2.50	0.41
1:A:358:PRO:HB2	1:A:361:LEU:HD21	2.02	0.41
1:A:483:GLU:HG2	1:A:483:GLU:H	1.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:544:LEU:HG	1:A:544:LEU:H	1.58	0.41
1:A:588:LEU:HD12	1:A:588:LEU:HA	1.89	0.41
1:B:315:ARG:HE	1:B:315:ARG:HB3	1.61	0.41
1:B:329:LYS:O	1:B:332:ASP:N	2.51	0.41
1:B:334:LEU:O	1:B:368:ALA:CB	2.60	0.41
1:B:447:TRP:CE3	1:B:448:GLU:HG3	2.53	0.41
1:B:647:PHE:CD1	1:B:647:PHE:N	2.88	0.41
1:B:71:GLU:N	1:B:71:GLU:OE1	2.35	0.41
1:A:202:TRP:HB3	1:A:244:VAL:HB	2.02	0.41
1:A:358:PRO:CG	1:A:360:PHE:HE1	2.33	0.41
1:A:661:ARG:HA	1:A:664:LYS:HD3	2.01	0.41
1:B:205:LEU:HB2	1:B:243:TRP:O	2.21	0.41
1:B:222:SER:O	1:B:226:TYR:N	2.51	0.41
1:B:281:LEU:HA	1:B:281:LEU:HD12	1.62	0.41
1:A:138:GLU:CB	1:A:141:ARG:HE	2.23	0.41
1:A:358:PRO:HB2	1:A:361:LEU:CD2	2.51	0.41
1:A:440:ARG:HH12	1:A:443:GLU:HB3	1.85	0.41
1:A:503:TRP:HB2	1:A:662:LEU:HD22	2.02	0.41
1:B:256:HIS:NE2	1:B:261:LEU:HD21	2.36	0.41
1:B:343:GLU:C	1:B:344:THR:CG2	2.89	0.41
1:B:640:ARG:HD3	1:B:649:PHE:CD1	2.56	0.41
1:B:657:HIS:O	1:B:657:HIS:HD2	2.03	0.41
1:A:210:GLU:HB2	1:A:215:LEU:CD1	2.51	0.41
1:A:531:ARG:HH11	1:A:537:LEU:HD23	1.84	0.41
1:B:137:ARG:O	1:B:148:LEU:HD12	2.21	0.41
1:B:301:LEU:HA	1:B:301:LEU:HD12	1.49	0.41
1:B:39:ARG:NH1	1:B:39:ARG:HG3	2.36	0.41
1:B:674:LEU:HD22	1:B:674:LEU:O	2.21	0.41
1:B:658:LEU:HD11	1:B:684:PHE:CE2	2.43	0.41
1:A:348:LEU:HB3	1:A:350:ARG:HH22	1.85	0.41
1:B:283:TRP:CZ3	1:B:287:ARG:NH2	2.88	0.41
1:B:406:VAL:O	1:B:454:LEU:HD13	2.21	0.41
1:A:419:ASN:O	1:A:423:ALA:N	2.45	0.41
1:A:440:ARG:HH12	1:A:443:GLU:CB	2.33	0.41
1:B:243:TRP:CZ3	1:B:255:PRO:HG3	2.56	0.41
1:B:435:LEU:HD12	1:B:436:ASN:O	2.21	0.41
1:B:439:LEU:HA	1:B:446:ARG:HH21	1.85	0.41
1:B:449:ASN:HD21	1:B:646:GLY:N	2.19	0.41
1:B:451:LEU:O	1:B:454:LEU:N	2.54	0.41
2:X:3:DA:N6	3:Y:16:DC:H42	2.18	0.41
1:A:234:GLN:N	1:A:234:GLN:CD	2.73	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:LYS:HB3	3:Y:19:DG:H3'	2.03	0.40
1:A:573:VAL:HG21	1:A:656:LEU:HD13	2.01	0.40
1:A:601:PHE:CE2	1:A:619:LEU:HD12	2.56	0.40
1:A:650:PRO:CB	1:A:657:HIS:ND1	2.72	0.40
1:B:349:LEU:CD1	1:B:349:LEU:C	2.85	0.40
1:B:361:LEU:H	1:B:361:LEU:HG	1.51	0.40
1:B:593:TYR:CE1	1:B:595:PRO:HD3	2.56	0.40
1:B:569:ASP:HA	1:B:624:GLY:HA3	2.03	0.40
1:A:246:ASP:OD1	1:A:247:PRO:HD2	2.21	0.40
1:A:321:LEU:CB	1:A:463:VAL:CG1	2.99	0.40
1:A:656:LEU:O	1:A:659:ALA:HB3	2.21	0.40
1:B:156:TRP:HE1	1:B:164:LEU:HD12	1.86	0.40
1:B:153:LEU:HD22	1:B:167:VAL:HG22	2.03	0.40
1:B:251:ARG:HA	1:B:252:LYS:HA	1.82	0.40
1:B:384:HIS:CE1	1:B:386:SER:HB3	2.55	0.40
1:B:12:ASN:O	1:B:14:PHE:CD1	2.74	0.40
1:B:345:ALA:CB	1:B:402:GLY:C	2.89	0.40
1:B:345:ALA:HB3	1:B:402:GLY:O	2.20	0.40
1:B:406:VAL:CG1	1:B:407:LEU:N	2.85	0.40
1:B:75:LEU:HD22	1:B:90:LEU:HB2	2.03	0.40
3:Y:4:DA:H8	3:Y:4:DA:O5'	2.04	0.40
1:A:49:VAL:HG12	1:A:64:LEU:HD21	2.03	0.40
1:A:457:LYS:HD2	1:A:685:VAL:CG2	2.52	0.40
1:B:479:ALA:HA	1:B:487:PHE:O	2.21	0.40
1:B:531:ARG:NH2	1:B:537:LEU:HA	2.32	0.40
1:A:205:LEU:HD11	1:A:245:ALA:HB3	2.02	0.40
1:A:75:LEU:HD22	1:A:90:LEU:HB2	2.03	0.40
1:B:209:GLU:HG2	1:B:209:GLU:H	1.58	0.40
1:B:503:TRP:CE2	1:B:679:ARG:HA	2.56	0.40
1:B:520:TRP:HB2	1:B:557:ALA:HA	2.02	0.40
1:B:631:LEU:O	1:B:635:ILE:CG1	2.70	0.40
1:B:7:THR:O	1:B:313:ALA:HB3	2.22	0.40
3:Y:13:DT:H1'	3:Y:14:DA:H5'	2.04	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:367:ARG:NH1	1:A:437:VAL:CG1[9_555]	1.75	0.45
1:A:353:GLY:O	1:A:370:GLY:CA[5_555]	2.18	0.02

5.3 Torsion angles

5.3.1 Protein backbone

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	675/685 (98%)	654 (97%)	18 (3%)	3 (0%)	34	68
1	B	675/685 (98%)	650 (96%)	22 (3%)	3 (0%)	34	68
All	All	1350/1370 (98%)	1304 (97%)	40 (3%)	6 (0%)	34	68

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	25	ARG
1	B	358	PRO
1	A	37	PRO
1	A	385	PRO
1	A	319	PRO
1	B	438	PRO

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.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	499/549 (91%)	393 (79%)	106 (21%)	1	4
1	B	498/549 (91%)	418 (84%)	80 (16%)	2	11
All	All	997/1098 (91%)	811 (81%)	186 (19%)	1	7

All (186) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	6	LYS
1	A	39	ARG
1	A	42	VAL
1	A	59	ARG
1	A	64	LEU
1	A	68	SER
1	A	85	THR
1	A	89	ARG
1	A	95	ARG
1	A	120	ARG
1	A	125	GLU
1	A	138	GLU
1	A	146	ARG
1	A	147	VAL
1	A	156	TRP
1	A	173	ILE
1	A	174	LEU
1	A	176	GLU
1	A	185	GLN
1	A	189	LEU
1	A	198	ASP
1	A	204	LEU
1	A	206	ARG
1	A	210	GLU
1	A	215	LEU
1	A	217	LEU
1	A	223	LEU
1	A	226	TYR
1	A	230	LYS
1	A	234	GLN
1	A	260	LEU
1	A	267	LEU
1	A	270	LEU
1	A	271	HIS
1	A	272	GLU
1	A	277	LEU
1	A	300	ARG
1	A	303	LEU
1	A	305	THR
1	A	317	SER
1	A	319	PRO
1	A	322	MET

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Mol	Chain	Res	Type
1	A	329	LYS
1	A	335	ARG
1	A	336	VAL
1	A	338	PHE
1	A	346	LEU
1	A	348	LEU
1	A	350	ARG
1	A	357	TRP
1	A	360	PHE
1	A	361	LEU
1	A	362	ARG
1	A	376	LEU
1	A	386	SER
1	A	389	LEU
1	A	409	LEU
1	A	415	TRP
1	A	420	ARG
1	A	422	LYS
1	A	426	LEU
1	A	435	LEU
1	A	439	LEU
1	A	440	ARG
1	A	444	ARG
1	A	447	TRP
1	A	451	LEU
1	A	452	LEU
1	A	455	LEU
1	A	457	LYS
1	A	463	VAL
1	A	483	GLU
1	A	512	GLU
1	A	517	GLU
1	A	532	ARG
1	A	536	ARG
1	A	537	LEU
1	A	548	ARG
1	A	564	GLU
1	A	574	ARG
1	A	580	ARG
1	A	592	LEU
1	A	593	TYR
1	A	598	ASP

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Mol	Chain	Res	Type
1	A	600	THR
1	A	604	LEU
1	A	608	ARG
1	A	625	ASP
1	A	631	LEU
1	A	639	THR
1	A	641	LEU
1	A	647	PHE
1	A	658	LEU
1	A	661	ARG
1	A	664	LYS
1	A	668	ARG
1	A	669	LEU
1	A	671	ILE
1	A	674	LEU
1	A	678	ASP
1	A	679	ARG
1	A	682	LEU
1	A	683	PHE
1	A	684	PHE
1	A	685	VAL
1	B	33	LEU
1	B	42	VAL
1	B	64	LEU
1	B	68	SER
1	B	85	THR
1	B	93	LYS
1	B	95	ARG
1	B	106	ARG
1	B	125	GLU
1	B	141	ARG
1	B	146	ARG
1	B	156	TRP
1	B	157	VAL
1	B	158	SER
1	B	174	LEU
1	B	176	GLU
1	B	177	MET
1	B	180	GLU
1	B	185	GLN
1	B	189	LEU
1	B	198	ASP

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Mol	Chain	Res	Type
1	B	205	LEU
1	B	206	ARG
1	B	207	LEU
1	B	209	GLU
1	B	210	GLU
1	B	230	LYS
1	B	232	ARG
1	B	260	LEU
1	B	271	HIS
1	B	281	LEU
1	B	287	ARG
1	B	318	ILE
1	B	322	MET
1	B	335	ARG
1	B	338	PHE
1	B	360	PHE
1	B	361	LEU
1	B	362	ARG
1	B	378	LEU
1	B	385	PRO
1	B	386	SER
1	B	389	LEU
1	B	396	ARG
1	B	399	LYS
1	B	409	LEU
1	B	415	TRP
1	B	420	ARG
1	B	421	LEU
1	B	424	LEU
1	B	426	LEU
1	B	434	ILE
1	B	437	VAL
1	B	440	ARG
1	B	441	GLU
1	B	443	GLU
1	B	444	ARG
1	B	452	LEU
1	B	463	VAL
1	B	465	LEU
1	B	514	ILE
1	B	528	TRP
1	B	531	ARG

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Mol	Chain	Res	Type
1	B	537	LEU
1	B	548	ARG
1	B	592	LEU
1	B	593	TYR
1	B	596	LEU
1	B	597	GLU
1	B	599	LYS
1	B	600	THR
1	B	658	LEU
1	B	662	LEU
1	B	669	LEU
1	B	671	ILE
1	B	672	ARG
1	B	678	ASP
1	B	682	LEU
1	B	683	PHE
1	B	685	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	312	GLN
1	A	387	GLN
1	A	436	ASN
1	A	633	HIS
1	A	657	HIS
1	B	379	HIS
1	B	384	HIS
1	B	633	HIS
1	B	657	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are 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	679/685 (99%)	0.23	14 (2%) 63 63	12, 56, 106, 149	0
1	B	679/685 (99%)	0.27	23 (3%) 45 44	12, 56, 103, 137	0
2	E	17/22 (77%)	-0.37	0 100 100	26, 40, 62, 63	0
2	X	17/22 (77%)	-0.28	0 100 100	25, 36, 60, 68	0
3	F	16/19 (84%)	-0.34	0 100 100	38, 54, 63, 71	0
3	Y	16/19 (84%)	-0.27	0 100 100	36, 48, 57, 60	0
4	C	3/3 (100%)	0.04	0 100 100	48, 48, 73, 100	0
4	D	3/3 (100%)	0.07	0 100 100	48, 48, 85, 110	0
All	All	1430/1458 (98%)	0.22	37 (2%) 56 54	12, 55, 104, 149	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	401	GLU	4.7
1	A	402	GLY	4.7
1	B	455	LEU	4.4
1	B	346	LEU	4.1
1	B	357	TRP	4.0
1	A	406	VAL	3.9
1	A	357	TRP	3.7
1	B	333	ALA	3.6
1	B	402	GLY	3.5
1	B	330	PRO	3.2
1	A	346	LEU	3.0
1	B	453	GLY	2.9
1	B	339	TYR	2.9
1	A	437	VAL	2.8
1	B	558	LEU	2.8
1	B	475	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	405	ALA	2.6
1	A	347	ALA	2.6
1	B	466	SER	2.5
1	B	474	ALA	2.5
1	A	432	SER	2.5
1	A	367	ARG	2.4
1	B	327	VAL	2.4
1	A	383	ALA	2.4
1	A	554	PHE	2.4
1	B	566	ILE	2.4
1	B	554	PHE	2.3
1	B	192	ARG	2.3
1	A	581	VAL	2.2
1	A	455	LEU	2.2
1	B	365	LEU	2.2
1	B	359	GLU	2.1
1	B	332	ASP	2.1
1	B	534	ALA	2.1
1	B	435	LEU	2.1
1	B	64	LEU	2.0
1	B	407	LEU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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(\AA^2)	Q<0.9
5	MG	X	101	1/1	0.87	0.15	51,51,51,51	0
5	MG	E	101	1/1	0.93	0.12	35,35,35,35	0

6.5 Other polymers

There are no such residues in this entry.