



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 01:31 am GMT

PDB ID : 2ACI  
Title : Structure of D166A arginine deiminase  
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Deposited on : 2005-07-18  
Resolution : 2.50 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

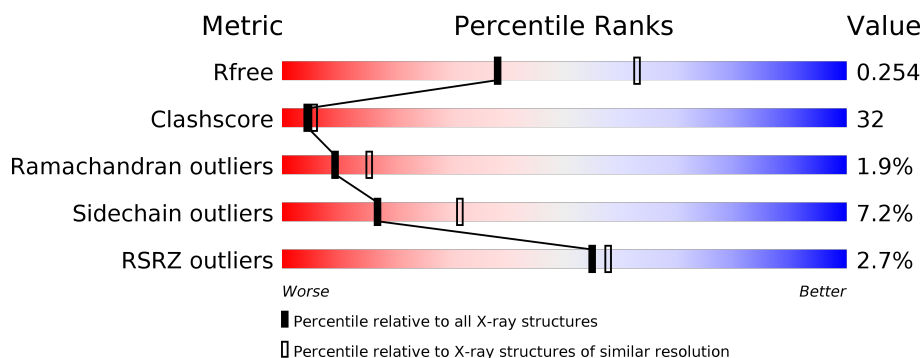
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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))
$R_{free}$	100719	3846 (2.50-2.50)
Clashscore	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)
RSRZ outliers	101464	3876 (2.50-2.50)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . 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	418	<div> <div>2%</div> <div> <div></div> <div>42%</div> <div>49%</div> <div>5%</div> <div></div> </div> </div>
1	B	418	<div> <div>3%</div> <div> <div></div> <div>61%</div> <div>32%</div> <div></div> </div> </div>
1	C	418	<div> <div>2%</div> <div> <div></div> <div>45%</div> <div>47%</div> <div></div> </div> </div>
1	D	418	<div> <div>3%</div> <div> <div></div> <div>46%</div> <div>46%</div> <div></div> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12953 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 Arginine deiminase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	402	Total	C	N	O	S	0	0	0
			3139	1988	546	588	17			
1	B	409	Total	C	N	O	S	0	0	0
			3193	2020	556	600	17			
1	C	403	Total	C	N	O	S	0	0	0
			3147	1992	547	591	17			
1	D	406	Total	C	N	O	S	0	0	0
			3174	2009	553	595	17			

There are 4 discrepancies between the modelled and reference sequences:

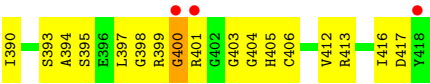
Chain	Residue	Modelled	Actual	Comment	Reference
A	166	ALA	ASP	ENGINEERED	UNP P13981
B	166	ALA	ASP	ENGINEERED	UNP P13981
C	166	ALA	ASP	ENGINEERED	UNP P13981
D	166	ALA	ASP	ENGINEERED	UNP P13981

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	60	Total	O	0	0
			60	60		
2	B	90	Total	O	0	0
			90	90		
2	C	86	Total	O	0	0
			86	86		
2	D	64	Total	O	0	0
			64	64		







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	91.20Å 123.90Å 150.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.50 19.96 – 2.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.50) 93.9 (19.96-2.90)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.16 (at 2.88Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.198 , 0.272 0.182 , 0.254	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	46.0	Xtriage
Anisotropy	0.128	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 63.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	12953	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.68% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

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	0.70	1/3205 (0.0%)	0.93	3/4346 (0.1%)
1	B	0.77	0/3261	0.96	3/4422 (0.1%)
1	C	0.74	3/3213 (0.1%)	0.92	1/4356 (0.0%)
1	D	0.73	0/3242	0.92	2/4396 (0.0%)
All	All	0.74	4/12921 (0.0%)	0.93	9/17520 (0.1%)

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	C	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	303	PRO	N-CD	10.53	1.62	1.47
1	C	214	PRO	N-CD	-5.74	1.39	1.47
1	A	37	CYS	CB-SG	-5.34	1.73	1.81
1	C	242	GLU	CG-CD	5.18	1.59	1.51

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	186	ARG	NE-CZ-NH2	-5.55	117.53	120.30
1	D	86	LEU	CA-CB-CG	5.33	127.55	115.30
1	C	339	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	B	306	LEU	CA-CB-CG	5.28	127.45	115.30
1	B	20	VAL	CB-CA-C	-5.19	101.54	111.40
1	B	290	LEU	CA-CB-CG	5.18	127.21	115.30
1	A	295	PRO	CA-N-CD	-5.11	104.34	111.50
1	A	107	LEU	CA-CB-CG	5.09	127.02	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	204	ASN	N-CA-CB	-5.03	101.55	110.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	144	TYR	Sidechain

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3139	0	3128	256	0
1	B	3193	0	3177	153	0
1	C	3147	0	3132	215	0
1	D	3174	0	3161	208	0
2	A	60	0	0	23	0
2	B	90	0	0	22	0
2	C	86	0	0	15	0
2	D	64	0	0	14	0
All	All	12953	0	12598	798	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 32.

All (798) 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:D:43:ASP:HB2	1:D:401:ARG:HH12	1.05	1.19
1:C:277:MET:HE2	1:C:281:THR:HG21	1.29	1.13
1:C:33:THR:HG22	1:C:35:SER:H	1.17	1.10
1:A:17:LEU:HD11	1:A:20:VAL:HG13	1.34	1.08
1:D:343:THR:HG21	1:D:358:GLY:N	1.69	1.07
1:D:343:THR:HG21	1:D:358:GLY:H	0.90	1.07
1:C:352:ARG:HB2	1:C:377:TYR:CE1	1.90	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:358:GLY:HA3	1:A:378:THR:HG21	1.34	1.04
1:D:343:THR:CG2	1:D:358:GLY:H	1.71	1.03
1:C:150:HIS:HA	2:C:442:HOH:O	1.59	1.01
1:A:293:VAL:HG23	1:A:295:PRO:HD3	1.02	0.99
1:C:352:ARG:HB2	1:C:377:TYR:CZ	1.98	0.98
1:A:320:ARG:HD3	1:D:143:MET:CE	1.94	0.97
1:D:77:THR:O	1:D:80:ILE:HG22	1.65	0.97
1:B:145:ARG:HD3	1:B:152:SER:HB3	1.50	0.94
1:B:358:GLY:HA3	1:B:378:THR:HG21	1.51	0.93
1:A:293:VAL:HG23	1:A:295:PRO:CD	1.96	0.93
1:C:277:MET:CE	1:C:281:THR:HG21	1.97	0.93
1:C:33:THR:HB	1:C:36:ASN:ND2	1.85	0.92
1:D:43:ASP:HB2	1:D:401:ARG:NH1	1.84	0.91
1:D:7:LYS:H	1:D:7:LYS:HD2	1.36	0.90
1:D:144:TYR:HB3	1:D:150:HIS:HD2	1.34	0.90
1:B:176:THR:HG23	2:B:503:HOH:O	1.71	0.90
1:C:44:ASP:HB3	2:C:498:HOH:O	1.70	0.90
1:D:103:LEU:HD13	1:D:154:LEU:HD23	1.51	0.88
1:B:104:THR:HG22	2:B:498:HOH:O	1.73	0.87
1:A:227:ASP:HB3	1:A:239:GLY:H	1.37	0.87
1:A:290:LEU:HB3	2:A:478:HOH:O	1.75	0.87
1:C:328:VAL:O	1:C:328:VAL:HG12	1.76	0.85
1:A:293:VAL:CG2	1:A:295:PRO:HD3	1.98	0.85
1:D:416:ILE:HG13	1:D:417:ASP:H	1.41	0.84
1:C:17:LEU:HD22	1:C:413:ARG:NH2	1.92	0.83
1:A:320:ARG:HD3	1:D:143:MET:HE1	1.61	0.82
1:D:238:ILE:HD12	1:D:265:VAL:HG11	1.61	0.82
1:A:94:ILE:HG12	1:A:107:LEU:HD13	1.59	0.82
1:C:33:THR:HG22	1:C:35:SER:N	1.95	0.82
1:A:12:SER:O	1:A:413:ARG:HD2	1.80	0.82
1:C:352:ARG:HB2	1:C:377:TYR:CD1	2.15	0.81
1:D:7:LYS:N	1:D:7:LYS:HD2	1.95	0.81
1:B:390:ILE:HD12	2:B:479:HOH:O	1.81	0.81
1:D:197:LYS:O	1:D:203:ALA:HB2	1.81	0.81
1:A:336:LYS:H	1:A:336:LYS:HD3	1.44	0.80
1:A:33:THR:HG22	1:A:36:ASN:H	1.45	0.80
1:A:202:PHE:HB2	2:A:463:HOH:O	1.81	0.80
1:B:404:GLY:HA3	2:B:483:HOH:O	1.81	0.80
1:A:320:ARG:HD3	1:D:143:MET:SD	2.20	0.80
1:C:314:TYR:HD2	1:C:314:TYR:H	1.30	0.79
1:D:25:PRO:HD3	1:D:55:HIS:CD2	2.17	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:293:VAL:HG22	1:D:298:VAL:HG21	1.66	0.78
1:B:177:LEU:O	1:B:179:PRO:HD3	1.82	0.78
1:B:99:VAL:HG13	1:B:154:LEU:HD22	1.64	0.78
1:C:180:MET:HA	1:C:180:MET:HE2	1.66	0.78
1:A:324:THR:O	1:A:328:VAL:HG23	1.83	0.77
1:A:90:LEU:HD22	1:A:94:ILE:CD1	2.14	0.77
1:B:69:VAL:HG13	2:B:492:HOH:O	1.83	0.77
1:A:264:ARG:HH11	1:A:266:ILE:HD11	1.49	0.77
1:D:93:LYS:HE3	1:D:155:LEU:HD23	1.65	0.77
1:A:10:VAL:HB	1:A:170:TRP:O	1.86	0.76
1:A:165:ARG:O	1:A:225:GLY:HA3	1.86	0.76
1:A:90:LEU:HD22	1:A:94:ILE:HD12	1.68	0.76
1:B:165:ARG:HD2	1:B:405:HIS:O	1.86	0.75
1:C:277:MET:CE	1:C:281:THR:CG2	2.65	0.75
1:D:399:ARG:HG3	1:D:399:ARG:HH11	1.51	0.75
1:A:278:HIS:O	1:A:281:THR:HB	1.87	0.75
1:D:124:ILE:HG23	1:D:161:THR:HG21	1.69	0.74
1:C:33:THR:HG21	2:C:489:HOH:O	1.86	0.74
1:D:307:ARG:HH11	1:D:307:ARG:HG2	1.52	0.74
1:C:74:ASN:O	1:C:78:GLU:HG3	1.88	0.74
1:A:94:ILE:HG23	1:A:99:VAL:HG21	1.70	0.74
1:D:284:SER:HB2	1:D:292:THR:OG1	1.86	0.74
1:C:87:LYS:HD3	1:C:91:ASP:OD2	1.87	0.73
1:B:352:ARG:HG3	1:B:377:TYR:CD2	2.23	0.73
1:C:21:MET:HB2	1:C:411:ILE:HD11	1.71	0.73
1:D:358:GLY:HA3	1:D:378:THR:HG21	1.69	0.73
1:A:264:ARG:NH1	1:A:332:SER:HB3	2.04	0.73
1:C:352:ARG:CB	1:C:377:TYR:CZ	2.72	0.72
1:D:145:ARG:HD3	1:D:152:SER:HB2	1.72	0.72
1:D:41:LEU:HD13	1:D:185:ARG:HD2	1.71	0.72
1:A:140:ILE:HD13	1:D:318:ILE:HG21	1.71	0.72
1:C:76:LEU:HD12	1:C:120:ALA:CB	2.20	0.72
1:B:242:GLU:HB2	1:B:275:ALA:O	1.90	0.72
1:D:153:PHE:HB3	1:D:155:LEU:O	1.89	0.72
1:D:80:ILE:HD11	1:D:119:LEU:HD23	1.70	0.72
1:D:307:ARG:HG2	1:D:307:ARG:NH1	2.04	0.72
1:C:301:ILE:O	1:C:303:PRO:HD3	1.90	0.72
1:B:374:ARG:HH11	1:B:374:ARG:HG3	1.55	0.71
1:D:25:PRO:HA	1:D:29:HIS:CE1	2.24	0.71
1:B:25:PRO:HA	1:B:29:HIS:CE1	2.25	0.71
1:A:402:GLY:HA2	2:A:470:HOH:O	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:142:LYS:HD2	1:B:145:ARG:NH2	2.05	0.71
1:D:24:SER:HA	1:D:55:HIS:CD2	2.25	0.70
1:B:290:LEU:HG	1:B:339:ARG:NH1	2.05	0.70
1:D:324:THR:O	1:D:328:VAL:HG23	1.91	0.70
1:C:76:LEU:HD12	1:C:120:ALA:HA	1.74	0.69
1:A:145:ARG:NH2	1:A:146:GLU:HG2	2.07	0.69
1:A:208:GLU:HG2	1:A:210:TRP:CZ3	2.27	0.69
1:B:274:ARG:HD3	1:B:297:VAL:HG22	1.74	0.69
1:D:79:THR:OG1	1:D:199:HIS:HB2	1.93	0.69
1:C:314:TYR:N	1:C:314:TYR:CD2	2.58	0.69
1:C:33:THR:CG2	1:C:35:SER:H	1.99	0.69
1:B:54:ASP:HB2	1:B:397:LEU:HD21	1.74	0.69
1:C:80:ILE:HD12	1:C:119:LEU:HD13	1.76	0.68
1:C:197:LYS:HD3	1:C:198:PHE:CE2	2.28	0.68
1:A:301:ILE:HD11	1:A:325:PHE:CD1	2.28	0.68
1:C:197:LYS:HD3	1:C:198:PHE:CZ	2.29	0.68
1:C:314:TYR:N	1:C:314:TYR:HD2	1.92	0.68
1:C:352:ARG:HB2	1:C:377:TYR:CE2	2.28	0.68
1:D:139:ASN:C	1:D:141:LEU:H	1.97	0.68
1:A:18:ARG:HB2	1:A:412:VAL:HG12	1.76	0.67
1:D:238:ILE:HD12	1:D:265:VAL:CG1	2.23	0.67
1:A:107:LEU:HD11	1:A:155:LEU:HD21	1.77	0.67
1:C:180:MET:HE2	1:C:224:GLU:HG3	1.76	0.67
1:D:36:ASN:O	1:D:40:LEU:HD13	1.95	0.67
1:C:180:MET:HA	1:C:180:MET:CE	2.24	0.67
1:C:86:LEU:HD22	1:C:90:LEU:HG	1.76	0.66
1:A:117:ARG:HA	2:A:453:HOH:O	1.96	0.66
1:D:103:LEU:HD11	1:D:141:LEU:HD22	1.77	0.66
1:A:94:ILE:HG12	1:A:107:LEU:CD1	2.25	0.66
1:A:145:ARG:HG3	1:A:152:SER:HB3	1.78	0.66
1:A:298:VAL:HG11	1:A:326:LEU:HD21	1.76	0.66
1:A:145:ARG:NH1	1:A:145:ARG:HB3	2.10	0.66
1:A:229:MET:CE	1:A:279:LEU:HD23	2.26	0.66
1:C:264:ARG:HD2	1:C:305:SER:HB2	1.75	0.66
1:A:320:ARG:CD	1:D:143:MET:CE	2.71	0.66
1:D:180:MET:O	1:D:186:ARG:NH1	2.29	0.66
1:D:122:TYR:CD1	1:D:127:VAL:HG22	2.29	0.66
1:C:324:THR:HG23	1:C:327:GLU:OE1	1.96	0.66
1:A:65:ARG:HB3	1:A:65:ARG:HH11	1.61	0.65
1:D:143:MET:O	1:D:146:GLU:HB3	1.96	0.65
1:D:290:LEU:HD12	2:D:447:HOH:O	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:VAL:HG21	1:D:147:TYR:HB2	1.76	0.65
1:A:145:ARG:CG	1:A:152:SER:HB3	2.26	0.65
1:C:145:ARG:HD3	1:C:152:SER:HB3	1.78	0.65
1:A:400:GLY:HA2	2:A:433:HOH:O	1.96	0.65
1:A:155:LEU:HD22	1:A:155:LEU:N	2.11	0.65
1:A:343:THR:HG21	1:A:378:THR:OG1	1.96	0.65
1:B:290:LEU:HG	1:B:339:ARG:HH12	1.62	0.65
1:C:260:GLY:HA2	2:C:476:HOH:O	1.97	0.65
1:D:62:MET:HB3	1:D:67:ILE:HD12	1.79	0.64
1:D:326:LEU:HD11	1:D:340:VAL:HG11	1.79	0.64
1:A:306:LEU:HD11	1:A:318:ILE:HG12	1.80	0.64
1:A:323:LYS:HG2	2:A:473:HOH:O	1.98	0.64
1:B:99:VAL:HG12	1:B:103:LEU:HB2	1.78	0.64
1:C:303:PRO:HG2	1:C:321:GLU:HB2	1.79	0.64
1:B:397:LEU:HB3	1:B:407:MET:CE	2.27	0.64
1:D:138:ALA:O	1:D:142:LYS:HG3	1.97	0.64
1:A:258:ALA:C	1:A:260:GLY:H	2.01	0.64
1:C:174:GLY:HA3	1:C:210:TRP:CE2	2.33	0.64
1:A:320:ARG:CD	1:D:143:MET:HE1	2.27	0.64
1:A:99:VAL:HG12	1:A:103:LEU:HB2	1.80	0.64
1:D:296:GLU:HA	1:D:299:LYS:HE3	1.79	0.64
1:A:154:LEU:C	1:A:155:LEU:HD22	2.18	0.64
1:B:363:CYS:O	1:B:413:ARG:NH2	2.31	0.64
1:C:399:ARG:HB3	2:C:498:HOH:O	1.97	0.64
1:B:217:ASP:O	1:B:218:HIS:HB2	1.98	0.63
1:B:58:PHE:CE1	1:B:370:VAL:HG11	2.32	0.63
1:B:58:PHE:HE1	1:B:370:VAL:HG11	1.62	0.63
1:D:151:SER:O	1:D:153:PHE:N	2.32	0.63
1:C:320:ARG:HG2	1:C:320:ARG:HH11	1.62	0.63
1:A:233:ASN:N	2:A:451:HOH:O	2.29	0.63
1:A:47:TRP:HA	1:B:354:GLN:HE22	1.62	0.63
1:C:67:ILE:HG22	1:C:68:ASP:N	2.13	0.63
1:D:165:ARG:HD2	1:D:405:HIS:O	1.98	0.63
1:A:233:ASN:ND2	1:A:233:ASN:O	2.30	0.63
1:B:397:LEU:HB3	1:B:407:MET:HE2	1.80	0.63
1:C:33:THR:HG23	1:C:34:PRO:HD2	1.81	0.63
1:C:372:TYR:OH	1:C:403:GLY:HA2	1.98	0.63
1:A:145:ARG:HH11	1:A:145:ARG:HB3	1.63	0.63
1:B:86:LEU:HD22	1:B:90:LEU:HG	1.81	0.63
1:B:20:VAL:HB	2:B:492:HOH:O	1.99	0.63
1:B:80:ILE:HG21	1:B:119:LEU:HD13	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:45:VAL:HG11	1:D:355:TRP:HE3	1.65	0.62
1:D:165:ARG:O	1:D:225:GLY:HA3	1.99	0.62
1:A:368:VAL:HG13	1:A:388:GLU:OE1	2.00	0.62
1:A:412:VAL:O	1:A:412:VAL:HG12	1.99	0.62
1:B:145:ARG:CD	1:B:152:SER:HB3	2.27	0.62
1:D:43:ASP:CB	1:D:401:ARG:HH12	1.97	0.62
1:C:33:THR:HB	1:C:36:ASN:HD21	1.61	0.62
1:D:96:ALA:O	1:D:100:GLY:HA2	1.99	0.62
1:A:88:TRP:NE1	1:A:92:ARG:NH2	2.48	0.61
1:C:352:ARG:CB	1:C:377:TYR:CE2	2.83	0.61
1:A:227:ASP:HB3	1:A:239:GLY:N	2.13	0.61
1:A:92:ARG:HH11	1:A:92:ARG:HG3	1.66	0.61
1:A:36:ASN:O	1:A:40:LEU:HB2	2.01	0.61
1:B:251:GLN:HG2	1:C:101:LEU:HD11	1.82	0.61
1:D:17:LEU:HD11	1:D:20:VAL:HG22	1.81	0.61
1:C:178:ASN:OD1	1:C:223:LEU:HD12	2.01	0.61
1:C:361:VAL:HB	1:C:369:VAL:HG12	1.83	0.61
1:C:9:GLY:O	1:C:412:VAL:HA	2.00	0.61
1:D:125:GLY:O	1:D:157:PRO:HB3	2.01	0.61
1:A:77:THR:O	1:A:81:GLN:HG3	2.00	0.61
1:B:76:LEU:HD22	1:B:80:ILE:HG12	1.82	0.60
1:C:25:PRO:HA	1:C:29:HIS:CE1	2.37	0.60
1:C:328:VAL:CG1	1:C:328:VAL:O	2.47	0.60
1:B:325:PHE:O	1:B:329:VAL:HG23	2.01	0.60
1:D:41:LEU:CD1	1:D:185:ARG:HD2	2.31	0.60
1:A:43:ASP:HA	1:A:401:ARG:NH2	2.16	0.60
1:B:94:ILE:HG22	2:B:498:HOH:O	2.02	0.60
1:D:321:GLU:HG3	1:D:328:VAL:HG11	1.82	0.60
1:C:352:ARG:HG3	1:C:377:TYR:CG	2.36	0.60
1:A:364:LEU:HD11	1:A:370:VAL:CG2	2.32	0.60
1:A:63:ARG:HH11	1:A:63:ARG:HG2	1.67	0.59
1:D:323:LYS:HB3	1:D:327:GLU:OE1	2.02	0.59
1:B:167:THR:HB	2:B:427:HOH:O	2.01	0.59
1:C:277:MET:HE1	1:C:281:THR:CG2	2.31	0.59
1:A:281:THR:HG22	1:A:282:VAL:HG13	1.84	0.59
1:A:319:ARG:HB3	2:A:421:HOH:O	2.02	0.59
1:B:145:ARG:HD3	1:B:152:SER:CB	2.30	0.59
1:B:169:CYS:HB2	1:B:176:THR:OG1	2.03	0.59
1:C:245:SER:HB2	1:C:247:GLN:OE1	2.03	0.59
1:A:313:PRO:HD2	2:A:471:HOH:O	2.02	0.59
1:A:320:ARG:HG2	1:A:320:ARG:HH11	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:CYS:N	2:A:478:HOH:O	2.35	0.59
1:A:319:ARG:HG3	1:A:320:ARG:N	2.18	0.59
1:C:187:GLN:O	1:C:190:LEU:HB3	2.02	0.59
1:C:165:ARG:O	1:C:225:GLY:HA3	2.03	0.58
1:A:174:GLY:HA3	1:A:210:TRP:NE1	2.17	0.58
1:B:132:LEU:HD22	1:B:133:PRO:HD2	1.85	0.58
1:C:60:THR:O	1:C:64:GLU:HG2	2.04	0.58
1:D:157:PRO:O	1:D:158:LEU:HD23	2.02	0.58
1:A:288:ARG:HG3	1:A:289:ASP:N	2.19	0.58
1:A:303:PRO:HG2	1:A:321:GLU:HB2	1.86	0.58
1:C:99:VAL:HG12	1:C:103:LEU:HB2	1.85	0.58
1:C:76:LEU:HD12	1:C:120:ALA:CA	2.32	0.58
1:C:416:ILE:HG22	1:C:417:ASP:N	2.18	0.58
1:D:80:ILE:HD11	1:D:119:LEU:CD2	2.32	0.58
1:A:354:GLN:HG3	1:A:355:TRP:N	2.18	0.58
1:C:352:ARG:HG3	1:C:377:TYR:CD2	2.38	0.58
1:C:58:PHE:CD1	1:C:392:ILE:HD13	2.38	0.58
1:C:82:ASN:O	1:C:85:ALA:N	2.36	0.58
1:D:28:ALA:HB2	1:D:125:GLY:HA2	1.85	0.58
1:A:110:TRP:CZ3	1:A:127:VAL:HG11	2.39	0.58
1:B:11:HIS:HB2	1:B:415:PRO:HB3	1.86	0.58
1:B:362:VAL:HG12	2:B:483:HOH:O	2.03	0.58
1:C:10:VAL:HG21	1:C:410:PRO:HB2	1.86	0.58
1:C:180:MET:CE	1:C:224:GLU:HG3	2.33	0.58
1:C:45:VAL:HG11	1:D:355:TRP:CE3	2.39	0.58
1:C:167:THR:HG23	1:C:168:THR:HG23	1.86	0.58
1:A:295:PRO:HG2	1:A:342:GLU:OE2	2.04	0.58
1:D:416:ILE:O	1:D:417:ASP:HB2	2.04	0.58
1:B:295:PRO:O	1:B:299:LYS:HG2	2.04	0.57
1:C:205:ALA:HB3	1:C:207:PHE:HE2	1.69	0.57
1:C:293:VAL:CG1	1:C:294:PHE:N	2.66	0.57
1:C:17:LEU:HD22	1:C:413:ARG:HH22	1.65	0.57
1:D:372:TYR:CD2	1:D:394:ALA:HB2	2.39	0.57
1:B:255:SER:O	1:B:259:LYS:HD3	2.04	0.57
1:C:294:PHE:HE1	1:C:296:GLU:HB3	1.69	0.57
1:C:277:MET:HE1	1:C:281:THR:HG22	1.85	0.57
1:A:247:GLN:HG2	1:D:97:ASP:O	2.04	0.57
1:A:379:ASN:O	1:A:383:ARG:HG3	2.04	0.57
1:D:168:THR:HG22	1:D:177:LEU:HA	1.86	0.57
1:A:242:GLU:HB3	1:A:243:ARG:NH1	2.19	0.57
1:A:264:ARG:NH1	1:A:266:ILE:HD11	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:320:ARG:HH12	1:B:322:GLU:HG2	1.70	0.57
1:C:13:GLU:CD	1:C:229:MET:HG2	2.25	0.57
1:B:277:MET:CE	1:B:297:VAL:HG21	2.34	0.57
1:C:369:VAL:HG23	1:C:387:VAL:CG1	2.35	0.57
1:B:72:MET:HE1	2:B:433:HOH:O	2.04	0.57
1:C:94:ILE:HD13	1:C:107:LEU:HD12	1.86	0.57
1:D:188:GLU:HB3	2:D:470:HOH:O	2.04	0.57
1:A:43:ASP:HA	1:A:401:ARG:HH21	1.69	0.56
1:B:167:THR:HG22	1:B:168:THR:HG23	1.87	0.56
1:A:264:ARG:HH12	1:A:332:SER:HB3	1.70	0.56
1:D:223:LEU:HD23	1:D:224:GLU:N	2.19	0.56
1:B:76:LEU:O	1:B:80:ILE:HG12	2.05	0.56
1:A:320:ARG:NH1	1:A:320:ARG:HG2	2.19	0.56
1:A:342:GLU:O	1:A:343:THR:HG23	2.05	0.56
1:D:321:GLU:HG3	1:D:328:VAL:CG1	2.35	0.56
1:A:17:LEU:CD1	1:A:20:VAL:HG13	2.23	0.56
1:D:224:GLU:HG3	1:D:243:ARG:HB3	1.87	0.56
1:C:355:TRP:HE3	1:D:45:VAL:HG11	1.71	0.56
1:A:42:PHE:HZ	2:A:447:HOH:O	1.88	0.56
1:C:18:ARG:HD2	1:C:414:ASP:OD2	2.06	0.56
1:D:118:LYS:O	1:D:121:GLU:HB2	2.05	0.56
1:A:17:LEU:HD21	1:A:20:VAL:CG1	2.35	0.56
1:C:288:ARG:HG3	1:C:416:ILE:HG21	1.87	0.56
1:B:398:GLY:C	1:B:400:GLY:H	2.10	0.56
1:C:17:LEU:HB2	1:C:413:ARG:NH1	2.21	0.56
1:C:33:THR:O	1:C:37:CYS:HB2	2.04	0.56
1:A:372:TYR:OH	1:A:403:GLY:HA2	2.06	0.55
1:A:63:ARG:NH1	1:A:63:ARG:HG2	2.20	0.55
1:D:165:ARG:NE	1:D:405:HIS:CE1	2.74	0.55
1:A:53:ARG:HD3	2:A:475:HOH:O	2.06	0.55
1:D:165:ARG:CZ	1:D:405:HIS:CE1	2.88	0.55
1:D:76:LEU:O	1:D:80:ILE:HB	2.07	0.55
1:C:293:VAL:HG13	1:C:298:VAL:HG21	1.88	0.55
1:C:416:ILE:CG2	1:C:417:ASP:H	2.19	0.55
1:A:145:ARG:HH22	1:A:146:GLU:HG2	1.71	0.55
1:B:142:LYS:HD2	1:B:145:ARG:HH22	1.70	0.55
1:C:354:GLN:HG3	1:C:355:TRP:O	2.06	0.55
1:B:43:ASP:HA	1:B:401:ARG:HH21	1.72	0.55
1:C:257:PHE:CG	1:C:308:PRO:HG3	2.41	0.55
1:A:101:LEU:HD12	1:A:102:GLY:N	2.22	0.55
1:D:233:ASN:ND2	1:D:332:SER:O	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:PHE:CD1	1:A:344:GLY:HA3	2.41	0.55
1:B:400:GLY:C	1:B:402:GLY:H	2.11	0.55
1:C:178:ASN:HB3	1:C:223:LEU:O	2.07	0.55
1:C:320:ARG:HG2	1:C:320:ARG:NH1	2.21	0.55
1:A:164:THR:O	1:A:409:CYS:HB2	2.08	0.54
1:C:76:LEU:CD1	1:C:120:ALA:HA	2.37	0.54
1:A:343:THR:HG21	1:A:378:THR:CG2	2.38	0.54
1:A:167:THR:HG23	2:A:438:HOH:O	2.08	0.54
1:B:309:ASP:OD1	1:B:311:SER:HB3	2.06	0.54
1:C:139:ASN:HD22	1:C:139:ASN:N	2.05	0.54
1:D:145:ARG:HD3	1:D:152:SER:CB	2.36	0.54
1:C:383:ARG:NH1	1:C:383:ARG:HG3	2.23	0.54
1:A:237:LEU:O	1:A:238:ILE:HG13	2.08	0.54
1:D:169:CYS:O	1:D:175:VAL:HA	2.06	0.54
1:B:12:SER:OG	1:B:13:GLU:N	2.37	0.54
1:C:383:ARG:HH11	1:C:383:ARG:HG3	1.73	0.54
1:C:416:ILE:CG2	1:C:417:ASP:N	2.71	0.54
1:D:80:ILE:HD11	1:D:119:LEU:CG	2.38	0.54
1:A:33:THR:HG23	1:A:35:SER:H	1.73	0.54
1:C:352:ARG:CG	1:C:377:TYR:CD2	2.90	0.54
1:D:216:LYS:HD3	1:D:218:HIS:CE1	2.42	0.54
1:A:174:GLY:HA3	1:A:210:TRP:CE2	2.42	0.54
1:A:264:ARG:HH21	1:A:307:ARG:HH22	1.55	0.53
1:B:317:ASN:HD22	1:B:318:ILE:H	1.55	0.53
1:B:86:LEU:HD22	1:B:90:LEU:CG	2.38	0.53
1:D:172:TYR:O	1:D:174:GLY:N	2.40	0.53
1:B:178:ASN:OD1	1:B:223:LEU:HD12	2.08	0.53
1:C:171:ILE:HG23	1:C:230:PRO:HB3	1.90	0.53
1:B:280:ASP:OD2	1:B:405:HIS:ND1	2.40	0.53
1:A:352:ARG:HD2	2:A:457:HOH:O	2.08	0.53
1:A:400:GLY:O	1:A:402:GLY:N	2.41	0.53
1:B:202:PHE:HZ	1:B:411:ILE:HD13	1.74	0.53
1:D:336:LYS:O	1:D:337:LYS:HB3	2.09	0.53
1:A:76:LEU:O	1:A:79:THR:HB	2.09	0.53
1:C:294:PHE:CE1	1:C:296:GLU:HB3	2.43	0.53
1:D:326:LEU:CD1	1:D:340:VAL:HG11	2.39	0.53
1:B:276:ALA:HB2	2:B:430:HOH:O	2.08	0.53
1:B:27:LEU:HD21	1:B:31:ARG:NH2	2.24	0.53
1:C:400:GLY:C	1:C:401:ARG:HG3	2.29	0.53
1:A:202:PHE:O	1:A:205:ALA:HB3	2.07	0.53
1:A:58:PHE:CE1	1:A:370:VAL:HG11	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:20:VAL:HG23	2:B:492:HOH:O	2.08	0.53
1:A:142:LYS:HA	1:A:145:ARG:HH11	1.73	0.53
1:A:169:CYS:SG	1:A:225:GLY:HA2	2.48	0.53
1:B:86:LEU:HD22	1:B:90:LEU:CD1	2.39	0.53
1:C:205:ALA:HB3	1:C:207:PHE:CE2	2.44	0.53
1:D:154:LEU:HD12	1:D:154:LEU:H	1.74	0.53
1:D:236:VAL:HG12	1:D:238:ILE:HG13	1.89	0.53
1:B:274:ARG:CD	1:B:297:VAL:HG22	2.39	0.53
1:B:277:MET:HB2	1:B:281:THR:HG21	1.90	0.53
1:D:8:LEU:HA	1:D:412:VAL:HG22	1.91	0.53
1:A:337:LYS:HD3	2:A:428:HOH:O	2.08	0.52
1:B:277:MET:HE3	1:B:297:VAL:HG21	1.90	0.52
1:D:72:MET:CE	1:D:192:THR:OG1	2.57	0.52
1:A:199:HIS:CE1	1:A:201:GLU:HG3	2.45	0.52
1:A:295:PRO:O	1:A:296:GLU:C	2.48	0.52
1:D:171:ILE:HG23	1:D:230:PRO:HB3	1.91	0.52
1:A:80:ILE:HB	1:A:86:LEU:HD13	1.91	0.52
1:B:397:LEU:HD22	1:B:397:LEU:N	2.24	0.52
1:B:20:VAL:CG2	2:B:492:HOH:O	2.58	0.52
1:B:374:ARG:HD2	1:B:394:ALA:HB3	1.91	0.52
1:B:80:ILE:CB	2:B:475:HOH:O	2.58	0.52
1:A:141:LEU:HD21	1:D:246:ARG:CZ	2.39	0.52
1:A:149:GLY:O	1:D:272:LYS:HG3	2.10	0.52
1:A:10:VAL:CG2	1:A:170:TRP:HB2	2.40	0.52
1:A:209:ILE:HG22	1:A:209:ILE:O	2.10	0.52
1:A:258:ALA:C	1:A:260:GLY:N	2.61	0.52
1:A:33:THR:HB	1:A:36:ASN:ND2	2.25	0.52
1:B:400:GLY:C	1:B:401:ARG:HG3	2.29	0.52
1:C:400:GLY:O	1:C:401:ARG:HG3	2.09	0.52
1:A:140:ILE:HA	1:A:143:MET:CE	2.40	0.52
1:A:309:ASP:HB2	1:A:317:ASN:HB2	1.92	0.52
1:B:167:THR:HG23	1:B:189:THR:HA	1.90	0.52
1:C:19:LYS:NZ	1:C:201:GLU:OE2	2.43	0.52
1:C:211:TYR:OH	1:C:221:SER:HB3	2.09	0.52
1:D:99:VAL:HG12	1:D:103:LEU:HB2	1.91	0.52
1:A:169:CYS:O	1:A:175:VAL:HA	2.09	0.51
1:A:199:HIS:CE1	1:A:201:GLU:CG	2.93	0.51
1:D:10:VAL:HG13	1:D:413:ARG:HB3	1.92	0.51
1:B:235:VAL:HG12	1:B:236:VAL:N	2.24	0.51
1:B:330:ALA:HB2	2:B:449:HOH:O	2.10	0.51
1:B:58:PHE:CD1	1:B:392:ILE:HD13	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:217:ASP:O	1:D:218:HIS:HB2	2.09	0.51
1:B:274:ARG:HB3	1:B:277:MET:HE1	1.90	0.51
1:D:165:ARG:HD3	1:D:405:HIS:ND1	2.25	0.51
1:A:17:LEU:HD21	1:A:20:VAL:HG11	1.91	0.51
1:A:218:HIS:O	1:A:221:SER:HB2	2.10	0.51
1:D:16:LYS:HD2	1:D:18:ARG:NH1	2.26	0.51
1:D:24:SER:HA	1:D:55:HIS:CG	2.46	0.51
1:A:60:THR:O	1:A:64:GLU:HG2	2.10	0.51
1:B:141:LEU:HD21	1:C:246:ARG:CZ	2.40	0.51
1:C:15:GLY:HA3	1:C:414:ASP:O	2.11	0.51
1:D:399:ARG:HG3	1:D:399:ARG:NH1	2.21	0.51
1:A:12:SER:O	1:A:413:ARG:CD	2.54	0.51
1:B:94:ILE:HD12	1:B:94:ILE:N	2.26	0.51
1:D:249:ILE:HD12	2:D:476:HOH:O	2.10	0.51
1:B:226:GLY:O	1:B:280:ASP:HB3	2.11	0.51
1:D:18:ARG:HG3	1:D:18:ARG:HH11	1.76	0.51
1:B:72:MET:HG2	1:B:124:ILE:HD11	1.92	0.51
1:B:70:LEU:HB3	1:B:75:LEU:HD11	1.92	0.51
1:A:253:ALA:CB	1:A:306:LEU:HD23	2.40	0.50
1:C:395:SER:OG	1:D:395:SER:HB3	2.11	0.50
1:A:248:ALA:O	1:A:252:VAL:HG23	2.11	0.50
1:A:338:LEU:O	1:A:340:VAL:HG23	2.11	0.50
1:C:54:ASP:HB2	1:C:397:LEU:CD1	2.42	0.50
1:A:142:LYS:HA	1:A:145:ARG:NH1	2.26	0.50
1:B:47:TRP:CD2	1:B:50:GLN:HB2	2.46	0.50
1:C:358:GLY:HA3	1:C:378:THR:HG21	1.92	0.50
1:A:372:TYR:CZ	1:A:403:GLY:HA2	2.47	0.50
1:B:17:LEU:HD21	1:B:20:VAL:CG1	2.41	0.50
1:B:304:PHE:CE1	1:C:143:MET:HE3	2.47	0.50
1:C:355:TRP:CE3	1:D:45:VAL:HG11	2.46	0.50
1:A:179:PRO:HB3	1:A:218:HIS:CD2	2.46	0.50
1:A:344:GLY:C	1:A:355:TRP:HE1	2.15	0.50
1:B:317:ASN:ND2	1:B:318:ILE:N	2.59	0.50
1:D:398:GLY:C	1:D:400:GLY:N	2.64	0.50
1:A:10:VAL:HG23	1:A:170:TRP:CB	2.42	0.50
1:B:317:ASN:HD22	1:B:318:ILE:N	2.10	0.50
1:D:199:HIS:HE1	1:D:201:GLU:HG3	1.77	0.50
1:B:167:THR:CG2	1:B:189:THR:HA	2.42	0.50
1:D:28:ALA:HB1	1:D:157:PRO:HB2	1.92	0.50
1:D:27:LEU:HA	1:D:30:GLN:OE1	2.12	0.50
1:D:23:CYS:O	1:D:55:HIS:NE2	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:304:PHE:HE1	1:C:143:MET:CE	2.25	0.49
1:C:76:LEU:O	1:C:80:ILE:HG12	2.12	0.49
1:A:318:ILE:O	1:A:318:ILE:HG22	2.11	0.49
1:A:336:LYS:HG2	1:A:337:LYS:HG2	1.95	0.49
1:B:288:ARG:HG3	1:B:289:ASP:N	2.26	0.49
1:A:22:VAL:O	1:A:71:GLU:HA	2.12	0.49
1:C:352:ARG:HB2	1:C:377:TYR:CG	2.47	0.49
1:D:295:PRO:HG2	1:D:342:GLU:OE2	2.12	0.49
1:D:94:ILE:N	1:D:94:ILE:HD12	2.27	0.49
1:A:115:GLU:HG2	1:A:118:LYS:HB2	1.94	0.49
1:A:10:VAL:HG23	1:A:170:TRP:HB3	1.94	0.49
1:A:72:MET:CE	1:A:192:THR:OG1	2.61	0.49
1:D:85:ALA:HA	1:D:198:PHE:CD2	2.48	0.49
1:D:131:ASP:N	1:D:131:ASP:OD2	2.44	0.49
1:C:307:ARG:NH1	1:C:307:ARG:HG2	2.27	0.49
1:C:153:PHE:HB2	2:C:436:HOH:O	2.11	0.49
1:A:18:ARG:HB2	1:A:412:VAL:O	2.13	0.49
1:A:90:LEU:HD22	1:A:94:ILE:HD11	1.95	0.49
1:C:373:ASP:OD2	1:C:374:ARG:N	2.45	0.49
1:D:169:CYS:SG	1:D:225:GLY:HA2	2.53	0.49
1:A:247:GLN:N	1:A:247:GLN:OE1	2.39	0.48
1:B:80:ILE:HB	2:B:475:HOH:O	2.11	0.48
1:D:231:ILE:HD12	1:D:333:LEU:HD21	1.94	0.48
1:A:86:LEU:O	1:A:86:LEU:HG	2.13	0.48
1:C:313:PRO:HD2	1:C:314:TYR:CE2	2.49	0.48
1:D:328:VAL:O	1:D:328:VAL:HG12	2.13	0.48
1:A:199:HIS:ND1	1:A:201:GLU:HB2	2.27	0.48
1:A:258:ALA:O	1:A:260:GLY:N	2.45	0.48
1:A:58:PHE:CD1	1:A:392:ILE:HD13	2.48	0.48
1:D:175:VAL:HG22	1:D:176:THR:N	2.28	0.48
1:A:257:PHE:CD2	1:A:316:MET:HG2	2.48	0.48
1:C:10:VAL:HB	1:C:170:TRP:O	2.14	0.48
1:A:140:ILE:HD13	1:D:318:ILE:CG2	2.41	0.48
1:D:24:SER:HB2	2:D:425:HOH:O	2.12	0.48
1:A:19:LYS:HB3	1:A:412:VAL:HB	1.95	0.48
1:A:356:ASP:HB2	1:A:375:ASN:OD1	2.13	0.48
1:B:76:LEU:HD22	1:B:80:ILE:CG1	2.44	0.48
1:C:180:MET:CA	1:C:180:MET:CE	2.92	0.48
1:A:140:ILE:O	1:A:143:MET:HB2	2.13	0.48
1:A:31:ARG:HH11	1:A:31:ARG:HG2	1.77	0.48
1:C:169:CYS:SG	1:C:225:GLY:HA2	2.54	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:277:MET:HE2	1:C:281:THR:CG2	2.18	0.48
1:D:88:TRP:NE1	1:D:92:ARG:CZ	2.77	0.48
1:A:323:LYS:HE2	1:A:327:GLU:O	2.14	0.47
1:B:374:ARG:HH11	1:B:374:ARG:CG	2.25	0.47
1:C:67:ILE:CG2	1:C:68:ASP:N	2.77	0.47
1:D:373:ASP:OD1	1:D:393:SER:HA	2.14	0.47
1:A:76:LEU:O	1:A:79:THR:N	2.47	0.47
1:C:153:PHE:HD2	2:C:436:HOH:O	1.96	0.47
1:C:183:PRO:HD2	2:C:441:HOH:O	2.13	0.47
1:D:37:CYS:HB2	1:D:42:PHE:O	2.14	0.47
1:A:28:ALA:CB	2:A:456:HOH:O	2.62	0.47
1:B:25:PRO:HA	1:B:29:HIS:HE1	1.77	0.47
1:A:242:GLU:OE1	1:A:243:ARG:NH1	2.47	0.47
1:A:343:THR:CG2	1:A:378:THR:OG1	2.61	0.47
1:A:10:VAL:HG21	1:A:170:TRP:HB2	1.95	0.47
1:C:264:ARG:HD3	1:C:307:ARG:CZ	2.44	0.47
1:A:17:LEU:HD11	1:A:20:VAL:CG1	2.24	0.47
1:B:304:PHE:CE1	1:C:143:MET:CE	2.97	0.47
1:D:208:GLU:OE1	1:D:259:LYS:NZ	2.48	0.47
1:D:25:PRO:HD3	1:D:55:HIS:CG	2.49	0.47
1:A:213:ASP:OD1	1:A:215:ASP:HB2	2.15	0.47
1:A:293:VAL:HB	1:A:298:VAL:HG21	1.97	0.47
1:A:71:GLU:OE2	1:A:73:HIS:ND1	2.48	0.47
1:D:88:TRP:HE1	1:D:92:ARG:NH2	2.12	0.47
1:A:155:LEU:N	1:A:155:LEU:CD2	2.76	0.47
1:A:165:ARG:NH2	1:A:405:HIS:CD2	2.82	0.47
1:A:394:ALA:HB1	1:A:398:GLY:HA3	1.96	0.47
1:A:132:LEU:HG	1:A:133:PRO:HD2	1.97	0.47
1:A:18:ARG:HE	1:A:414:ASP:CG	2.19	0.47
1:C:282:VAL:O	1:C:298:VAL:CG2	2.63	0.47
1:D:416:ILE:HG23	1:D:417:ASP:N	2.29	0.47
1:A:33:THR:HG22	1:A:36:ASN:N	2.23	0.46
1:C:76:LEU:HD12	1:C:120:ALA:HB1	1.94	0.46
1:C:264:ARG:NH2	1:C:332:SER:HB2	2.30	0.46
1:C:381:LEU:HG	2:C:484:HOH:O	2.14	0.46
1:C:48:VAL:O	1:C:52:LYS:HG3	2.15	0.46
1:D:292:THR:O	1:D:293:VAL:HG23	2.16	0.46
1:D:343:THR:HG22	1:D:357:ASP:HA	1.97	0.46
1:D:58:PHE:CE1	1:D:370:VAL:HG11	2.50	0.46
1:A:397:LEU:HD23	1:A:407:MET:HE1	1.98	0.46
1:C:370:VAL:HA	1:C:390:ILE:O	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:331:GLU:C	1:D:331:GLU:CD	2.74	0.46
1:C:313:PRO:HD2	1:C:314:TYR:HE2	1.80	0.46
1:D:247:GLN:O	1:D:251:GLN:HG3	2.16	0.46
1:D:271:PRO:HG3	1:D:300:GLU:HB2	1.97	0.46
1:D:372:TYR:OH	1:D:403:GLY:HA2	2.15	0.46
1:A:139:ASN:O	1:A:143:MET:HE3	2.16	0.46
1:A:156:PRO:HD2	2:A:468:HOH:O	2.15	0.46
1:A:88:TRP:CZ3	1:A:194:ALA:HB2	2.50	0.46
1:B:17:LEU:HD12	1:B:412:VAL:O	2.15	0.46
1:B:274:ARG:HB3	1:B:297:VAL:HG22	1.97	0.46
1:C:166:ALA:HA	1:C:225:GLY:HA3	1.98	0.46
1:C:397:LEU:HD13	2:C:419:HOH:O	2.15	0.46
1:D:15:GLY:O	1:D:413:ARG:NH1	2.43	0.46
1:A:320:ARG:HE	1:D:143:MET:HE2	1.81	0.46
1:B:208:GLU:HG2	1:B:210:TRP:CZ3	2.51	0.46
1:C:416:ILE:HG22	1:C:417:ASP:H	1.79	0.46
1:D:17:LEU:HD21	1:D:20:VAL:HG21	1.97	0.46
1:D:245:SER:O	1:D:249:ILE:HG13	2.15	0.46
1:B:302:VAL:HB	1:C:148:LEU:HD21	1.96	0.46
1:A:61:LYS:O	1:A:65:ARG:HG2	2.15	0.46
1:B:222:THR:O	1:B:244:SER:HA	2.16	0.46
1:B:411:ILE:HG22	1:B:412:VAL:HG23	1.98	0.46
1:C:352:ARG:HB2	1:C:377:TYR:CD2	2.51	0.46
1:C:372:TYR:CZ	1:C:403:GLY:HA2	2.51	0.46
1:C:45:VAL:HG12	1:C:45:VAL:O	2.16	0.46
1:D:293:VAL:O	1:D:295:PRO:HD3	2.16	0.46
1:C:65:ARG:O	1:C:65:ARG:HG3	2.15	0.46
1:D:140:ILE:HG13	1:D:140:ILE:O	2.14	0.46
1:D:373:ASP:OD2	1:D:374:ARG:N	2.46	0.46
1:D:90:LEU:HD13	1:D:108:ARG:HG3	1.98	0.46
1:A:301:ILE:HD11	1:A:325:PHE:HB2	1.98	0.45
1:B:17:LEU:HD21	1:B:20:VAL:HG13	1.98	0.45
1:C:64:GLU:C	1:C:66:GLY:H	2.19	0.45
1:D:307:ARG:HH11	1:D:307:ARG:CG	2.19	0.45
1:D:291:VAL:HG23	1:D:340:VAL:HG12	1.97	0.45
1:A:237:LEU:C	1:A:238:ILE:HG13	2.36	0.45
1:A:59:VAL:HG13	1:A:69:VAL:HG11	1.98	0.45
1:B:176:THR:N	2:B:503:HOH:O	2.48	0.45
1:B:36:ASN:O	1:B:40:LEU:HB2	2.16	0.45
1:D:136:GLU:O	1:D:140:ILE:HG12	2.16	0.45
1:D:58:PHE:HE1	1:D:370:VAL:HG11	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:VAL:HG21	1:A:332:SER:HB2	1.97	0.45
1:B:372:TYR:OH	1:B:407:MET:CE	2.64	0.45
1:C:396:GLU:N	2:C:419:HOH:O	2.40	0.45
1:A:18:ARG:NH2	1:A:414:ASP:OD1	2.48	0.45
1:A:294:PHE:CE1	1:A:344:GLY:HA3	2.50	0.45
1:A:165:ARG:CZ	1:A:405:HIS:CE1	2.99	0.45
1:B:102:GLY:C	1:B:103:LEU:HD23	2.37	0.45
1:B:17:LEU:HD21	1:B:20:VAL:CG2	2.46	0.45
1:B:288:ARG:HH11	1:B:288:ARG:HG2	1.82	0.45
1:C:119:LEU:HD22	1:C:123:LEU:HG	1.99	0.45
1:C:267:VAL:HB	1:C:304:PHE:HB2	1.99	0.45
1:C:335:LEU:HD21	2:C:473:HOH:O	2.16	0.45
1:C:54:ASP:HB2	1:C:397:LEU:HD11	1.97	0.45
1:D:169:CYS:HA	2:D:448:HOH:O	2.16	0.45
1:D:290:LEU:HG	1:D:339:ARG:NH2	2.31	0.45
1:D:401:ARG:NH2	2:D:460:HOH:O	2.49	0.45
1:A:267:VAL:HB	1:A:304:PHE:HB2	1.99	0.45
1:A:88:TRP:CE2	1:A:92:ARG:CZ	3.00	0.45
1:C:307:ARG:HG2	1:C:307:ARG:HH11	1.81	0.45
1:A:264:ARG:HD3	1:A:266:ILE:CG1	2.47	0.45
1:A:304:PHE:HE1	1:D:143:MET:SD	2.40	0.45
1:B:103:LEU:HD13	1:B:154:LEU:HD21	1.99	0.45
1:B:132:LEU:CD2	1:B:133:PRO:HD2	2.47	0.45
1:D:179:PRO:HB3	2:D:469:HOH:O	2.17	0.45
1:A:233:ASN:O	1:A:235:VAL:N	2.50	0.45
1:A:286:CYS:HB2	2:A:478:HOH:O	2.17	0.45
1:B:164:THR:O	1:B:409:CYS:HB2	2.16	0.45
1:C:306:LEU:N	1:C:306:LEU:HD12	2.32	0.45
1:C:355:TRP:CG	1:C:356:ASP:N	2.85	0.45
1:C:51:ALA:O	1:C:397:LEU:HD11	2.17	0.45
1:C:89:ILE:HD11	1:C:194:ALA:CB	2.47	0.45
1:C:93:LYS:HE3	1:C:155:LEU:HD12	1.99	0.45
1:D:144:TYR:HB3	1:D:150:HIS:CD2	2.27	0.45
1:D:17:LEU:HB2	1:D:413:ARG:NH1	2.31	0.45
1:A:120:ALA:HB3	2:A:453:HOH:O	2.17	0.45
1:A:199:HIS:HE1	1:A:201:GLU:CG	2.30	0.45
1:B:169:CYS:SG	1:B:225:GLY:HA2	2.57	0.45
1:C:178:ASN:HA	1:C:179:PRO:HD3	1.83	0.45
1:D:158:LEU:O	1:D:161:THR:HG23	2.17	0.45
1:D:240:MET:HG3	2:D:476:HOH:O	2.17	0.45
1:A:257:PHE:CE2	1:A:316:MET:HG2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:365:GLU:O	1:B:366:PRO:C	2.54	0.44
1:B:372:TYR:OH	1:B:407:MET:HE2	2.16	0.44
1:C:155:LEU:N	1:C:155:LEU:HD22	2.32	0.44
1:C:129:ALA:HA	1:C:154:LEU:HD11	1.98	0.44
1:D:256:LEU:HB3	1:D:262:ALA:HB3	1.98	0.44
1:A:235:VAL:HB	2:A:451:HOH:O	2.18	0.44
1:C:122:TYR:O	1:C:123:LEU:C	2.54	0.44
1:C:199:HIS:CG	1:C:200:PRO:HD2	2.53	0.44
1:C:94:ILE:HD13	1:C:107:LEU:CD1	2.48	0.44
1:D:42:PHE:O	1:D:43:ASP:C	2.55	0.44
1:B:372:TYR:CD2	1:B:394:ALA:HB2	2.52	0.44
1:C:177:LEU:O	1:C:212:GLY:HA3	2.17	0.44
1:C:374:ARG:HH22	1:D:399:ARG:HH21	1.64	0.44
1:B:320:ARG:HG2	1:B:320:ARG:NH1	2.31	0.44
1:B:372:TYR:CG	1:B:394:ALA:HB2	2.51	0.44
1:A:140:ILE:HA	1:A:143:MET:HE3	1.99	0.44
1:A:307:ARG:NE	2:A:421:HOH:O	2.44	0.44
1:A:324:THR:O	1:A:327:GLU:HB2	2.17	0.44
1:A:33:THR:HB	1:A:36:ASN:HD21	1.81	0.44
1:B:86:LEU:HD22	1:B:90:LEU:HD11	2.00	0.44
1:D:111:LEU:HA	1:D:114:LEU:CD1	2.47	0.44
1:D:291:VAL:HG21	1:D:338:LEU:HD13	2.00	0.44
1:D:82:ASN:HB3	1:D:85:ALA:CB	2.48	0.44
1:A:13:GLU:HG3	1:A:229:MET:HB2	1.99	0.44
1:A:92:ARG:HH11	1:A:92:ARG:CG	2.30	0.44
1:B:85:ALA:HB2	1:B:198:PHE:CG	2.53	0.44
1:B:209:ILE:O	1:B:209:ILE:HG22	2.16	0.44
1:B:20:VAL:CB	2:B:492:HOH:O	2.61	0.44
1:B:364:LEU:HD12	2:B:479:HOH:O	2.17	0.44
1:C:374:ARG:NH2	1:D:399:ARG:HH21	2.16	0.44
1:A:29:HIS:ND1	1:A:29:HIS:N	2.66	0.44
1:B:80:ILE:HG21	1:B:119:LEU:CD1	2.47	0.44
1:C:216:LYS:HG2	1:C:217:ASP:N	2.32	0.44
1:C:210:TRP:CH2	1:C:261:ALA:HB2	2.52	0.44
1:C:295:PRO:HG3	1:C:342:GLU:HG2	1.99	0.44
1:D:227:ASP:OD1	1:D:244:SER:OG	2.23	0.44
1:D:39:GLU:C	1:D:40:LEU:HD12	2.38	0.44
1:A:264:ARG:HG2	1:A:265:VAL:N	2.33	0.44
1:A:27:LEU:HD21	1:A:31:ARG:HH21	1.83	0.44
1:B:254:GLN:HB2	1:B:316:MET:CE	2.48	0.44
1:D:107:LEU:O	1:D:111:LEU:HG	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:294:PHE:CD2	1:D:297:VAL:HG23	2.52	0.44
1:D:14:ALA:O	1:D:366:PRO:HG3	2.18	0.44
1:D:41:LEU:CD2	2:D:460:HOH:O	2.65	0.44
1:A:202:PHE:O	1:A:205:ALA:N	2.50	0.43
1:A:229:MET:SD	1:A:279:LEU:HD23	2.59	0.43
1:A:233:ASN:O	1:A:235:VAL:HG23	2.18	0.43
1:A:279:LEU:C	1:A:281:THR:H	2.21	0.43
1:A:290:LEU:HD23	1:A:339:ARG:O	2.19	0.43
1:A:8:LEU:O	1:A:173:GLY:HA2	2.17	0.43
1:C:33:THR:HG23	1:C:34:PRO:CD	2.47	0.43
1:C:397:LEU:HD12	1:C:397:LEU:N	2.33	0.43
1:A:239:GLY:O	1:A:244:SER:HB2	2.18	0.43
1:A:264:ARG:HD3	1:A:266:ILE:HG13	2.00	0.43
1:A:320:ARG:NE	1:D:143:MET:CE	2.82	0.43
1:C:169:CYS:O	1:C:175:VAL:HA	2.18	0.43
1:C:63:ARG:HD2	2:C:471:HOH:O	2.17	0.43
1:A:280:ASP:HA	1:A:283:PHE:O	2.19	0.43
1:B:342:GLU:O	1:B:343:THR:HG22	2.17	0.43
1:A:268:ALA:HB2	1:A:325:PHE:CE1	2.54	0.43
1:A:270:LEU:HA	1:A:271:PRO:HD3	1.73	0.43
1:A:329:VAL:CG1	1:A:338:LEU:HD11	2.49	0.43
1:A:387:VAL:HG12	1:A:388:GLU:N	2.33	0.43
1:A:20:VAL:HG12	1:A:410:PRO:HA	2.00	0.43
1:A:19:LYS:NZ	1:A:68:ASP:OD2	2.43	0.43
1:B:31:ARG:HG2	1:B:31:ARG:HH11	1.84	0.43
1:C:284:SER:O	1:C:291:VAL:HA	2.18	0.43
1:C:372:TYR:CG	1:C:394:ALA:HB2	2.53	0.43
1:A:364:LEU:HD11	1:A:370:VAL:HG23	2.00	0.43
1:B:80:ILE:CG1	2:B:475:HOH:O	2.65	0.43
1:D:174:GLY:HA3	1:D:210:TRP:CE2	2.53	0.43
1:A:15:GLY:HA3	1:A:414:ASP:O	2.19	0.43
1:C:267:VAL:N	1:C:304:PHE:O	2.49	0.43
1:D:284:SER:O	1:D:291:VAL:HA	2.19	0.43
1:A:74:ASN:O	1:A:77:THR:HB	2.18	0.43
1:C:141:LEU:HD22	1:C:141:LEU:HA	1.79	0.43
1:C:229:MET:HE1	1:C:279:LEU:HG	2.01	0.43
1:C:80:ILE:HD12	1:C:119:LEU:CD1	2.47	0.43
1:D:80:ILE:HD11	1:D:119:LEU:HG	2.00	0.43
1:D:245:SER:C	2:D:476:HOH:O	2.57	0.43
1:A:303:PRO:CG	1:A:321:GLU:HB2	2.48	0.43
1:D:240:MET:CG	2:D:476:HOH:O	2.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:377:TYR:O	1:D:380:THR:HB	2.19	0.43
1:A:24:SER:HA	1:A:55:HIS:CE1	2.54	0.42
1:A:320:ARG:NH1	1:A:321:GLU:O	2.52	0.42
1:A:384:LYS:C	1:A:386:GLY:H	2.22	0.42
1:A:93:LYS:HE3	1:A:93:LYS:HB3	1.84	0.42
1:C:295:PRO:O	1:C:299:LYS:HG2	2.19	0.42
1:C:396:GLU:HA	1:C:399:ARG:HG3	2.00	0.42
1:D:274:ARG:HD2	2:D:479:HOH:O	2.18	0.42
1:D:80:ILE:HG21	1:D:80:ILE:HD13	1.72	0.42
1:A:143:MET:O	1:A:147:TYR:HB2	2.19	0.42
1:B:361:VAL:HG21	1:B:369:VAL:HG11	2.01	0.42
1:C:407:MET:HB3	2:C:428:HOH:O	2.18	0.42
1:D:88:TRP:NE1	1:D:92:ARG:NH2	2.67	0.42
1:B:400:GLY:O	1:B:402:GLY:N	2.52	0.42
1:B:251:GLN:CG	1:C:101:LEU:HD11	2.47	0.42
1:C:323:LYS:HB3	1:C:327:GLU:OE1	2.20	0.42
1:C:92:ARG:HG3	1:C:92:ARG:HH11	1.84	0.42
1:D:198:PHE:O	1:D:199:HIS:C	2.57	0.42
1:D:416:ILE:HA	1:D:416:ILE:HD12	1.84	0.42
1:D:99:VAL:HG12	1:D:99:VAL:O	2.18	0.42
1:A:233:ASN:C	1:A:235:VAL:H	2.22	0.42
1:A:65:ARG:CB	1:A:65:ARG:HH11	2.29	0.42
1:B:154:LEU:HD23	1:B:154:LEU:HA	1.90	0.42
1:C:414:ASP:HA	1:C:415:PRO:HD3	1.75	0.42
1:D:230:PRO:HG2	1:D:230:PRO:O	2.18	0.42
1:B:9:GLY:HA2	1:B:172:TYR:O	2.19	0.42
1:C:118:LYS:HE3	1:C:118:LYS:HB2	1.68	0.42
1:D:111:LEU:HA	1:D:114:LEU:HD12	2.01	0.42
1:D:72:MET:HE1	1:D:192:THR:OG1	2.19	0.42
1:D:416:ILE:HG13	1:D:417:ASP:N	2.20	0.42
1:B:147:TYR:HB3	1:C:302:VAL:HG21	2.00	0.42
1:B:267:VAL:HB	1:B:304:PHE:HB2	2.02	0.42
1:C:312:SER:HA	1:C:313:PRO:HD3	1.86	0.42
1:C:336:LYS:HB3	1:C:336:LYS:HE3	1.88	0.42
1:D:399:ARG:CG	1:D:399:ARG:NH1	2.83	0.42
1:B:165:ARG:O	1:B:225:GLY:HA3	2.20	0.42
1:B:80:ILE:HG23	1:B:86:LEU:HG	2.02	0.42
1:C:21:MET:HE3	1:C:21:MET:HB3	1.79	0.42
1:C:25:PRO:HG3	1:C:162:GLN:OE1	2.19	0.42
1:A:295:PRO:HG3	1:A:299:LYS:HZ1	1.84	0.42
1:C:80:ILE:CD1	1:C:119:LEU:HD13	2.46	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:242:GLU:CD	1:C:276:ALA:HA	2.40	0.42
1:C:282:VAL:O	1:C:298:VAL:HG21	2.19	0.42
1:C:31:ARG:HG2	1:C:31:ARG:HH11	1.85	0.42
1:D:186:ARG:HG2	1:D:186:ARG:HH11	1.84	0.42
1:A:170:TRP:CE2	1:A:411:ILE:HG23	2.55	0.42
1:A:286:CYS:CB	2:A:478:HOH:O	2.68	0.42
1:A:397:LEU:HD23	1:A:407:MET:CE	2.49	0.42
1:B:69:VAL:HA	2:B:492:HOH:O	2.20	0.42
1:D:266:ILE:HA	1:D:304:PHE:O	2.19	0.42
1:A:65:ARG:NH2	1:A:390:ILE:HD11	2.35	0.42
1:B:55:HIS:HE1	2:B:487:HOH:O	2.02	0.42
1:B:87:LYS:HG2	1:B:91:ASP:OD2	2.20	0.42
1:C:206:GLU:O	1:C:207:PHE:HB3	2.20	0.42
1:D:287:ASP:CB	1:D:290:LEU:HB2	2.50	0.42
1:A:245:SER:O	1:A:249:ILE:HG13	2.20	0.41
1:A:246:ARG:HG2	1:A:247:GLN:OE1	2.20	0.41
1:B:101:LEU:HD22	1:C:254:GLN:OE1	2.19	0.41
1:B:317:ASN:ND2	1:B:318:ILE:H	2.17	0.41
1:C:23:CYS:O	1:C:162:GLN:HA	2.20	0.41
1:C:351:GLU:HB2	1:C:352:ARG:H	1.41	0.41
1:C:355:TRP:N	2:C:479:HOH:O	2.53	0.41
1:A:141:LEU:HD21	1:D:246:ARG:NE	2.35	0.41
1:A:271:PRO:O	1:A:272:LYS:C	2.58	0.41
1:A:58:PHE:HE1	1:A:370:VAL:HG11	1.83	0.41
1:A:88:TRP:HE1	1:A:92:ARG:NH2	2.18	0.41
1:B:50:GLN:OE1	1:B:53:ARG:NH2	2.40	0.41
1:A:320:ARG:HE	1:D:143:MET:CE	2.33	0.41
1:D:248:ALA:O	1:D:252:VAL:HG23	2.20	0.41
1:D:306:LEU:N	1:D:306:LEU:CD1	2.84	0.41
1:A:231:ILE:HD13	1:A:237:LEU:HD11	2.02	0.41
1:A:228:VAL:HG22	1:A:238:ILE:HG12	2.01	0.41
1:B:309:ASP:CG	1:B:311:SER:HB3	2.41	0.41
1:B:397:LEU:HB3	1:B:407:MET:HE1	2.02	0.41
1:B:43:ASP:CA	1:B:401:ARG:HH21	2.33	0.41
1:D:222:THR:O	1:D:244:SER:HA	2.20	0.41
1:A:8:LEU:HD12	1:A:207:PHE:CD2	2.54	0.41
1:C:231:ILE:HD11	1:C:235:VAL:HG11	2.02	0.41
1:C:8:LEU:HA	1:C:412:VAL:HG22	2.02	0.41
1:C:267:VAL:HG23	1:C:306:LEU:CD1	2.51	0.41
1:C:292:THR:HA	1:C:341:VAL:O	2.21	0.41
1:D:379:ASN:HA	1:D:382:LEU:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:84:GLU:O	1:D:85:ALA:C	2.58	0.41
1:A:120:ALA:HA	1:A:123:LEU:HD12	2.02	0.41
1:C:12:SER:O	1:C:413:ARG:HD2	2.20	0.41
1:C:77:THR:O	1:C:81:GLN:HG3	2.20	0.41
1:D:188:GLU:O	1:D:191:LEU:N	2.54	0.41
1:A:353:GLU:OE2	1:A:353:GLU:HA	2.19	0.41
1:A:384:LYS:C	1:A:386:GLY:N	2.74	0.41
1:A:63:ARG:CG	1:A:63:ARG:HH11	2.33	0.41
1:B:65:ARG:NH1	1:B:390:ILE:HD11	2.35	0.41
1:C:169:CYS:SG	1:C:228:VAL:HB	2.61	0.41
1:C:22:VAL:HG12	1:C:408:THR:HG22	2.02	0.41
1:D:139:ASN:C	1:D:141:LEU:N	2.66	0.41
1:D:370:VAL:HA	1:D:390:ILE:O	2.21	0.41
1:A:265:VAL:O	1:A:306:LEU:HB2	2.21	0.41
1:A:306:LEU:CD1	1:A:318:ILE:HG12	2.48	0.41
1:A:336:LYS:N	1:A:336:LYS:HD3	2.23	0.41
1:C:137:GLY:O	1:C:138:ALA:C	2.59	0.41
1:D:187:GLN:OE1	1:D:187:GLN:HA	2.20	0.41
1:D:270:LEU:HD12	1:D:301:ILE:HG12	2.02	0.41
1:D:354:GLN:HB2	2:D:465:HOH:O	2.21	0.41
1:B:257:PHE:HB3	1:B:308:PRO:HB3	2.02	0.41
1:B:361:VAL:HB	1:B:369:VAL:HG13	2.02	0.41
1:B:374:ARG:NH1	1:B:374:ARG:CG	2.82	0.41
1:C:199:HIS:HA	1:C:200:PRO:HD3	1.84	0.41
1:C:213:ASP:OD1	1:C:214:PRO:HD2	2.21	0.41
1:A:142:LYS:O	1:A:146:GLU:HB2	2.21	0.41
1:A:301:ILE:C	1:A:301:ILE:HD12	2.41	0.41
1:B:141:LEU:HD21	1:C:246:ARG:NE	2.35	0.41
1:B:169:CYS:O	1:B:175:VAL:HA	2.21	0.41
1:B:297:VAL:O	1:B:301:ILE:HG13	2.21	0.41
1:B:99:VAL:HG13	1:B:154:LEU:CD2	2.44	0.41
1:C:364:LEU:N	1:C:364:LEU:HD23	2.36	0.41
1:C:288:ARG:HB2	1:C:288:ARG:HE	1.68	0.41
1:D:138:ALA:O	1:D:141:LEU:HB3	2.20	0.41
1:D:324:THR:OG1	1:D:327:GLU:HG3	2.21	0.41
1:D:335:LEU:HD12	1:D:335:LEU:HA	1.93	0.41
1:A:110:TRP:HZ3	1:A:127:VAL:HG11	1.86	0.40
1:C:293:VAL:HG13	1:C:298:VAL:CG2	2.50	0.40
1:C:65:ARG:HE	1:C:65:ARG:HB2	1.51	0.40
1:A:24:SER:CA	1:A:55:HIS:CE1	3.05	0.40
1:C:199:HIS:O	1:C:202:PHE:N	2.48	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:322:GLU:O	1:D:323:LYS:O	2.39	0.40
1:A:103:LEU:HD13	1:A:141:LEU:HD11	2.03	0.40
1:A:290:LEU:C	2:A:478:HOH:O	2.59	0.40
1:D:286:CYS:SG	1:D:292:THR:HG23	2.62	0.40
1:C:289:ASP:O	1:C:339:ARG:N	2.45	0.40
1:C:294:PHE:H	1:C:298:VAL:HG21	1.86	0.40
1:C:92:ARG:HG3	1:C:92:ARG:NH1	2.37	0.40
1:D:138:ALA:O	1:D:142:LYS:N	2.55	0.40
1:A:18:ARG:HG2	1:A:18:ARG:HH11	1.86	0.40
1:B:361:VAL:HB	1:B:369:VAL:CG1	2.52	0.40
1:D:249:ILE:CD1	2:D:476:HOH:O	2.68	0.40
1:D:388:GLU:OE2	1:D:390:ILE:HD11	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	396/418 (95%)	342 (86%)	45 (11%)	9 (2%)	7	11
1	B	405/418 (97%)	366 (90%)	36 (9%)	3 (1%)	25	43
1	C	397/418 (95%)	346 (87%)	45 (11%)	6 (2%)	12	21
1	D	402/418 (96%)	336 (84%)	53 (13%)	13 (3%)	5	6
All	All	1600/1672 (96%)	1390 (87%)	179 (11%)	31 (2%)	9	15

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	43	ASP
1	D	152	SER
1	D	276	ALA

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Mol	Chain	Res	Type
1	D	323	LYS
1	A	172	TYR
1	A	225	GLY
1	B	272	LYS
1	C	164	THR
1	D	146	GLU
1	D	173	GLY
1	A	258	ALA
1	A	271	PRO
1	A	328	VAL
1	A	401	ARG
1	C	401	ARG
1	D	296	GLU
1	D	337	LYS
1	B	43	ASP
1	C	272	LYS
1	C	330	ALA
1	D	101	LEU
1	A	234	GLY
1	C	313	PRO
1	D	116	PRO
1	B	401	ARG
1	D	400	GLY
1	C	365	GLU
1	D	404	GLY
1	D	140	ILE
1	A	400	GLY
1	D	137	GLY

### 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	342/354 (97%)	314 (92%)	28 (8%)	13	25
1	B	346/354 (98%)	315 (91%)	31 (9%)	11	21
1	C	343/354 (97%)	321 (94%)	22 (6%)	20	38

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	345/354 (98%)	327 (95%)	18 (5%)	27	49
All	All	1376/1416 (97%)	1277 (93%)	99 (7%)	17	31

All (99) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	SER
1	A	20	VAL
1	A	33	THR
1	A	39	GLU
1	A	40	LEU
1	A	65	ARG
1	A	71	GLU
1	A	76	LEU
1	A	107	LEU
1	A	109	SER
1	A	118	LYS
1	A	119	LEU
1	A	176	THR
1	A	178	ASN
1	A	223	LEU
1	A	233	ASN
1	A	242	GLU
1	A	287	ASP
1	A	290	LEU
1	A	306	LEU
1	A	310	PRO
1	A	333	LEU
1	A	336	LYS
1	A	353	GLU
1	A	369	VAL
1	A	382	LEU
1	A	406	CYS
1	A	417	ASP
1	B	12	SER
1	B	20	VAL
1	B	25	PRO
1	B	39	GLU
1	B	40	LEU
1	B	60	THR
1	B	76	LEU
1	B	86	LEU

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Mol	Chain	Res	Type
1	B	107	LEU
1	B	109	SER
1	B	117	ARG
1	B	119	LEU
1	B	165	ARG
1	B	200	PRO
1	B	220	SER
1	B	242	GLU
1	B	274	ARG
1	B	277	MET
1	B	280	ASP
1	B	281	THR
1	B	287	ASP
1	B	288	ARG
1	B	290	LEU
1	B	336	LYS
1	B	352	ARG
1	B	356	ASP
1	B	363	CYS
1	B	374	ARG
1	B	382	LEU
1	B	401	ARG
1	B	406	CYS
1	C	20	VAL
1	C	21	MET
1	C	33	THR
1	C	86	LEU
1	C	101	LEU
1	C	115	GLU
1	C	119	LEU
1	C	139	ASN
1	C	141	LEU
1	C	162	GLN
1	C	206	GLU
1	C	259	LYS
1	C	280	ASP
1	C	290	LEU
1	C	307	ARG
1	C	311	SER
1	C	314	TYR
1	C	331	GLU
1	C	351	GLU

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Mol	Chain	Res	Type
1	C	352	ARG
1	C	376	THR
1	C	401	ARG
1	D	7	LYS
1	D	42	PHE
1	D	76	LEU
1	D	116	PRO
1	D	131	ASP
1	D	147	TYR
1	D	154	LEU
1	D	165	ARG
1	D	189	THR
1	D	200	PRO
1	D	221	SER
1	D	291	VAL
1	D	295	PRO
1	D	296	GLU
1	D	306	LEU
1	D	307	ARG
1	D	397	LEU
1	D	406	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	GLN
1	B	317	ASN
1	C	139	ASN
1	D	81	GLN
1	D	150	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](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	402/418 (96%)	-0.05	10 (2%) 58 60	18, 41, 64, 78	0
1	B	409/418 (97%)	-0.20	12 (2%) 52 55	16, 30, 60, 78	0
1	C	403/418 (96%)	-0.21	9 (2%) 62 64	17, 36, 62, 78	0
1	D	406/418 (97%)	-0.07	12 (2%) 51 53	17, 39, 66, 79	0
All	All	1620/1672 (96%)	-0.13	43 (2%) 55 58	16, 37, 64, 79	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	275	ALA	5.8
1	D	418	TYR	5.6
1	A	6	THR	5.0
1	D	274	ARG	4.3
1	C	352	ARG	4.2
1	D	314	TYR	4.2
1	D	400	GLY	3.8
1	B	274	ARG	3.7
1	D	147	TYR	3.7
1	C	401	ARG	3.6
1	D	313	PRO	3.0
1	A	7	LYS	3.0
1	B	149	GLY	2.9
1	C	313	PRO	2.9
1	D	401	ARG	2.9
1	B	400	GLY	2.9
1	C	400	GLY	2.8
1	D	311	SER	2.7
1	D	276	ALA	2.7
1	B	43	ASP	2.6
1	A	401	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	12	SER	2.5
1	B	136	GLU	2.5
1	C	312	SER	2.5
1	B	417	ASP	2.5
1	A	147	TYR	2.5
1	C	204	ASN	2.4
1	B	6	THR	2.4
1	D	277	MET	2.4
1	A	311	SER	2.4
1	D	146	GLU	2.4
1	B	351	GLU	2.3
1	A	386	GLY	2.3
1	B	418	TYR	2.3
1	C	353	GLU	2.2
1	B	134	ALA	2.2
1	A	313	PRO	2.2
1	C	311	SER	2.2
1	B	133	PRO	2.1
1	B	275	ALA	2.1
1	A	309	ASP	2.1
1	C	273	SER	2.1
1	A	400	GLY	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.